Supporting Information

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General information.

All manipulations were performed under an inert argon or nitrogen atmosphere using standard Schlenk-line and glovebox techniques. Dry, oxygen-free solvents were employed. Reagents were obtained from commercial suppliers unless otherwise stated. *N*-(2,6-dimethylphenyl)acetamide,[1] *N*-(2,6-dimethylphenyl)acetimidoyl chloride,[1] *N,N'*-(naphthalene-1,8-diyl)bis(2,2-dimethylpropanamide),[2] *N,N'*(naphthalene-1,8-diyl)bis(2,2-dimethylpropanimidoyl chloride),[2] L$_1$[3], and L$_2$[2] were synthesized following reported procedures. The Lappert germanium(II) and tin (II) derivatives were prepared according to literature procedures.[4] 1D and 2D NMR spectra were recorded with the following spectrometers for ^{1}H, ^{13}C and ^{119}Sn: Bruker Avance II 300MHz, Avance III HD 400 MHz, and Avance I and II 500 MHz spectrometers. The chemical shift has been counted positively verse the low field and expressed in part per million (ppm). The mass spectrometric analysis was done using three techniques, direct chemical ionization (DCI-CH$_4$) methods and recorded on a GCT Premier Waters mass spectrometer; electrospray ionization (ESI), recorded on a Waters Xevo G2 Q-TOF mass spectrometer; and a Maldi micro-MX micro–Mass in a pyrene matrix (ratio product/matrix:1/100). Melting points were measured with a capillary Electrothermal Stuart SMP40 apparatus, and samples were prepared in the glovebox before the analysis. FT-IR spectra were measured on a ThermoNicolet 6700, Nexus and recovered in solid state (KBr). Single-crystal X-ray data were collected at low temperature (193(2)K) on a Bruker APEX II Quazar diffractometer equipped with a 30W air-cooled microfocus source [**(L2Sn)2, L$_2$Ge, 2a** and **3b**] or on a Bruker D8 VENTURE diffractometer equipped with a PHOTON III detector [**L$_3$H$_2$, L$_1$Sn, (L$_1$Ge)$_2$, 1a** and **1b**], using MoKα radiation (λ= 0.71037 Å). The structure were solved by intrinsic phasing method (SHELXT)[5] and refined by full-matrix least- squares method on F2.[6] All non-H atoms were refined with anisotropic displacement parameters and all the hydrogen atoms were refined isotropically at calculated positions using a riding model. For **2a**, some solvent molecules were highly disordered and difficult to model correctly. Therefore the SQUEEZE function of PLATON[7] was used to eliminate the contribution of the electron density of those solvent molecules from the intensity data.

CCDC-2303009 (**L$_3$H$_2$**), CCDC-2266345 (**L$_1$Sn**), CCDC-2266346 [(**L$_2$Sn)$_2$**], CCDC-2266347 [(**L$_1$Ge)$_2$**], CCDC-2266348 (**L$_2$Ge**), CCDC-2266349 (**1a**), CCDC-2266350 (**1b**) CCDC-2266351 (**2a**) and CCDC-2266352 (**3b**) contain the supplementary

crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

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(7) Van der Sluis, P.; Spek, A. L. BYPASS: an effective method for the refinement of crystal structures containing disordered solvent regions. *Acta Cryst., Sect. A*, **1990**, 46, 194-201. https://doi.org/10.1107/S0108767389011189

^{1}H NMR spectrum of compound **L$_3$H$_2$** (DMSO-d$_6$, 500 MHz)

161.35
160.69
147.20
146.55
138.60
137.28
135.57
131.25
130.42
128.74
127.99
127.66
124.83
121.40
120.91
119.77
116.49
114.76
39.52 Dimethyl Sulfoxide-d6
28.79
28.28
20.29

$^{13}C\{^1H\}$ NMR spectrum of compound **L₃H₂** (DMSO-d₆, 125 MHz)

6

^{1}H NMR spectrum of compound **L₁Sn** (THF-d₈, 500 MHz)

7.43
7.43
7.41
7.31
7.29
7.28
7.08
7.08
7.07
7.07
7.06
6.97
6.95
6.84
6.83
6.81

3.58 Tetrahydrofuran-d8

2.18
1.97

2.22
2.28
2.33
4.30
2.32

12.04
6.00

$^{13}C\{^1H\}$ NMR spectrum of compound $\textbf{L}_1\textbf{Sn}$ (THF-d$_8$, 125 MHz)

$^{119}\text{Sn}\{^{1}\text{H}\}$ NMR spectrum of compound $\mathbf{L_1Sn}$ (THF-d$_8$, 186 MHz)

9

^{1}H NMR spectrum of compound **L₃Sn** (THF-d₈, 400 MHz)

$^{13}C\{^{1}H\}$ NMR spectrum of compound **L₃Sn** (THF-d₈, 125 MHz)

^{119}Sn{^{1}H} NMR spectrum of compound **L₃Sn** (THF-d₈, 186 MHz)

—−254.87

^{1}H NMR spectrum of compound **L₂Ge** (C₆D₆, 300 MHz)

$^{13}C\{^1H\}$ NMR spectrum of compound **L₂Ge** (C_6D_6, 125 MHz)
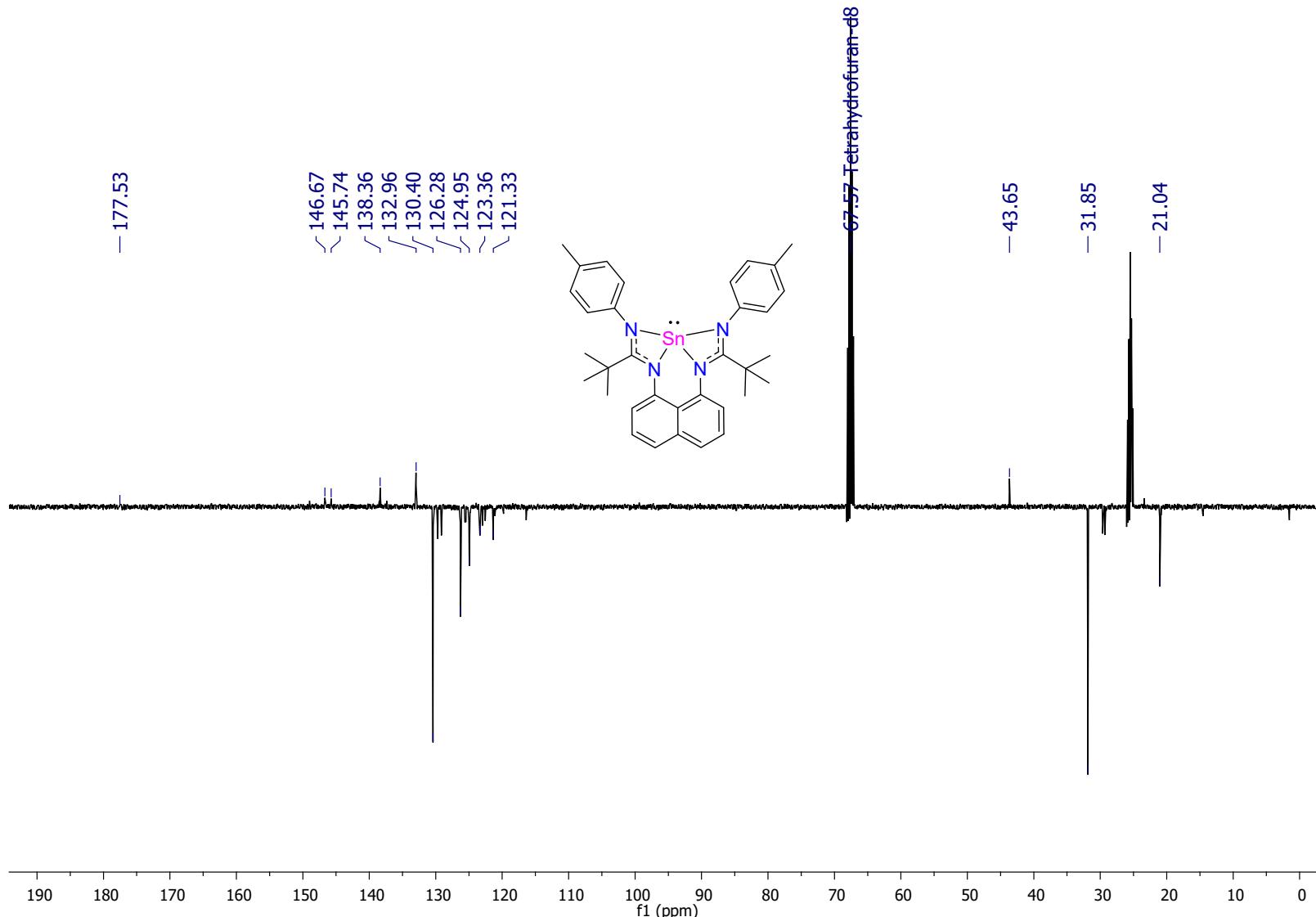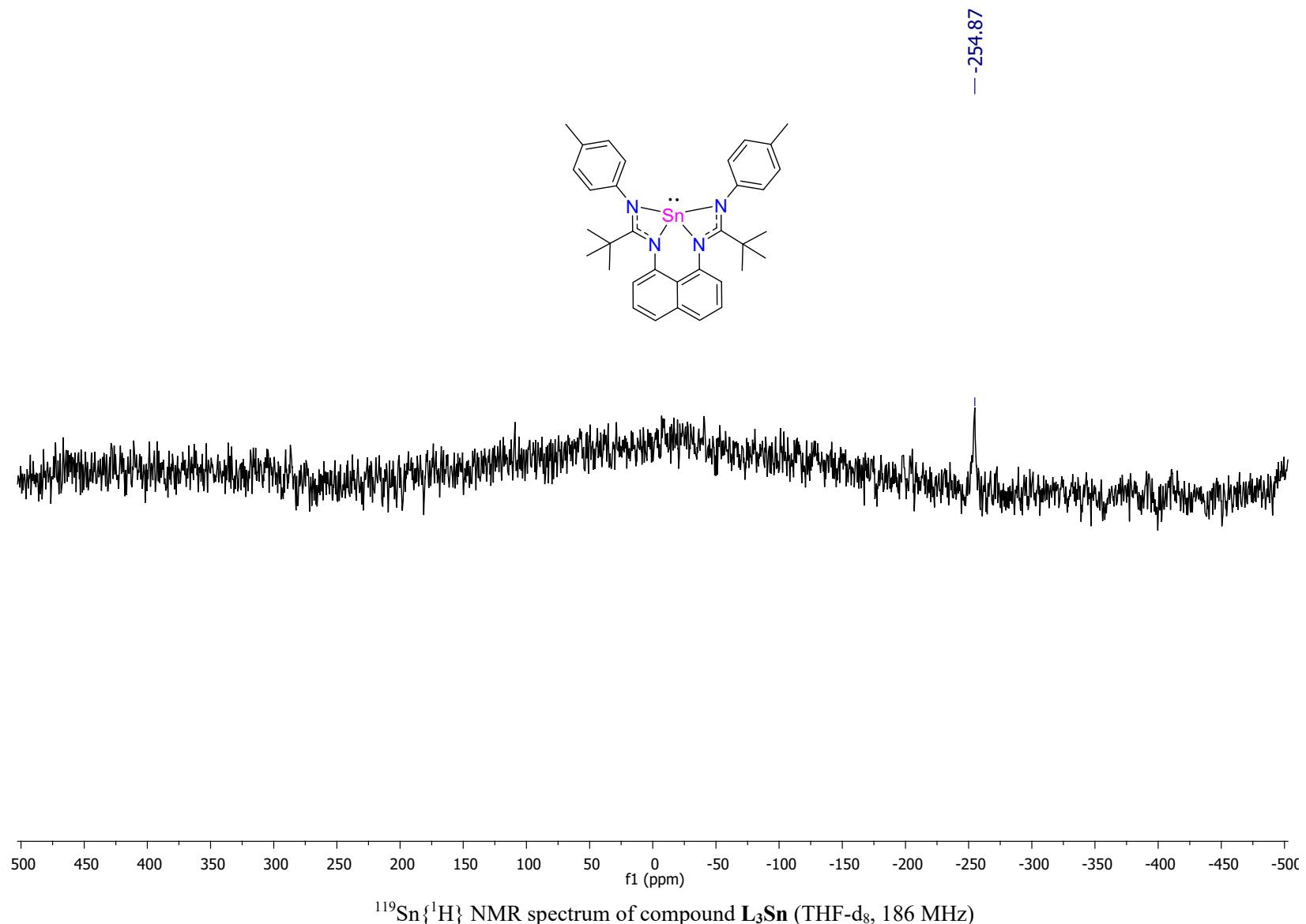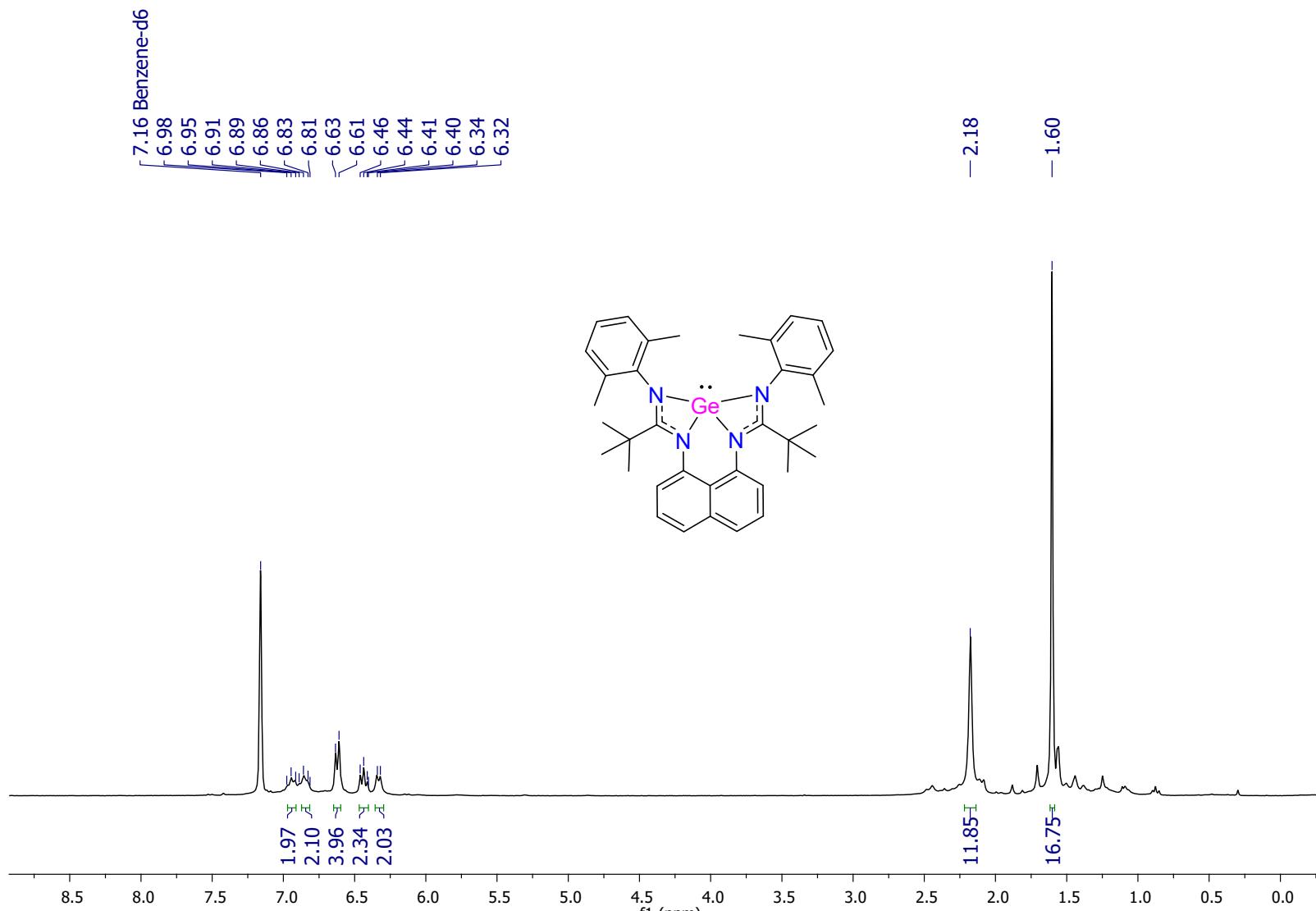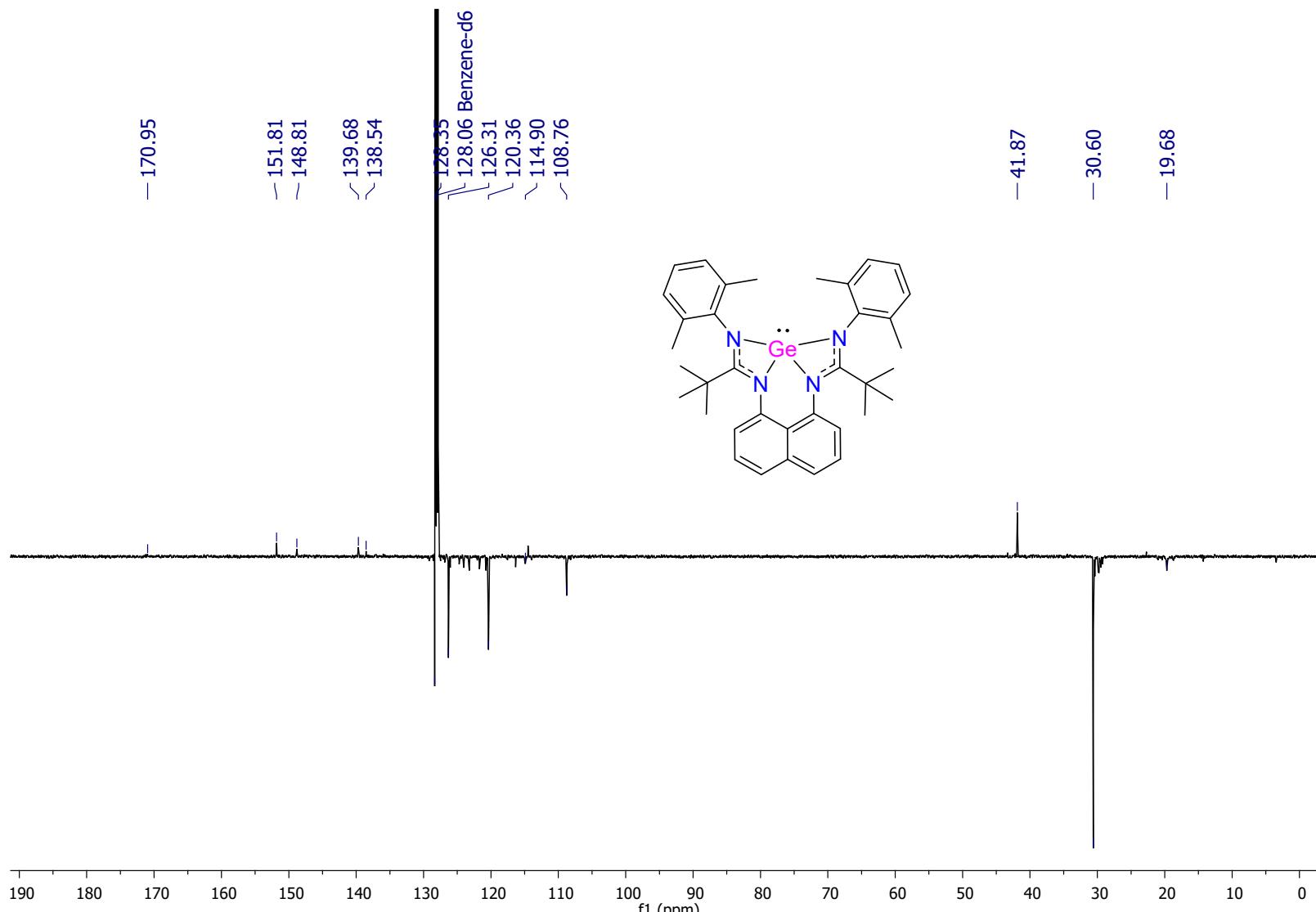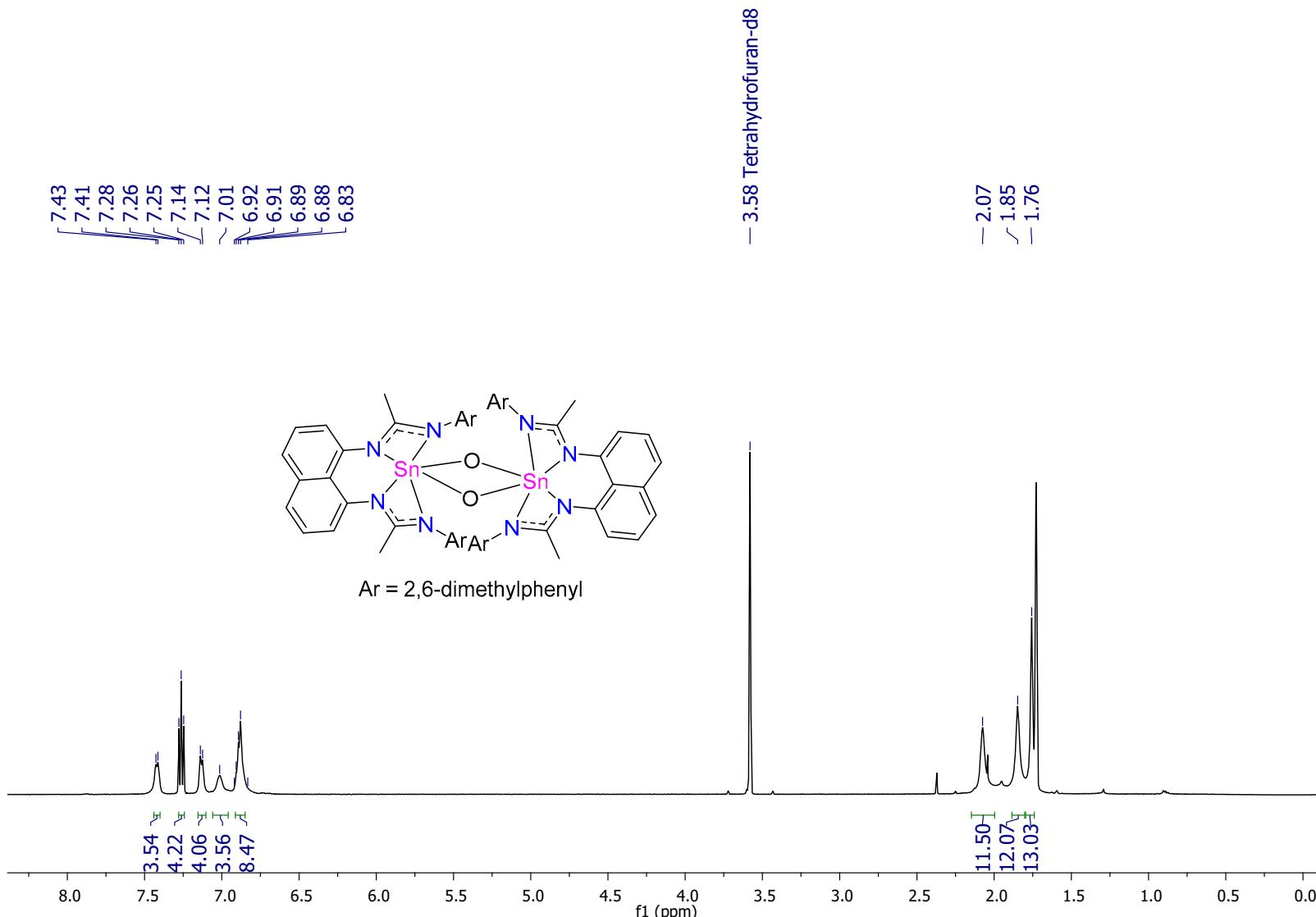
^{1}H NMR spectrum of compound **1a** (THF-d$_8$, 500 MHz)

Ar = 2,6-dimethylphenyl

168.70

143.64
142.68
138.50
136.98
135.26
128.74
128.31
126.26
125.69
124.81
120.59

67.57 Tetrahydrofuran-d8

19.81
19.03
15.76

Ar = 2,6-dimethylphenyl

$^{13}C\{^1H\}$ NMR spectrum of compound **1a** (THF-d$_8$, 125 MHz)

—494.50
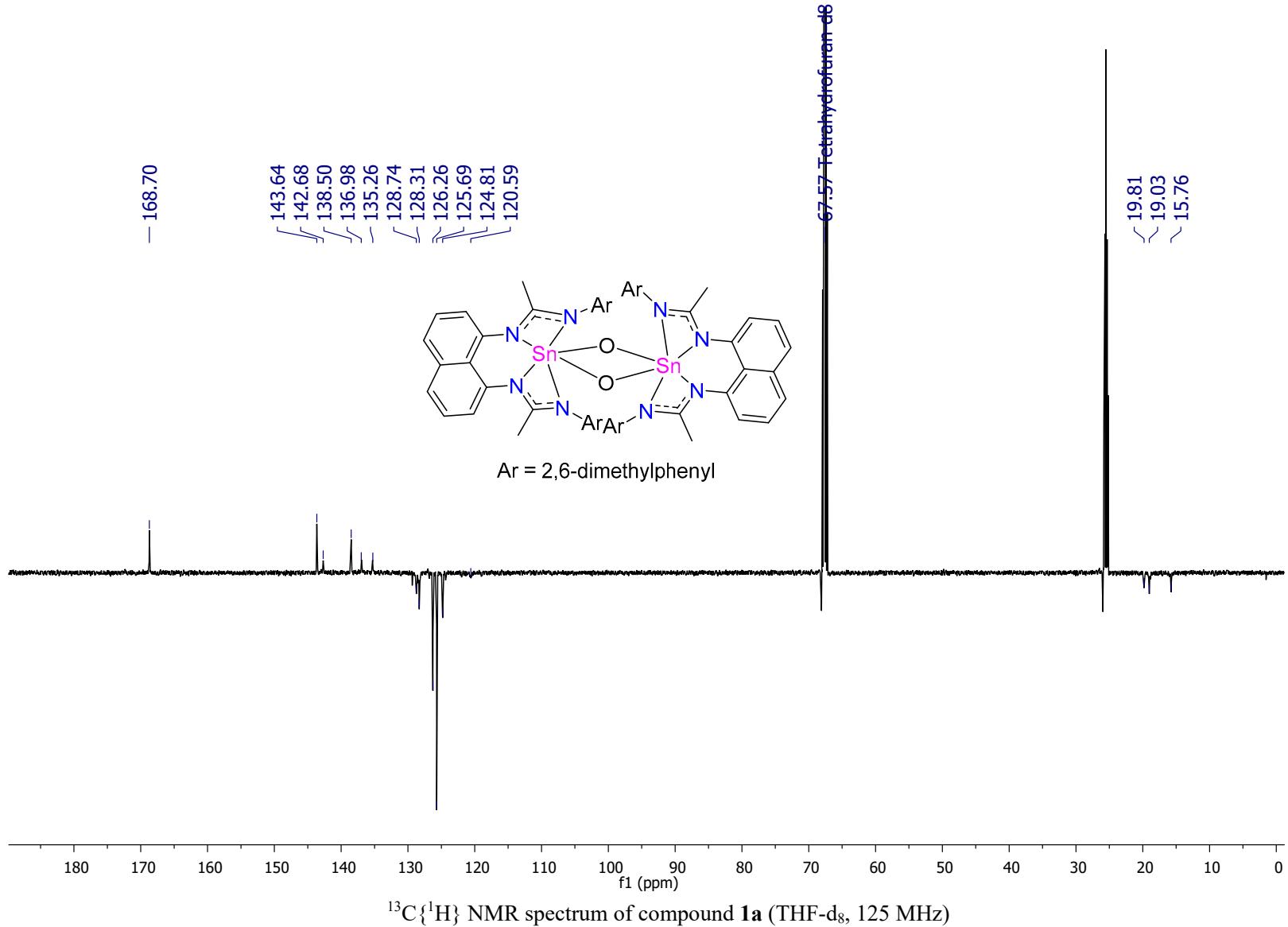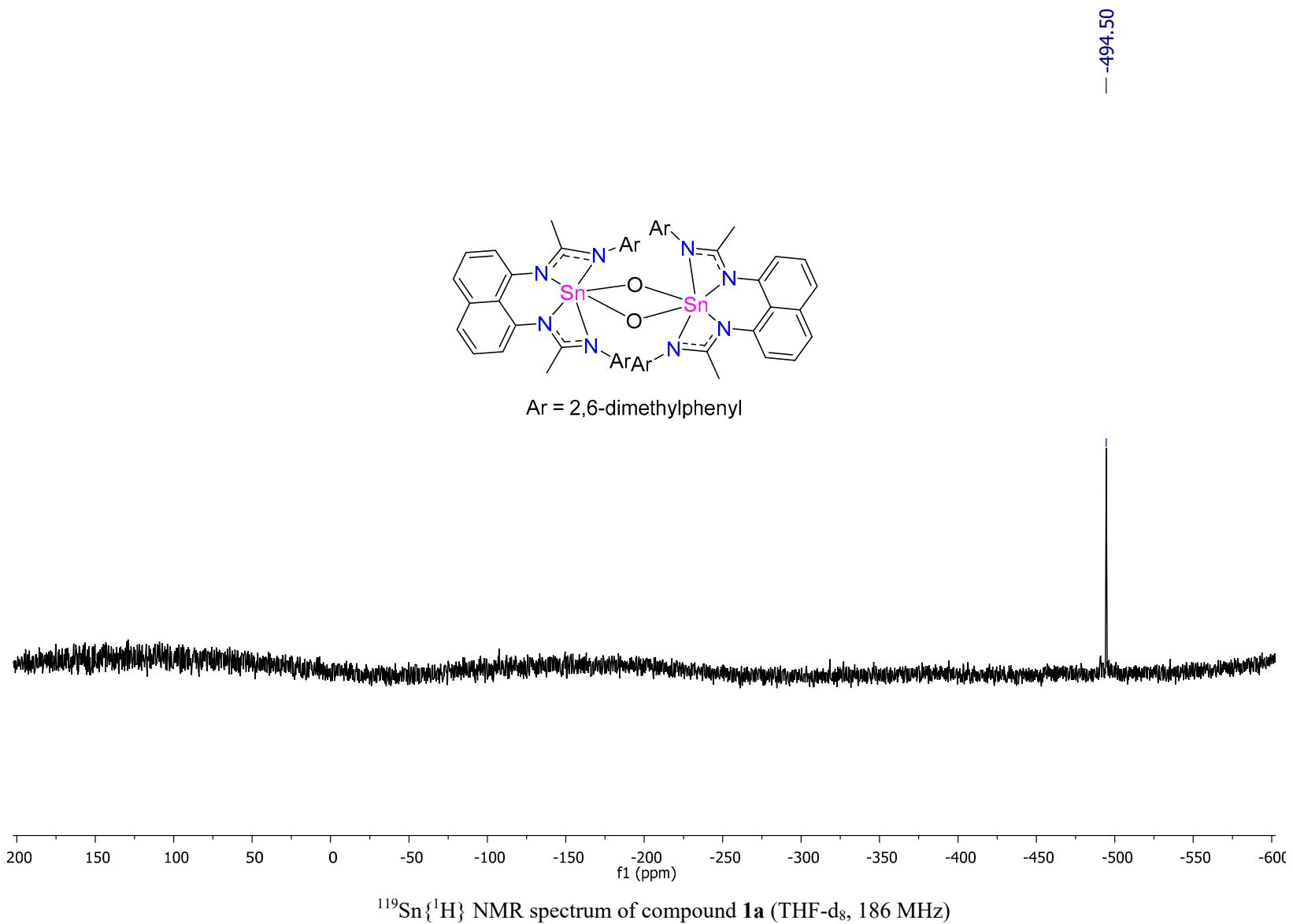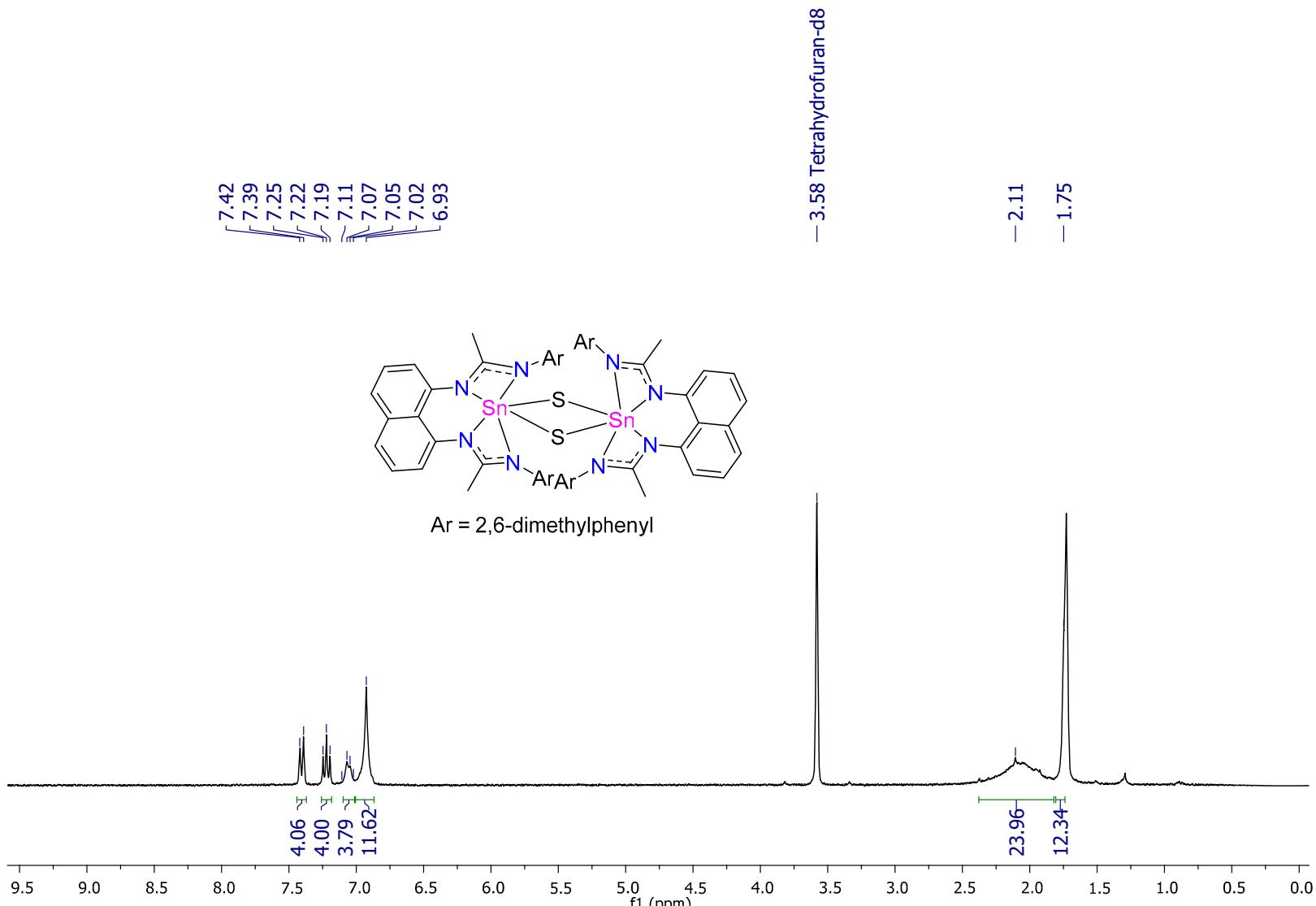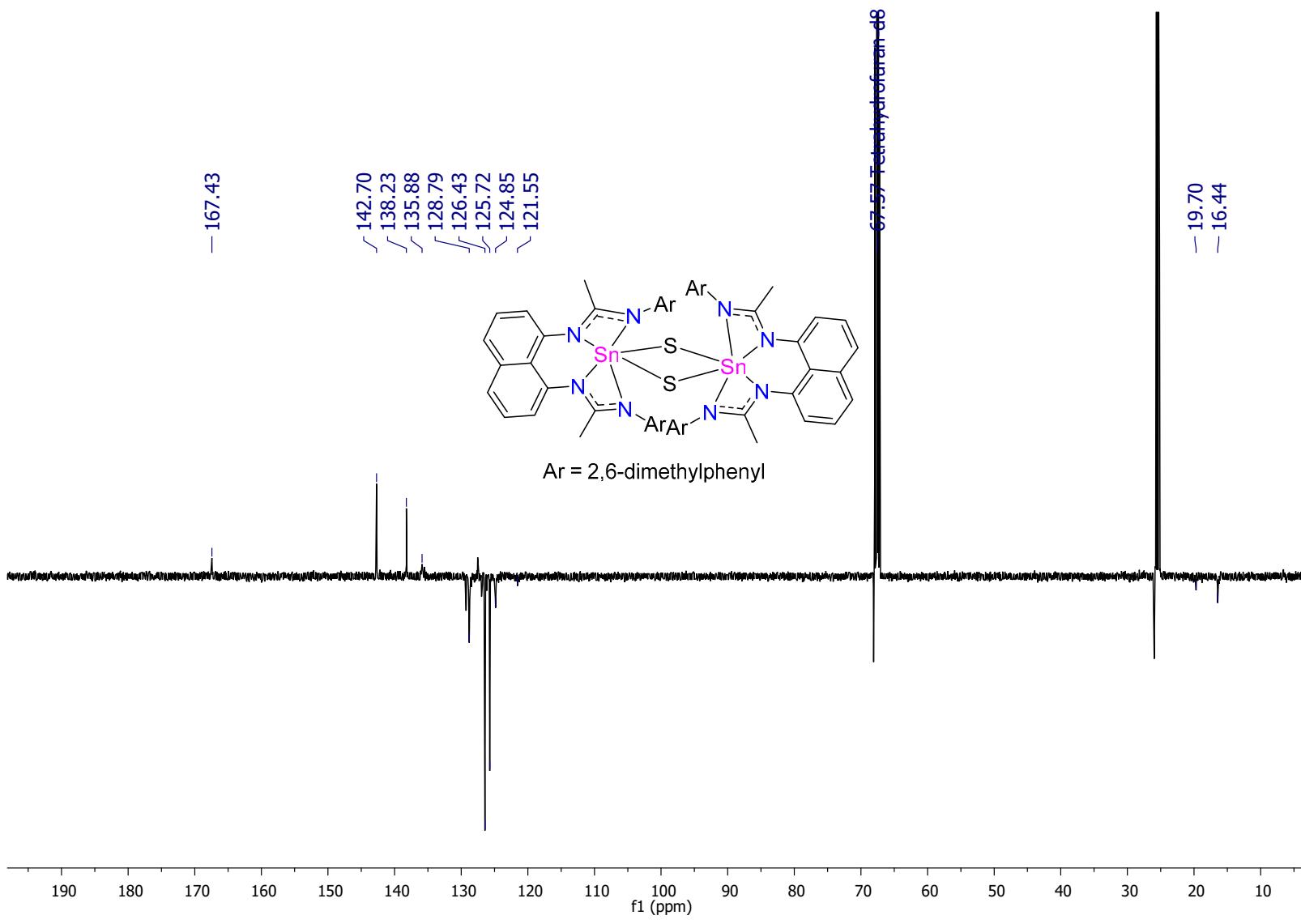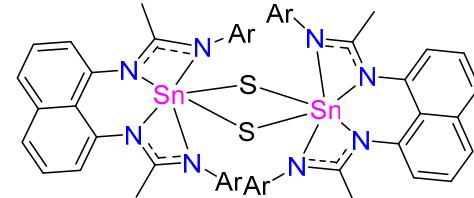
Ar = 2,6-dimethylphenyl

^{119}Sn{^{1}H} NMR spectrum of compound **1a** (THF-d$_8$, 186 MHz)

7.42
7.39
7.25
7.22
7.19
7.11
7.07
7.05
7.02
6.93

3.58 Tetrahydrofuran-d8

2.11

1.75

Ar = 2,6-dimethylphenyl

4.06
4.00
3.79
11.62

23.96
12.34

^{1}H NMR spectrum of compound **1b** (THF-d$_8$, 300 MHz)

167.43

142.70
138.23
135.88
128.79
126.43
125.72
124.85
121.55

67.57 Tetrahydrofuran-d8

19.70
16.44

Ar = 2,6-dimethylphenyl

$^{13}C\{^{1}H\}$ NMR spectrum of compound **1b** (THF-d$_8$, 125 MHz)

Ar = 2,6-dimethylphenyl

—−647.99

-520 -530 -540 -550 -560 -570 -580 -590 -600 -610 -620 -630 -640 -650 -660 -670 -680 -690
f1 (ppm)

^{119}Sn{^{1}H} NMR spectrum of compound **1b** (THF-d$_8$, 186 MHz)

20

7.41
7.40
7.39
7.39
7.25
7.23
7.21
7.18
7.18
7.17
7.16
7.04
7.02
7.00
6.99
6.98
6.97
6.96
6.64
6.62
6.45
6.43

— 3.58 Tetrahydrofuran-d8

2.19
2.09
1.79

1.97
2.09
2.03
6.25
3.89
3.90

11.86
5.94
6.02

8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

^{1}H NMR spectrum of compound **2a** (THF-d$_8$, 500 MHz)

$^{13}C\{^1H\}$ NMR spectrum of compound **2a** (THF-d$_8$, 125 MHz)

—456.70

^{119}Sn{^{1}H} NMR spectrum of compound **2a** (THF-d$_8$, 186 MHz)

23

^{1}H NMR spectrum of compound **2b** (THF-d$_8$, 500 MHz)
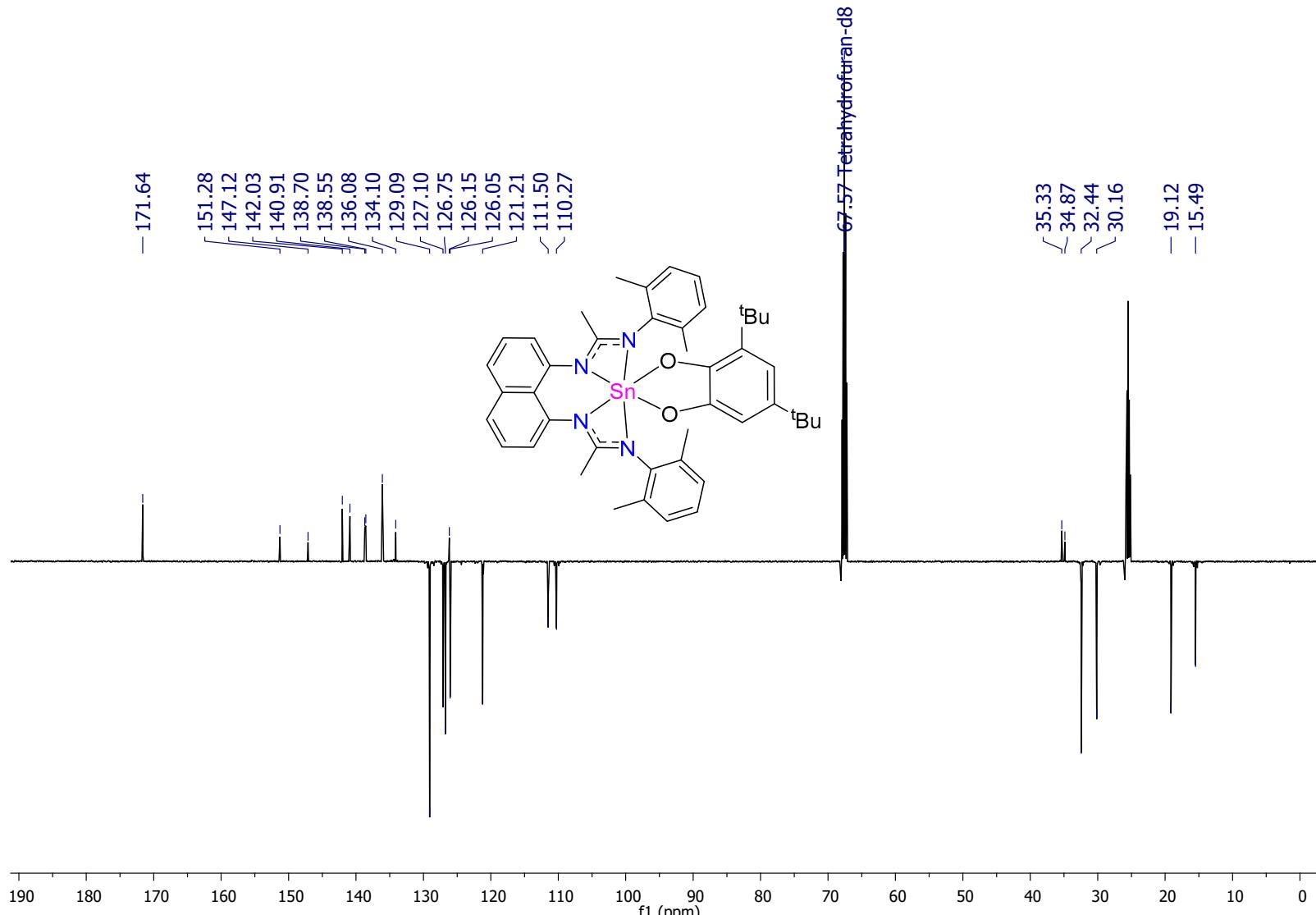
$^{13}C\{^1H\}$ NMR spectrum of compound **2b** (THF-d$_8$, 125 MHz)
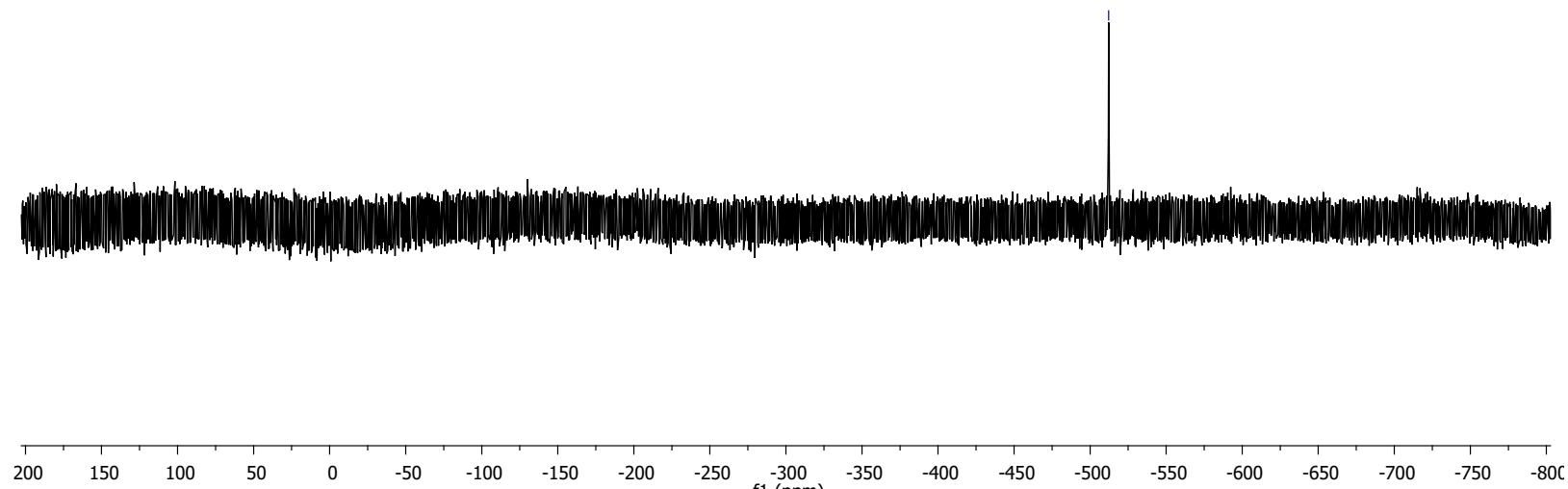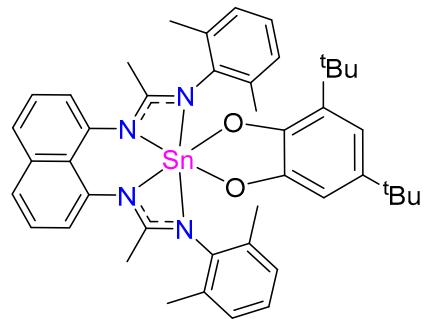
25

^{119}Sn{^{1}H} NMR spectrum of compound **2b** (THF-d$_8$, 186 MHz)
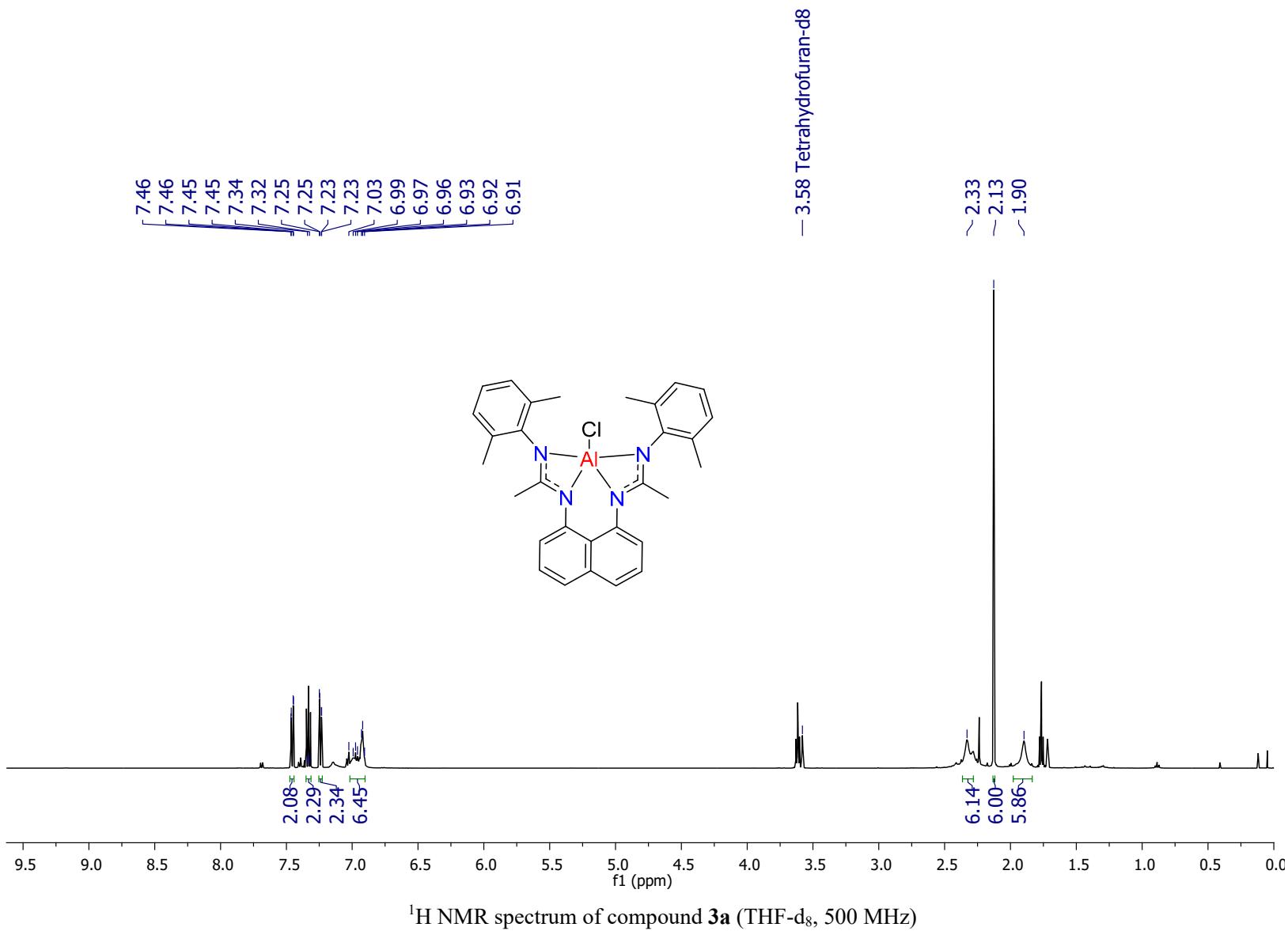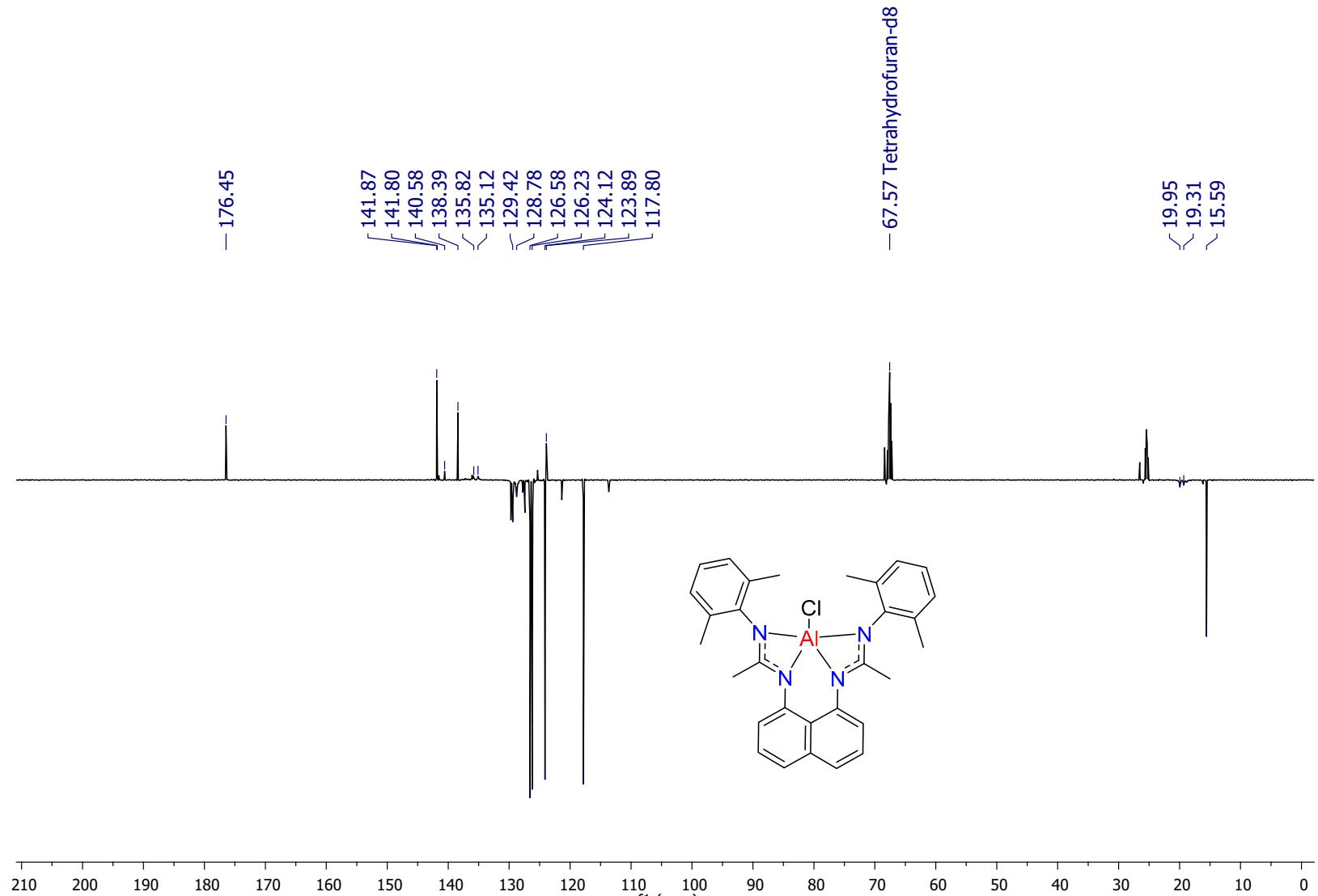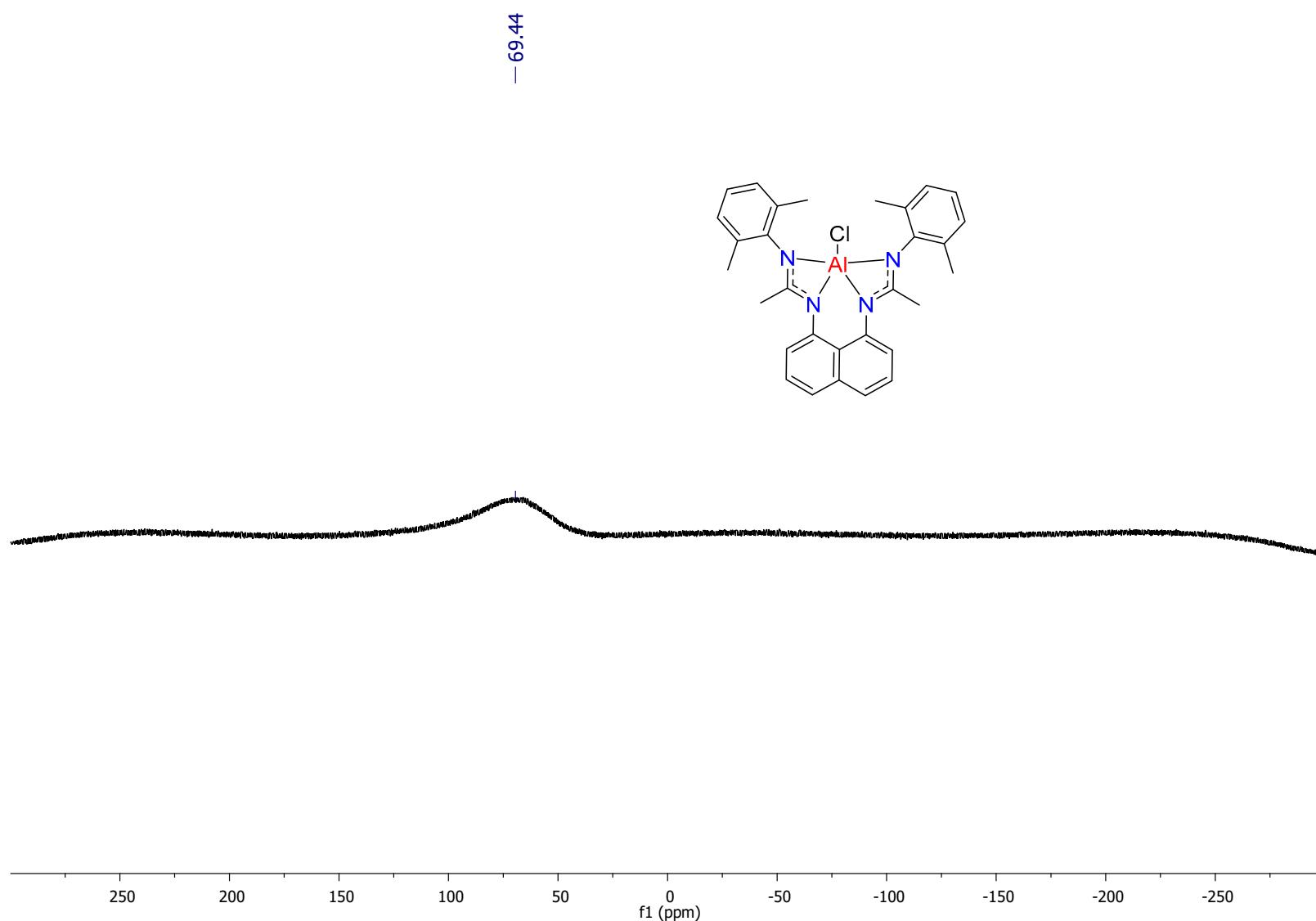
— −512.16

^{1}H NMR spectrum of compound **3a** (THF-d$_8$, 500 MHz)

$^{13}C\{^1H\}$ NMR spectrum of compound **3a** (THF-d$_8$, 125 MHz)

Peak labels: 176.45, 141.87, 141.80, 140.58, 138.39, 135.82, 135.12, 129.42, 128.78, 126.58, 126.23, 124.12, 123.89, 117.80, 67.57 Tetrahydrofuran-d8, 19.95, 19.31, 15.59

f1 (ppm)

28

—69.44

^{27}Al{^{1}H} NMR spectrum of compound **3a** (THF-d$_8$, 130 MHz)

^{1}H NMR spectrum of compound **3b** (THF-d$_8$, 500 MHz)

$^{13}C\{^1H\}$ NMR spectrum of compound **3b** (THF-d$_8$, 125 MHz)

31
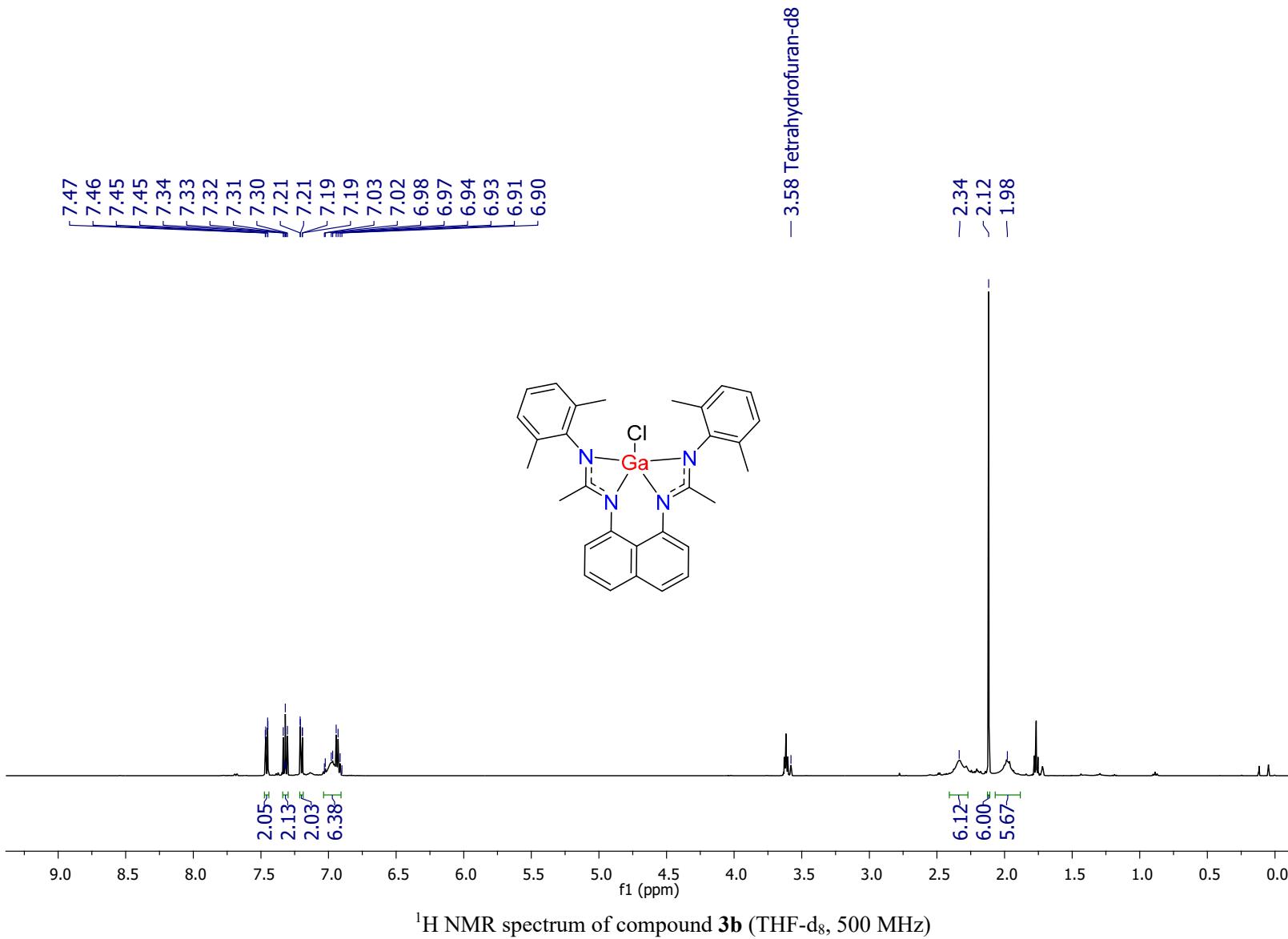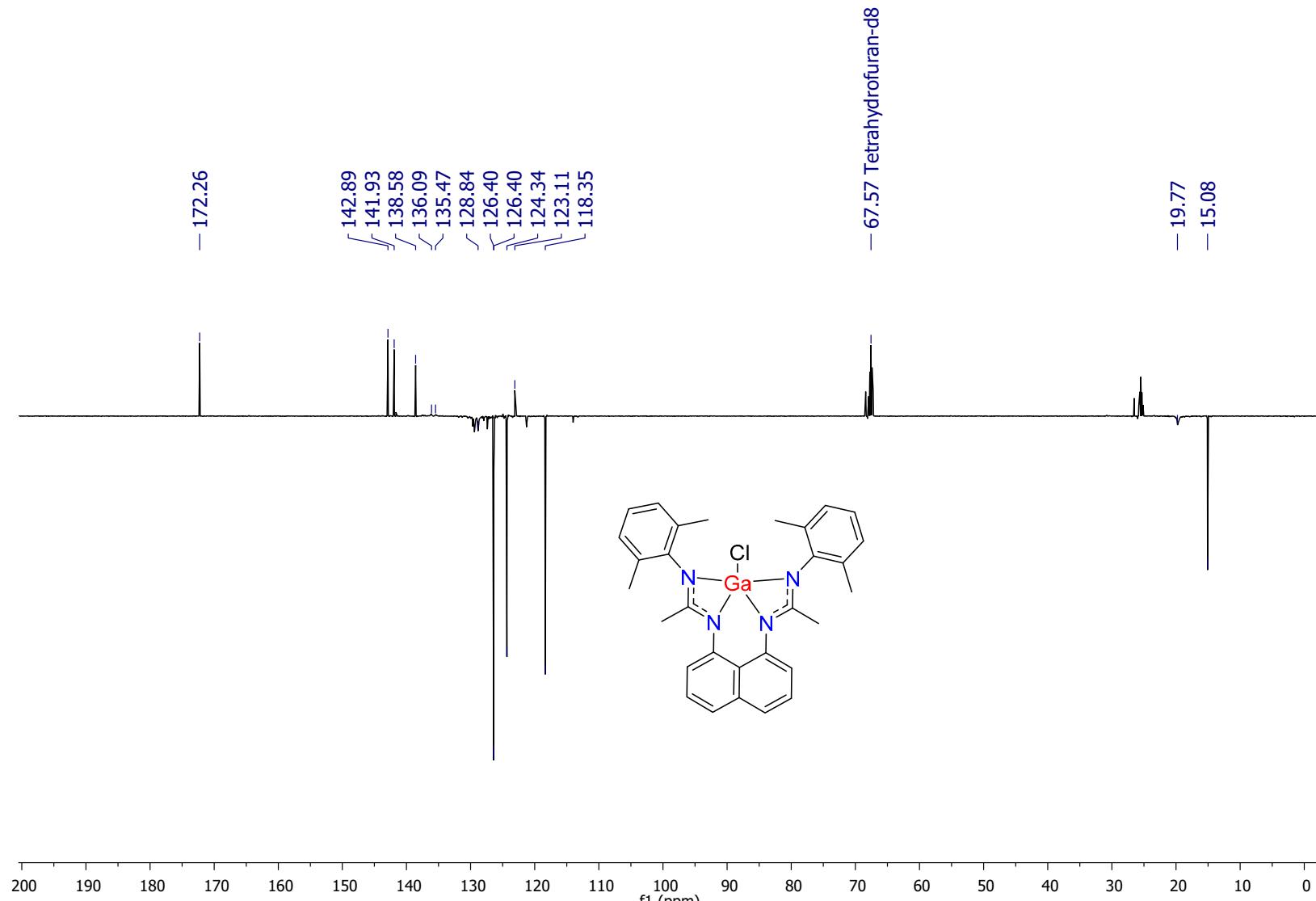
Crystal data and structure refinement of compound L₃H₂
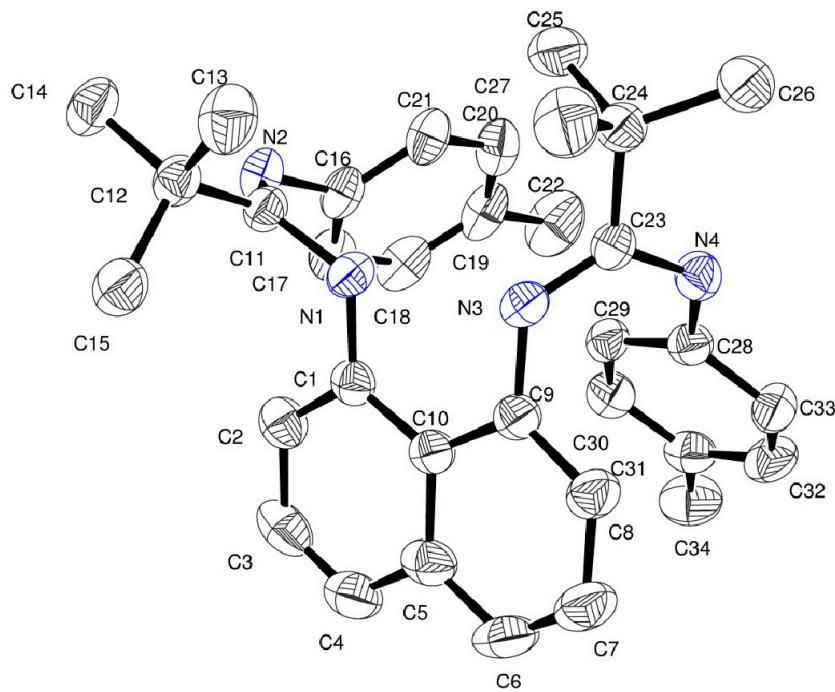
Figure S1. Asymmetric Unit

Table S1. Crystal data and structure refinement for R104.

Identification code	R104
Empirical formula	C34 H40 N4
Formula weight	504.70
Temperature	193(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, P 21 21 21
Unit cell dimensions	a = 10.4214(4) A alpha = 90 deg.
	b = 16.1580(7) A beta = 90 deg.
	c = 17.5675(8) A gamma = 90 deg.
Volume	2958.2(2) A^3
Z, Calculated density	4, 1.133 Mg/m^3
Absorption coefficient	0.067 mm^-1

```
F(000)                           1088

Crystal size                     0.180 x 0.160 x 0.100 mm

Theta range for data collection  2.639 to 25.376 deg.

Limiting indices                 -12<=h<=12, -18<=k<=19,
                                  -21<=l<=21

Reflections collected / unique   45826 / 5433 [R(int) = 0.1088]

Completeness to theta = 25.242   99.8 %

Refinement method                Full-matrix least-squares on F^2

Data / restraints / parameters   5433 / 0 / 359

Goodness-of-fit on F^2           1.030

Final R indices [I>2sigma(I)]    R1 = 0.0510, wR2 = 0.1244

R indices (all data)             R1 = 0.0756, wR2 = 0.1404

Largest diff. peak and hole      0.762 and -0.156 e.A^-3
```

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic
displacement parameters (A^2 x 10^3) for R104.
U(eq) is defined as one third of the trace of the orthogonalized
Uij tensor.

_____

	x	y	z	U(eq)
C(1)	8472(3)	3199(2)	2197(2)	35(1)
C(2)	9235(4)	3678(3)	2654(2)	44(1)
C(3)	10477(4)	3409(3)	2863(3)	54(1)
C(4)	10944(4)	2678(3)	2617(3)	53(1)
C(5)	10202(4)	2163(3)	2141(2)	45(1)
C(6)	10697(4)	1404(3)	1870(3)	55(1)
C(7)	10001(4)	909(3)	1406(3)	55(1)
C(8)	8753(4)	1127(2)	1200(2)	43(1)
C(9)	8213(3)	1856(2)	1457(2)	35(1)
C(10)	8935(3)	2410(2)	1926(2)	34(1)
C(11)	6840(4)	4297(2)	2095(2)	36(1)
C(12)	6932(4)	4882(2)	1420(2)	39(1)
C(13)	6144(5)	4531(3)	759(2)	59(1)
C(14)	6417(4)	5738(3)	1612(3)	52(1)
C(15)	8333(4)	4955(3)	1176(3)	52(1)
C(16)	6200(4)	3962(2)	3331(2)	40(1)
C(17)	6953(4)	3963(3)	3975(2)	47(1)
C(18)	6691(5)	3425(3)	4572(2)	54(1)
C(19)	5651(5)	2901(3)	4557(2)	53(1)
C(20)	4872(5)	2921(3)	3916(3)	53(1)
C(21)	5146(5)	3436(2)	3314(2)	46(1)
C(22)	5392(6)	2320(3)	5212(3)	80(2)
C(23)	5993(3)	1598(2)	1292(2)	32(1)
C(24)	4758(4)	1812(2)	863(2)	38(1)
C(25)	4060(4)	2476(3)	1336(3)	56(1)
C(26)	3865(4)	1068(3)	774(2)	48(1)
C(27)	5077(5)	2145(3)	71(3)	59(1)
C(28)	6650(3)	812(2)	2451(2)	34(1)
C(29)	6898(3)	1451(2)	2950(2)	36(1)
C(30)	7495(4)	1292(3)	3637(2)	43(1)
C(31)	7850(4)	501(3)	3853(2)	43(1)
C(32)	7610(4)	-132(3)	3347(3)	49(1)
C(33)	7035(4)	16(2)	2651(2)	42(1)
C(34)	8437(5)	340(3)	4628(3)	65(1)
N(1)	7260(3)	3472(2)	1969(2)	36(1)
N(2)	6394(3)	4539(2)	2732(2)	40(1)
N(3)	6974(3)	2068(2)	1191(2)	34(1)
N(4)	5926(3)	932(2)	1777(2)	39(1)

_____

Table S3. Bond lengths [A] and angles [deg] for R104.
_____

C(1)-C(2)	1.371(5)
C(1)-N(1)	1.397(5)
C(1)-C(10)	1.443(5)
C(2)-C(3)	1.414(6)
C(2)-H(2)	0.9500
C(3)-C(4)	1.349(7)
C(3)-H(3)	0.9500
C(4)-C(5)	1.409(6)
C(4)-H(4)	0.9500
C(5)-C(6)	1.414(6)
C(5)-C(10)	1.431(5)
C(6)-C(7)	1.352(7)
C(6)-H(6)	0.9500
C(7)-C(8)	1.395(6)
C(7)-H(7)	0.9500
C(8)-C(9)	1.381(5)
C(8)-H(8)	0.9500
C(9)-N(3)	1.416(5)
C(9)-C(10)	1.430(5)
C(11)-N(2)	1.272(5)
C(11)-N(1)	1.421(5)
C(11)-C(12)	1.519(5)
C(12)-C(14)	1.521(5)
C(12)-C(15)	1.526(6)
C(12)-C(13)	1.531(6)
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(16)-C(17)	1.378(6)
C(16)-C(21)	1.389(6)
C(16)-N(2)	1.421(5)
C(17)-C(18)	1.389(6)
C(17)-H(17)	0.9500
C(18)-C(19)	1.376(7)
C(18)-H(18)	0.9500
C(19)-C(20)	1.389(7)
C(19)-C(22)	1.509(6)
C(20)-C(21)	1.376(6)
C(20)-H(20)	0.9500
C(21)-H(21)	0.9500
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(23)-N(3)	1.286(5)
C(23)-N(4)	1.373(5)

```
C(23)-C(24)              1.531(5)
C(24)-C(27)              1.528(6)
C(24)-C(26)              1.529(5)
C(24)-C(25)              1.540(6)
C(25)-H(25A)             0.9800
C(25)-H(25B)             0.9800
C(25)-H(25C)             0.9800
C(26)-H(26A)             0.9800
C(26)-H(26B)             0.9800
C(26)-H(26C)             0.9800
C(27)-H(27A)             0.9800
C(27)-H(27B)             0.9800
C(27)-H(27C)             0.9800
C(28)-C(29)              1.380(5)
C(28)-C(33)              1.392(5)
C(28)-N(4)               1.419(5)
C(29)-C(30)              1.382(5)
C(29)-H(29)              0.9500
C(30)-C(31)              1.383(6)
C(30)-H(30)              0.9500
C(31)-C(32)              1.378(6)
C(31)-C(34)              1.515(6)
C(32)-C(33)              1.383(6)
C(32)-H(32)              0.9500
C(33)-H(33)              0.9500
C(34)-H(34A)             0.9800
C(34)-H(34B)             0.9800
C(34)-H(34C)             0.9800
N(1)-H(1)                0.89(5)
N(4)-H(4A)               0.89(5)

C(2)-C(1)-N(1)           120.9(4)
C(2)-C(1)-C(10)          119.9(3)
N(1)-C(1)-C(10)          119.1(3)
C(1)-C(2)-C(3)           120.6(4)
C(1)-C(2)-H(2)           119.7
C(3)-C(2)-H(2)           119.7
C(4)-C(3)-C(2)           121.1(4)
C(4)-C(3)-H(3)           119.5
C(2)-C(3)-H(3)           119.5
C(3)-C(4)-C(5)           120.6(4)
C(3)-C(4)-H(4)           119.7
C(5)-C(4)-H(4)           119.7
C(4)-C(5)-C(6)           120.8(4)
C(4)-C(5)-C(10)          119.9(4)
C(6)-C(5)-C(10)          119.3(4)
C(7)-C(6)-C(5)           121.4(4)
C(7)-C(6)-H(6)           119.3
C(5)-C(6)-H(6)           119.3
C(6)-C(7)-C(8)           120.5(4)
C(6)-C(7)-H(7)           119.8
C(8)-C(7)-H(7)           119.8
C(9)-C(8)-C(7)           120.7(4)
C(9)-C(8)-H(8)           119.7
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C(7)-C(8)-H(8)              119.7
C(8)-C(9)-N(3)              118.0(3)
C(8)-C(9)-C(10)             120.5(3)
N(3)-C(9)-C(10)             121.2(3)
C(9)-C(10)-C(5)             117.6(3)
C(9)-C(10)-C(1)             124.5(3)
C(5)-C(10)-C(1)             117.8(4)
N(2)-C(11)-N(1)             122.5(3)
N(2)-C(11)-C(12)            121.2(3)
N(1)-C(11)-C(12)            116.2(3)
C(11)-C(12)-C(14)           111.7(3)
C(11)-C(12)-C(15)           109.1(3)
C(14)-C(12)-C(15)           109.2(3)
C(11)-C(12)-C(13)           109.2(3)
C(14)-C(12)-C(13)           108.4(4)
C(15)-C(12)-C(13)           109.2(4)
C(12)-C(13)-H(13A)          109.5
C(12)-C(13)-H(13B)          109.5
H(13A)-C(13)-H(13B)         109.5
C(12)-C(13)-H(13C)          109.5
H(13A)-C(13)-H(13C)         109.5
H(13B)-C(13)-H(13C)         109.5
C(12)-C(14)-H(14A)          109.5
C(12)-C(14)-H(14B)          109.5
H(14A)-C(14)-H(14B)         109.5
C(12)-C(14)-H(14C)          109.5
H(14A)-C(14)-H(14C)         109.5
H(14B)-C(14)-H(14C)         109.5
C(12)-C(15)-H(15A)          109.5
C(12)-C(15)-H(15B)          109.5
H(15A)-C(15)-H(15B)         109.5
C(12)-C(15)-H(15C)          109.5
H(15A)-C(15)-H(15C)         109.5
H(15B)-C(15)-H(15C)         109.5
C(17)-C(16)-C(21)           118.0(4)
C(17)-C(16)-N(2)            121.8(4)
C(21)-C(16)-N(2)            119.9(4)
C(16)-C(17)-C(18)           120.5(4)
C(16)-C(17)-H(17)           119.7
C(18)-C(17)-H(17)           119.7
C(19)-C(18)-C(17)           121.7(4)
C(19)-C(18)-H(18)           119.1
C(17)-C(18)-H(18)           119.1
C(18)-C(19)-C(20)           117.5(4)
C(18)-C(19)-C(22)           120.6(5)
C(20)-C(19)-C(22)           121.9(5)
C(21)-C(20)-C(19)           121.0(4)
C(21)-C(20)-H(20)           119.5
C(19)-C(20)-H(20)           119.5
C(20)-C(21)-C(16)           121.2(4)
C(20)-C(21)-H(21)           119.4
C(16)-C(21)-H(21)           119.4
C(19)-C(22)-H(22A)          109.5
C(19)-C(22)-H(22B)          109.5
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H(22A)-C(22)-H(22B)          109.5
C(19)-C(22)-H(22C)           109.5
H(22A)-C(22)-H(22C)          109.5
H(22B)-C(22)-H(22C)          109.5
N(3)-C(23)-N(4)              126.1(3)
N(3)-C(23)-C(24)             117.8(3)
N(4)-C(23)-C(24)             116.1(3)
C(27)-C(24)-C(26)            108.4(3)
C(27)-C(24)-C(23)            110.2(3)
C(26)-C(24)-C(23)            112.6(3)
C(27)-C(24)-C(25)            110.4(4)
C(26)-C(24)-C(25)            108.4(3)
C(23)-C(24)-C(25)            106.8(3)
C(24)-C(25)-H(25A)           109.5
C(24)-C(25)-H(25B)           109.5
H(25A)-C(25)-H(25B)          109.5
C(24)-C(25)-H(25C)           109.5
H(25A)-C(25)-H(25C)          109.5
H(25B)-C(25)-H(25C)          109.5
C(24)-C(26)-H(26A)           109.5
C(24)-C(26)-H(26B)           109.5
H(26A)-C(26)-H(26B)          109.5
C(24)-C(26)-H(26C)           109.5
H(26A)-C(26)-H(26C)          109.5
H(26B)-C(26)-H(26C)          109.5
C(24)-C(27)-H(27A)           109.5
C(24)-C(27)-H(27B)           109.5
H(27A)-C(27)-H(27B)          109.5
C(24)-C(27)-H(27C)           109.5
H(27A)-C(27)-H(27C)          109.5
H(27B)-C(27)-H(27C)          109.5
C(29)-C(28)-C(33)            118.6(3)
C(29)-C(28)-N(4)             121.8(3)
C(33)-C(28)-N(4)             119.4(3)
C(28)-C(29)-C(30)            120.0(3)
C(28)-C(29)-H(29)            120.0
C(30)-C(29)-H(29)            120.0
C(29)-C(30)-C(31)            122.2(4)
C(29)-C(30)-H(30)            118.9
C(31)-C(30)-H(30)            118.9
C(32)-C(31)-C(30)            117.4(4)
C(32)-C(31)-C(34)            121.7(4)
C(30)-C(31)-C(34)            120.9(4)
C(31)-C(32)-C(33)            121.5(4)
C(31)-C(32)-H(32)            119.3
C(33)-C(32)-H(32)            119.3
C(32)-C(33)-C(28)            120.4(4)
C(32)-C(33)-H(33)            119.8
C(28)-C(33)-H(33)            119.8
C(31)-C(34)-H(34A)           109.5
C(31)-C(34)-H(34B)           109.5
H(34A)-C(34)-H(34B)          109.5
C(31)-C(34)-H(34C)           109.5
H(34A)-C(34)-H(34C)          109.5
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H(34B)-C(34)-H(34C)        109.5
C(1)-N(1)-C(11)            122.0(3)
C(1)-N(1)-H(1)             111(3)
C(11)-N(1)-H(1)            119(3)
C(11)-N(2)-C(16)           120.1(3)
C(23)-N(3)-C(9)            122.5(3)
C(23)-N(4)-C(28)           126.8(3)
C(23)-N(4)-H(4A)           115(3)
C(28)-N(4)-H(4A)           115(3)
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Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters (A^2 x 10^3) for R104.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

_____

	U11	U22	U33	U23	U13	U12
C(1)	34(2)	37(2)	32(2)	7(2)	3(2)	-3(2)
C(2)	44(2)	47(2)	39(2)	3(2)	0(2)	-6(2)
C(3)	42(2)	73(3)	46(2)	9(2)	-7(2)	-18(2)
C(4)	36(2)	67(3)	56(3)	16(2)	0(2)	1(2)
C(5)	35(2)	56(3)	42(2)	16(2)	6(2)	2(2)
C(6)	39(2)	63(3)	62(3)	19(2)	9(2)	21(2)
C(7)	49(3)	50(3)	64(3)	4(2)	19(2)	17(2)
C(8)	41(2)	40(2)	49(2)	3(2)	12(2)	6(2)
C(9)	33(2)	36(2)	35(2)	6(2)	8(2)	2(2)
C(10)	32(2)	37(2)	32(2)	11(2)	8(2)	1(2)
C(11)	38(2)	30(2)	39(2)	-1(2)	-1(2)	2(2)
C(12)	44(2)	35(2)	38(2)	5(2)	7(2)	4(2)
C(13)	76(3)	56(3)	44(2)	14(2)	-3(2)	-4(2)
C(14)	61(3)	41(2)	55(3)	15(2)	18(2)	12(2)
C(15)	54(3)	48(2)	54(3)	12(2)	18(2)	7(2)
C(16)	60(3)	30(2)	31(2)	-5(2)	5(2)	5(2)
C(17)	59(3)	43(2)	38(2)	-4(2)	-1(2)	1(2)
C(18)	79(3)	50(2)	31(2)	-1(2)	2(2)	16(3)
C(19)	83(3)	38(2)	40(2)	4(2)	17(2)	11(2)
C(20)	68(3)	38(2)	53(3)	3(2)	10(2)	-4(2)
C(21)	67(3)	33(2)	39(2)	-3(2)	1(2)	2(2)
C(22)	110(5)	72(4)	58(3)	23(3)	19(3)	11(3)
C(23)	37(2)	29(2)	30(2)	-2(2)	1(2)	2(2)
C(24)	38(2)	37(2)	39(2)	-4(2)	-9(2)	1(2)
C(25)	44(2)	48(2)	74(3)	-16(2)	-13(2)	8(2)
C(26)	48(2)	48(2)	48(2)	-6(2)	-11(2)	-1(2)
C(27)	71(3)	59(3)	47(3)	15(2)	-18(2)	-5(2)
C(28)	31(2)	35(2)	35(2)	5(2)	2(2)	2(2)
C(29)	37(2)	32(2)	39(2)	7(2)	7(2)	2(2)
C(30)	42(2)	47(2)	38(2)	-1(2)	4(2)	0(2)
C(31)	36(2)	53(2)	41(2)	8(2)	1(2)	4(2)
C(32)	49(2)	44(2)	54(3)	16(2)	0(2)	12(2)
C(33)	46(2)	32(2)	49(2)	1(2)	2(2)	1(2)
C(34)	61(3)	79(3)	54(3)	11(3)	-8(2)	12(3)
N(1)	40(2)	32(2)	38(2)	-2(1)	-4(1)	6(1)
N(2)	56(2)	31(2)	34(2)	1(1)	2(2)	1(1)
N(3)	36(2)	32(2)	35(2)	2(1)	2(1)	6(1)
N(4)	40(2)	35(2)	41(2)	6(1)	-3(2)	-2(2)

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Crystal data and structure refinement of compound L₁Sn
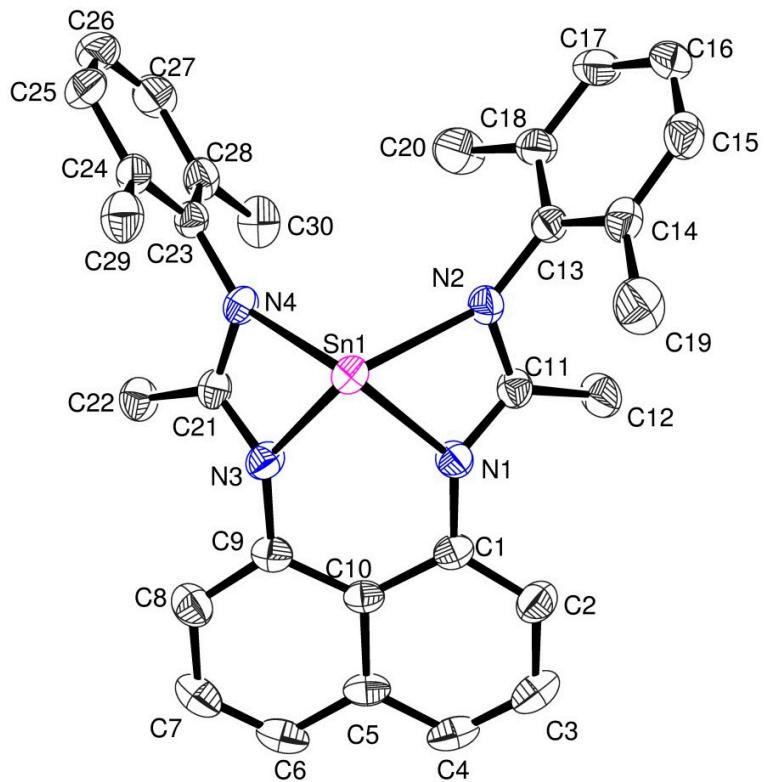
Figure S2. Asymmetric Unit

Table S5. Crystal data and structure refinement for R29.

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Identification code            R29

Empirical formula              C30 H30 N4 Sn

Formula weight                 565.29

Temperature                    193(2) K

Wavelength                     0.71073 A

Crystal system, space group    Monoclinic,  C 2/c

Unit cell dimensions     a = 20.6812(9) A    alpha = 90 deg.
                         b = 12.6563(5) A     beta = 96.409(2) deg.
                         c = 20.1577(8) A    gamma = 90 deg.

Volume                         5243.3(4) A^3
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Z, Calculated density              8,  1.432 Mg/m^3

Absorption coefficient             1.000 mm^-1

F(000)                             2304

Crystal size                       0.120 x 0.100 x 0.080 mm

Theta range for data collection    2.677 to 35.008 deg.

Limiting indices                   -33<=h<=33, -20<=k<=19,
                                    -31<=l<=32

Reflections collected / unique     95894 / 11564 [R(int) = 0.0699]

Completeness to theta = 25.242     99.9 %

Refinement method                  Full-matrix least-squares on F^2

Data / restraints / parameters     11564 / 0 / 322

Goodness-of-fit on F^2             1.029

Final R indices [I>2sigma(I)]      R1 = 0.0403, wR2 = 0.0747

R indices (all data)               R1 = 0.0784, wR2 = 0.0867

Largest diff. peak and hole        0.588 and -0.596 e.A^-3
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Table S6. Atomic coordinates (x 10^4) and equivalent isotropic
displacement parameters (A^2 x 10^3) for R29.
U(eq) is defined as one third of the trace of the orthogonalized
Uij tensor.

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	x	y	z	U(eq)
Sn(1)	7150(1)	5482(1)	5806(1)	25(1)
N(4)	6571(1)	4738(1)	4870(1)	26(1)
C(6)	5812(1)	9560(2)	5074(1)	40(1)
N(2)	6556(1)	4643(1)	6572(1)	29(1)
C(13)	6597(1)	3738(2)	6994(1)	28(1)
C(14)	7039(1)	3723(2)	7579(1)	33(1)
C(5)	5874(1)	8979(2)	5682(1)	32(1)
N(1)	6434(1)	6341(1)	6368(1)	29(1)
C(12)	5794(1)	5558(2)	7243(1)	41(1)
C(15)	7088(1)	2815(2)	7967(1)	38(1)
C(7)	5987(1)	9129(2)	4508(1)	43(1)
C(22)	5955(1)	5806(2)	3973(1)	36(1)
N(3)	6518(1)	6438(1)	5071(1)	30(1)
C(4)	5690(1)	9446(2)	6268(1)	40(1)
C(16)	6706(1)	1946(2)	7796(1)	43(1)
C(10)	6121(1)	7917(2)	5698(1)	26(1)
C(25)	7039(1)	2465(2)	3872(1)	42(1)
C(18)	6225(1)	2845(2)	6807(1)	34(1)
C(24)	7087(1)	3392(2)	4248(1)	31(1)
C(9)	6281(1)	7478(2)	5077(1)	29(1)
C(21)	6347(1)	5667(2)	4640(1)	27(1)
C(19)	7462(1)	4663(2)	7776(1)	52(1)
C(29)	7736(1)	3935(2)	4402(1)	40(1)
C(11)	6272(1)	5533(2)	6734(1)	29(1)
C(17)	6282(1)	1959(2)	7220(1)	43(1)
C(8)	6228(1)	8093(2)	4507(1)	38(1)
C(3)	5764(1)	8922(2)	6856(1)	46(1)
C(28)	5926(1)	3267(2)	4352(1)	33(1)
C(26)	6453(2)	1946(2)	3740(1)	48(1)
C(2)	6022(1)	7892(2)	6893(1)	38(1)
C(23)	6524(1)	3800(2)	4482(1)	26(1)
C(1)	6179(1)	7367(2)	6331(1)	28(1)
C(27)	5905(1)	2334(2)	3978(1)	43(1)
C(20)	5777(1)	2848(2)	6164(1)	52(1)
C(30)	5309(1)	3669(2)	4599(1)	43(1)

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Table S7. Bond lengths [A] and angles [deg] for R29.

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Sn(1)-N(3)	2.2232(17)
Sn(1)-N(1)	2.2435(17)
Sn(1)-N(4)	2.3181(16)
Sn(1)-N(2)	2.3327(17)
N(4)-C(21)	1.329(3)
N(4)-C(23)	1.420(2)
C(6)-C(7)	1.350(4)
C(6)-C(5)	1.422(3)
C(6)-H(6)	0.9500
N(2)-C(11)	1.328(3)
N(2)-C(13)	1.423(3)
C(13)-C(18)	1.395(3)
C(13)-C(14)	1.409(3)
C(14)-C(15)	1.387(3)
C(14)-C(19)	1.505(3)
C(5)-C(4)	1.410(3)
C(5)-C(10)	1.437(3)
N(1)-C(11)	1.326(3)
N(1)-C(1)	1.400(3)
C(12)-C(11)	1.503(3)
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(15)-C(16)	1.375(4)
C(15)-H(15)	0.9500
C(7)-C(8)	1.403(3)
C(7)-H(7)	0.9500
C(22)-C(21)	1.500(3)
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
N(3)-C(21)	1.328(3)
N(3)-C(9)	1.405(3)
C(4)-C(3)	1.352(4)
C(4)-H(4)	0.9500
C(16)-C(17)	1.375(4)
C(16)-H(16)	0.9500
C(10)-C(9)	1.442(3)
C(10)-C(1)	1.447(3)
C(25)-C(26)	1.379(4)
C(25)-C(24)	1.394(3)
C(25)-H(25)	0.9500
C(18)-C(17)	1.392(3)
C(18)-C(20)	1.507(3)
C(24)-C(23)	1.404(3)
C(24)-C(29)	1.509(3)
C(9)-C(8)	1.380(3)
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(29)-H(29A)	0.9800

```
C(29)-H(29B)                    0.9800
C(29)-H(29C)                    0.9800
C(17)-H(17)                     0.9500
C(8)-H(8)                       0.9500
C(3)-C(2)                       1.408(3)
C(3)-H(3)                       0.9500
C(28)-C(27)                     1.399(3)
C(28)-C(23)                     1.406(3)
C(28)-C(30)                     1.509(3)
C(26)-C(27)                     1.369(4)
C(26)-H(26)                     0.9500
C(2)-C(1)                       1.383(3)
C(2)-H(2)                       0.9500
C(27)-H(27)                     0.9500
C(20)-H(20A)                    0.9800
C(20)-H(20B)                    0.9800
C(20)-H(20C)                    0.9800
C(30)-H(30A)                    0.9800
C(30)-H(30B)                    0.9800
C(30)-H(30C)                    0.9800

N(3)-Sn(1)-N(1)                 72.57(6)
N(3)-Sn(1)-N(4)                 57.74(6)
N(1)-Sn(1)-N(4)                107.35(6)
N(3)-Sn(1)-N(2)                112.07(6)
N(1)-Sn(1)-N(2)                 57.38(6)
N(4)-Sn(1)-N(2)                 95.29(6)
C(21)-N(4)-C(23)               123.17(17)
C(21)-N(4)-Sn(1)                93.11(12)
C(23)-N(4)-Sn(1)               141.84(13)
C(7)-C(6)-C(5)                 120.8(2)
C(7)-C(6)-H(6)                 119.6
C(5)-C(6)-H(6)                 119.6
C(11)-N(2)-C(13)               122.30(17)
C(11)-N(2)-Sn(1)                93.22(12)
C(13)-N(2)-Sn(1)               139.58(13)
C(18)-C(13)-C(14)              120.13(19)
C(18)-C(13)-N(2)               119.73(18)
C(14)-C(13)-N(2)               120.04(19)
C(15)-C(14)-C(13)              118.9(2)
C(15)-C(14)-C(19)              120.2(2)
C(13)-C(14)-C(19)              120.9(2)
C(4)-C(5)-C(6)                 119.9(2)
C(4)-C(5)-C(10)                120.1(2)
C(6)-C(5)-C(10)                120.0(2)
C(11)-N(1)-C(1)                128.94(17)
C(11)-N(1)-Sn(1)                97.36(12)
C(1)-N(1)-Sn(1)                133.51(13)
C(11)-C(12)-H(12A)             109.5
C(11)-C(12)-H(12B)             109.5
H(12A)-C(12)-H(12B)            109.5
C(11)-C(12)-H(12C)             109.5
H(12A)-C(12)-H(12C)            109.5
H(12B)-C(12)-H(12C)            109.5
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C(16)-C(15)-C(14)        121.1(2)
C(16)-C(15)-H(15)        119.4
C(14)-C(15)-H(15)        119.4
C(6)-C(7)-C(8)           120.5(2)
C(6)-C(7)-H(7)           119.8
C(8)-C(7)-H(7)           119.8
C(21)-C(22)-H(22A)       109.5
C(21)-C(22)-H(22B)       109.5
H(22A)-C(22)-H(22B)      109.5
C(21)-C(22)-H(22C)       109.5
H(22A)-C(22)-H(22C)      109.5
H(22B)-C(22)-H(22C)      109.5
C(21)-N(3)-C(9)          128.79(18)
C(21)-N(3)-Sn(1)          97.47(13)
C(9)-N(3)-Sn(1)          133.17(14)
C(3)-C(4)-C(5)           120.9(2)
C(3)-C(4)-H(4)           119.5
C(5)-C(4)-H(4)           119.5
C(17)-C(16)-C(15)        119.8(2)
C(17)-C(16)-H(16)        120.1
C(15)-C(16)-H(16)        120.1
C(5)-C(10)-C(9)          117.16(19)
C(5)-C(10)-C(1)          117.60(19)
C(9)-C(10)-C(1)          125.23(18)
C(26)-C(25)-C(24)        120.9(2)
C(26)-C(25)-H(25)        119.6
C(24)-C(25)-H(25)        119.6
C(17)-C(18)-C(13)        118.9(2)
C(17)-C(18)-C(20)        121.3(2)
C(13)-C(18)-C(20)        119.9(2)
C(25)-C(24)-C(23)        118.7(2)
C(25)-C(24)-C(29)        120.2(2)
C(23)-C(24)-C(29)        121.06(19)
C(8)-C(9)-N(3)           121.1(2)
C(8)-C(9)-C(10)          120.02(19)
N(3)-C(9)-C(10)          118.82(18)
N(3)-C(21)-N(4)          111.37(17)
N(3)-C(21)-C(22)         125.31(19)
N(4)-C(21)-C(22)         123.32(19)
C(14)-C(19)-H(19A)       109.5
C(14)-C(19)-H(19B)       109.5
H(19A)-C(19)-H(19B)      109.5
C(14)-C(19)-H(19C)       109.5
H(19A)-C(19)-H(19C)      109.5
H(19B)-C(19)-H(19C)      109.5
C(24)-C(29)-H(29A)       109.5
C(24)-C(29)-H(29B)       109.5
H(29A)-C(29)-H(29B)      109.5
C(24)-C(29)-H(29C)       109.5
H(29A)-C(29)-H(29C)      109.5
H(29B)-C(29)-H(29C)      109.5
N(1)-C(11)-N(2)          111.85(17)
N(1)-C(11)-C(12)         126.14(19)
N(2)-C(11)-C(12)         121.89(19)
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C(16)-C(17)-C(18)          121.2(2)
C(16)-C(17)-H(17)          119.4
C(18)-C(17)-H(17)          119.4
C(9)-C(8)-C(7)             121.4(2)
C(9)-C(8)-H(8)             119.3
C(7)-C(8)-H(8)             119.3
C(4)-C(3)-C(2)             120.4(2)
C(4)-C(3)-H(3)             119.8
C(2)-C(3)-H(3)             119.8
C(27)-C(28)-C(23)          118.6(2)
C(27)-C(28)-C(30)          119.1(2)
C(23)-C(28)-C(30)          122.3(2)
C(27)-C(26)-C(25)          120.4(2)
C(27)-C(26)-H(26)          119.8
C(25)-C(26)-H(26)          119.8
C(1)-C(2)-C(3)             121.5(2)
C(1)-C(2)-H(2)             119.2
C(3)-C(2)-H(2)             119.2
C(24)-C(23)-C(28)          120.44(19)
C(24)-C(23)-N(4)           118.90(18)
C(28)-C(23)-N(4)           120.63(18)
C(2)-C(1)-N(1)             121.5(2)
C(2)-C(1)-C(10)            119.24(19)
N(1)-C(1)-C(10)            119.12(18)
C(26)-C(27)-C(28)          120.9(2)
C(26)-C(27)-H(27)          119.5
C(28)-C(27)-H(27)          119.5
C(18)-C(20)-H(20A)         109.5
C(18)-C(20)-H(20B)         109.5
H(20A)-C(20)-H(20B)        109.5
C(18)-C(20)-H(20C)         109.5
H(20A)-C(20)-H(20C)        109.5
H(20B)-C(20)-H(20C)        109.5
C(28)-C(30)-H(30A)         109.5
C(28)-C(30)-H(30B)         109.5
H(30A)-C(30)-H(30B)        109.5
C(28)-C(30)-H(30C)         109.5
H(30A)-C(30)-H(30C)        109.5
H(30B)-C(30)-H(30C)        109.5
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Symmetry transformations used to generate equivalent atoms:

Table S8. Anisotropic displacement parameters (A^2 x 10^3) for R29.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Sn(1)	20(1)	28(1)	26(1)	-4(1)	1(1)	-1(1)
N(4)	24(1)	30(1)	24(1)	-4(1)	1(1)	0(1)
C(6)	33(1)	25(1)	61(2)	9(1)	2(1)	1(1)
N(2)	32(1)	30(1)	27(1)	2(1)	7(1)	2(1)
C(13)	29(1)	28(1)	27(1)	1(1)	7(1)	5(1)
C(14)	32(1)	40(1)	29(1)	-2(1)	6(1)	3(1)
C(5)	25(1)	23(1)	47(1)	-3(1)	0(1)	-2(1)
N(1)	28(1)	28(1)	30(1)	2(1)	6(1)	3(1)
C(12)	43(1)	42(1)	43(1)	8(1)	22(1)	10(1)
C(15)	40(1)	46(1)	29(1)	2(1)	1(1)	13(1)
C(7)	41(1)	38(1)	51(2)	17(1)	7(1)	1(1)
C(22)	35(1)	42(1)	29(1)	2(1)	-2(1)	2(1)
N(3)	32(1)	30(1)	29(1)	-4(1)	1(1)	5(1)
C(4)	38(1)	26(1)	56(1)	-12(1)	-2(1)	4(1)
C(16)	60(2)	33(1)	37(1)	7(1)	8(1)	16(1)
C(10)	21(1)	23(1)	35(1)	-2(1)	2(1)	-4(1)
C(25)	57(2)	36(1)	35(1)	-5(1)	10(1)	13(1)
C(18)	38(1)	28(1)	35(1)	0(1)	0(1)	2(1)
C(24)	36(1)	33(1)	25(1)	2(1)	6(1)	4(1)
C(9)	24(1)	27(1)	37(1)	1(1)	4(1)	-1(1)
C(21)	22(1)	34(1)	26(1)	-2(1)	5(1)	2(1)
C(19)	50(2)	59(2)	43(1)	0(1)	-9(1)	-14(1)
C(29)	32(1)	51(2)	39(1)	0(1)	11(1)	2(1)
C(11)	27(1)	32(1)	27(1)	1(1)	5(1)	4(1)
C(17)	58(2)	26(1)	45(1)	0(1)	0(1)	0(1)
C(8)	37(1)	39(1)	40(1)	8(1)	10(1)	2(1)
C(3)	48(1)	41(1)	48(1)	-19(1)	3(1)	3(1)
C(28)	35(1)	38(1)	25(1)	-1(1)	0(1)	-10(1)
C(26)	77(2)	32(1)	33(1)	-6(1)	-2(1)	-1(1)
C(2)	43(1)	37(1)	33(1)	-7(1)	1(1)	2(1)
C(23)	27(1)	28(1)	22(1)	-1(1)	1(1)	-1(1)
C(1)	24(1)	27(1)	33(1)	-4(1)	0(1)	-1(1)
C(27)	55(2)	37(1)	35(1)	-2(1)	-6(1)	-16(1)
C(20)	56(2)	45(1)	50(2)	1(1)	-16(1)	-6(1)
C(30)	27(1)	61(2)	41(1)	-1(1)	1(1)	-8(1)

Crystal data and structure refinement of compound (L₂Sn)₂
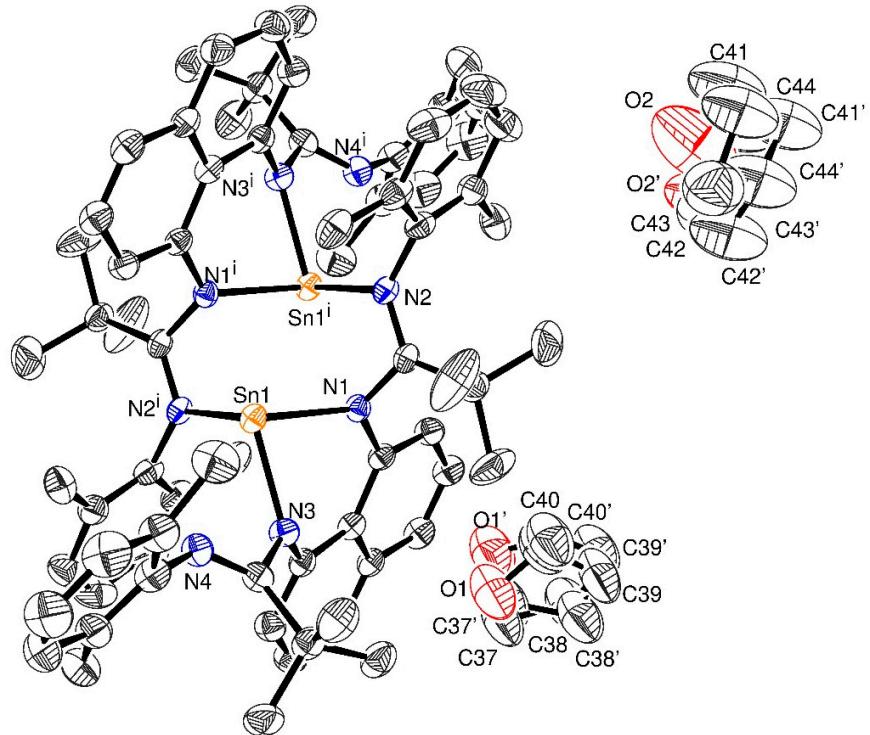
Figure S3. Asymmetric Unit (Symmetry code (i) : 2-x,1-y,1-z)
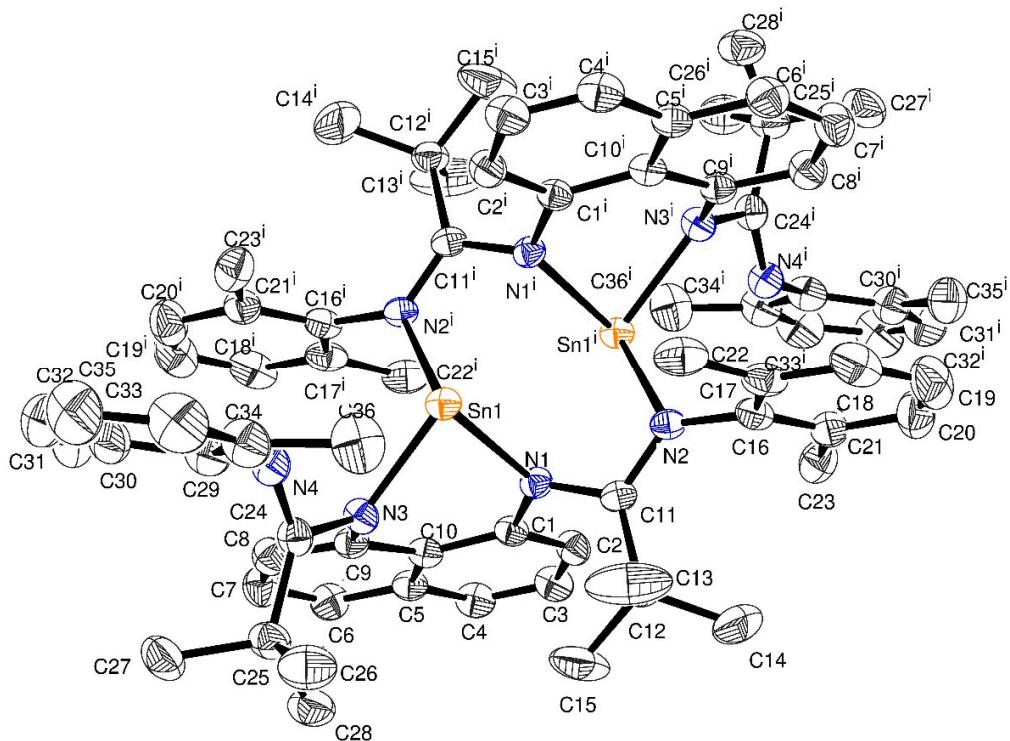
Figure S4. Compound
Table S9. Crystal data and structure refinement for R102.

Identification code	R102
Empirical formula	C72 H84 N8 Sn2, 4(C4 H8 O)
Formula weight	1587.31
Temperature	193(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P -1
Unit cell dimensions	a = 11.2468(7) A alpha = 86.510(2) deg.
	b = 12.6512(7) A beta = 78.588(2) deg.
	c = 14.5050(9) A gamma = 79.579(2) deg.
Volume	1989.0(2) A^3
Z, Calculated density	1, 1.325 Mg/m^3
Absorption coefficient	0.683 mm^-1

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F(000)                              832

Crystal size                        0.080 x 0.060 x 0.040 mm

Theta range for data collection     3.327 to 29.622 deg.

Limiting indices                    -15<=h<=15, -17<=k<=17,
                                     -20<=l<=20

Reflections collected / unique      75976 / 11128 [R(int) = 0.0936]

Completeness to theta = 25.242      99.4 %

Refinement method                   Full-matrix least-squares on F^2

Data / restraints / parameters      11128 / 277 / 564

Goodness-of-fit on F^2              1.015

Final R indices [I>2sigma(I)]       R1 = 0.0461, wR2 = 0.1054

R indices (all data)                R1 = 0.0747, wR2 = 0.1209

Extinction coefficient              0.0126(10)

Largest diff. peak and hole         1.132 and -0.909 e.A^-3
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Table S10. Atomic coordinates (x 10^4) and equivalent isotropic
displacement parameters (A^2 x 10^3) for R102.
U(eq) is defined as one third of the trace of the orthogonalized
Uij tensor.

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	x	y	z	U(eq)
C(1)	7596(3)	5785(2)	4640(2)	25(1)
C(2)	7495(3)	5731(3)	3707(2)	31(1)
C(3)	6786(3)	6554(3)	3259(2)	35(1)
C(4)	6215(3)	7465(3)	3729(2)	34(1)
C(5)	6292(3)	7571(3)	4678(2)	28(1)
C(6)	5712(3)	8527(3)	5142(3)	36(1)
C(7)	5787(3)	8659(3)	6059(3)	39(1)
C(8)	6402(3)	7829(3)	6555(2)	34(1)
C(9)	6931(3)	6843(2)	6151(2)	27(1)
C(10)	6958(3)	6705(2)	5169(2)	25(1)
C(11)	8587(3)	3925(2)	4711(2)	24(1)
C(12)	7481(3)	3306(3)	4982(2)	32(1)
C(13)	7679(4)	2623(5)	5846(4)	80(2)
C(14)	7341(4)	2573(5)	4212(4)	79(2)
C(15)	6253(3)	4048(3)	5221(4)	65(1)
C(16)	10183(3)	2413(2)	4079(2)	30(1)
C(17)	10704(3)	1681(3)	4708(3)	35(1)
C(18)	11205(3)	642(3)	4407(3)	48(1)
C(19)	11215(4)	349(3)	3503(3)	56(1)
C(20)	10720(4)	1087(3)	2882(3)	47(1)
C(21)	10205(3)	2130(3)	3149(2)	35(1)
C(22)	10750(3)	1953(3)	5701(3)	42(1)
C(23)	9669(4)	2923(3)	2451(2)	42(1)
C(24)	7082(3)	5931(3)	7667(2)	29(1)
C(25)	5716(3)	5845(3)	8102(2)	35(1)
C(26)	5707(4)	4703(3)	8496(3)	53(1)
C(27)	5164(4)	6631(4)	8912(3)	49(1)
C(28)	4837(3)	6045(4)	7398(3)	45(1)
C(29)	8024(3)	5543(3)	9082(2)	36(1)
C(30)	7876(3)	6404(3)	9679(2)	40(1)
C(31)	8031(4)	6178(4)	10607(3)	51(1)
C(32)	8340(4)	5144(4)	10931(3)	61(1)
C(33)	8536(4)	4304(4)	10327(3)	55(1)
C(34)	8402(3)	4493(3)	9383(2)	42(1)
C(35)	7613(4)	7554(3)	9352(3)	49(1)
C(36)	8753(4)	3560(3)	8711(3)	54(1)
O(1)	4578(11)	9100(6)	2166(8)	109(2)
C(37)	4034(16)	9949(9)	1700(12)	105(3)
C(38)	3512(15)	9554(9)	922(11)	110(3)
C(39)	3615(14)	8390(9)	1182(10)	109(3)
C(40)	4680(20)	8175(9)	1660(20)	112(3)
O(1')	5176(17)	8998(13)	1611(15)	113(3)
C(37')	4250(20)	9830(16)	1450(20)	111(3)
C(38')	3190(20)	9323(18)	1210(20)	111(3)

C(39')	4020(20)	8359(17)	810(18)	109(3)
C(40')	4720(40)	8043(15)	1570(40)	110(3)
C(43)	7733(10)	41(8)	2503(7)	117(3)
C(42)	7580(11)	919(8)	1851(10)	121(4)
O(2)	8651(14)	719(8)	1069(7)	203(5)
C(41)	9022(13)	-427(9)	1098(8)	146(4)
C(44)	8468(11)	-823(8)	1925(8)	135(4)
C(43')	7380(60)	-270(30)	2190(30)	140(5)
C(42')	7010(60)	830(30)	2100(40)	140(6)
O(2')	7840(50)	1200(30)	1290(30)	142(6)
C(41')	8420(60)	220(40)	780(30)	143(5)
C(44')	7930(60)	-620(30)	1250(40)	141(5)
N(1)	8441(2)	4967(2)	4998(2)	24(1)
N(2)	9719(2)	3514(2)	4329(2)	25(1)
N(3)	7461(2)	6003(2)	6691(2)	27(1)
N(4)	7988(3)	5748(2)	8112(2)	31(1)
Sn(1)	9263(1)	5074(1)	6270(1)	25(1)

Table S11. Bond lengths [A] and angles [deg] for R102.
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C(1)-C(2)                    1.387(4)
C(1)-N(1)                    1.421(4)
C(1)-C(10)                   1.431(4)
C(2)-C(3)                    1.401(4)
C(2)-H(2)                    0.9500
C(3)-C(4)                    1.364(5)
C(3)-H(3)                    0.9500
C(4)-C(5)                    1.412(4)
C(4)-H(4)                    0.9500
C(5)-C(6)                    1.408(5)
C(5)-C(10)                   1.444(4)
C(6)-C(7)                    1.371(5)
C(6)-H(6)                    0.9500
C(7)-C(8)                    1.394(5)
C(7)-H(7)                    0.9500
C(8)-C(9)                    1.391(5)
C(8)-H(8)                    0.9500
C(9)-N(3)                    1.397(4)
C(9)-C(10)                   1.440(4)
C(11)-N(2)                   1.309(4)
C(11)-N(1)                   1.378(4)
C(11)-C(12)                  1.561(4)
C(12)-C(13)                  1.508(5)
C(12)-C(15)                  1.513(5)
C(12)-C(14)                  1.543(6)
C(13)-H(13A)                 0.9800
C(13)-H(13B)                 0.9800
C(13)-H(13C)                 0.9800
C(14)-H(14A)                 0.9800
C(14)-H(14B)                 0.9800
C(14)-H(14C)                 0.9800
C(15)-H(15A)                 0.9800
C(15)-H(15B)                 0.9800
C(15)-H(15C)                 0.9800
C(16)-C(17)                  1.395(4)
C(16)-C(21)                  1.410(5)
C(16)-N(2)                   1.438(4)
C(17)-C(18)                  1.393(5)
C(17)-C(22)                  1.515(5)
C(18)-C(19)                  1.381(6)
C(18)-H(18)                  0.9500
C(19)-C(20)                  1.379(6)
C(19)-H(19)                  0.9500
C(20)-C(21)                  1.386(5)
C(20)-H(20)                  0.9500
C(21)-C(23)                  1.515(5)
C(22)-H(22A)                 0.9800
C(22)-H(22B)                 0.9800
C(22)-H(22C)                 0.9800
C(23)-H(23A)                 0.9800
C(23)-H(23B)                 0.9800
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C(23)-H(23C)            0.9800
C(24)-N(4)              1.291(4)
C(24)-N(3)              1.398(4)
C(24)-C(25)             1.562(4)
C(25)-C(26)             1.522(5)
C(25)-C(28)             1.538(5)
C(25)-C(27)             1.544(5)
C(26)-H(26A)            0.9800
C(26)-H(26B)            0.9800
C(26)-H(26C)            0.9800
C(27)-H(27A)            0.9800
C(27)-H(27B)            0.9800
C(27)-H(27C)            0.9800
C(28)-H(28A)            0.9800
C(28)-H(28B)            0.9800
C(28)-H(28C)            0.9800
C(29)-C(34)             1.391(5)
C(29)-C(30)             1.398(5)
C(29)-N(4)              1.422(4)
C(30)-C(31)             1.397(5)
C(30)-C(35)             1.498(5)
C(31)-C(32)             1.370(6)
C(31)-H(31)             0.9500
C(32)-C(33)             1.377(6)
C(32)-H(32)             0.9500
C(33)-C(34)             1.408(5)
C(33)-H(33)             0.9500
C(34)-C(36)             1.523(6)
C(35)-H(35A)            0.9800
C(35)-H(35B)            0.9800
C(35)-H(35C)            0.9800
C(36)-H(36A)            0.9800
C(36)-H(36B)            0.9800
C(36)-H(36C)            0.9800
O(1)-C(37)              1.349(11)
O(1)-C(40)              1.395(14)
C(37)-C(38)             1.519(13)
C(37)-H(37A)            0.9900
C(37)-H(37B)            0.9900
C(38)-C(39)             1.486(14)
C(38)-H(38A)            0.9900
C(38)-H(38B)            0.9900
C(39)-C(40)             1.470(13)
C(39)-H(39A)            0.9900
C(39)-H(39B)            0.9900
C(40)-H(40A)            0.9900
C(40)-H(40B)            0.9900
O(1')-C(37')            1.385(15)
O(1')-C(40')            1.41(2)
C(37')-C(38')           1.557(18)
C(37')-H(37C)           0.9900
C(37')-H(37D)           0.9900
C(38')-C(39')           1.469(18)
C(38')-H(38C)           0.9900
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C(38')-H(38D)                0.9900
C(39')-C(40')                1.466(18)
C(39')-H(39C)                0.9900
C(39')-H(39D)                0.9900
C(40')-H(40C)                0.9900
C(40')-H(40D)                0.9900
C(43)-C(42)                  1.423(12)
C(43)-C(44)                  1.446(13)
C(43)-H(43A)                 0.9900
C(43)-H(43B)                 0.9900
C(42)-O(2)                   1.478(12)
C(42)-H(42A)                 0.9900
C(42)-H(42B)                 0.9900
O(2)-C(41)                   1.435(12)
C(41)-C(44)                  1.350(12)
C(41)-H(41A)                 0.9900
C(41)-H(41B)                 0.9900
C(44)-H(44A)                 0.9900
C(44)-H(44B)                 0.9900
C(43')-C(42')                1.389(18)
C(43')-C(44')                1.44(2)
C(43')-H(43C)                0.9900
C(43')-H(43D)                0.9900
C(42')-O(2')                 1.454(19)
C(42')-H(42C)                0.9900
C(42')-H(42D)                0.9900
O(2')-C(41')                 1.464(18)
C(41')-C(44')                1.374(18)
C(41')-H(41C)                0.9900
C(41')-H(41D)                0.9900
C(44')-H(44C)                0.9900
C(44')-H(44D)                0.9900
N(1)-Sn(1)                   2.243(2)
N(2)-Sn(1)#1                 2.327(2)
N(3)-Sn(1)                   2.144(3)

C(2)-C(1)-N(1)               117.6(3)
C(2)-C(1)-C(10)              119.5(3)
N(1)-C(1)-C(10)              122.6(3)
C(1)-C(2)-C(3)               122.1(3)
C(1)-C(2)-H(2)               119.0
C(3)-C(2)-H(2)               119.0
C(4)-C(3)-C(2)               119.9(3)
C(4)-C(3)-H(3)               120.0
C(2)-C(3)-H(3)               120.0
C(3)-C(4)-C(5)               120.5(3)
C(3)-C(4)-H(4)               119.7
C(5)-C(4)-H(4)               119.7
C(6)-C(5)-C(4)               119.4(3)
C(6)-C(5)-C(10)              120.3(3)
C(4)-C(5)-C(10)              120.3(3)
C(7)-C(6)-C(5)               120.7(3)
C(7)-C(6)-H(6)               119.6
C(5)-C(6)-H(6)               119.6
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C(6)-C(7)-C(8)            120.2(3)
C(6)-C(7)-H(7)            119.9
C(8)-C(7)-H(7)            119.9
C(9)-C(8)-C(7)            121.7(3)
C(9)-C(8)-H(8)            119.2
C(7)-C(8)-H(8)            119.2
C(8)-C(9)-N(3)            120.0(3)
C(8)-C(9)-C(10)           119.6(3)
N(3)-C(9)-C(10)           120.4(3)
C(1)-C(10)-C(9)           125.3(3)
C(1)-C(10)-C(5)           117.5(3)
C(9)-C(10)-C(5)           117.2(3)
N(2)-C(11)-N(1)           114.2(3)
N(2)-C(11)-C(12)          126.3(3)
N(1)-C(11)-C(12)          119.0(3)
C(13)-C(12)-C(15)         108.0(4)
C(13)-C(12)-C(14)         108.7(4)
C(15)-C(12)-C(14)         105.5(4)
C(13)-C(12)-C(11)         106.9(3)
C(15)-C(12)-C(11)         112.8(3)
C(14)-C(12)-C(11)         114.7(3)
C(12)-C(13)-H(13A)        109.5
C(12)-C(13)-H(13B)        109.5
H(13A)-C(13)-H(13B)       109.5
C(12)-C(13)-H(13C)        109.5
H(13A)-C(13)-H(13C)       109.5
H(13B)-C(13)-H(13C)       109.5
C(12)-C(14)-H(14A)        109.5
C(12)-C(14)-H(14B)        109.5
H(14A)-C(14)-H(14B)       109.5
C(12)-C(14)-H(14C)        109.5
H(14A)-C(14)-H(14C)       109.5
H(14B)-C(14)-H(14C)       109.5
C(12)-C(15)-H(15A)        109.5
C(12)-C(15)-H(15B)        109.5
H(15A)-C(15)-H(15B)       109.5
C(12)-C(15)-H(15C)        109.5
H(15A)-C(15)-H(15C)       109.5
H(15B)-C(15)-H(15C)       109.5
C(17)-C(16)-C(21)         121.3(3)
C(17)-C(16)-N(2)          120.7(3)
C(21)-C(16)-N(2)          117.7(3)
C(18)-C(17)-C(16)         118.2(3)
C(18)-C(17)-C(22)         118.2(3)
C(16)-C(17)-C(22)         123.6(3)
C(19)-C(18)-C(17)         121.1(4)
C(19)-C(18)-H(18)         119.4
C(17)-C(18)-H(18)         119.4
C(20)-C(19)-C(18)         120.1(4)
C(20)-C(19)-H(19)         120.0
C(18)-C(19)-H(19)         120.0
C(19)-C(20)-C(21)         121.0(4)
C(19)-C(20)-H(20)         119.5
C(21)-C(20)-H(20)         119.5
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C(20)-C(21)-C(16)          118.3(3)
C(20)-C(21)-C(23)          119.8(3)
C(16)-C(21)-C(23)          121.9(3)
C(17)-C(22)-H(22A)         109.5
C(17)-C(22)-H(22B)         109.5
H(22A)-C(22)-H(22B)        109.5
C(17)-C(22)-H(22C)         109.5
H(22A)-C(22)-H(22C)        109.5
H(22B)-C(22)-H(22C)        109.5
C(21)-C(23)-H(23A)         109.5
C(21)-C(23)-H(23B)         109.5
H(23A)-C(23)-H(23B)        109.5
C(21)-C(23)-H(23C)         109.5
H(23A)-C(23)-H(23C)        109.5
H(23B)-C(23)-H(23C)        109.5
N(4)-C(24)-N(3)            113.1(3)
N(4)-C(24)-C(25)           125.5(3)
N(3)-C(24)-C(25)           120.2(3)
C(26)-C(25)-C(28)          107.2(3)
C(26)-C(25)-C(27)          108.4(3)
C(28)-C(25)-C(27)          106.9(3)
C(26)-C(25)-C(24)          107.2(3)
C(28)-C(25)-C(24)          114.6(3)
C(27)-C(25)-C(24)          112.4(3)
C(25)-C(26)-H(26A)         109.5
C(25)-C(26)-H(26B)         109.5
H(26A)-C(26)-H(26B)        109.5
C(25)-C(26)-H(26C)         109.5
H(26A)-C(26)-H(26C)        109.5
H(26B)-C(26)-H(26C)        109.5
C(25)-C(27)-H(27A)         109.5
C(25)-C(27)-H(27B)         109.5
H(27A)-C(27)-H(27B)        109.5
C(25)-C(27)-H(27C)         109.5
H(27A)-C(27)-H(27C)        109.5
H(27B)-C(27)-H(27C)        109.5
C(25)-C(28)-H(28A)         109.5
C(25)-C(28)-H(28B)         109.5
H(28A)-C(28)-H(28B)        109.5
C(25)-C(28)-H(28C)         109.5
H(28A)-C(28)-H(28C)        109.5
H(28B)-C(28)-H(28C)        109.5
C(34)-C(29)-C(30)          120.8(3)
C(34)-C(29)-N(4)           118.6(3)
C(30)-C(29)-N(4)           119.7(3)
C(31)-C(30)-C(29)          118.4(4)
C(31)-C(30)-C(35)          118.9(4)
C(29)-C(30)-C(35)          122.6(3)
C(32)-C(31)-C(30)          121.6(4)
C(32)-C(31)-H(31)          119.2
C(30)-C(31)-H(31)          119.2
C(31)-C(32)-C(33)          119.7(4)
C(31)-C(32)-H(32)          120.2
C(33)-C(32)-H(32)          120.2
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C(32)-C(33)-C(34)          120.8(4)
C(32)-C(33)-H(33)          119.6
C(34)-C(33)-H(33)          119.6
C(29)-C(34)-C(33)          118.6(4)
C(29)-C(34)-C(36)          122.0(3)
C(33)-C(34)-C(36)          119.3(4)
C(30)-C(35)-H(35A)         109.5
C(30)-C(35)-H(35B)         109.5
H(35A)-C(35)-H(35B)        109.5
C(30)-C(35)-H(35C)         109.5
H(35A)-C(35)-H(35C)        109.5
H(35B)-C(35)-H(35C)        109.5
C(34)-C(36)-H(36A)         109.5
C(34)-C(36)-H(36B)         109.5
H(36A)-C(36)-H(36B)        109.5
C(34)-C(36)-H(36C)         109.5
H(36A)-C(36)-H(36C)        109.5
H(36B)-C(36)-H(36C)        109.5
C(37)-O(1)-C(40)           108.7(9)
O(1)-C(37)-C(38)           109.6(8)
O(1)-C(37)-H(37A)          109.7
C(38)-C(37)-H(37A)         109.7
O(1)-C(37)-H(37B)          109.7
C(38)-C(37)-H(37B)         109.7
H(37A)-C(37)-H(37B)        108.2
C(39)-C(38)-C(37)          100.4(10)
C(39)-C(38)-H(38A)         111.7
C(37)-C(38)-H(38A)         111.7
C(39)-C(38)-H(38B)         111.7
C(37)-C(38)-H(38B)         111.7
H(38A)-C(38)-H(38B)        109.5
C(40)-C(39)-C(38)          103.6(10)
C(40)-C(39)-H(39A)         111.0
C(38)-C(39)-H(39A)         111.0
C(40)-C(39)-H(39B)         111.0
C(38)-C(39)-H(39B)         111.0
H(39A)-C(39)-H(39B)        109.0
O(1)-C(40)-C(39)           104.5(11)
O(1)-C(40)-H(40A)          110.9
C(39)-C(40)-H(40A)         110.9
O(1)-C(40)-H(40B)          110.9
C(39)-C(40)-H(40B)         110.9
H(40A)-C(40)-H(40B)        108.9
C(37')-O(1')-C(40')        106.0(16)
O(1')-C(37')-C(38')        107.7(13)
O(1')-C(37')-H(37C)        110.2
C(38')-C(37')-H(37C)       110.2
O(1')-C(37')-H(37D)        110.2
C(38')-C(37')-H(37D)       110.2
H(37C)-C(37')-H(37D)       108.5
C(39')-C(38')-C(37')        93.6(15)
C(39')-C(38')-H(38C)       113.0
C(37')-C(38')-H(38C)       113.0
C(39')-C(38')-H(38D)       113.0
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C(37')-C(38')-H(38D)        113.0
H(38C)-C(38')-H(38D)        110.4
C(40')-C(39')-C(38')        100.3(18)
C(40')-C(39')-H(39C)        111.7
C(38')-C(39')-H(39C)        111.7
C(40')-C(39')-H(39D)        111.7
C(38')-C(39')-H(39D)        111.7
H(39C)-C(39')-H(39D)        109.5
O(1')-C(40')-C(39')          99.1(18)
O(1')-C(40')-H(40C)         111.9
C(39')-C(40')-H(40C)        111.9
O(1')-C(40')-H(40D)         111.9
C(39')-C(40')-H(40D)        111.9
H(40C)-C(40')-H(40D)        109.6
C(42)-C(43)-C(44)           103.6(9)
C(42)-C(43)-H(43A)          111.0
C(44)-C(43)-H(43A)          111.0
C(42)-C(43)-H(43B)          111.0
C(44)-C(43)-H(43B)          111.0
H(43A)-C(43)-H(43B)         109.0
C(43)-C(42)-O(2)            106.2(8)
C(43)-C(42)-H(42A)          110.5
O(2)-C(42)-H(42A)           110.5
C(43)-C(42)-H(42B)          110.5
O(2)-C(42)-H(42B)           110.5
H(42A)-C(42)-H(42B)         108.7
C(41)-O(2)-C(42)            103.7(9)
C(44)-C(41)-O(2)            108.9(8)
C(44)-C(41)-H(41A)          109.9
O(2)-C(41)-H(41A)           109.9
C(44)-C(41)-H(41B)          109.9
O(2)-C(41)-H(41B)           109.9
H(41A)-C(41)-H(41B)         108.3
C(41)-C(44)-C(43)           110.4(8)
C(41)-C(44)-H(44A)          109.6
C(43)-C(44)-H(44A)          109.6
C(41)-C(44)-H(44B)          109.6
C(43)-C(44)-H(44B)          109.6
H(44A)-C(44)-H(44B)         108.1
C(42')-C(43')-C(44')        105(2)
C(42')-C(43')-H(43C)        110.7
C(44')-C(43')-H(43C)        110.7
C(42')-C(43')-H(43D)        110.7
C(44')-C(43')-H(43D)        110.7
H(43C)-C(43')-H(43D)        108.8
C(43')-C(42')-O(2')         107(2)
C(43')-C(42')-H(42C)        110.4
O(2')-C(42')-H(42C)         110.4
C(43')-C(42')-H(42D)        110.4
O(2')-C(42')-H(42D)         110.4
H(42C)-C(42')-H(42D)        108.6
C(42')-O(2')-C(41')         104(2)
C(44')-C(41')-O(2')         107.8(18)
C(44')-C(41')-H(41C)        110.1
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O(2')-C(41')-H(41C)          110.2
C(44')-C(41')-H(41D)         110.2
O(2')-C(41')-H(41D)          110.2
H(41C)-C(41')-H(41D)         108.5
C(41')-C(44')-C(43')         106.7(19)
C(41')-C(44')-H(44C)         110.4
C(43')-C(44')-H(44C)         110.4
C(41')-C(44')-H(44D)         110.4
C(43')-C(44')-H(44D)         110.4
H(44C)-C(44')-H(44D)         108.6
C(11)-N(1)-C(1)              119.7(2)
C(11)-N(1)-Sn(1)            112.43(18)
C(1)-N(1)-Sn(1)             126.11(19)
C(11)-N(2)-C(16)            126.8(3)
C(11)-N(2)-Sn(1)#1          107.94(19)
C(16)-N(2)-Sn(1)#1          123.20(19)
C(9)-N(3)-C(24)             121.8(3)
C(9)-N(3)-Sn(1)             124.34(19)
C(24)-N(3)-Sn(1)            110.35(19)
C(24)-N(4)-C(29)            131.6(3)
N(3)-Sn(1)-N(1)             78.80(9)
N(3)-Sn(1)-N(2)#1           97.73(9)
N(1)-Sn(1)-N(2)#1           95.21(9)
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Symmetry transformations used to generate equivalent atoms:
#1 -x+2,-y+1,-z+1

Table S12. Anisotropic displacement parameters (A^2 x 10^3) for R102.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	22(1)	29(2)	24(1)	3(1)	-6(1)	-3(1)
C(2)	30(2)	38(2)	24(2)	-1(1)	-6(1)	-2(1)
C(3)	33(2)	47(2)	24(2)	6(1)	-9(1)	-3(2)
C(4)	34(2)	40(2)	30(2)	10(1)	-12(1)	-3(1)
C(5)	25(2)	31(2)	29(2)	5(1)	-8(1)	-5(1)
C(6)	36(2)	31(2)	42(2)	4(1)	-13(2)	0(1)
C(7)	41(2)	32(2)	41(2)	-2(2)	-9(2)	0(2)
C(8)	35(2)	37(2)	29(2)	-1(1)	-6(1)	-5(1)
C(9)	25(1)	30(2)	26(1)	2(1)	-6(1)	-6(1)
C(10)	23(1)	28(2)	24(1)	6(1)	-4(1)	-5(1)
C(11)	24(1)	27(2)	24(1)	6(1)	-10(1)	-5(1)
C(12)	25(2)	33(2)	38(2)	0(1)	-5(1)	-7(1)
C(13)	51(3)	112(4)	85(4)	63(3)	-27(3)	-44(3)
C(14)	52(3)	103(4)	89(4)	-41(3)	8(3)	-46(3)
C(15)	26(2)	44(2)	117(4)	6(2)	6(2)	-10(2)
C(16)	22(1)	26(2)	39(2)	2(1)	-3(1)	-4(1)
C(17)	25(2)	30(2)	49(2)	9(1)	-5(1)	-7(1)
C(18)	38(2)	32(2)	65(3)	13(2)	0(2)	-3(2)
C(19)	58(3)	26(2)	75(3)	-4(2)	6(2)	-5(2)
C(20)	54(2)	36(2)	50(2)	-9(2)	3(2)	-12(2)
C(21)	30(2)	34(2)	39(2)	-3(1)	-1(1)	-10(1)
C(22)	35(2)	44(2)	50(2)	15(2)	-15(2)	-9(2)
C(23)	51(2)	43(2)	34(2)	-3(2)	-10(2)	-14(2)
C(24)	33(2)	30(2)	22(1)	1(1)	-2(1)	-6(1)
C(25)	30(2)	50(2)	26(2)	2(1)	-3(1)	-8(2)
C(26)	45(2)	58(3)	56(2)	13(2)	-5(2)	-20(2)
C(27)	37(2)	73(3)	33(2)	-10(2)	2(2)	-3(2)
C(28)	32(2)	69(3)	34(2)	1(2)	-4(2)	-13(2)
C(29)	33(2)	48(2)	25(2)	6(1)	-6(1)	-5(2)
C(30)	41(2)	50(2)	27(2)	-1(2)	-5(1)	-5(2)
C(31)	55(2)	75(3)	25(2)	-4(2)	-12(2)	-8(2)
C(32)	69(3)	86(3)	25(2)	7(2)	-17(2)	1(3)
C(33)	60(3)	66(3)	36(2)	18(2)	-16(2)	1(2)
C(34)	43(2)	52(2)	29(2)	7(2)	-6(2)	-5(2)
C(35)	56(2)	50(2)	40(2)	-6(2)	-7(2)	-8(2)
C(36)	66(3)	44(2)	48(2)	8(2)	-15(2)	1(2)
O(1)	152(5)	77(3)	112(5)	-14(4)	-65(4)	-7(4)
C(37)	145(6)	65(4)	119(6)	-22(4)	-58(5)	-9(4)
C(38)	148(6)	75(4)	117(6)	-9(4)	-63(5)	-2(4)
C(39)	151(6)	71(4)	121(6)	-20(4)	-64(5)	-15(4)
C(40)	149(5)	71(4)	122(6)	-8(4)	-56(5)	-3(4)
O(1')	145(6)	78(4)	128(6)	-15(5)	-57(5)	-14(4)
C(37')	151(6)	71(4)	123(7)	-16(5)	-59(5)	-10(4)
C(38')	147(6)	75(5)	119(7)	-19(5)	-60(5)	-1(5)
C(39')	149(6)	70(4)	118(7)	-21(5)	-56(5)	-4(5)

C(40')	148(6)	70(4)	122(6)	-13(5)	-56(5)	-7(5)
C(43)	113(8)	98(7)	134(9)	-3(6)	-9(6)	-15(6)
C(42)	111(9)	99(7)	150(11)	-4(8)	-26(8)	-8(6)
O(2)	331(16)	133(8)	126(7)	-4(6)	5(9)	-46(10)
C(41)	175(9)	118(7)	114(6)	-25(6)	27(6)	10(6)
C(44)	170(9)	106(6)	102(6)	-17(5)	13(6)	10(6)
C(43')	172(11)	115(9)	106(8)	-18(8)	16(8)	9(8)
C(42')	171(13)	116(10)	103(10)	-14(9)	17(10)	14(10)
O(2')	170(12)	118(9)	104(10)	-12(9)	17(10)	17(10)
C(41')	173(11)	117(9)	106(8)	-18(8)	17(8)	15(8)
C(44')	172(10)	116(8)	107(8)	-22(7)	18(8)	10(8)
N(1)	25(1)	27(1)	22(1)	0(1)	-7(1)	-5(1)
N(2)	22(1)	26(1)	26(1)	2(1)	-7(1)	-5(1)
N(3)	28(1)	33(1)	19(1)	3(1)	-5(1)	-3(1)
N(4)	35(2)	37(2)	21(1)	3(1)	-8(1)	-5(1)
Sn(1)	25(1)	28(1)	21(1)	4(1)	-7(1)	-5(1)

Crystal data and structure refinement of compound (L₁Ge)₂
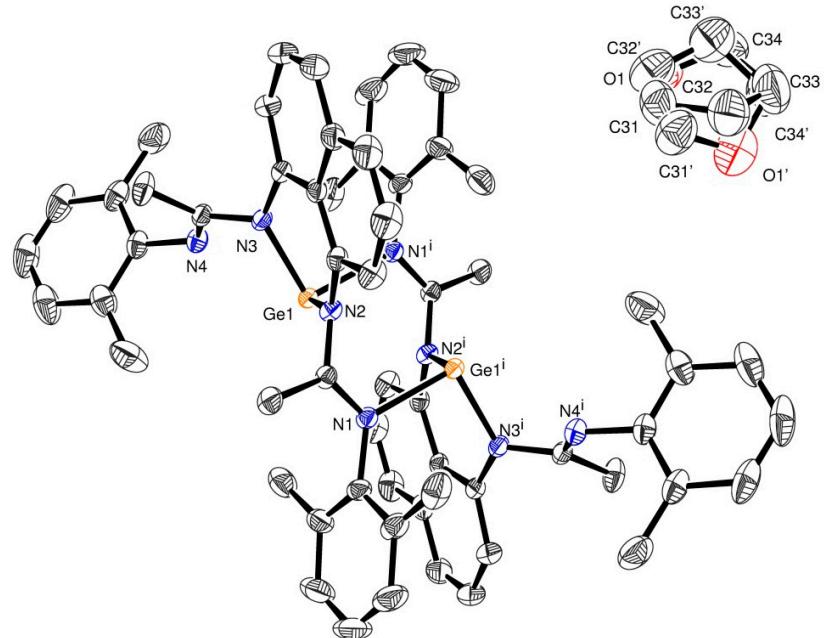
Figure S5. Asymmetric Unit [Symmetry code : (i) 1-x, 1-y, 1-z]
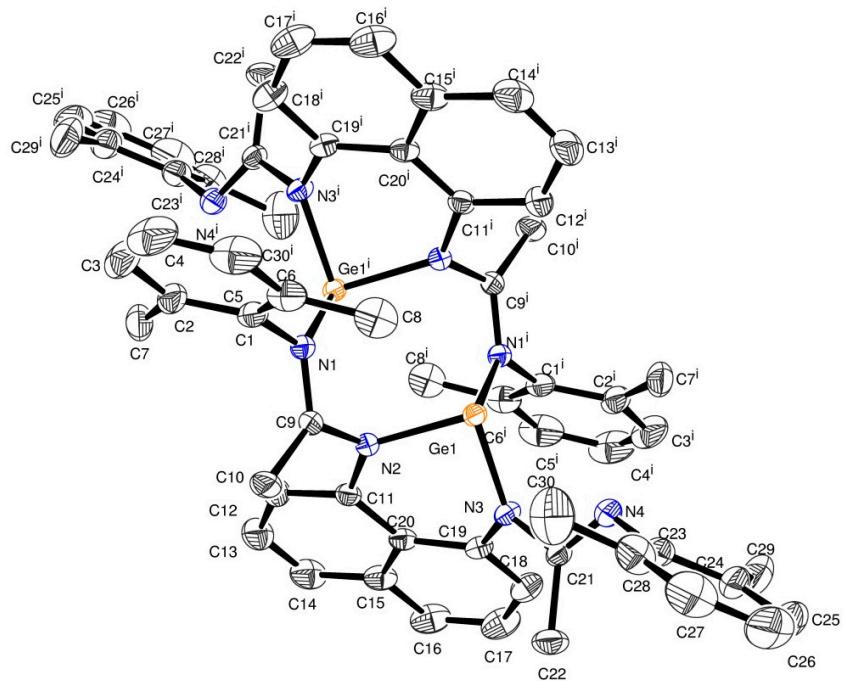
Figure S6. Compound [Symmetry code : (i) 1-x, 1-y, 1-z]

Table S13. Crystal data and structure refinement for AA-R34.

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Identification code              AA-R34

Empirical formula                C60 H60 Ge2 N8, 2(C4 H8 O)

Formula weight                   1182.59

Temperature                      193(2) K

Wavelength                       0.71073 A

Crystal system, space group      Triclinic,  P -1

Unit cell dimensions      a = 9.1577(4) A    alpha = 65.967(2) deg.
                          b = 12.9975(5) A    beta = 73.850(2) deg.
                          c = 14.4975(5) A    gamma = 83.201(2) deg.

Volume                           1513.79(11) A^3

Z, Calculated density            1,  1.297 Mg/m^3

Absorption coefficient           1.044 mm^-1

F(000)                           620

Crystal size                     0.200 x 0.080 x 0.060 mm

Theta range for data collection  2.874 to 34.433 deg.

Limiting indices                 -14<=h<=14, -20<=k<=20,
                                 -23<=l<=21

Reflections collected / unique   62134 / 12689 [R(int) = 0.0398]

Completeness to theta = 25.242   99.5 %

Refinement method                Full-matrix least-squares on F^2

Data / restraints / parameters   12689 / 186 / 414

Goodness-of-fit on F^2           1.051

Final R indices [I>2sigma(I)]    R1 = 0.0381, wR2 = 0.0898

R indices (all data)             R1 = 0.0527, wR2 = 0.0964

Largest diff. peak and hole      0.674 and -0.468 e.A^-3
```

Table S14. Atomic coordinates (x 10^4) and equivalent isotropic
displacement parameters (A^2 x 10^3) for AA-R34.
U(eq) is defined as one third of the trace of the orthogonalized
Uij tensor.

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	x	y	z	U(eq)
C(1)	5002(2)	4429(1)	7510(1)	26(1)
C(2)	5066(2)	3390(2)	8339(1)	35(1)
C(3)	4578(2)	3367(2)	9350(1)	51(1)
C(4)	4064(2)	4323(2)	9526(2)	59(1)
C(5)	4052(2)	5347(2)	8696(2)	50(1)
C(6)	4523(2)	5419(2)	7669(1)	33(1)
C(7)	5668(2)	2348(2)	8151(1)	42(1)
C(8)	4540(2)	6536(2)	6771(2)	40(1)
C(9)	6772(1)	4662(1)	5873(1)	20(1)
C(10)	8088(2)	4774(1)	6255(1)	30(1)
C(11)	8077(1)	4261(1)	4369(1)	21(1)
C(12)	8404(2)	3167(1)	4984(1)	30(1)
C(13)	9418(2)	2482(1)	4552(2)	39(1)
C(14)	10050(2)	2866(1)	3507(2)	38(1)
C(15)	9725(2)	3965(1)	2840(1)	29(1)
C(16)	10386(2)	4347(2)	1752(1)	39(1)
C(17)	10089(2)	5406(2)	1096(1)	40(1)
C(18)	9133(2)	6137(1)	1500(1)	31(1)
C(19)	8510(1)	5817(1)	2560(1)	22(1)
C(20)	8744(1)	4698(1)	3267(1)	21(1)
C(21)	8118(1)	7709(1)	2521(1)	21(1)
C(22)	9799(2)	7948(1)	2184(1)	35(1)
C(23)	7531(2)	9586(1)	2280(1)	28(1)
C(24)	7771(2)	10359(1)	1239(1)	36(1)
C(25)	8141(2)	11472(2)	1003(2)	52(1)
C(26)	8267(3)	11801(2)	1762(2)	60(1)
C(27)	7999(2)	11041(2)	2785(2)	55(1)
C(28)	7608(2)	9924(2)	3071(2)	39(1)
C(29)	7619(3)	9999(2)	413(1)	50(1)
C(30)	7269(3)	9095(2)	4187(2)	59(1)
O(1)	2910(4)	1766(2)	1930(2)	76(1)
C(31)	3761(5)	1192(4)	2702(4)	74(1)
C(32)	3318(5)	-47(4)	3259(4)	81(1)
C(33)	2147(10)	-147(6)	2799(5)	93(2)
C(34)	2378(5)	886(4)	1778(4)	79(1)
O(1')	2125(11)	254(9)	3602(7)	97(2)
C(31')	3548(13)	772(13)	3286(8)	78(2)
C(32')	3854(18)	1449(13)	2118(10)	81(2)
C(33')	3102(19)	812(15)	1777(10)	90(2)
C(34')	1980(30)	50(20)	2741(11)	88(3)
Ge(1)	5879(1)	6276(1)	4108(1)	18(1)
N(1)	5383(1)	4465(1)	6463(1)	20(1)
N(2)	6962(1)	4871(1)	4839(1)	20(1)
N(3)	7640(1)	6605(1)	2931(1)	21(1)

N(4)	7093(1)	8469(1)	2558(1)	25(1)

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          Table S15.  Bond lengths [A] and angles [deg] for AA-R34.
        _____

          C(1)-C(6)                        1.397(2)
          C(1)-C(2)                        1.403(2)
          C(1)-N(1)                        1.4419(16)
          C(2)-C(3)                        1.397(2)
          C(2)-C(7)                        1.502(3)
          C(3)-C(4)                        1.372(4)
          C(3)-H(3)                        0.9500
          C(4)-C(5)                        1.386(3)
          C(4)-H(4)                        0.9500
          C(5)-C(6)                        1.397(2)
          C(5)-H(5)                        0.9500
          C(6)-C(8)                        1.502(3)
          C(7)-H(7A)                       0.9800
          C(7)-H(7B)                       0.9800
          C(7)-H(7C)                       0.9800
          C(8)-H(8A)                       0.9800
          C(8)-H(8B)                       0.9800
          C(8)-H(8C)                       0.9800
          C(9)-N(1)                        1.3074(16)
          C(9)-N(2)                        1.3740(16)
          C(9)-C(10)                       1.5027(18)
          C(10)-H(10A)                     0.9800
          C(10)-H(10B)                     0.9800
          C(10)-H(10C)                     0.9800
          C(11)-C(12)                      1.3867(18)
          C(11)-N(2)                       1.4125(16)
          C(11)-C(20)                      1.4317(18)
          C(12)-C(13)                      1.408(2)
          C(12)-H(12)                      0.9500
          C(13)-C(14)                      1.358(3)
          C(13)-H(13)                      0.9500
          C(14)-C(15)                      1.414(2)
          C(14)-H(14)                      0.9500
          C(15)-C(16)                      1.416(2)
          C(15)-C(20)                      1.4373(18)
          C(16)-C(17)                      1.364(3)
          C(16)-H(16)                      0.9500
          C(17)-C(18)                      1.408(2)
          C(17)-H(17)                      0.9500
          C(18)-C(19)                      1.3815(18)
          C(18)-H(18)                      0.9500
          C(19)-N(3)                       1.4102(16)
          C(19)-C(20)                      1.4305(18)
          C(21)-N(4)                       1.2869(17)
          C(21)-N(3)                       1.3831(16)
          C(21)-C(22)                      1.5089(19)
          C(22)-H(22A)                     0.9800
          C(22)-H(22B)                     0.9800
          C(22)-H(22C)                     0.9800
          C(23)-C(24)                      1.402(2)
          C(23)-C(28)                      1.404(2)
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C(23)-N(4)              1.4153(18)
C(24)-C(25)             1.406(2)
C(24)-C(29)             1.496(3)
C(25)-C(26)             1.368(4)
C(25)-H(25)             0.9500
C(26)-C(27)             1.377(4)
C(26)-H(26)             0.9500
C(27)-C(28)             1.400(3)
C(27)-H(27)             0.9500
C(28)-C(30)             1.502(3)
C(29)-H(29A)            0.9800
C(29)-H(29B)            0.9800
C(29)-H(29C)            0.9800
C(30)-H(30A)            0.9800
C(30)-H(30B)            0.9800
C(30)-H(30C)            0.9800
O(1)-C(34)              1.410(5)
O(1)-C(31)              1.443(5)
C(31)-C(32)             1.524(6)
C(31)-H(31A)            0.9900
C(31)-H(31B)            0.9900
C(32)-C(33)             1.454(8)
C(32)-H(32A)            0.9900
C(32)-H(32B)            0.9900
C(33)-C(34)             1.521(7)
C(33)-H(33A)            0.9900
C(33)-H(33B)            0.9900
C(34)-H(34A)            0.9900
C(34)-H(34B)            0.9900
O(1')-C(31')            1.410(9)
O(1')-C(34')            1.421(11)
C(31')-C(32')           1.517(10)
C(31')-H(31C)           0.9900
C(31')-H(31D)           0.9900
C(32')-C(33')           1.436(11)
C(32')-H(32C)           0.9900
C(32')-H(32D)           0.9900
C(33')-C(34')           1.517(10)
C(33')-H(33C)           0.9900
C(33')-H(33D)           0.9900
C(34')-H(34C)           0.9900
C(34')-H(34D)           0.9900
Ge(1)-N(3)              1.9332(10)
Ge(1)-N(2)              2.0048(10)
Ge(1)-N(1)#1            2.0961(11)

C(6)-C(1)-C(2)          122.28(14)
C(6)-C(1)-N(1)          118.95(13)
C(2)-C(1)-N(1)          118.71(14)
C(3)-C(2)-C(1)          117.35(18)
C(3)-C(2)-C(7)          121.06(16)
C(1)-C(2)-C(7)          121.57(14)
C(4)-C(3)-C(2)          121.36(19)
C(4)-C(3)-H(3)          119.3
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C(2)-C(3)-H(3)            119.3
C(3)-C(4)-C(5)            120.39(17)
C(3)-C(4)-H(4)            119.8
C(5)-C(4)-H(4)            119.8
C(4)-C(5)-C(6)            120.7(2)
C(4)-C(5)-H(5)            119.7
C(6)-C(5)-H(5)            119.7
C(5)-C(6)-C(1)            117.91(17)
C(5)-C(6)-C(8)            120.38(17)
C(1)-C(6)-C(8)            121.70(13)
C(2)-C(7)-H(7A)           109.5
C(2)-C(7)-H(7B)           109.5
H(7A)-C(7)-H(7B)          109.5
C(2)-C(7)-H(7C)           109.5
H(7A)-C(7)-H(7C)          109.5
H(7B)-C(7)-H(7C)          109.5
C(6)-C(8)-H(8A)           109.5
C(6)-C(8)-H(8B)           109.5
H(8A)-C(8)-H(8B)          109.5
C(6)-C(8)-H(8C)           109.5
H(8A)-C(8)-H(8C)          109.5
H(8B)-C(8)-H(8C)          109.5
N(1)-C(9)-N(2)            116.31(11)
N(1)-C(9)-C(10)           123.05(12)
N(2)-C(9)-C(10)           120.36(11)
C(9)-C(10)-H(10A)         109.5
C(9)-C(10)-H(10B)         109.5
H(10A)-C(10)-H(10B)       109.5
C(9)-C(10)-H(10C)         109.5
H(10A)-C(10)-H(10C)       109.5
H(10B)-C(10)-H(10C)       109.5
C(12)-C(11)-N(2)          118.31(12)
C(12)-C(11)-C(20)         119.64(12)
N(2)-C(11)-C(20)          121.69(11)
C(11)-C(12)-C(13)         121.36(14)
C(11)-C(12)-H(12)         119.3
C(13)-C(12)-H(12)         119.3
C(14)-C(13)-C(12)         120.31(15)
C(14)-C(13)-H(13)         119.8
C(12)-C(13)-H(13)         119.8
C(13)-C(14)-C(15)         120.67(14)
C(13)-C(14)-H(14)         119.7
C(15)-C(14)-H(14)         119.7
C(14)-C(15)-C(16)         119.79(14)
C(14)-C(15)-C(20)         120.10(14)
C(16)-C(15)-C(20)         120.10(14)
C(17)-C(16)-C(15)         120.61(14)
C(17)-C(16)-H(16)         119.7
C(15)-C(16)-H(16)         119.7
C(16)-C(17)-C(18)         120.10(15)
C(16)-C(17)-H(17)         119.9
C(18)-C(17)-H(17)         119.9
C(19)-C(18)-C(17)         121.36(15)
C(19)-C(18)-H(18)         119.3
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C(17)-C(18)-H(18)          119.3
C(18)-C(19)-N(3)           119.18(12)
C(18)-C(19)-C(20)          120.04(12)
N(3)-C(19)-C(20)           120.77(11)
C(19)-C(20)-C(11)          124.53(11)
C(19)-C(20)-C(15)          117.63(12)
C(11)-C(20)-C(15)          117.85(12)
N(4)-C(21)-N(3)            117.45(11)
N(4)-C(21)-C(22)           123.03(12)
N(3)-C(21)-C(22)           119.03(11)
C(21)-C(22)-H(22A)         109.5
C(21)-C(22)-H(22B)         109.5
H(22A)-C(22)-H(22B)        109.5
C(21)-C(22)-H(22C)         109.5
H(22A)-C(22)-H(22C)        109.5
H(22B)-C(22)-H(22C)        109.5
C(24)-C(23)-C(28)          121.00(14)
C(24)-C(23)-N(4)           119.86(14)
C(28)-C(23)-N(4)           118.97(14)
C(23)-C(24)-C(25)          118.11(18)
C(23)-C(24)-C(29)          120.42(14)
C(25)-C(24)-C(29)          121.47(17)
C(26)-C(25)-C(24)          121.3(2)
C(26)-C(25)-H(25)          119.3
C(24)-C(25)-H(25)          119.3
C(25)-C(26)-C(27)          120.03(17)
C(25)-C(26)-H(26)          120.0
C(27)-C(26)-H(26)          120.0
C(26)-C(27)-C(28)          121.3(2)
C(26)-C(27)-H(27)          119.4
C(28)-C(27)-H(27)          119.4
C(27)-C(28)-C(23)          118.17(19)
C(27)-C(28)-C(30)          121.82(19)
C(23)-C(28)-C(30)          120.01(16)
C(24)-C(29)-H(29A)         109.5
C(24)-C(29)-H(29B)         109.5
H(29A)-C(29)-H(29B)        109.5
C(24)-C(29)-H(29C)         109.5
H(29A)-C(29)-H(29C)        109.5
H(29B)-C(29)-H(29C)        109.5
C(28)-C(30)-H(30A)         109.5
C(28)-C(30)-H(30B)         109.5
H(30A)-C(30)-H(30B)        109.5
C(28)-C(30)-H(30C)         109.5
H(30A)-C(30)-H(30C)        109.5
H(30B)-C(30)-H(30C)        109.5
C(34)-O(1)-C(31)           103.9(3)
O(1)-C(31)-C(32)           109.8(3)
O(1)-C(31)-H(31A)          109.7
C(32)-C(31)-H(31A)         109.7
O(1)-C(31)-H(31B)          109.7
C(32)-C(31)-H(31B)         109.7
H(31A)-C(31)-H(31B)        108.2
C(33)-C(32)-C(31)          104.2(4)
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C(33)-C(32)-H(32A)           110.9
C(31)-C(32)-H(32A)           110.9
C(33)-C(32)-H(32B)           110.9
C(31)-C(32)-H(32B)           110.9
H(32A)-C(32)-H(32B)          108.9
C(32)-C(33)-C(34)            103.8(4)
C(32)-C(33)-H(33A)           111.0
C(34)-C(33)-H(33A)           111.0
C(32)-C(33)-H(33B)           111.0
C(34)-C(33)-H(33B)           111.0
H(33A)-C(33)-H(33B)          109.0
O(1)-C(34)-C(33)             108.1(4)
O(1)-C(34)-H(34A)            110.1
C(33)-C(34)-H(34A)           110.1
O(1)-C(34)-H(34B)            110.1
C(33)-C(34)-H(34B)           110.1
H(34A)-C(34)-H(34B)          108.4
C(31')-O(1')-C(34')          106.1(9)
O(1')-C(31')-C(32')          106.7(8)
O(1')-C(31')-H(31C)          110.4
C(32')-C(31')-H(31C)         110.4
O(1')-C(31')-H(31D)          110.4
C(32')-C(31')-H(31D)         110.4
H(31C)-C(31')-H(31D)         108.6
C(33')-C(32')-C(31')         103.2(9)
C(33')-C(32')-H(32C)         111.1
C(31')-C(32')-H(32C)         111.1
C(33')-C(32')-H(32D)         111.1
C(31')-C(32')-H(32D)         111.1
H(32C)-C(32')-H(32D)         109.1
C(32')-C(33')-C(34')         106.5(9)
C(32')-C(33')-H(33C)         110.4
C(34')-C(33')-H(33C)         110.4
C(32')-C(33')-H(33D)         110.4
C(34')-C(33')-H(33D)         110.4
H(33C)-C(33')-H(33D)         108.6
O(1')-C(34')-C(33')          107.3(10)
O(1')-C(34')-H(34C)          110.3
C(33')-C(34')-H(34C)         110.2
O(1')-C(34')-H(34D)          110.2
C(33')-C(34')-H(34D)         110.2
H(34C)-C(34')-H(34D)         108.5
N(3)-Ge(1)-N(2)               87.48(4)
N(3)-Ge(1)-N(1)#1             95.69(4)
N(2)-Ge(1)-N(1)#1             96.79(4)
C(9)-N(1)-C(1)               121.22(11)
C(9)-N(1)-Ge(1)#1            110.44(8)
C(1)-N(1)-Ge(1)#1            125.38(8)
C(9)-N(2)-C(11)              119.28(10)
C(9)-N(2)-Ge(1)             112.38(8)
C(11)-N(2)-Ge(1)            126.95(8)
C(21)-N(3)-C(19)             120.24(10)
C(21)-N(3)-Ge(1)            113.24(8)
C(19)-N(3)-Ge(1)            126.15(8)
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 C(21)-N(4)-C(23)                   119.68(12)
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Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+1,-z+1

Table S16. Anisotropic displacement parameters (A^2 x 10^3) for AA-R34.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

_____

	U11	U22	U33	U23	U13	U12

_____

C(1)	20(1)	39(1)	19(1)	-11(1)	-4(1)	-6(1)
C(2)	29(1)	47(1)	22(1)	-3(1)	-9(1)	-11(1)
C(3)	46(1)	77(1)	20(1)	-5(1)	-9(1)	-20(1)
C(4)	48(1)	107(2)	26(1)	-32(1)	0(1)	-20(1)
C(5)	40(1)	84(2)	42(1)	-44(1)	-4(1)	-6(1)
C(6)	27(1)	49(1)	31(1)	-23(1)	-5(1)	-4(1)
C(7)	40(1)	36(1)	38(1)	4(1)	-20(1)	-7(1)
C(8)	44(1)	39(1)	48(1)	-28(1)	-12(1)	1(1)
C(9)	18(1)	22(1)	20(1)	-6(1)	-7(1)	-1(1)
C(10)	21(1)	42(1)	28(1)	-10(1)	-9(1)	-7(1)
C(11)	16(1)	21(1)	25(1)	-9(1)	-5(1)	-1(1)
C(12)	27(1)	23(1)	33(1)	-6(1)	-7(1)	3(1)
C(13)	34(1)	25(1)	52(1)	-12(1)	-11(1)	7(1)
C(14)	30(1)	29(1)	56(1)	-23(1)	-5(1)	6(1)
C(15)	23(1)	29(1)	38(1)	-20(1)	-1(1)	-2(1)
C(16)	35(1)	42(1)	43(1)	-29(1)	6(1)	-4(1)
C(17)	42(1)	46(1)	30(1)	-23(1)	8(1)	-9(1)
C(18)	34(1)	34(1)	23(1)	-12(1)	1(1)	-7(1)
C(19)	19(1)	24(1)	22(1)	-10(1)	-1(1)	-5(1)
C(20)	17(1)	22(1)	26(1)	-12(1)	-3(1)	-3(1)
C(21)	21(1)	20(1)	20(1)	-5(1)	-4(1)	-4(1)
C(22)	21(1)	28(1)	52(1)	-13(1)	-3(1)	-5(1)
C(23)	24(1)	21(1)	37(1)	-10(1)	-6(1)	-1(1)
C(24)	32(1)	23(1)	41(1)	-3(1)	-4(1)	-3(1)
C(25)	42(1)	23(1)	68(1)	-3(1)	-1(1)	-5(1)
C(26)	48(1)	26(1)	102(2)	-25(1)	-10(1)	-5(1)
C(27)	50(1)	41(1)	92(2)	-42(1)	-22(1)	4(1)
C(28)	39(1)	34(1)	54(1)	-23(1)	-17(1)	4(1)
C(29)	58(1)	43(1)	33(1)	1(1)	-8(1)	-10(1)
C(30)	85(2)	59(1)	49(1)	-29(1)	-31(1)	5(1)
O(1)	84(2)	59(1)	68(2)	-22(1)	6(1)	-3(1)
C(31)	57(2)	81(2)	99(3)	-45(2)	-21(2)	-9(2)
C(32)	65(2)	91(2)	92(2)	-37(2)	-24(2)	-8(2)
C(33)	82(3)	94(3)	124(3)	-60(2)	-23(2)	-19(3)
C(34)	67(2)	108(3)	78(2)	-51(2)	-21(2)	0(2)
O(1')	89(4)	88(4)	100(4)	-26(3)	-15(4)	-15(3)
C(31')	66(4)	89(5)	72(4)	-19(4)	-21(4)	-14(4)
C(32')	59(4)	93(4)	77(4)	-22(4)	-13(4)	-2(3)
C(33')	79(4)	96(4)	92(4)	-36(4)	-13(4)	-7(4)
C(34')	72(4)	84(5)	113(4)	-42(4)	-20(4)	-15(4)
Ge(1)	17(1)	17(1)	17(1)	-6(1)	-3(1)	-1(1)
N(1)	18(1)	22(1)	18(1)	-6(1)	-5(1)	-2(1)
N(2)	17(1)	21(1)	18(1)	-5(1)	-4(1)	0(1)
N(3)	20(1)	19(1)	20(1)	-6(1)	0(1)	-4(1)
N(4)	24(1)	20(1)	26(1)	-6(1)	-5(1)	-2(1)

Crystal data and structure refinement of compound L₂Ge
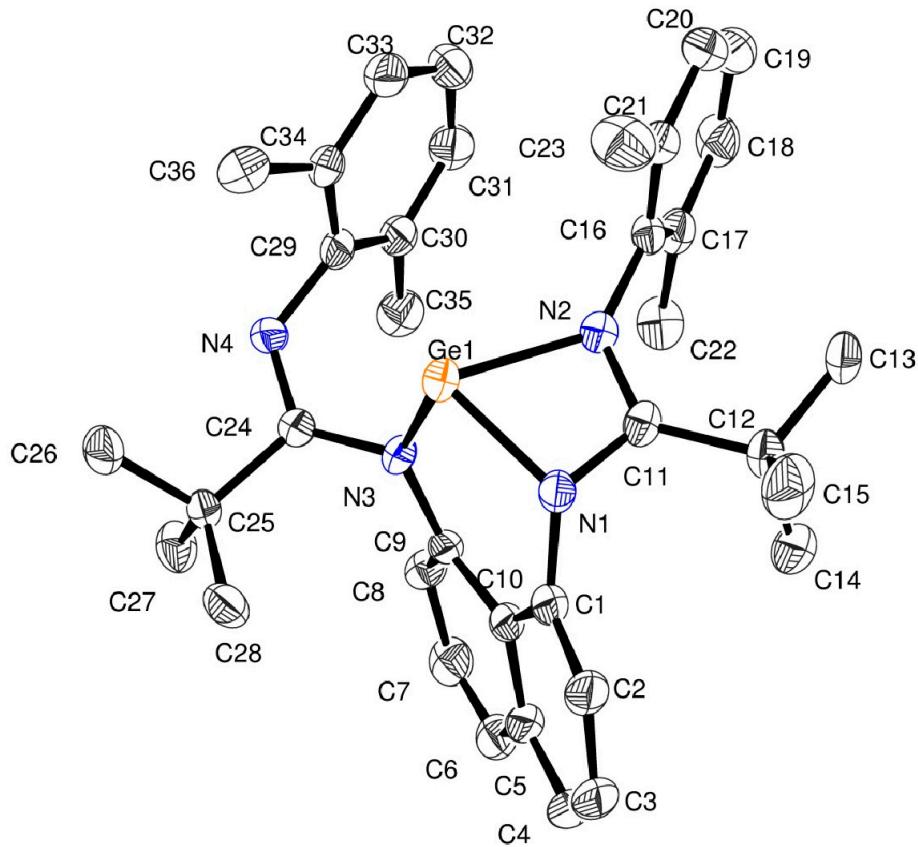
Figure S7. Asymmetric Unit

Table S17. Crystal data and structure refinement for R109.

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Identification code            R109

Empirical formula              C36 H42 Ge N4

Formula weight                 603.35

Temperature                    193(2) K

Wavelength                     0.71073 A

Crystal system, space group    Monoclinic,  P 21/n

Unit cell dimensions       a = 10.879(2) A   alpha = 90 deg.
                           b = 14.307(2) A    beta = 97.332(6) deg.
                           c = 20.235(4) A   gamma = 90 deg.

Volume                         3123.7(10) A^3
```

```
Z, Calculated density              4,  1.283 Mg/m^3

Absorption coefficient             1.011 mm^-1

F(000)                             1272

Crystal size                       0.180 x 0.040 x 0.010 mm

Theta range for data collection    1.748 to 24.129 deg.

Limiting indices                   -12<=h<=12, -14<=k<=16,
                                    -23<=l<=23

Reflections collected / unique     56977 / 4948 [R(int) = 0.1415]

Completeness to theta = 24.129     99.2 %

Refinement method                  Full-matrix least-squares on F^2

Data / restraints / parameters     4948 / 0 / 380

Goodness-of-fit on F^2             1.051

Final R indices [I>2sigma(I)]      R1 = 0.0485, wR2 = 0.1040

R indices (all data)               R1 = 0.0920, wR2 = 0.1230

Largest diff. peak and hole        0.527 and -0.577 e.A^-3
```

Table S18. Atomic coordinates (x 10^4) and equivalent isotropic
displacement parameters (A^2 x 10^3) for R109.
U(eq) is defined as one third of the trace of the orthogonalized
Uij tensor.

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	x	y	z	U(eq)
C(1)	8505(4)	5352(3)	1746(2)	28(1)
C(2)	9492(4)	5021(3)	1465(2)	35(1)
C(3)	9754(4)	5372(3)	855(2)	44(1)
C(4)	9044(4)	6073(3)	543(2)	44(1)
C(5)	7952(4)	6386(3)	786(2)	34(1)
C(6)	7179(4)	7072(3)	447(2)	38(1)
C(7)	6102(5)	7309(3)	666(2)	39(1)
C(8)	5718(4)	6860(3)	1216(2)	30(1)
C(9)	6409(4)	6167(3)	1556(2)	24(1)
C(10)	7623(4)	5967(3)	1382(2)	28(1)
C(11)	8690(4)	5728(3)	2941(2)	25(1)
C(12)	10019(4)	6107(3)	3089(2)	31(1)
C(13)	10277(4)	6598(3)	3770(2)	40(1)
C(14)	10290(4)	6810(3)	2554(2)	44(1)
C(15)	10897(4)	5256(3)	3106(3)	49(1)
C(16)	7704(4)	6242(3)	3925(2)	25(1)
C(17)	7389(4)	7194(3)	3923(2)	31(1)
C(18)	7273(4)	7612(3)	4527(2)	40(1)
C(19)	7448(4)	7109(3)	5113(2)	45(1)
C(20)	7739(4)	6171(3)	5105(2)	41(1)
C(21)	7852(4)	5718(3)	4507(2)	31(1)
C(22)	7182(4)	7739(3)	3283(2)	40(1)
C(23)	8152(5)	4689(3)	4498(2)	48(1)
C(24)	4593(4)	5390(2)	1884(2)	21(1)
C(25)	4093(4)	4904(3)	1212(2)	26(1)
C(26)	3245(4)	4092(3)	1381(2)	38(1)
C(27)	3282(4)	5564(3)	745(2)	38(1)
C(28)	5124(4)	4488(3)	856(2)	37(1)
C(29)	4105(4)	5776(3)	2966(2)	28(1)
C(30)	4070(4)	6748(3)	3095(2)	31(1)
C(31)	4200(4)	7034(3)	3752(2)	40(1)
C(32)	4357(4)	6419(4)	4276(2)	43(1)
C(33)	4339(4)	5459(3)	4141(2)	38(1)
C(34)	4187(4)	5125(3)	3489(2)	29(1)
C(35)	3853(4)	7445(3)	2541(2)	42(1)
C(36)	4033(4)	4092(3)	3363(2)	41(1)
N(1)	8322(3)	5144(2)	2415(2)	26(1)
N(2)	7773(3)	5801(2)	3298(2)	24(1)
N(3)	5867(3)	5612(2)	2030(2)	24(1)
N(4)	3822(3)	5429(2)	2308(2)	26(1)
Ge(1)	6714(1)	4836(1)	2710(1)	25(1)

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Table S19. Bond lengths [A] and angles [deg] for R109.
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```
C(1)-C(2)             1.362(6)
C(1)-N(1)             1.424(5)
C(1)-C(10)            1.435(6)
C(2)-C(3)             1.396(6)
C(2)-H(2)             0.9500
C(3)-C(4)             1.370(6)
C(3)-H(3)             0.9500
C(4)-C(5)             1.416(6)
C(4)-H(4)             0.9500
C(5)-C(6)             1.411(6)
C(5)-C(10)            1.431(6)
C(6)-C(7)             1.349(6)
C(6)-H(6)             0.9500
C(7)-C(8)             1.395(6)
C(7)-H(7)             0.9500
C(8)-C(9)             1.375(5)
C(8)-H(8)             0.9500
C(9)-N(3)             1.428(5)
C(9)-C(10)            1.439(5)
C(11)-N(2)            1.308(5)
C(11)-N(1)            1.374(5)
C(11)-C(12)           1.537(5)
C(12)-C(14)           1.534(6)
C(12)-C(13)           1.541(5)
C(12)-C(15)           1.545(6)
C(13)-H(13A)          0.9800
C(13)-H(13B)          0.9800
C(13)-H(13C)          0.9800
C(14)-H(14A)          0.9800
C(14)-H(14B)          0.9800
C(14)-H(14C)          0.9800
C(15)-H(15A)          0.9800
C(15)-H(15B)          0.9800
C(15)-H(15C)          0.9800
C(16)-C(21)           1.388(5)
C(16)-C(17)           1.404(5)
C(16)-N(2)            1.427(5)
C(17)-C(18)           1.381(6)
C(17)-C(22)           1.503(6)
C(18)-C(19)           1.379(6)
C(18)-H(18)           0.9500
C(19)-C(20)           1.380(6)
C(19)-H(19)           0.9500
C(20)-C(21)           1.392(6)
C(20)-H(20)           0.9500
C(21)-C(23)           1.508(6)
C(22)-H(22A)          0.9800
C(22)-H(22B)          0.9800
C(22)-H(22C)          0.9800
C(23)-H(23A)          0.9800
C(23)-H(23B)          0.9800
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C(23)-H(23C)                    0.9800
C(24)-N(4)                      1.275(5)
C(24)-N(3)                      1.417(5)
C(24)-C(25)                     1.561(5)
C(25)-C(28)                     1.530(6)
C(25)-C(27)                     1.532(6)
C(25)-C(26)                     1.548(5)
C(26)-H(26A)                    0.9800
C(26)-H(26B)                    0.9800
C(26)-H(26C)                    0.9800
C(27)-H(27A)                    0.9800
C(27)-H(27B)                    0.9800
C(27)-H(27C)                    0.9800
C(28)-H(28A)                    0.9800
C(28)-H(28B)                    0.9800
C(28)-H(28C)                    0.9800
C(29)-C(34)                     1.403(6)
C(29)-C(30)                     1.417(6)
C(29)-N(4)                      1.417(5)
C(30)-C(31)                     1.380(6)
C(30)-C(35)                     1.497(6)
C(31)-C(32)                     1.372(6)
C(31)-H(31)                     0.9500
C(32)-C(33)                     1.400(6)
C(32)-H(32)                     0.9500
C(33)-C(34)                     1.392(6)
C(33)-H(33)                     0.9500
C(34)-C(36)                     1.506(6)
C(35)-H(35A)                    0.9800
C(35)-H(35B)                    0.9800
C(35)-H(35C)                    0.9800
C(36)-H(36A)                    0.9800
C(36)-H(36B)                    0.9800
C(36)-H(36C)                    0.9800
N(1)-Ge(1)                      1.969(3)
N(2)-Ge(1)                      2.073(3)
N(3)-Ge(1)                      1.912(3)

C(2)-C(1)-N(1)                  122.5(4)
C(2)-C(1)-C(10)                 120.6(4)
N(1)-C(1)-C(10)                 116.9(4)
C(1)-C(2)-C(3)                  120.4(4)
C(1)-C(2)-H(2)                  119.8
C(3)-C(2)-H(2)                  119.8
C(4)-C(3)-C(2)                  120.3(4)
C(4)-C(3)-H(3)                  119.9
C(2)-C(3)-H(3)                  119.9
C(3)-C(4)-C(5)                  121.4(4)
C(3)-C(4)-H(4)                  119.3
C(5)-C(4)-H(4)                  119.3
C(6)-C(5)-C(4)                  121.6(4)
C(6)-C(5)-C(10)                 120.2(4)
C(4)-C(5)-C(10)                 118.1(4)
C(7)-C(6)-C(5)                  120.2(4)
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C(7)-C(6)-H(6)          119.9
C(5)-C(6)-H(6)          119.9
C(6)-C(7)-C(8)          120.5(4)
C(6)-C(7)-H(7)          119.7
C(8)-C(7)-H(7)          119.7
C(9)-C(8)-C(7)          122.1(4)
C(9)-C(8)-H(8)          118.9
C(7)-C(8)-H(8)          118.9
C(8)-C(9)-N(3)          119.4(4)
C(8)-C(9)-C(10)         118.7(4)
N(3)-C(9)-C(10)         121.7(3)
C(5)-C(10)-C(1)         117.9(4)
C(5)-C(10)-C(9)         117.4(4)
C(1)-C(10)-C(9)         124.7(4)
N(2)-C(11)-N(1)         108.0(3)
N(2)-C(11)-C(12)        129.0(4)
N(1)-C(11)-C(12)        122.6(4)
C(14)-C(12)-C(11)       110.7(3)
C(14)-C(12)-C(13)       107.6(3)
C(11)-C(12)-C(13)       113.2(3)
C(14)-C(12)-C(15)       111.0(4)
C(11)-C(12)-C(15)       106.9(3)
C(13)-C(12)-C(15)       107.4(4)
C(12)-C(13)-H(13A)      109.5
C(12)-C(13)-H(13B)      109.5
H(13A)-C(13)-H(13B)     109.5
C(12)-C(13)-H(13C)      109.5
H(13A)-C(13)-H(13C)     109.5
H(13B)-C(13)-H(13C)     109.5
C(12)-C(14)-H(14A)      109.5
C(12)-C(14)-H(14B)      109.5
H(14A)-C(14)-H(14B)     109.5
C(12)-C(14)-H(14C)      109.5
H(14A)-C(14)-H(14C)     109.5
H(14B)-C(14)-H(14C)     109.5
C(12)-C(15)-H(15A)      109.5
C(12)-C(15)-H(15B)      109.5
H(15A)-C(15)-H(15B)     109.5
C(12)-C(15)-H(15C)      109.5
H(15A)-C(15)-H(15C)     109.5
H(15B)-C(15)-H(15C)     109.5
C(21)-C(16)-C(17)       121.9(4)
C(21)-C(16)-N(2)        120.1(3)
C(17)-C(16)-N(2)        117.8(3)
C(18)-C(17)-C(16)       117.9(4)
C(18)-C(17)-C(22)       121.1(4)
C(16)-C(17)-C(22)       121.0(4)
C(19)-C(18)-C(17)       121.1(4)
C(19)-C(18)-H(18)       119.5
C(17)-C(18)-H(18)       119.5
C(18)-C(19)-C(20)       120.3(4)
C(18)-C(19)-H(19)       119.8
C(20)-C(19)-H(19)       119.8
C(19)-C(20)-C(21)       120.6(4)
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C(19)-C(20)-H(20)         119.7
C(21)-C(20)-H(20)         119.7
C(16)-C(21)-C(20)         118.2(4)
C(16)-C(21)-C(23)         121.3(4)
C(20)-C(21)-C(23)         120.5(4)
C(17)-C(22)-H(22A)        109.5
C(17)-C(22)-H(22B)        109.5
H(22A)-C(22)-H(22B)       109.5
C(17)-C(22)-H(22C)        109.5
H(22A)-C(22)-H(22C)       109.5
H(22B)-C(22)-H(22C)       109.5
C(21)-C(23)-H(23A)        109.5
C(21)-C(23)-H(23B)        109.5
H(23A)-C(23)-H(23B)       109.5
C(21)-C(23)-H(23C)        109.5
H(23A)-C(23)-H(23C)       109.5
H(23B)-C(23)-H(23C)       109.5
N(4)-C(24)-N(3)           124.0(3)
N(4)-C(24)-C(25)          114.8(3)
N(3)-C(24)-C(25)          120.3(3)
C(28)-C(25)-C(27)         110.4(3)
C(28)-C(25)-C(26)         107.8(3)
C(27)-C(25)-C(26)         106.6(3)
C(28)-C(25)-C(24)         112.8(3)
C(27)-C(25)-C(24)         111.8(3)
C(26)-C(25)-C(24)         107.0(3)
C(25)-C(26)-H(26A)        109.5
C(25)-C(26)-H(26B)        109.5
H(26A)-C(26)-H(26B)       109.5
C(25)-C(26)-H(26C)        109.5
H(26A)-C(26)-H(26C)       109.5
H(26B)-C(26)-H(26C)       109.5
C(25)-C(27)-H(27A)        109.5
C(25)-C(27)-H(27B)        109.5
H(27A)-C(27)-H(27B)       109.5
C(25)-C(27)-H(27C)        109.5
H(27A)-C(27)-H(27C)       109.5
H(27B)-C(27)-H(27C)       109.5
C(25)-C(28)-H(28A)        109.5
C(25)-C(28)-H(28B)        109.5
H(28A)-C(28)-H(28B)       109.5
C(25)-C(28)-H(28C)        109.5
H(28A)-C(28)-H(28C)       109.5
H(28B)-C(28)-H(28C)       109.5
C(34)-C(29)-C(30)         120.8(4)
C(34)-C(29)-N(4)          117.5(4)
C(30)-C(29)-N(4)          120.6(4)
C(31)-C(30)-C(29)         117.8(4)
C(31)-C(30)-C(35)         120.7(4)
C(29)-C(30)-C(35)         121.4(4)
C(32)-C(31)-C(30)         122.8(4)
C(32)-C(31)-H(31)         118.6
C(30)-C(31)-H(31)         118.6
C(31)-C(32)-C(33)         118.7(4)
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C(31)-C(32)-H(32)            120.6
C(33)-C(32)-H(32)            120.6
C(34)-C(33)-C(32)            121.2(4)
C(34)-C(33)-H(33)            119.4
C(32)-C(33)-H(33)            119.4
C(33)-C(34)-C(29)            118.4(4)
C(33)-C(34)-C(36)            119.6(4)
C(29)-C(34)-C(36)            121.9(4)
C(30)-C(35)-H(35A)           109.5
C(30)-C(35)-H(35B)           109.5
H(35A)-C(35)-H(35B)          109.5
C(30)-C(35)-H(35C)           109.5
H(35A)-C(35)-H(35C)          109.5
H(35B)-C(35)-H(35C)          109.5
C(34)-C(36)-H(36A)           109.5
C(34)-C(36)-H(36B)           109.5
H(36A)-C(36)-H(36B)          109.5
C(34)-C(36)-H(36C)           109.5
H(36A)-C(36)-H(36C)          109.5
H(36B)-C(36)-H(36C)          109.5
C(11)-N(1)-C(1)              123.2(3)
C(11)-N(1)-Ge(1)              94.7(2)
C(1)-N(1)-Ge(1)             125.0(3)
C(11)-N(2)-C(16)            131.0(3)
C(11)-N(2)-Ge(1)             92.1(2)
C(16)-N(2)-Ge(1)           135.7(3)
C(24)-N(3)-C(9)             117.5(3)
C(24)-N(3)-Ge(1)           112.9(2)
C(9)-N(3)-Ge(1)            127.1(3)
C(24)-N(4)-C(29)           124.4(3)
N(3)-Ge(1)-N(1)             90.95(13)
N(3)-Ge(1)-N(2)            102.00(13)
N(1)-Ge(1)-N(2)             64.89(13)
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Symmetry transformations used to generate equivalent atoms:

Table S20. Anisotropic displacement parameters (A^2 x 10^3) for R109.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

_____

	U11	U22	U33	U23	U13	U12
C(1)	27(3)	29(3)	28(2)	-7(2)	5(2)	-6(2)
C(2)	28(3)	37(3)	42(3)	-16(2)	13(2)	-4(2)
C(3)	31(3)	60(4)	44(3)	-21(3)	19(2)	-10(3)
C(4)	40(3)	58(3)	38(3)	-12(3)	19(2)	-18(3)
C(5)	36(3)	37(3)	32(3)	-8(2)	12(2)	-15(2)
C(6)	44(3)	37(3)	33(3)	5(2)	4(2)	-14(2)
C(7)	48(3)	27(3)	42(3)	3(2)	4(3)	-8(2)
C(8)	33(3)	22(2)	35(3)	1(2)	10(2)	-1(2)
C(9)	27(3)	23(2)	21(2)	-4(2)	6(2)	-6(2)
C(10)	28(3)	28(2)	30(2)	-12(2)	8(2)	-8(2)
C(11)	20(2)	22(2)	32(2)	5(2)	0(2)	1(2)
C(12)	21(3)	35(3)	35(3)	-2(2)	-1(2)	-3(2)
C(13)	26(3)	51(3)	40(3)	0(2)	-3(2)	-12(2)
C(14)	43(3)	45(3)	46(3)	-3(2)	11(2)	-20(2)
C(15)	26(3)	57(3)	64(3)	-4(3)	2(2)	8(2)
C(16)	23(3)	27(2)	26(2)	-5(2)	2(2)	-6(2)
C(17)	28(3)	27(2)	38(3)	-3(2)	5(2)	-4(2)
C(18)	44(3)	28(3)	48(3)	-13(2)	7(2)	-8(2)
C(19)	52(3)	45(3)	39(3)	-17(3)	14(2)	-15(2)
C(20)	46(3)	49(3)	27(3)	0(2)	4(2)	-15(2)
C(21)	30(3)	34(3)	29(3)	1(2)	4(2)	-6(2)
C(22)	40(3)	31(3)	47(3)	3(2)	-1(2)	4(2)
C(23)	64(4)	39(3)	40(3)	11(2)	2(3)	4(3)
C(24)	26(2)	14(2)	24(2)	2(2)	3(2)	1(2)
C(25)	26(2)	29(2)	23(2)	-2(2)	0(2)	-6(2)
C(26)	46(3)	31(3)	36(3)	-4(2)	3(2)	-12(2)
C(27)	35(3)	37(3)	37(3)	4(2)	-9(2)	-3(2)
C(28)	35(3)	44(3)	30(3)	-12(2)	2(2)	1(2)
C(29)	17(2)	35(3)	31(2)	-3(2)	4(2)	-3(2)
C(30)	19(3)	40(3)	33(3)	-4(2)	5(2)	0(2)
C(31)	35(3)	42(3)	45(3)	-13(2)	14(2)	0(2)
C(32)	35(3)	61(4)	34(3)	-11(3)	4(2)	-5(2)
C(33)	29(3)	53(3)	33(3)	4(2)	2(2)	-4(2)
C(34)	18(2)	38(3)	31(2)	-1(2)	3(2)	-3(2)
C(35)	40(3)	38(3)	49(3)	-3(2)	11(2)	1(2)
C(36)	43(3)	43(3)	39(3)	5(2)	11(2)	-4(2)
N(1)	21(2)	26(2)	29(2)	-5(2)	3(2)	-2(2)
N(2)	22(2)	22(2)	27(2)	2(2)	2(2)	1(2)
N(3)	18(2)	25(2)	28(2)	0(2)	4(2)	-2(2)
N(4)	23(2)	31(2)	23(2)	-2(2)	4(2)	-1(2)
Ge(1)	22(1)	23(1)	31(1)	0(1)	2(1)	-2(1)

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Crystal data and structure refinement of compound 1a
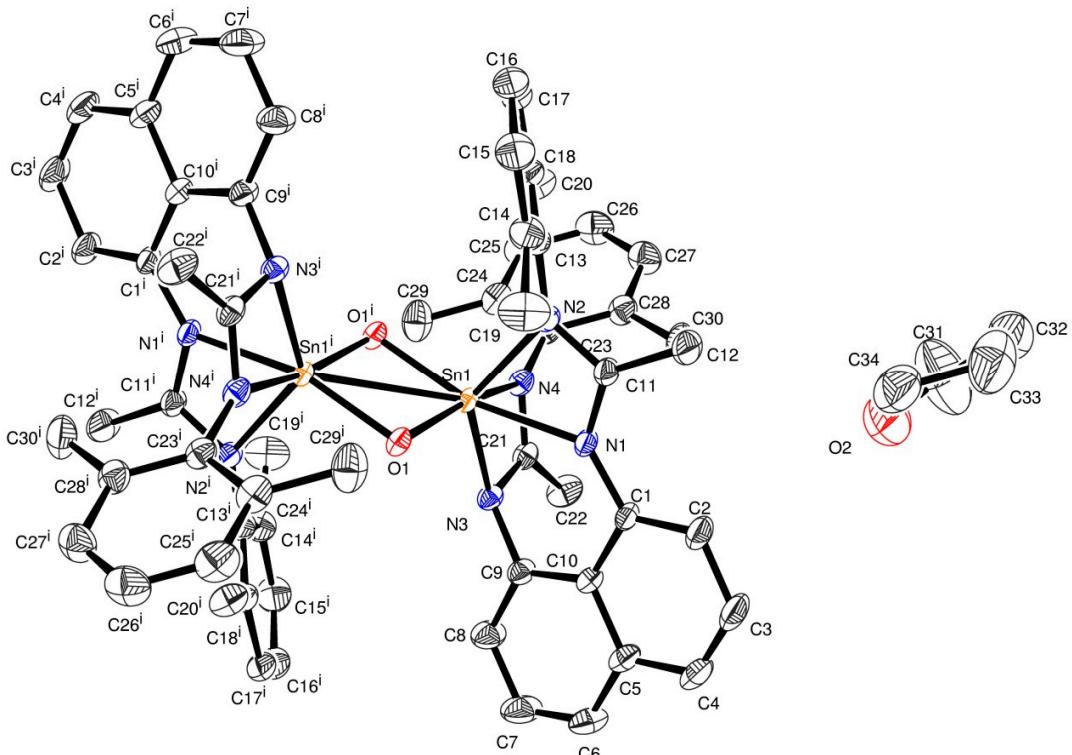
Figure S8. Asymmetric Unit

Table S21. Crystal data and structure refinement for R126.

Identification code	R126
Empirical formula	C60 H60 N8 O2 Sn2, 2(C4 H8 O)
Formula weight	1306.79
Temperature	193(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P -1
Unit cell dimensions	a = 11.0951(5) A alpha = 88.337(2) deg.
	b = 11.8481(6) A beta = 88.326(2) deg.
	c = 12.8106(6) A gamma = 65.647(2) deg.
Volume	1533.27(13) A^3
Z, Calculated density	1, 1.415 Mg/m^3
Absorption coefficient	0.870 mm^-1

```
F(000)                            672

Crystal size                      0.120 x 0.120 x 0.080 mm

Theta range for data collection   3.182 to 36.438 deg.

Limiting indices                  -18<=h<=18, -19<=k<=19,
                                   -21<=l<=21

Reflections collected / unique    122943 / 14935 [R(int) = 0.0430]

Completeness to theta = 25.242    99.7 %

Refinement method                 Full-matrix least-squares on F^2

Data / restraints / parameters    14935 / 0 / 376

Goodness-of-fit on F^2            1.061

Final R indices [I>2sigma(I)]     R1 = 0.0272, wR2 = 0.0652

R indices (all data)              R1 = 0.0361, wR2 = 0.0703

Largest diff. peak and hole       1.016 and -0.944 e.A^-3
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Table S22. Atomic coordinates (x 10^4) and equivalent isotropic
displacement parameters (A^2 x 10^3) for R126.
U(eq) is defined as one third of the trace of the orthogonalized
Uij tensor.

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	x	y	z	U(eq)
C(1)	1225(1)	5332(1)	8431(1)	22(1)
C(2)	581(1)	4715(2)	7943(1)	33(1)
C(3)	-758(2)	4974(2)	8162(2)	38(1)
C(4)	-1470(1)	5842(2)	8865(1)	34(1)
C(5)	-884(1)	6531(1)	9367(1)	28(1)
C(6)	-1641(2)	7429(2)	10105(2)	38(1)
C(7)	-1111(2)	8092(2)	10630(2)	43(1)
C(8)	205(2)	7926(2)	10406(1)	34(1)
C(9)	961(1)	7097(1)	9665(1)	23(1)
C(10)	470(1)	6319(1)	9142(1)	22(1)
C(11)	3519(1)	4161(1)	7727(1)	24(1)
C(12)	3330(2)	3412(2)	6877(2)	46(1)
C(13)	5954(1)	3202(1)	7614(1)	24(1)
C(14)	6330(2)	1970(1)	7966(1)	31(1)
C(15)	7575(2)	1088(2)	7666(1)	37(1)
C(16)	8441(2)	1419(2)	7069(1)	36(1)
C(17)	8087(1)	2646(2)	6775(1)	31(1)
C(18)	6842(1)	3554(1)	7034(1)	25(1)
C(19)	5448(2)	1609(2)	8691(2)	47(1)
C(20)	6454(2)	4881(2)	6702(2)	35(1)
C(21)	2328(1)	7708(1)	8523(1)	22(1)
C(22)	1220(2)	8870(1)	8143(1)	34(1)
C(23)	3877(1)	7715(1)	7170(1)	23(1)
C(24)	4677(2)	8352(1)	7317(1)	29(1)
C(25)	5098(2)	8821(2)	6435(2)	39(1)
C(26)	4741(2)	8659(2)	5440(2)	41(1)
C(27)	3956(2)	8027(2)	5305(1)	36(1)
C(28)	3512(1)	7541(1)	6167(1)	28(1)
C(29)	5065(2)	8512(2)	8401(2)	41(1)
C(30)	2698(2)	6815(2)	6002(1)	41(1)
C(31)	853(6)	3423(4)	4475(3)	112(2)
C(32)	1106(3)	2388(3)	3786(2)	74(1)
C(33)	1235(3)	1337(3)	4558(3)	86(1)
C(34)	1539(3)	1780(3)	5565(2)	65(1)
N(1)	2600(1)	4968(1)	8340(1)	21(1)
N(2)	4712(1)	4140(1)	7914(1)	23(1)
N(3)	2221(1)	7087(1)	9390(1)	20(1)
N(4)	3484(1)	7180(1)	8050(1)	22(1)
O(1)	4297(1)	4403(1)	10413(1)	20(1)
O(2)	883(2)	3071(2)	5526(2)	72(1)
Sn(1)	4040(1)	5497(1)	9137(1)	16(1)

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Table S23. Bond lengths [A] and angles [deg] for R126
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```
C(1)-C(2)              1.3849(18)
C(1)-N(1)              1.4063(16)
C(1)-C(10)             1.4515(18)
C(2)-C(3)              1.409(2)
C(2)-H(2)              0.9500
C(3)-C(4)              1.354(3)
C(3)-H(3)              0.9500
C(4)-C(5)              1.414(2)
C(4)-H(4)              0.9500
C(5)-C(6)              1.417(2)
C(5)-C(10)             1.4388(18)
C(6)-C(7)              1.361(3)
C(6)-H(6)              0.9500
C(7)-C(8)              1.412(2)
C(7)-H(7)              0.9500
C(8)-C(9)              1.3772(19)
C(8)-H(8)              0.9500
C(9)-N(3)              1.4267(16)
C(9)-C(10)             1.4371(18)
C(11)-N(1)             1.3285(16)
C(11)-N(2)             1.3415(16)
C(11)-C(12)            1.497(2)
C(11)-Sn(1)            2.6612(12)
C(12)-H(12A)           0.9800
C(12)-H(12B)           0.9800
C(12)-H(12C)           0.9800
C(13)-C(18)            1.405(2)
C(13)-C(14)            1.407(2)
C(13)-N(2)             1.4186(16)
C(14)-C(15)            1.397(2)
C(14)-C(19)            1.508(3)
C(15)-C(16)            1.383(3)
C(15)-H(15)            0.9500
C(16)-C(17)            1.383(2)
C(16)-H(16)            0.9500
C(17)-C(18)            1.3949(19)
C(17)-H(17)            0.9500
C(18)-C(20)            1.501(2)
C(19)-H(19A)           0.9800
C(19)-H(19B)           0.9800
C(19)-H(19C)           0.9800
C(20)-H(20A)           0.9800
C(20)-H(20B)           0.9800
C(20)-H(20C)           0.9800
C(21)-N(4)             1.3113(17)
C(21)-N(3)             1.3439(17)
C(21)-C(22)            1.4978(18)
C(21)-Sn(1)            2.6374(12)
C(22)-H(22A)           0.9800
C(22)-H(22B)           0.9800
C(22)-H(22C)           0.9800
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C(23)-C(24)                  1.401(2)
C(23)-C(28)                  1.404(2)
C(23)-N(4)                   1.4213(17)
C(24)-C(25)                  1.397(2)
C(24)-C(29)                  1.505(2)
C(25)-C(26)                  1.387(3)
C(25)-H(25)                  0.9500
C(26)-C(27)                  1.380(3)
C(26)-H(26)                  0.9500
C(27)-C(28)                  1.400(2)
C(27)-H(27)                  0.9500
C(28)-C(30)                  1.504(2)
C(29)-H(29A)                 0.9800
C(29)-H(29B)                 0.9800
C(29)-H(29C)                 0.9800
C(30)-H(30A)                 0.9800
C(30)-H(30B)                 0.9800
C(30)-H(30C)                 0.9800
C(31)-O(2)                   1.395(4)
C(31)-C(32)                  1.458(5)
C(31)-H(31A)                 0.9900
C(31)-H(31B)                 0.9900
C(32)-C(33)                  1.530(5)
C(32)-H(32A)                 0.9900
C(32)-H(32B)                 0.9900
C(33)-C(34)                  1.504(4)
C(33)-H(33A)                 0.9900
C(33)-H(33B)                 0.9900
C(34)-O(2)                   1.397(3)
C(34)-H(34A)                 0.9900
C(34)-H(34B)                 0.9900
N(1)-Sn(1)                   2.2236(10)
N(2)-Sn(1)                   2.1644(11)
N(3)-Sn(1)                   2.1423(10)
N(4)-Sn(1)                   2.2742(10)
O(1)-Sn(1)#1                 1.9996(8)
O(1)-Sn(1)                   2.0079(9)
Sn(1)-Sn(1)#1                2.97787(19)

C(2)-C(1)-N(1)               122.61(12)
C(2)-C(1)-C(10)              118.62(12)
N(1)-C(1)-C(10)              118.51(10)
C(1)-C(2)-C(3)               121.84(15)
C(1)-C(2)-H(2)               119.1
C(3)-C(2)-H(2)               119.1
C(4)-C(3)-C(2)               120.95(14)
C(4)-C(3)-H(3)               119.5
C(2)-C(3)-H(3)               119.5
C(3)-C(4)-C(5)               120.05(13)
C(3)-C(4)-H(4)               120.0
C(5)-C(4)-H(4)               120.0
C(4)-C(5)-C(6)               119.19(13)
C(4)-C(5)-C(10)              120.64(14)
C(6)-C(5)-C(10)              120.16(14)
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C(7)-C(6)-C(5)            121.41(14)
C(7)-C(6)-H(6)            119.3
C(5)-C(6)-H(6)            119.3
C(6)-C(7)-C(8)            119.61(15)
C(6)-C(7)-H(7)            120.2
C(8)-C(7)-H(7)            120.2
C(9)-C(8)-C(7)            120.89(15)
C(9)-C(8)-H(8)            119.6
C(7)-C(8)-H(8)            119.6
C(8)-C(9)-N(3)            117.66(12)
C(8)-C(9)-C(10)           121.30(12)
N(3)-C(9)-C(10)           120.95(11)
C(9)-C(10)-C(5)           116.42(12)
C(9)-C(10)-C(1)           125.86(11)
C(5)-C(10)-C(1)           117.71(12)
N(1)-C(11)-N(2)           110.50(11)
N(1)-C(11)-C(12)          127.95(12)
N(2)-C(11)-C(12)          121.42(12)
N(1)-C(11)-Sn(1)           56.50(6)
N(2)-C(11)-Sn(1)           54.00(6)
C(12)-C(11)-Sn(1)         174.81(11)
C(11)-C(12)-H(12A)        109.5
C(11)-C(12)-H(12B)        109.5
H(12A)-C(12)-H(12B)       109.5
C(11)-C(12)-H(12C)        109.5
H(12A)-C(12)-H(12C)       109.5
H(12B)-C(12)-H(12C)       109.5
C(18)-C(13)-C(14)         120.86(12)
C(18)-C(13)-N(2)          118.26(12)
C(14)-C(13)-N(2)          120.64(13)
C(15)-C(14)-C(13)         118.33(15)
C(15)-C(14)-C(19)         120.20(15)
C(13)-C(14)-C(19)         121.40(14)
C(16)-C(15)-C(14)         121.13(15)
C(16)-C(15)-H(15)         119.4
C(14)-C(15)-H(15)         119.4
C(15)-C(16)-C(17)         119.94(14)
C(15)-C(16)-H(16)         120.0
C(17)-C(16)-H(16)         120.0
C(16)-C(17)-C(18)         120.96(15)
C(16)-C(17)-H(17)         119.5
C(18)-C(17)-H(17)         119.5
C(17)-C(18)-C(13)         118.63(13)
C(17)-C(18)-C(20)         120.86(14)
C(13)-C(18)-C(20)         120.51(12)
C(14)-C(19)-H(19A)        109.5
C(14)-C(19)-H(19B)        109.5
H(19A)-C(19)-H(19B)       109.5
C(14)-C(19)-H(19C)        109.5
H(19A)-C(19)-H(19C)       109.5
H(19B)-C(19)-H(19C)       109.5
C(18)-C(20)-H(20A)        109.5
C(18)-C(20)-H(20B)        109.5
H(20A)-C(20)-H(20B)       109.5
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C(18)-C(20)-H(20C)          109.5
H(20A)-C(20)-H(20C)         109.5
H(20B)-C(20)-H(20C)         109.5
N(4)-C(21)-N(3)             112.95(11)
N(4)-C(21)-C(22)            124.42(13)
N(3)-C(21)-C(22)            122.62(12)
N(4)-C(21)-Sn(1)             59.57(6)
N(3)-C(21)-Sn(1)             53.94(6)
C(22)-C(21)-Sn(1)           171.30(10)
C(21)-C(22)-H(22A)          109.5
C(21)-C(22)-H(22B)          109.5
H(22A)-C(22)-H(22B)         109.5
C(21)-C(22)-H(22C)          109.5
H(22A)-C(22)-H(22C)         109.5
H(22B)-C(22)-H(22C)         109.5
C(24)-C(23)-C(28)           121.39(13)
C(24)-C(23)-N(4)            119.17(12)
C(28)-C(23)-N(4)            119.36(12)
C(25)-C(24)-C(23)           118.07(15)
C(25)-C(24)-C(29)           121.70(15)
C(23)-C(24)-C(29)           120.23(14)
C(26)-C(25)-C(24)           121.11(16)
C(26)-C(25)-H(25)           119.4
C(24)-C(25)-H(25)           119.4
C(27)-C(26)-C(25)           120.25(15)
C(27)-C(26)-H(26)           119.9
C(25)-C(26)-H(26)           119.9
C(26)-C(27)-C(28)           120.55(16)
C(26)-C(27)-H(27)           119.7
C(28)-C(27)-H(27)           119.7
C(27)-C(28)-C(23)           118.63(14)
C(27)-C(28)-C(30)           119.79(14)
C(23)-C(28)-C(30)           121.55(13)
C(24)-C(29)-H(29A)          109.5
C(24)-C(29)-H(29B)          109.5
H(29A)-C(29)-H(29B)         109.5
C(24)-C(29)-H(29C)          109.5
H(29A)-C(29)-H(29C)         109.5
H(29B)-C(29)-H(29C)         109.5
C(28)-C(30)-H(30A)          109.5
C(28)-C(30)-H(30B)          109.5
H(30A)-C(30)-H(30B)         109.5
C(28)-C(30)-H(30C)          109.5
H(30A)-C(30)-H(30C)         109.5
H(30B)-C(30)-H(30C)         109.5
O(2)-C(31)-C(32)            112.0(3)
O(2)-C(31)-H(31A)           109.2
C(32)-C(31)-H(31A)          109.2
O(2)-C(31)-H(31B)           109.2
C(32)-C(31)-H(31B)          109.2
H(31A)-C(31)-H(31B)         107.9
C(31)-C(32)-C(33)           102.4(3)
C(31)-C(32)-H(32A)          111.3
C(33)-C(32)-H(32A)          111.3
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C(31)-C(32)-H(32B)            111.3
C(33)-C(32)-H(32B)            111.3
H(32A)-C(32)-H(32B)           109.2
C(34)-C(33)-C(32)             102.9(2)
C(34)-C(33)-H(33A)            111.2
C(32)-C(33)-H(33A)            111.2
C(34)-C(33)-H(33B)            111.2
C(32)-C(33)-H(33B)            111.2
H(33A)-C(33)-H(33B)           109.1
O(2)-C(34)-C(33)              106.0(2)
O(2)-C(34)-H(34A)             110.5
C(33)-C(34)-H(34A)            110.5
O(2)-C(34)-H(34B)             110.5
C(33)-C(34)-H(34B)            110.5
H(34A)-C(34)-H(34B)           108.7
C(11)-N(1)-C(1)               132.08(11)
C(11)-N(1)-Sn(1)               93.61(7)
C(1)-N(1)-Sn(1)               134.30(8)
C(11)-N(2)-C(13)              126.28(11)
C(11)-N(2)-Sn(1)               95.91(8)
C(13)-N(2)-Sn(1)              134.66(8)
C(21)-N(3)-C(9)               118.61(10)
C(21)-N(3)-Sn(1)               95.58(8)
C(9)-N(3)-Sn(1)               127.19(8)
C(21)-N(4)-C(23)              123.45(11)
C(21)-N(4)-Sn(1)               90.62(8)
C(23)-N(4)-Sn(1)              145.85(9)
Sn(1)#1-O(1)-Sn(1)             95.98(4)
C(31)-O(2)-C(34)              106.4(3)
O(1)#1-Sn(1)-O(1)              84.01(4)
O(1)#1-Sn(1)-N(3)            117.25(4)
O(1)-Sn(1)-N(3)              106.26(4)
O(1)#1-Sn(1)-N(2)            103.51(4)
O(1)-Sn(1)-N(2)              101.24(4)
N(3)-Sn(1)-N(2)              132.38(4)
O(1)#1-Sn(1)-N(1)            163.46(4)
O(1)-Sn(1)-N(1)               97.84(4)
N(3)-Sn(1)-N(1)               78.15(4)
N(2)-Sn(1)-N(1)               59.97(4)
O(1)#1-Sn(1)-N(4)             93.43(4)
O(1)-Sn(1)-N(4)              162.99(4)
N(3)-Sn(1)-N(4)               60.07(4)
N(2)-Sn(1)-N(4)               95.71(4)
N(1)-Sn(1)-N(4)               89.39(4)
O(1)#1-Sn(1)-C(21)           109.70(4)
O(1)-Sn(1)-C(21)             136.53(4)
N(3)-Sn(1)-C(21)              30.47(4)
N(2)-Sn(1)-C(21)             114.25(4)
N(1)-Sn(1)-C(21)              80.27(4)
N(4)-Sn(1)-C(21)              29.81(4)
O(1)#1-Sn(1)-C(11)           133.59(4)
O(1)-Sn(1)-C(11)             100.72(4)
N(3)-Sn(1)-C(11)             105.72(4)
N(2)-Sn(1)-C(11)              30.09(4)
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N(1)-Sn(1)-C(11)              29.88(4)
N(4)-Sn(1)-C(11)              93.23(4)
C(21)-Sn(1)-C(11)             98.20(4)
O(1)#1-Sn(1)-Sn(1)#1          42.11(3)
O(1)-Sn(1)-Sn(1)#1            41.90(2)
N(3)-Sn(1)-Sn(1)#1           119.75(3)
N(2)-Sn(1)-Sn(1)#1           106.75(3)
N(1)-Sn(1)-Sn(1)#1           137.37(3)
N(4)-Sn(1)-Sn(1)#1           133.24(3)
C(21)-Sn(1)-Sn(1)#1          135.70(3)
C(11)-Sn(1)-Sn(1)#1          126.04(3)
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Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+1,-z+2

Table S24. Anisotropic displacement parameters (A^2 x 10^3) for R126.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	16(1)	24(1)	25(1)	-1(1)	-5(1)	-9(1)
C(2)	23(1)	40(1)	39(1)	-10(1)	-5(1)	-16(1)
C(3)	26(1)	48(1)	46(1)	-4(1)	-9(1)	-22(1)
C(4)	19(1)	43(1)	43(1)	5(1)	-6(1)	-16(1)
C(5)	16(1)	31(1)	35(1)	3(1)	-2(1)	-9(1)
C(6)	20(1)	42(1)	48(1)	-4(1)	8(1)	-10(1)
C(7)	28(1)	42(1)	55(1)	-17(1)	15(1)	-10(1)
C(8)	26(1)	31(1)	42(1)	-13(1)	7(1)	-10(1)
C(9)	18(1)	21(1)	28(1)	-2(1)	0(1)	-6(1)
C(10)	15(1)	23(1)	26(1)	1(1)	-2(1)	-7(1)
C(11)	20(1)	26(1)	27(1)	-8(1)	-2(1)	-9(1)
C(12)	30(1)	60(1)	51(1)	-36(1)	2(1)	-19(1)
C(13)	19(1)	23(1)	26(1)	-7(1)	-2(1)	-5(1)
C(14)	31(1)	24(1)	34(1)	-5(1)	0(1)	-8(1)
C(15)	35(1)	24(1)	42(1)	-4(1)	-3(1)	-1(1)
C(16)	24(1)	33(1)	37(1)	-7(1)	-2(1)	3(1)
C(17)	19(1)	36(1)	30(1)	-5(1)	-2(1)	-5(1)
C(18)	18(1)	26(1)	27(1)	-4(1)	-3(1)	-5(1)
C(19)	48(1)	32(1)	58(1)	0(1)	12(1)	-15(1)
C(20)	25(1)	31(1)	46(1)	2(1)	0(1)	-10(1)
C(21)	19(1)	16(1)	28(1)	0(1)	-5(1)	-6(1)
C(22)	25(1)	22(1)	46(1)	9(1)	-5(1)	0(1)
C(23)	20(1)	21(1)	27(1)	6(1)	-3(1)	-7(1)
C(24)	29(1)	24(1)	37(1)	6(1)	-5(1)	-13(1)
C(25)	40(1)	35(1)	48(1)	11(1)	-1(1)	-22(1)
C(26)	47(1)	38(1)	39(1)	11(1)	5(1)	-20(1)
C(27)	41(1)	36(1)	29(1)	8(1)	-1(1)	-14(1)
C(28)	26(1)	29(1)	28(1)	7(1)	-4(1)	-10(1)
C(29)	53(1)	38(1)	43(1)	6(1)	-14(1)	-29(1)
C(30)	45(1)	54(1)	33(1)	8(1)	-13(1)	-30(1)
C(31)	195(5)	94(3)	72(2)	-11(2)	-7(3)	-84(3)
C(32)	53(1)	90(2)	66(2)	-21(2)	-8(1)	-14(1)
C(33)	64(2)	57(2)	122(3)	-37(2)	-28(2)	-6(1)
C(34)	43(1)	68(2)	77(2)	-8(1)	-9(1)	-15(1)
N(1)	16(1)	22(1)	24(1)	-4(1)	-4(1)	-7(1)
N(2)	17(1)	24(1)	26(1)	-8(1)	-1(1)	-6(1)
N(3)	17(1)	18(1)	25(1)	-2(1)	-1(1)	-6(1)
N(4)	18(1)	20(1)	25(1)	5(1)	-5(1)	-6(1)
O(1)	17(1)	22(1)	24(1)	3(1)	-5(1)	-10(1)
O(2)	74(1)	70(1)	71(1)	-24(1)	2(1)	-27(1)
Sn(1)	13(1)	16(1)	20(1)	0(1)	-4(1)	-5(1)

Crystal data and structure refinement of compound 1b
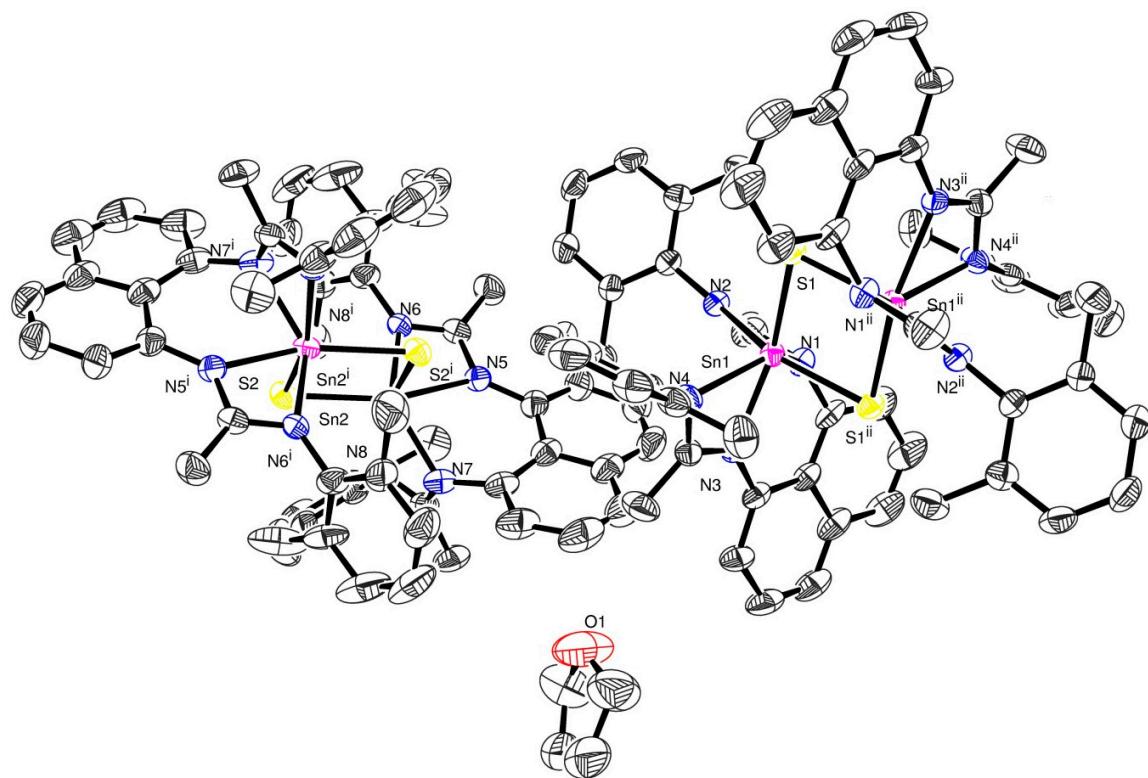
Figure S9. Asymmetric unit (Symmetry code : i = -x, -y, 1-z ; ii =-x, 1-y, 2-z)
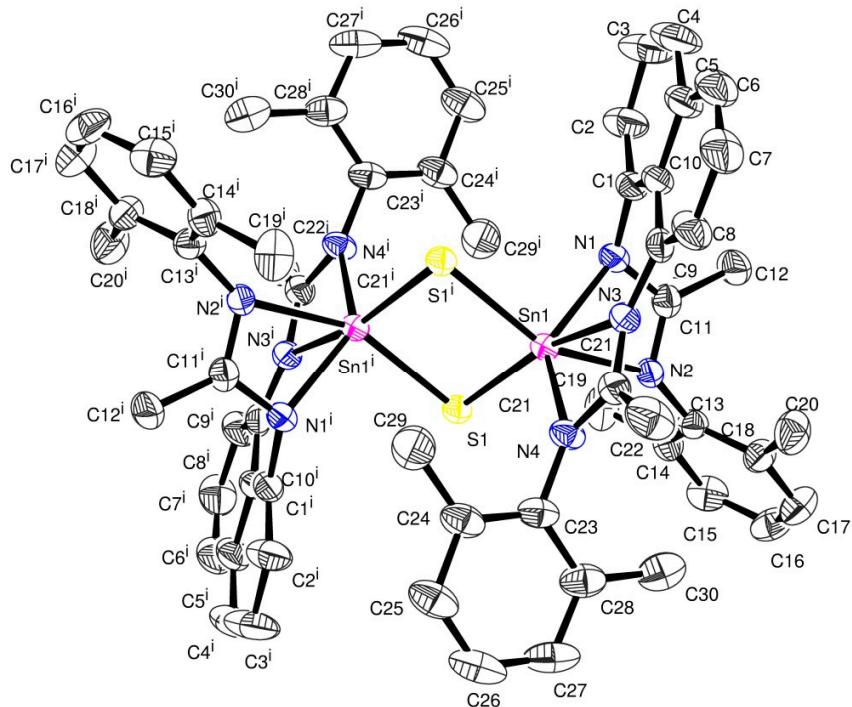
Figure S10. Compound (Symmetry code : i= -x, 1-y, 2-z)

Table S25. Crystal data and structure refinement for R200.

Identification code	R200
Empirical formula	C60 H60 N8 S2 Sn2, C4 H8 O
Formula weight	1266.80
Temperature	193(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P -1
Unit cell dimensions	a = 12.269(5) A alpha = 95.205(15) deg. b = 12.952(7) A beta = 94.892(14) deg. c = 19.923(6) A gamma = 110.382(19) deg.
Volume	2932(2) A^3
Z, Calculated density	2, 1.435 Mg/m^3

```
Absorption coefficient              0.972 mm^-1

F(000)                              1296

Crystal size                        0.100 x 0.080 x 0.060 mm

Theta range for data collection     2.837 to 28.722 deg.

Limiting indices                    -16<=h<=16, -17<=k<=17,
                                    -26<=l<=26

Reflections collected / unique      75605 / 15114 [R(int) = 0.1174]

Completeness to theta = 25.242      99.9 %

Refinement method                   Full-matrix least-squares on F^2

Data / restraints / parameters      15114 / 0 / 706

Goodness-of-fit on F^2              1.008

Final R indices [I>2sigma(I)]       R1 = 0.0515, wR2 = 0.0893

R indices (all data)                R1 = 0.1157, wR2 = 0.1092

Largest diff. peak and hole         0.687 and -0.593 e.A^-3
```

Table S26. Atomic coordinates (x 10^4) and equivalent isotropic
displacement parameters (A^2 x 10^3) for R200.
U(eq) is defined as one third of the trace of the orthogonalized
Uij tensor.

_____

	x	y	z	U(eq)
C(1)	2592(4)	6749(4)	8920(2)	37(1)
C(2)	2884(5)	7875(4)	8972(3)	52(1)
C(3)	4065(5)	8594(5)	9071(3)	71(2)
C(4)	4919(5)	8150(5)	9100(3)	65(2)
C(5)	4674(4)	6991(5)	9059(3)	48(1)
C(6)	5589(4)	6578(5)	9095(3)	56(2)
C(7)	5369(4)	5471(5)	9085(3)	55(2)
C(8)	4211(4)	4720(4)	9051(3)	44(1)
C(9)	3262(4)	5068(4)	9008(2)	34(1)
C(10)	3473(4)	6245(4)	8993(2)	34(1)
C(11)	837(4)	5695(4)	8142(2)	33(1)
C(12)	1231(4)	6306(4)	7553(2)	47(1)
C(13)	-836(4)	4290(4)	7492(2)	31(1)
C(14)	-1886(4)	4487(4)	7392(2)	36(1)
C(15)	-2644(4)	3987(4)	6802(3)	45(1)
C(16)	-2363(5)	3323(4)	6313(3)	49(1)
C(17)	-1319(5)	3151(4)	6410(3)	48(1)
C(18)	-544(4)	3612(4)	7000(2)	36(1)
C(19)	-2172(5)	5265(5)	7905(3)	50(1)
C(20)	609(4)	3436(5)	7086(3)	53(1)
C(21)	1632(4)	3272(4)	9070(2)	33(1)
C(22)	2207(4)	2417(4)	9001(3)	54(2)
C(23)	-212(4)	1913(4)	9313(3)	35(1)
C(24)	-244(4)	1663(4)	9986(3)	41(1)
C(25)	-1004(4)	626(4)	10091(3)	50(1)
C(26)	-1696(4)	-134(4)	9560(4)	56(2)
C(27)	-1649(4)	105(4)	8906(3)	54(2)
C(28)	-914(4)	1137(4)	8765(3)	44(1)
C(29)	512(5)	2461(4)	10574(3)	56(2)
C(30)	-856(5)	1396(5)	8045(3)	59(2)
C(31)	2199(4)	3911(4)	5415(3)	41(1)
C(32)	2329(5)	4999(4)	5368(3)	54(1)
C(33)	2942(5)	5857(5)	5898(4)	69(2)
C(34)	3394(5)	5607(5)	6482(4)	66(2)
C(35)	3345(4)	4525(5)	6546(3)	54(2)
C(36)	3794(5)	4291(7)	7156(3)	72(2)
C(37)	3753(5)	3248(7)	7234(3)	77(2)
C(38)	3336(5)	2384(6)	6677(3)	66(2)
C(39)	2929(4)	2608(5)	6054(3)	43(1)
C(40)	2817(4)	3657(4)	5991(3)	43(1)
C(41)	648(4)	2940(4)	4426(2)	35(1)
C(42)	309(5)	3879(4)	4194(3)	54(1)
C(43)	-829(4)	1495(4)	3612(3)	44(1)
C(44)	-1937(5)	1388(5)	3776(3)	59(2)

C(45)	-2875(6)	970(6)	3285(4)	88(2)
C(46)	-2746(7)	594(6)	2632(4)	90(3)
C(47)	-1646(6)	666(5)	2467(3)	72(2)
C(48)	-672(5)	1126(4)	2961(3)	52(1)
C(49)	-2124(6)	1727(7)	4493(4)	92(3)
C(50)	537(6)	1232(6)	2779(3)	71(2)
C(51)	3373(4)	1988(4)	4987(3)	38(1)
C(52)	4675(4)	2597(5)	5127(3)	57(2)
C(53)	3345(4)	1555(4)	3769(3)	41(1)
C(54)	3623(4)	610(5)	3577(3)	56(2)
C(55)	4058(5)	543(6)	2963(4)	80(2)
C(56)	4220(5)	1373(8)	2554(4)	90(3)
C(57)	3967(5)	2293(6)	2752(3)	71(2)
C(58)	3542(4)	2424(5)	3366(3)	51(1)
C(59)	3487(5)	-271(5)	4043(4)	88(3)
C(60)	3339(5)	3469(5)	3601(3)	65(2)
C(61)	5681(8)	2215(8)	8124(5)	115(3)
C(62)	6549(9)	1870(10)	8452(5)	145(5)
C(63)	6224(7)	1656(6)	9147(6)	108(3)
C(64)	5219(8)	2057(8)	9169(4)	116(3)
N(1)	1386(3)	6079(3)	8778(2)	32(1)
N(2)	-56(3)	4756(3)	8109(2)	29(1)
N(3)	2106(3)	4357(3)	9033(2)	30(1)
N(4)	523(3)	2992(3)	9188(2)	32(1)
N(5)	1442(3)	3001(3)	4947(2)	35(1)
N(6)	167(3)	1905(3)	4119(2)	33(1)
N(7)	2683(3)	1793(3)	5474(2)	39(1)
N(8)	2808(3)	1605(3)	4370(2)	37(1)
S(1)	-1432(1)	4460(1)	9574(1)	30(1)
S(2)	268(1)	-759(1)	4290(1)	36(1)
Sn(1)	496(1)	4687(1)	9270(1)	26(1)
Sn(2)	1041(1)	1155(1)	4825(1)	30(1)
O(1)	4754(5)	2050(6)	8513(3)	126(2)

Table S27. Bond lengths [A] and angles [deg] for R200.
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```
C(1)-C(2)                    1.367(7)
C(1)-N(1)                    1.419(5)
C(1)-C(10)                   1.447(7)
C(2)-C(3)                    1.409(7)
C(2)-H(2)                    0.9500
C(3)-C(4)                    1.359(9)
C(3)-H(3)                    0.9500
C(4)-C(5)                    1.417(8)
C(4)-H(4)                    0.9500
C(5)-C(6)                    1.401(8)
C(5)-C(10)                   1.441(6)
C(6)-C(7)                    1.361(8)
C(6)-H(6)                    0.9500
C(7)-C(8)                    1.406(7)
C(7)-H(7)                    0.9500
C(8)-C(9)                    1.387(6)
C(8)-H(8)                    0.9500
C(9)-N(3)                    1.404(5)
C(9)-C(10)                   1.459(7)
C(11)-N(2)                   1.315(5)
C(11)-N(1)                   1.345(6)
C(11)-C(12)                  1.496(6)
C(12)-H(12A)                 0.9800
C(12)-H(12B)                 0.9800
C(12)-H(12C)                 0.9800
C(13)-C(14)                  1.399(6)
C(13)-C(18)                  1.408(6)
C(13)-N(2)                   1.433(5)
C(14)-C(15)                  1.385(6)
C(14)-C(19)                  1.519(6)
C(15)-C(16)                  1.385(7)
C(15)-H(15)                  0.9500
C(16)-C(17)                  1.376(7)
C(16)-H(16)                  0.9500
C(17)-C(18)                  1.390(6)
C(17)-H(17)                  0.9500
C(18)-C(20)                  1.507(6)
C(19)-H(19A)                 0.9800
C(19)-H(19B)                 0.9800
C(19)-H(19C)                 0.9800
C(20)-H(20A)                 0.9800
C(20)-H(20B)                 0.9800
C(20)-H(20C)                 0.9800
C(21)-N(4)                   1.328(5)
C(21)-N(3)                   1.332(5)
C(21)-C(22)                  1.508(6)
C(22)-H(22A)                 0.9800
C(22)-H(22B)                 0.9800
C(22)-H(22C)                 0.9800
C(23)-C(28)                  1.408(7)
C(23)-C(24)                  1.409(7)
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C(23)-N(4)	1.433(5)
C(24)-C(25)	1.390(6)
C(24)-C(29)	1.492(7)
C(25)-C(26)	1.372(8)
C(25)-H(25)	0.9500
C(26)-C(27)	1.368(8)
C(26)-H(26)	0.9500
C(27)-C(28)	1.397(7)
C(27)-H(27)	0.9500
C(28)-C(30)	1.504(8)
C(29)-H(29A)	0.9800
C(29)-H(29B)	0.9800
C(29)-H(29C)	0.9800
C(30)-H(30A)	0.9800
C(30)-H(30B)	0.9800
C(30)-H(30C)	0.9800
C(31)-C(32)	1.376(7)
C(31)-N(5)	1.418(6)
C(31)-C(40)	1.446(7)
C(32)-C(33)	1.409(8)
C(32)-H(32)	0.9500
C(33)-C(34)	1.361(9)
C(33)-H(33)	0.9500
C(34)-C(35)	1.399(9)
C(34)-H(34)	0.9500
C(35)-C(36)	1.393(9)
C(35)-C(40)	1.433(7)
C(36)-C(37)	1.358(10)
C(36)-H(36)	0.9500
C(37)-C(38)	1.423(9)
C(37)-H(37)	0.9500
C(38)-C(39)	1.391(7)
C(38)-H(38)	0.9500
C(39)-C(40)	1.427(7)
C(39)-N(7)	1.427(6)
C(41)-N(6)	1.326(6)
C(41)-N(5)	1.339(6)
C(41)-C(42)	1.513(7)
C(42)-H(42A)	0.9800
C(42)-H(42B)	0.9800
C(42)-H(42C)	0.9800
C(43)-C(44)	1.388(7)
C(43)-C(48)	1.395(7)
C(43)-N(6)	1.426(6)
C(44)-C(45)	1.362(8)
C(44)-C(49)	1.516(9)
C(45)-C(46)	1.389(11)
C(45)-H(45)	0.9500
C(46)-C(47)	1.390(10)
C(46)-H(46)	0.9500
C(47)-C(48)	1.396(8)
C(47)-H(47)	0.9500
C(48)-C(50)	1.519(8)
C(49)-H(49A)	0.9800

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C(49)-H(49B)              0.9800
C(49)-H(49C)              0.9800
C(50)-H(50A)              0.9800
C(50)-H(50B)              0.9800
C(50)-H(50C)              0.9800
C(51)-N(8)                1.319(6)
C(51)-N(7)                1.326(6)
C(51)-C(52)               1.503(6)
C(51)-Sn(2)               2.662(5)
C(52)-H(52A)              0.9800
C(52)-H(52B)              0.9800
C(52)-H(52C)              0.9800
C(53)-C(58)               1.405(7)
C(53)-C(54)               1.411(7)
C(53)-N(8)                1.422(6)
C(54)-C(55)               1.384(9)
C(54)-C(59)               1.509(9)
C(55)-C(56)               1.377(11)
C(55)-H(55)               0.9500
C(56)-C(57)               1.365(10)
C(56)-H(56)               0.9500
C(57)-C(58)               1.389(8)
C(57)-H(57)               0.9500
C(58)-C(60)               1.502(8)
C(59)-H(59A)              0.9800
C(59)-H(59B)              0.9800
C(59)-H(59C)              0.9800
C(60)-H(60A)              0.9800
C(60)-H(60B)              0.9800
C(60)-H(60C)              0.9800
C(61)-O(1)                1.396(9)
C(61)-C(62)               1.423(11)
C(61)-H(61A)              0.9900
C(61)-H(61B)              0.9900
C(62)-C(63)               1.498(13)
C(62)-H(62A)              0.9900
C(62)-H(62B)              0.9900
C(63)-C(64)               1.498(11)
C(63)-H(63A)              0.9900
C(63)-H(63B)              0.9900
C(64)-O(1)                1.378(9)
C(64)-H(64A)              0.9900
C(64)-H(64B)              0.9900
N(1)-Sn(1)                2.130(4)
N(2)-Sn(1)                2.374(3)
N(3)-Sn(1)                2.240(3)
N(4)-Sn(1)                2.198(4)
N(5)-Sn(2)                2.252(4)
N(6)-Sn(2)                2.189(4)
N(7)-Sn(2)                2.148(4)
N(8)-Sn(2)                2.327(4)
S(1)-Sn(1)                2.4172(14)
S(1)-Sn(1)#1              2.4585(13)
S(2)-Sn(2)                2.4271(17)
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S(2)-Sn(2)#2                       2.4546(13)

C(2)-C(1)-N(1)                     117.6(5)
C(2)-C(1)-C(10)                    121.9(4)
N(1)-C(1)-C(10)                    120.5(4)
C(1)-C(2)-C(3)                     121.0(6)
C(1)-C(2)-H(2)                     119.5
C(3)-C(2)-H(2)                     119.5
C(4)-C(3)-C(2)                     118.9(6)
C(4)-C(3)-H(3)                     120.6
C(2)-C(3)-H(3)                     120.6
C(3)-C(4)-C(5)                     122.8(5)
C(3)-C(4)-H(4)                     118.6
C(5)-C(4)-H(4)                     118.6
C(6)-C(5)-C(4)                     120.5(5)
C(6)-C(5)-C(10)                    120.4(5)
C(4)-C(5)-C(10)                    119.1(5)
C(7)-C(6)-C(5)                     121.1(5)
C(7)-C(6)-H(6)                     119.4
C(5)-C(6)-H(6)                     119.4
C(6)-C(7)-C(8)                     120.2(5)
C(6)-C(7)-H(7)                     119.9
C(8)-C(7)-H(7)                     119.9
C(9)-C(8)-C(7)                     121.8(5)
C(9)-C(8)-H(8)                     119.1
C(7)-C(8)-H(8)                     119.1
C(8)-C(9)-N(3)                     123.2(4)
C(8)-C(9)-C(10)                    118.9(4)
N(3)-C(9)-C(10)                    117.7(4)
C(5)-C(10)-C(1)                    116.1(4)
C(5)-C(10)-C(9)                    117.4(4)
C(1)-C(10)-C(9)                    126.5(4)
N(2)-C(11)-N(1)                    112.8(4)
N(2)-C(11)-C(12)                   125.4(4)
N(1)-C(11)-C(12)                   121.8(4)
C(11)-C(12)-H(12A)                 109.5
C(11)-C(12)-H(12B)                 109.5
H(12A)-C(12)-H(12B)                109.5
C(11)-C(12)-H(12C)                 109.5
H(12A)-C(12)-H(12C)                109.5
H(12B)-C(12)-H(12C)                109.5
C(14)-C(13)-C(18)                  120.9(4)
C(14)-C(13)-N(2)                   120.1(4)
C(18)-C(13)-N(2)                   119.0(4)
C(15)-C(14)-C(13)                  118.7(4)
C(15)-C(14)-C(19)                  120.4(4)
C(13)-C(14)-C(19)                  120.9(4)
C(16)-C(15)-C(14)                  121.0(5)
C(16)-C(15)-H(15)                  119.5
C(14)-C(15)-H(15)                  119.5
C(17)-C(16)-C(15)                  120.0(5)
C(17)-C(16)-H(16)                  120.0
C(15)-C(16)-H(16)                  120.0
C(16)-C(17)-C(18)                  121.1(5)
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C(16)-C(17)-H(17)          119.5
C(18)-C(17)-H(17)          119.5
C(17)-C(18)-C(13)          118.4(4)
C(17)-C(18)-C(20)          120.1(4)
C(13)-C(18)-C(20)          121.5(4)
C(14)-C(19)-H(19A)         109.5
C(14)-C(19)-H(19B)         109.5
H(19A)-C(19)-H(19B)        109.5
C(14)-C(19)-H(19C)         109.5
H(19A)-C(19)-H(19C)        109.5
H(19B)-C(19)-H(19C)        109.5
C(18)-C(20)-H(20A)         109.5
C(18)-C(20)-H(20B)         109.5
H(20A)-C(20)-H(20B)        109.5
C(18)-C(20)-H(20C)         109.5
H(20A)-C(20)-H(20C)        109.5
H(20B)-C(20)-H(20C)        109.5
N(4)-C(21)-N(3)            110.9(4)
N(4)-C(21)-C(22)           121.1(4)
N(3)-C(21)-C(22)           128.0(4)
C(21)-C(22)-H(22A)         109.5
C(21)-C(22)-H(22B)         109.5
H(22A)-C(22)-H(22B)        109.5
C(21)-C(22)-H(22C)         109.5
H(22A)-C(22)-H(22C)        109.5
H(22B)-C(22)-H(22C)        109.5
C(28)-C(23)-C(24)          121.4(4)
C(28)-C(23)-N(4)           119.5(4)
C(24)-C(23)-N(4)           119.1(4)
C(25)-C(24)-C(23)          117.5(5)
C(25)-C(24)-C(29)          120.1(5)
C(23)-C(24)-C(29)          122.4(4)
C(26)-C(25)-C(24)          121.6(6)
C(26)-C(25)-H(25)          119.2
C(24)-C(25)-H(25)          119.2
C(27)-C(26)-C(25)          120.8(5)
C(27)-C(26)-H(26)          119.6
C(25)-C(26)-H(26)          119.6
C(26)-C(27)-C(28)          120.7(5)
C(26)-C(27)-H(27)          119.6
C(28)-C(27)-H(27)          119.6
C(27)-C(28)-C(23)          118.1(5)
C(27)-C(28)-C(30)          120.7(5)
C(23)-C(28)-C(30)          121.2(5)
C(24)-C(29)-H(29A)         109.5
C(24)-C(29)-H(29B)         109.5
H(29A)-C(29)-H(29B)        109.5
C(24)-C(29)-H(29C)         109.5
H(29A)-C(29)-H(29C)        109.5
H(29B)-C(29)-H(29C)        109.5
C(28)-C(30)-H(30A)         109.5
C(28)-C(30)-H(30B)         109.5
H(30A)-C(30)-H(30B)        109.5
C(28)-C(30)-H(30C)         109.5
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H(30A)-C(30)-H(30C)        109.5
H(30B)-C(30)-H(30C)        109.5
C(32)-C(31)-N(5)           123.8(5)
C(32)-C(31)-C(40)          119.0(5)
N(5)-C(31)-C(40)           117.1(4)
C(31)-C(32)-C(33)          121.8(6)
C(31)-C(32)-H(32)          119.1
C(33)-C(32)-H(32)          119.1
C(34)-C(33)-C(32)          119.6(6)
C(34)-C(33)-H(33)          120.2
C(32)-C(33)-H(33)          120.2
C(33)-C(34)-C(35)          121.1(6)
C(33)-C(34)-H(34)          119.4
C(35)-C(34)-H(34)          119.4
C(36)-C(35)-C(34)          119.8(6)
C(36)-C(35)-C(40)          120.0(6)
C(34)-C(35)-C(40)          120.2(6)
C(37)-C(36)-C(35)          121.1(6)
C(37)-C(36)-H(36)          119.4
C(35)-C(36)-H(36)          119.4
C(36)-C(37)-C(38)          120.6(6)
C(36)-C(37)-H(37)          119.7
C(38)-C(37)-H(37)          119.7
C(39)-C(38)-C(37)          119.3(6)
C(39)-C(38)-H(38)          120.4
C(37)-C(38)-H(38)          120.4
C(38)-C(39)-C(40)          120.4(5)
C(38)-C(39)-N(7)           118.8(5)
C(40)-C(39)-N(7)           120.8(4)
C(39)-C(40)-C(35)          117.5(5)
C(39)-C(40)-C(31)          125.3(5)
C(35)-C(40)-C(31)          117.2(5)
N(6)-C(41)-N(5)            110.2(4)
N(6)-C(41)-C(42)           122.6(4)
N(5)-C(41)-C(42)           127.3(4)
C(41)-C(42)-H(42A)         109.5
C(41)-C(42)-H(42B)         109.5
H(42A)-C(42)-H(42B)        109.5
C(41)-C(42)-H(42C)         109.5
H(42A)-C(42)-H(42C)        109.5
H(42B)-C(42)-H(42C)        109.5
C(44)-C(43)-C(48)          120.9(5)
C(44)-C(43)-N(6)           120.8(5)
C(48)-C(43)-N(6)           118.1(4)
C(45)-C(44)-C(43)          119.5(6)
C(45)-C(44)-C(49)          119.2(6)
C(43)-C(44)-C(49)          121.3(5)
C(44)-C(45)-C(46)          120.7(7)
C(44)-C(45)-H(45)          119.6
C(46)-C(45)-H(45)          119.6
C(45)-C(46)-C(47)          120.2(6)
C(45)-C(46)-H(46)          119.9
C(47)-C(46)-H(46)          119.9
C(46)-C(47)-C(48)          119.5(7)
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C(46)-C(47)-H(47)          120.3
C(48)-C(47)-H(47)          120.3
C(43)-C(48)-C(47)          119.0(6)
C(43)-C(48)-C(50)          121.2(5)
C(47)-C(48)-C(50)          119.8(6)
C(44)-C(49)-H(49A)         109.5
C(44)-C(49)-H(49B)         109.5
H(49A)-C(49)-H(49B)        109.5
C(44)-C(49)-H(49C)         109.5
H(49A)-C(49)-H(49C)        109.5
H(49B)-C(49)-H(49C)        109.5
C(48)-C(50)-H(50A)         109.5
C(48)-C(50)-H(50B)         109.5
H(50A)-C(50)-H(50B)        109.5
C(48)-C(50)-H(50C)         109.5
H(50A)-C(50)-H(50C)        109.5
H(50B)-C(50)-H(50C)        109.5
N(8)-C(51)-N(7)            113.7(4)
N(8)-C(51)-C(52)           123.4(4)
N(7)-C(51)-C(52)           122.9(5)
N(8)-C(51)-Sn(2)            60.9(2)
N(7)-C(51)-Sn(2)            53.2(2)
C(52)-C(51)-Sn(2)          172.2(4)
C(51)-C(52)-H(52A)         109.5
C(51)-C(52)-H(52B)         109.5
H(52A)-C(52)-H(52B)        109.5
C(51)-C(52)-H(52C)         109.5
H(52A)-C(52)-H(52C)        109.5
H(52B)-C(52)-H(52C)        109.5
C(58)-C(53)-C(54)          121.6(5)
C(58)-C(53)-N(8)           119.5(5)
C(54)-C(53)-N(8)           118.9(5)
C(55)-C(54)-C(53)          117.7(6)
C(55)-C(54)-C(59)          121.7(6)
C(53)-C(54)-C(59)          120.5(5)
C(56)-C(55)-C(54)          121.2(7)
C(56)-C(55)-H(55)          119.4
C(54)-C(55)-H(55)          119.4
C(57)-C(56)-C(55)          120.5(6)
C(57)-C(56)-H(56)          119.8
C(55)-C(56)-H(56)          119.8
C(56)-C(57)-C(58)          121.5(7)
C(56)-C(57)-H(57)          119.2
C(58)-C(57)-H(57)          119.2
C(57)-C(58)-C(53)          117.5(6)
C(57)-C(58)-C(60)          121.3(6)
C(53)-C(58)-C(60)          121.2(5)
C(54)-C(59)-H(59A)         109.5
C(54)-C(59)-H(59B)         109.5
H(59A)-C(59)-H(59B)        109.5
C(54)-C(59)-H(59C)         109.5
H(59A)-C(59)-H(59C)        109.5
H(59B)-C(59)-H(59C)        109.5
C(58)-C(60)-H(60A)         109.5
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C(58)-C(60)-H(60B)      109.5
H(60A)-C(60)-H(60B)     109.5
C(58)-C(60)-H(60C)      109.5
H(60A)-C(60)-H(60C)     109.5
H(60B)-C(60)-H(60C)     109.5
O(1)-C(61)-C(62)        109.7(9)
O(1)-C(61)-H(61A)       109.7
C(62)-C(61)-H(61A)      109.7
O(1)-C(61)-H(61B)       109.7
C(62)-C(61)-H(61B)      109.7
H(61A)-C(61)-H(61B)     108.2
C(61)-C(62)-C(63)       106.7(8)
C(61)-C(62)-H(62A)      110.4
C(63)-C(62)-H(62A)      110.4
C(61)-C(62)-H(62B)      110.4
C(63)-C(62)-H(62B)      110.4
H(62A)-C(62)-H(62B)     108.6
C(62)-C(63)-C(64)       101.4(7)
C(62)-C(63)-H(63A)      111.5
C(64)-C(63)-H(63A)      111.5
C(62)-C(63)-H(63B)      111.5
C(64)-C(63)-H(63B)      111.5
H(63A)-C(63)-H(63B)     109.3
O(1)-C(64)-C(63)        108.8(8)
O(1)-C(64)-H(64A)       109.9
C(63)-C(64)-H(64A)      109.9
O(1)-C(64)-H(64B)       109.9
C(63)-C(64)-H(64B)      109.9
H(64A)-C(64)-H(64B)     108.3
C(11)-N(1)-C(1)         123.0(4)
C(11)-N(1)-Sn(1)         99.0(3)
C(1)-N(1)-Sn(1)         125.9(3)
C(11)-N(2)-C(13)        120.9(4)
C(11)-N(2)-Sn(1)         88.9(3)
C(13)-N(2)-Sn(1)        150.1(3)
C(21)-N(3)-C(9)         132.6(4)
C(21)-N(3)-Sn(1)         93.9(3)
C(9)-N(3)-Sn(1)         132.2(3)
C(21)-N(4)-C(23)        125.3(4)
C(21)-N(4)-Sn(1)         95.9(3)
C(23)-N(4)-Sn(1)        138.0(3)
C(41)-N(5)-C(31)        131.7(4)
C(41)-N(5)-Sn(2)         93.7(3)
C(31)-N(5)-Sn(2)        134.5(3)
C(41)-N(6)-C(43)        125.7(4)
C(41)-N(6)-Sn(2)         97.0(3)
C(43)-N(6)-Sn(2)        135.1(3)
C(51)-N(7)-C(39)        119.4(4)
C(51)-N(7)-Sn(2)         97.2(3)
C(39)-N(7)-Sn(2)        123.8(3)
C(51)-N(8)-C(53)        125.2(4)
C(51)-N(8)-Sn(2)         89.4(3)
C(53)-N(8)-Sn(2)        145.3(3)
Sn(1)-S(1)-Sn(1)#1       87.92(4)
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Sn(2)-S(2)-Sn(2)#2            87.14(4)
N(1)-Sn(1)-N(4)             131.38(14)
N(1)-Sn(1)-N(3)              77.63(14)
N(4)-Sn(1)-N(3)              59.16(13)
N(1)-Sn(1)-N(2)              58.65(13)
N(4)-Sn(1)-N(2)              99.06(13)
N(3)-Sn(1)-N(2)              91.81(12)
N(1)-Sn(1)-S(1)            118.91(10)
N(4)-Sn(1)-S(1)            103.69(10)
N(3)-Sn(1)-S(1)            162.73(10)
N(2)-Sn(1)-S(1)             93.17(9)
N(1)-Sn(1)-S(1)#1           96.05(10)
N(4)-Sn(1)-S(1)#1          105.19(10)
N(3)-Sn(1)-S(1)#1           90.90(10)
N(2)-Sn(1)-S(1)#1          153.19(9)
S(1)-Sn(1)-S(1)#1           92.08(4)
N(7)-Sn(2)-N(6)            132.85(15)
N(7)-Sn(2)-N(5)             77.24(15)
N(6)-Sn(2)-N(5)             58.93(14)
N(7)-Sn(2)-N(8)             59.18(14)
N(6)-Sn(2)-N(8)             97.54(14)
N(5)-Sn(2)-N(8)             84.40(13)
N(7)-Sn(2)-S(2)            120.77(12)
N(6)-Sn(2)-S(2)            100.09(10)
N(5)-Sn(2)-S(2)            158.57(10)
N(8)-Sn(2)-S(2)             95.04(10)
N(7)-Sn(2)-S(2)#2           98.24(11)
N(6)-Sn(2)-S(2)#2          102.43(10)
N(5)-Sn(2)-S(2)#2           95.94(10)
N(8)-Sn(2)-S(2)#2          156.87(11)
S(2)-Sn(2)-S(2)#2           92.86(4)
N(7)-Sn(2)-C(51)            29.63(14)
N(6)-Sn(2)-C(51)           116.03(15)
N(5)-Sn(2)-C(51)            77.16(14)
N(8)-Sn(2)-C(51)            29.71(14)
S(2)-Sn(2)-C(51)           112.22(11)
S(2)#2-Sn(2)-C(51)         127.86(12)
C(64)-O(1)-C(61)           105.8(6)
```

Symmetry transformations used to generate equivalent atoms:
#1 -x,-y+1,-z+2   #2 -x,-y,-z+1

Table S28. Anisotropic displacement parameters (A^2 x 10^3) for R200.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

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	U11	U22	U33	U23	U13	U12
C(1)	28(2)	45(3)	24(2)	7(2)	-3(2)	-4(2)
C(2)	48(3)	34(3)	64(4)	13(3)	3(3)	0(2)
C(3)	54(4)	40(3)	94(5)	16(3)	-3(4)	-13(3)
C(4)	38(3)	57(4)	74(4)	18(3)	0(3)	-15(3)
C(5)	33(3)	55(3)	38(3)	11(2)	3(2)	-5(2)
C(6)	30(3)	73(4)	48(3)	9(3)	1(2)	-4(3)
C(7)	25(3)	83(5)	52(3)	7(3)	2(2)	14(3)
C(8)	25(2)	55(3)	48(3)	10(3)	7(2)	10(2)
C(9)	26(2)	49(3)	22(2)	3(2)	4(2)	7(2)
C(10)	28(2)	38(3)	27(2)	7(2)	2(2)	-1(2)
C(11)	38(3)	36(3)	29(2)	7(2)	7(2)	15(2)
C(12)	52(3)	48(3)	32(3)	14(2)	6(2)	5(3)
C(13)	30(2)	31(2)	30(2)	5(2)	2(2)	8(2)
C(14)	38(3)	41(3)	31(2)	11(2)	6(2)	17(2)
C(15)	35(3)	47(3)	52(3)	11(3)	-8(2)	16(2)
C(16)	52(3)	43(3)	41(3)	-4(2)	-16(2)	12(3)
C(17)	51(3)	50(3)	39(3)	-9(2)	-6(2)	22(3)
C(18)	35(2)	38(3)	34(3)	-2(2)	2(2)	13(2)
C(19)	55(3)	67(4)	43(3)	13(3)	9(3)	39(3)
C(20)	43(3)	68(4)	50(3)	-4(3)	9(3)	27(3)
C(21)	31(2)	33(3)	34(2)	4(2)	8(2)	10(2)
C(22)	38(3)	48(3)	86(4)	14(3)	21(3)	22(3)
C(23)	22(2)	26(2)	56(3)	4(2)	4(2)	10(2)
C(24)	35(3)	29(3)	64(3)	12(2)	10(2)	13(2)
C(25)	42(3)	37(3)	76(4)	24(3)	13(3)	15(2)
C(26)	33(3)	34(3)	99(5)	24(3)	6(3)	6(2)
C(27)	32(3)	30(3)	89(5)	-2(3)	-11(3)	6(2)
C(28)	31(3)	36(3)	62(4)	1(3)	-3(2)	11(2)
C(29)	77(4)	42(3)	52(3)	13(3)	11(3)	22(3)
C(30)	54(3)	50(3)	61(4)	-6(3)	-7(3)	11(3)
C(31)	34(3)	39(3)	45(3)	5(2)	10(2)	7(2)
C(32)	48(3)	37(3)	68(4)	4(3)	6(3)	8(3)
C(33)	54(4)	44(4)	97(5)	-10(4)	10(4)	6(3)
C(34)	41(3)	65(4)	71(4)	-18(4)	7(3)	0(3)
C(35)	31(3)	76(4)	47(3)	-3(3)	11(2)	10(3)
C(36)	57(4)	109(6)	42(4)	-5(4)	6(3)	24(4)
C(37)	60(4)	137(7)	30(3)	11(4)	-1(3)	31(4)
C(38)	63(4)	106(5)	38(3)	25(3)	1(3)	39(4)
C(39)	30(2)	60(3)	39(3)	16(3)	8(2)	13(2)
C(40)	31(3)	55(3)	39(3)	5(2)	10(2)	8(2)
C(41)	37(3)	38(3)	36(3)	16(2)	10(2)	17(2)
C(42)	66(4)	47(3)	57(4)	13(3)	2(3)	30(3)
C(43)	43(3)	44(3)	45(3)	13(2)	-7(2)	19(2)
C(44)	38(3)	81(4)	63(4)	36(3)	-4(3)	23(3)
C(45)	46(4)	106(6)	103(6)	51(5)	-16(4)	15(4)

C(46)	67(5)	72(5)	100(6)	27(4)	-44(5)	-5(4)
C(47)	87(5)	56(4)	60(4)	5(3)	-28(4)	19(4)
C(48)	62(4)	49(3)	44(3)	4(3)	-12(3)	25(3)
C(49)	61(4)	164(8)	86(5)	65(5)	29(4)	69(5)
C(50)	92(5)	85(5)	42(3)	-6(3)	5(3)	42(4)
C(51)	30(2)	41(3)	47(3)	8(2)	5(2)	17(2)
C(52)	27(3)	78(4)	59(4)	9(3)	5(2)	11(3)
C(53)	26(2)	49(3)	41(3)	-3(2)	7(2)	6(2)
C(54)	23(2)	48(3)	84(4)	-19(3)	2(3)	3(2)
C(55)	31(3)	91(5)	91(5)	-50(4)	14(3)	2(3)
C(56)	41(4)	147(8)	52(4)	-37(5)	10(3)	7(4)
C(57)	45(3)	104(6)	43(4)	7(4)	5(3)	1(4)
C(58)	35(3)	69(4)	41(3)	5(3)	8(2)	9(3)
C(59)	49(4)	41(4)	177(8)	10(4)	40(4)	14(3)
C(60)	69(4)	65(4)	64(4)	32(3)	24(3)	20(3)
C(61)	107(7)	126(8)	137(8)	25(6)	25(6)	68(6)
C(62)	118(8)	194(11)	127(9)	-94(8)	-55(7)	106(8)
C(63)	81(6)	44(4)	176(10)	15(5)	-34(6)	5(4)
C(64)	130(8)	159(9)	88(6)	13(6)	-8(6)	93(7)
N(1)	32(2)	29(2)	30(2)	7(2)	6(2)	5(2)
N(2)	27(2)	33(2)	25(2)	5(2)	5(2)	8(2)
N(3)	23(2)	33(2)	32(2)	1(2)	6(2)	7(2)
N(4)	28(2)	24(2)	45(2)	6(2)	10(2)	10(2)
N(5)	32(2)	32(2)	39(2)	10(2)	4(2)	10(2)
N(6)	34(2)	30(2)	36(2)	6(2)	2(2)	16(2)
N(7)	32(2)	55(3)	35(2)	16(2)	8(2)	17(2)
N(8)	34(2)	35(2)	44(2)	7(2)	13(2)	11(2)
S(1)	24(1)	32(1)	29(1)	3(1)	3(1)	6(1)
S(2)	37(1)	34(1)	40(1)	7(1)	13(1)	14(1)
Sn(1)	25(1)	24(1)	27(1)	4(1)	5(1)	6(1)
Sn(2)	26(1)	32(1)	35(1)	10(1)	6(1)	12(1)
O(1)	88(4)	234(8)	82(4)	11(4)	0(3)	92(5)

Crystal data and structure refinement of compound 2a
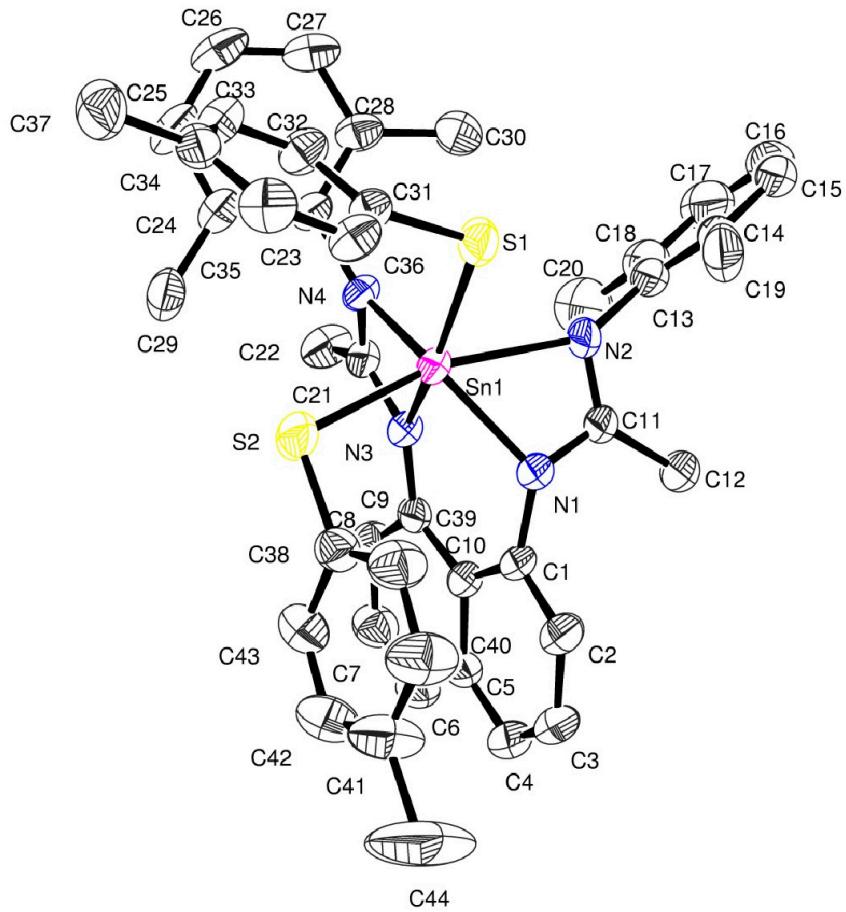
Figure S11. Asymmetric unit

Table S29. Crystal data and structure refinement for R202.

Identification code	R202
Empirical formula	C44 H44 N4 S2 Sn
Formula weight	811.64
Temperature	193(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P 21/c
Unit cell dimensions	a = 19.655(17) A alpha = 90 deg.
	b = 11.760(8) A beta = 104.67(4) deg.
	c = 20.040(17) A gamma = 90 deg.

Volume   4481(6) A^3

Z, Calculated density   4, 1.203 Mg/m^3

Absorption coefficient   0.695 mm^-1

F(000)   1672

Crystal size   0.120 x 0.060 x 0.060 mm

Theta range for data collection   2.723 to 29.596 deg.

Limiting indices   -26<=h<=27, -16<=k<=16,
                                      -27<=l<=27

Reflections collected / unique   124683 / 12518 [R(int) = 0.1184]

Completeness to theta = 25.242   99.5 %

Refinement method   Full-matrix least-squares on F^2

Data / restraints / parameters   12518 / 0 / 468

Goodness-of-fit on F^2   0.996

Final R indices [I>2sigma(I)]   R1 = 0.0473, wR2 = 0.1191

R indices (all data)   R1 = 0.0947, wR2 = 0.1422

Largest diff. peak and hole   0.537 and -0.874 e.A^-3

Table S30. Atomic coordinates (x 10^4) and equivalent isotropic
displacement parameters (A^2 x 10^3) for R202.
U(eq) is defined as one third of the trace of the orthogonalized
Uij tensor.

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	x	y	z	U(eq)
C(1)	1960(2)	7174(3)	5651(2)	40(1)
C(2)	1523(2)	7951(3)	5862(2)	49(1)
C(3)	1459(2)	9075(3)	5605(2)	55(1)
C(4)	1823(2)	9403(3)	5142(2)	52(1)
C(5)	2296(2)	8642(3)	4937(2)	41(1)
C(6)	2675(2)	9027(3)	4466(2)	47(1)
C(7)	3132(2)	8320(3)	4261(2)	51(1)
C(8)	3244(2)	7209(3)	4523(2)	44(1)
C(9)	2893(2)	6784(3)	4991(2)	35(1)
C(10)	2384(2)	7498(3)	5205(2)	36(1)
C(11)	1506(2)	5294(3)	5435(2)	41(1)
C(12)	849(2)	5699(3)	4941(2)	63(1)
C(13)	1325(2)	3333(3)	5118(2)	53(1)
C(14)	865(2)	2741(3)	5436(3)	63(1)
C(15)	478(2)	1848(4)	5068(4)	84(2)
C(16)	538(3)	1553(4)	4422(4)	90(2)
C(17)	989(3)	2136(4)	4125(3)	89(2)
C(18)	1396(2)	3043(4)	4464(2)	66(1)
C(19)	777(2)	3073(4)	6129(3)	80(2)
C(20)	1857(3)	3691(4)	4121(2)	84(2)
C(21)	3498(2)	4900(3)	5253(2)	37(1)
C(22)	3888(2)	4762(3)	4700(2)	55(1)
C(23)	4033(2)	3193(3)	5890(2)	37(1)
C(24)	4737(2)	3402(3)	6228(2)	43(1)
C(25)	5187(2)	2466(4)	6404(2)	54(1)
C(26)	4948(2)	1369(4)	6262(2)	61(1)
C(27)	4251(2)	1182(3)	5937(2)	54(1)
C(28)	3778(2)	2082(3)	5743(2)	43(1)
C(29)	5011(2)	4575(3)	6449(2)	54(1)
C(30)	3014(2)	1866(3)	5398(2)	58(1)
C(31)	3336(2)	3378(3)	7696(2)	39(1)
C(32)	3925(2)	2785(3)	7626(2)	45(1)
C(33)	4500(2)	2663(3)	8181(2)	46(1)
C(34)	4512(2)	3111(3)	8825(2)	42(1)
C(35)	3921(2)	3687(3)	8889(2)	52(1)
C(36)	3335(2)	3834(3)	8335(2)	47(1)
C(37)	5143(2)	2959(4)	9431(2)	62(1)
C(38)	3226(2)	7381(3)	7131(2)	43(1)
C(39)	2722(2)	7433(3)	7504(2)	57(1)
C(40)	2420(3)	8455(4)	7605(2)	73(1)
C(41)	2608(3)	9444(4)	7331(3)	79(2)
C(42)	3103(3)	9390(4)	6958(2)	67(1)
C(43)	3412(2)	8391(3)	6857(2)	53(1)
C(44)	2222(4)	10570(5)	7417(4)	153(3)

N(1)	1928(1)	6031(2)	5877(1)	38(1)
N(2)	1743(1)	4257(2)	5488(2)	44(1)
N(3)	3053(1)	5725(2)	5316(1)	35(1)
N(4)	3544(1)	4119(2)	5747(1)	35(1)
S(1)	2568(1)	3477(1)	7001(1)	48(1)
S(2)	3685(1)	6111(1)	7058(1)	57(1)
Sn(1)	2816(1)	4955(1)	6249(1)	34(1)

Table S31. Bond lengths [A] and angles [deg] for R202.
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C(1)-C(2)            1.391(5)
C(1)-C(10)           1.420(5)
C(1)-N(1)            1.425(4)
C(2)-C(3)            1.412(5)
C(2)-H(2)            0.9500
C(3)-C(4)            1.362(5)
C(3)-H(3)            0.9500
C(4)-C(5)            1.424(5)
C(4)-H(4)            0.9500
C(5)-C(6)            1.418(5)
C(5)-C(10)           1.442(4)
C(6)-C(7)            1.362(5)
C(6)-H(6)            0.9500
C(7)-C(8)            1.404(5)
C(7)-H(7)            0.9500
C(8)-C(9)            1.391(5)
C(8)-H(8)            0.9500
C(9)-N(3)            1.403(4)
C(9)-C(10)           1.451(5)
C(11)-N(2)           1.301(4)
C(11)-N(1)           1.361(4)
C(11)-C(12)          1.493(5)
C(12)-H(12A)         0.9800
C(12)-H(12B)         0.9800
C(12)-H(12C)         0.9800
C(13)-C(18)          1.394(6)
C(13)-C(14)          1.415(6)
C(13)-N(2)           1.448(5)
C(14)-C(15)          1.392(6)
C(14)-C(19)          1.494(7)
C(15)-C(16)          1.375(8)
C(15)-H(15)          0.9500
C(16)-C(17)          1.369(8)
C(16)-H(16)          0.9500
C(17)-C(18)          1.401(6)
C(17)-H(17)          0.9500
C(18)-C(20)          1.481(6)
C(19)-H(19A)         0.9800
C(19)-H(19B)         0.9800
C(19)-H(19C)         0.9800
C(20)-H(20A)         0.9800
C(20)-H(20B)         0.9800
C(20)-H(20C)         0.9800
C(21)-N(3)           1.334(4)
C(21)-N(4)           1.337(4)
C(21)-C(22)          1.506(5)
C(22)-H(22A)         0.9800
C(22)-H(22B)         0.9800
C(22)-H(22C)         0.9800
C(23)-C(24)          1.400(5)
C(23)-C(28)          1.405(5)
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C(23)-N(4)            1.432(4)
C(24)-C(25)           1.400(5)
C(24)-C(29)           1.507(5)
C(25)-C(26)           1.378(6)
C(25)-H(25)           0.9500
C(26)-C(27)           1.377(6)
C(26)-H(26)           0.9500
C(27)-C(28)           1.398(5)
C(27)-H(27)           0.9500
C(28)-C(30)           1.506(5)
C(29)-H(29A)          0.9800
C(29)-H(29B)          0.9800
C(29)-H(29C)          0.9800
C(30)-H(30A)          0.9800
C(30)-H(30B)          0.9800
C(30)-H(30C)          0.9800
C(31)-C(36)           1.389(5)
C(31)-C(32)           1.389(5)
C(31)-S(1)            1.779(4)
C(32)-C(33)           1.378(5)
C(32)-H(32)           0.9500
C(33)-C(34)           1.389(5)
C(33)-H(33)           0.9500
C(34)-C(35)           1.380(5)
C(34)-C(37)           1.510(5)
C(35)-C(36)           1.393(5)
C(35)-H(35)           0.9500
C(36)-H(36)           0.9500
C(37)-H(37A)          0.9800
C(37)-H(37B)          0.9800
C(37)-H(37C)          0.9800
C(38)-C(39)           1.387(5)
C(38)-C(43)           1.395(5)
C(38)-S(2)            1.771(4)
C(39)-C(40)           1.378(5)
C(39)-H(39)           0.9500
C(40)-C(41)           1.377(6)
C(40)-H(40)           0.9500
C(41)-C(42)           1.369(6)
C(41)-C(44)           1.558(7)
C(42)-C(43)           1.362(6)
C(42)-H(42)           0.9500
C(43)-H(43)           0.9500
C(44)-H(44A)          0.9800
C(44)-H(44B)          0.9800
C(44)-H(44C)          0.9800
N(1)-Sn(1)            2.132(3)
N(2)-Sn(1)            2.411(3)
N(3)-Sn(1)            2.230(3)
N(4)-Sn(1)            2.180(3)
S(1)-Sn(1)            2.4297(15)
S(2)-Sn(1)            2.4483(16)

C(2)-C(1)-C(10)       121.4(3)
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C(2)-C(1)-N(1)            116.2(3)
C(10)-C(1)-N(1)           122.3(3)
C(1)-C(2)-C(3)            120.6(4)
C(1)-C(2)-H(2)            119.7
C(3)-C(2)-H(2)            119.7
C(4)-C(3)-C(2)            120.0(3)
C(4)-C(3)-H(3)            120.0
C(2)-C(3)-H(3)            120.0
C(3)-C(4)-C(5)            120.7(3)
C(3)-C(4)-H(4)            119.6
C(5)-C(4)-H(4)            119.6
C(6)-C(5)-C(4)            118.9(3)
C(6)-C(5)-C(10)           120.7(3)
C(4)-C(5)-C(10)           120.4(3)
C(7)-C(6)-C(5)            120.3(3)
C(7)-C(6)-H(6)            119.9
C(5)-C(6)-H(6)            119.9
C(6)-C(7)-C(8)            120.6(3)
C(6)-C(7)-H(7)            119.7
C(8)-C(7)-H(7)            119.7
C(9)-C(8)-C(7)            122.0(3)
C(9)-C(8)-H(8)            119.0
C(7)-C(8)-H(8)            119.0
C(8)-C(9)-N(3)            122.8(3)
C(8)-C(9)-C(10)           119.2(3)
N(3)-C(9)-C(10)           117.8(3)
C(1)-C(10)-C(5)           116.7(3)
C(1)-C(10)-C(9)           126.1(3)
C(5)-C(10)-C(9)           117.2(3)
N(2)-C(11)-N(1)           113.5(3)
N(2)-C(11)-C(12)          125.8(3)
N(1)-C(11)-C(12)          120.7(3)
C(11)-C(12)-H(12A)        109.5
C(11)-C(12)-H(12B)        109.5
H(12A)-C(12)-H(12B)       109.5
C(11)-C(12)-H(12C)        109.5
H(12A)-C(12)-H(12C)       109.5
H(12B)-C(12)-H(12C)       109.5
C(18)-C(13)-C(14)         122.0(4)
C(18)-C(13)-N(2)          119.0(4)
C(14)-C(13)-N(2)          118.9(4)
C(15)-C(14)-C(13)         117.3(5)
C(15)-C(14)-C(19)         120.8(5)
C(13)-C(14)-C(19)         121.9(4)
C(16)-C(15)-C(14)         121.6(5)
C(16)-C(15)-H(15)         119.2
C(14)-C(15)-H(15)         119.2
C(17)-C(16)-C(15)         120.1(5)
C(17)-C(16)-H(16)         120.0
C(15)-C(16)-H(16)         120.0
C(16)-C(17)-C(18)         121.6(6)
C(16)-C(17)-H(17)         119.2
C(18)-C(17)-H(17)         119.2
C(13)-C(18)-C(17)         117.5(5)
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C(13)-C(18)-C(20)          122.0(4)
C(17)-C(18)-C(20)          120.5(5)
C(14)-C(19)-H(19A)         109.5
C(14)-C(19)-H(19B)         109.5
H(19A)-C(19)-H(19B)        109.5
C(14)-C(19)-H(19C)         109.5
H(19A)-C(19)-H(19C)        109.5
H(19B)-C(19)-H(19C)        109.5
C(18)-C(20)-H(20A)         109.5
C(18)-C(20)-H(20B)         109.5
H(20A)-C(20)-H(20B)        109.5
C(18)-C(20)-H(20C)         109.5
H(20A)-C(20)-H(20C)        109.5
H(20B)-C(20)-H(20C)        109.5
N(3)-C(21)-N(4)            110.6(3)
N(3)-C(21)-C(22)           128.0(3)
N(4)-C(21)-C(22)           121.3(3)
C(21)-C(22)-H(22A)         109.5
C(21)-C(22)-H(22B)         109.5
H(22A)-C(22)-H(22B)        109.5
C(21)-C(22)-H(22C)         109.5
H(22A)-C(22)-H(22C)        109.5
H(22B)-C(22)-H(22C)        109.5
C(24)-C(23)-C(28)          121.4(3)
C(24)-C(23)-N(4)           119.7(3)
C(28)-C(23)-N(4)           118.6(3)
C(25)-C(24)-C(23)          118.0(3)
C(25)-C(24)-C(29)          119.4(3)
C(23)-C(24)-C(29)          122.5(3)
C(26)-C(25)-C(24)          121.5(4)
C(26)-C(25)-H(25)          119.3
C(24)-C(25)-H(25)          119.3
C(27)-C(26)-C(25)          119.6(3)
C(27)-C(26)-H(26)          120.2
C(25)-C(26)-H(26)          120.2
C(26)-C(27)-C(28)          121.5(4)
C(26)-C(27)-H(27)          119.2
C(28)-C(27)-H(27)          119.2
C(27)-C(28)-C(23)          118.0(4)
C(27)-C(28)-C(30)          121.1(3)
C(23)-C(28)-C(30)          121.0(3)
C(24)-C(29)-H(29A)         109.5
C(24)-C(29)-H(29B)         109.5
H(29A)-C(29)-H(29B)        109.5
C(24)-C(29)-H(29C)         109.5
H(29A)-C(29)-H(29C)        109.5
H(29B)-C(29)-H(29C)        109.5
C(28)-C(30)-H(30A)         109.5
C(28)-C(30)-H(30B)         109.5
H(30A)-C(30)-H(30B)        109.5
C(28)-C(30)-H(30C)         109.5
H(30A)-C(30)-H(30C)        109.5
H(30B)-C(30)-H(30C)        109.5
C(36)-C(31)-C(32)          118.8(3)
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C(36)-C(31)-S(1)          119.8(3)
C(32)-C(31)-S(1)          121.2(3)
C(33)-C(32)-C(31)         120.3(3)
C(33)-C(32)-H(32)         119.9
C(31)-C(32)-H(32)         119.9
C(32)-C(33)-C(34)         122.0(3)
C(32)-C(33)-H(33)         119.0
C(34)-C(33)-H(33)         119.0
C(35)-C(34)-C(33)         117.1(3)
C(35)-C(34)-C(37)         121.6(4)
C(33)-C(34)-C(37)         121.3(4)
C(34)-C(35)-C(36)         122.2(3)
C(34)-C(35)-H(35)         118.9
C(36)-C(35)-H(35)         118.9
C(31)-C(36)-C(35)         119.6(3)
C(31)-C(36)-H(36)         120.2
C(35)-C(36)-H(36)         120.2
C(34)-C(37)-H(37A)        109.5
C(34)-C(37)-H(37B)        109.5
H(37A)-C(37)-H(37B)       109.5
C(34)-C(37)-H(37C)        109.5
H(37A)-C(37)-H(37C)       109.5
H(37B)-C(37)-H(37C)       109.5
C(39)-C(38)-C(43)         118.0(3)
C(39)-C(38)-S(2)          122.0(3)
C(43)-C(38)-S(2)          119.7(3)
C(40)-C(39)-C(38)         120.7(4)
C(40)-C(39)-H(39)         119.7
C(38)-C(39)-H(39)         119.7
C(41)-C(40)-C(39)         120.6(4)
C(41)-C(40)-H(40)         119.7
C(39)-C(40)-H(40)         119.7
C(42)-C(41)-C(40)         118.6(4)
C(42)-C(41)-C(44)         122.2(5)
C(40)-C(41)-C(44)         119.1(5)
C(43)-C(42)-C(41)         121.7(4)
C(43)-C(42)-H(42)         119.1
C(41)-C(42)-H(42)         119.1
C(42)-C(43)-C(38)         120.3(4)
C(42)-C(43)-H(43)         119.8
C(38)-C(43)-H(43)         119.8
C(41)-C(44)-H(44A)        109.5
C(41)-C(44)-H(44B)        109.5
H(44A)-C(44)-H(44B)       109.5
C(41)-C(44)-H(44C)        109.5
H(44A)-C(44)-H(44C)       109.5
H(44B)-C(44)-H(44C)       109.5
C(11)-N(1)-C(1)           117.5(3)
C(11)-N(1)-Sn(1)           99.1(2)
C(1)-N(1)-Sn(1)           124.9(2)
C(11)-N(2)-C(13)          121.1(3)
C(11)-N(2)-Sn(1)           88.3(2)
C(13)-N(2)-Sn(1)          150.6(2)
C(21)-N(3)-C(9)           132.6(3)
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C(21)-N(3)-Sn(1)                    93.8(2)
C(9)-N(3)-Sn(1)                    132.8(2)
C(21)-N(4)-C(23)                   125.9(3)
C(21)-N(4)-Sn(1)                    95.9(2)
C(23)-N(4)-Sn(1)                   137.4(2)
C(31)-S(1)-Sn(1)                   105.59(12)
C(38)-S(2)-Sn(1)                   103.78(13)
N(1)-Sn(1)-N(4)                    132.96(11)
N(1)-Sn(1)-N(3)                     78.01(11)
N(4)-Sn(1)-N(3)                     59.72(10)
N(1)-Sn(1)-N(2)                     58.27(11)
N(4)-Sn(1)-N(2)                     97.20(12)
N(3)-Sn(1)-N(2)                     86.71(11)
N(1)-Sn(1)-S(1)                    111.48(9)
N(4)-Sn(1)-S(1)                    102.83(8)
N(3)-Sn(1)-S(1)                    158.14(7)
N(2)-Sn(1)-S(1)                     82.44(9)
N(1)-Sn(1)-S(2)                    105.90(9)
N(4)-Sn(1)-S(2)                     97.26(9)
N(3)-Sn(1)-S(2)                     94.06(9)
N(2)-Sn(1)-S(2)                    163.67(8)
S(1)-Sn(1)-S(2)                    101.67(7)
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Symmetry transformations used to generate equivalent atoms:

Table S32. Anisotropic displacement parameters (A^2 x 10^3) for R202.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

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	U11	U22	U33	U23	U13	U12
C(1)	29(2)	30(2)	57(2)	10(2)	2(2)	6(1)
C(2)	40(2)	42(2)	66(3)	9(2)	13(2)	8(2)
C(3)	43(2)	38(2)	86(3)	7(2)	17(2)	11(2)
C(4)	44(2)	35(2)	72(3)	11(2)	8(2)	7(2)
C(5)	37(2)	32(2)	49(2)	5(1)	-1(2)	-2(1)
C(6)	52(2)	36(2)	50(2)	10(2)	4(2)	-1(2)
C(7)	57(2)	46(2)	50(2)	8(2)	14(2)	-6(2)
C(8)	47(2)	39(2)	44(2)	4(2)	7(2)	0(2)
C(9)	30(2)	32(2)	37(2)	3(1)	-5(1)	-3(1)
C(10)	30(2)	32(2)	41(2)	5(1)	-1(1)	2(1)
C(11)	27(2)	34(2)	55(2)	11(2)	-1(2)	0(1)
C(12)	37(2)	42(2)	91(3)	18(2)	-17(2)	1(2)
C(13)	34(2)	36(2)	74(3)	6(2)	-13(2)	1(2)
C(14)	30(2)	36(2)	107(4)	20(2)	-10(2)	0(2)
C(15)	39(2)	42(2)	151(5)	13(3)	-16(3)	-1(2)
C(16)	58(3)	46(3)	139(5)	-4(3)	-29(3)	-3(2)
C(17)	71(3)	59(3)	107(4)	-11(3)	-34(3)	4(3)
C(18)	55(3)	52(2)	70(3)	4(2)	-20(2)	2(2)
C(19)	37(2)	78(3)	118(5)	32(3)	9(3)	-8(2)
C(20)	91(4)	89(4)	57(3)	-1(3)	-8(3)	-2(3)
C(21)	29(2)	37(2)	42(2)	-1(1)	2(1)	1(1)
C(22)	61(3)	55(2)	54(2)	9(2)	22(2)	16(2)
C(23)	36(2)	37(2)	36(2)	0(1)	6(1)	10(1)
C(24)	37(2)	50(2)	39(2)	0(2)	7(2)	12(2)
C(25)	44(2)	70(3)	44(2)	1(2)	6(2)	27(2)
C(26)	69(3)	55(2)	57(3)	4(2)	14(2)	34(2)
C(27)	76(3)	37(2)	53(2)	3(2)	21(2)	15(2)
C(28)	54(2)	36(2)	40(2)	-2(2)	12(2)	10(2)
C(29)	33(2)	65(2)	60(2)	-9(2)	5(2)	3(2)
C(30)	56(3)	42(2)	73(3)	-14(2)	9(2)	-2(2)
C(31)	37(2)	37(2)	41(2)	7(1)	6(2)	2(1)
C(32)	48(2)	49(2)	36(2)	1(2)	8(2)	11(2)
C(33)	39(2)	54(2)	44(2)	9(2)	12(2)	12(2)
C(34)	41(2)	41(2)	41(2)	10(2)	3(2)	-4(2)
C(35)	64(3)	55(2)	35(2)	-4(2)	13(2)	1(2)
C(36)	48(2)	46(2)	48(2)	1(2)	14(2)	14(2)
C(37)	55(3)	70(3)	49(2)	12(2)	-5(2)	-8(2)
C(38)	45(2)	40(2)	42(2)	-5(2)	7(2)	-2(2)
C(39)	69(3)	48(2)	58(3)	12(2)	27(2)	2(2)
C(40)	99(4)	57(3)	81(3)	0(2)	55(3)	8(2)
C(41)	117(4)	39(2)	91(4)	-6(2)	45(3)	5(3)
C(42)	87(3)	42(2)	75(3)	8(2)	24(3)	-10(2)
C(43)	58(2)	48(2)	54(2)	-1(2)	16(2)	-11(2)
C(44)	228(9)	47(3)	225(9)	-10(4)	133(7)	29(4)
N(1)	30(1)	32(1)	49(2)	8(1)	3(1)	2(1)

|						
N(2)	28(1)	39(2)	56(2)	10(1)	-4(1)	-3(1)
N(3)	30(1)	33(1)	39(2)	4(1)	3(1)	3(1)
N(4)	31(1)	32(1)	39(2)	2(1)	4(1)	7(1)
S(1)	35(1)	54(1)	51(1)	14(1)	0(1)	-2(1)
S(2)	41(1)	51(1)	66(1)	-16(1)	-10(1)	4(1)
Sn(1)	26(1)	33(1)	38(1)	2(1)	1(1)	4(1)

Crystal data and structure refinement of compound 3b
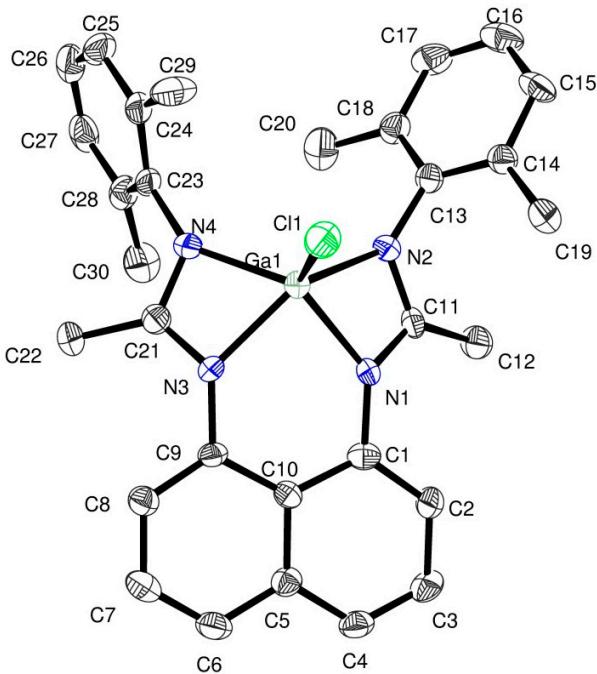
Figure S12. Asymmetric Unit

Table S33. Crystal data and structure refinement for R229.

Identification code	R229
Empirical formula	C30 H30 Cl Ga N4
Formula weight	551.75
Temperature	193(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P 21/c
Unit cell dimensions	a = 10.208(2) A alpha = 90 deg.
	b = 19.494(4) A beta = 90.929(7) deg.
	c = 13.220(3) A gamma = 90 deg.
Volume	2630.4(10) A^3
Z, Calculated density	4, 1.393 Mg/m^3
Absorption coefficient	1.174 mm^-1

```
F(000)                              1144

Crystal size                        0.100 x 0.040 x 0.040 mm

Theta range for data collection     3.255 to 24.147 deg.

Limiting indices                    -11<=h<=11, -22<=k<=21,
                                     -15<=l<=15

Reflections collected / unique      26145 / 4150 [R(int) = 0.1436]

Completeness to theta = 24.147      98.7 %

Refinement method                   Full-matrix least-squares on F^2

Data / restraints / parameters      4150 / 0 / 331

Goodness-of-fit on F^2              1.010

Final R indices [I>2sigma(I)]       R1 = 0.0502, wR2 = 0.0863

R indices (all data)                R1 = 0.1078, wR2 = 0.1079

Largest diff. peak and hole         0.447 and -0.523 e.A^-3
```

Table S34. Atomic coordinates (x 10^4) and equivalent isotropic
displacement parameters (A^2 x 10^3) for R229.
U(eq) is defined as one third of the trace of the orthogonalized
Uij tensor.

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	x	y	z	U(eq)
C(1)	794(5)	4090(2)	5502(3)	24(1)
C(2)	-495(5)	4091(3)	5177(4)	29(1)
C(3)	-864(5)	4177(2)	4165(4)	30(1)
C(4)	81(5)	4279(2)	3470(4)	31(1)
C(5)	1417(5)	4316(2)	3747(4)	26(1)
C(6)	2352(5)	4442(3)	2991(4)	33(1)
C(7)	3651(5)	4491(3)	3232(4)	34(1)
C(8)	4072(5)	4419(2)	4234(4)	27(1)
C(9)	3212(5)	4270(2)	5002(3)	23(1)
C(10)	1825(5)	4219(2)	4782(3)	21(1)
C(11)	580(5)	3659(2)	7257(4)	24(1)
C(12)	-697(5)	3284(3)	7223(4)	34(1)
C(13)	1038(5)	3471(2)	9078(4)	26(1)
C(14)	121(5)	3868(2)	9593(4)	26(1)
C(15)	-103(5)	3716(3)	10601(4)	36(1)
C(16)	541(6)	3193(3)	11090(4)	43(2)
C(17)	1426(6)	2799(3)	10565(4)	40(2)
C(18)	1695(5)	2930(3)	9559(4)	31(1)
C(19)	-607(5)	4450(3)	9077(4)	35(1)
C(20)	2662(5)	2501(3)	9001(4)	46(2)
C(21)	4693(5)	3837(2)	6356(4)	26(1)
C(22)	5883(5)	3640(3)	5775(4)	33(1)
C(23)	5439(5)	3287(3)	7938(4)	28(1)
C(24)	6011(5)	3565(3)	8807(4)	32(1)
C(25)	6882(5)	3166(3)	9366(4)	40(2)
C(26)	7205(5)	2516(3)	9069(4)	43(2)
C(27)	6589(5)	2231(3)	8240(4)	40(2)
C(28)	5671(5)	2600(3)	7668(4)	32(1)
C(29)	5666(6)	4275(3)	9151(4)	46(2)
C(30)	4939(6)	2248(3)	6824(4)	45(2)
N(1)	1147(4)	4005(2)	6526(3)	24(1)
N(2)	1397(4)	3646(2)	8065(3)	25(1)
N(3)	3659(4)	4180(2)	6006(3)	24(1)
N(4)	4550(4)	3696(2)	7342(3)	25(1)
Cl(1)	2899(1)	5202(1)	8016(1)	35(1)
Ga(1)	2771(1)	4185(1)	7328(1)	24(1)

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Table S35. Bond lengths [A] and angles [deg] for R229.
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C(1)-C(2)                        1.378(6)
C(1)-N(1)                        1.406(6)
C(1)-C(10)                       1.452(6)
C(2)-C(3)                        1.394(6)
C(2)-H(2)                        0.9500
C(3)-C(4)                        1.359(6)
C(3)-H(3)                        0.9500
C(4)-C(5)                        1.408(7)
C(4)-H(4)                        0.9500
C(5)-C(6)                        1.414(6)
C(5)-C(10)                       1.437(6)
C(6)-C(7)                        1.362(7)
C(6)-H(6)                        0.9500
C(7)-C(8)                        1.393(7)
C(7)-H(7)                        0.9500
C(8)-C(9)                        1.384(6)
C(8)-H(8)                        0.9500
C(9)-N(3)                        1.408(6)
C(9)-C(10)                       1.445(6)
C(11)-N(1)                       1.320(5)
C(11)-N(2)                       1.345(6)
C(11)-C(12)                      1.494(6)
C(11)-Ga(1)                      2.462(5)
C(12)-H(12A)                     0.9800
C(12)-H(12B)                     0.9800
C(12)-H(12C)                     0.9800
C(13)-C(18)                      1.397(7)
C(13)-C(14)                      1.399(6)
C(13)-N(2)                       1.435(6)
C(14)-C(15)                      1.388(6)
C(14)-C(19)                      1.513(7)
C(15)-C(16)                      1.370(7)
C(15)-H(15)                      0.9500
C(16)-C(17)                      1.382(7)
C(16)-H(16)                      0.9500
C(17)-C(18)                      1.386(7)
C(17)-H(17)                      0.9500
C(18)-C(20)                      1.498(7)
C(19)-H(19A)                     0.9800
C(19)-H(19B)                     0.9800
C(19)-H(19C)                     0.9800
C(20)-H(20A)                     0.9800
C(20)-H(20B)                     0.9800
C(20)-H(20C)                     0.9800
C(21)-N(3)                       1.327(6)
C(21)-N(4)                       1.342(6)
C(21)-C(22)                      1.498(6)
C(21)-Ga(1)                      2.458(5)
C(22)-H(22A)                     0.9800
C(22)-H(22B)                     0.9800
C(22)-H(22C)                     0.9800
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C(23)-C(24)              1.391(7)
C(23)-C(28)              1.407(7)
C(23)-N(4)               1.433(6)
C(24)-C(25)              1.385(7)
C(24)-C(29)              1.501(7)
C(25)-C(26)              1.368(8)
C(25)-H(25)              0.9500
C(26)-C(27)              1.373(8)
C(26)-H(26)              0.9500
C(27)-C(28)              1.395(7)
C(27)-H(27)              0.9500
C(28)-C(30)              1.499(7)
C(29)-H(29A)             0.9800
C(29)-H(29B)             0.9800
C(29)-H(29C)             0.9800
C(30)-H(30A)             0.9800
C(30)-H(30B)             0.9800
C(30)-H(30C)             0.9800
N(1)-Ga(1)               1.984(4)
N(2)-Ga(1)               2.017(4)
N(3)-Ga(1)               1.981(4)
N(4)-Ga(1)               2.051(4)
Cl(1)-Ga(1)              2.1828(14)

C(2)-C(1)-N(1)           121.9(4)
C(2)-C(1)-C(10)          119.6(4)
N(1)-C(1)-C(10)          118.3(4)
C(1)-C(2)-C(3)           122.7(5)
C(1)-C(2)-H(2)           118.6
C(3)-C(2)-H(2)           118.6
C(4)-C(3)-C(2)           118.9(5)
C(4)-C(3)-H(3)           120.5
C(2)-C(3)-H(3)           120.5
C(3)-C(4)-C(5)           121.8(5)
C(3)-C(4)-H(4)           119.1
C(5)-C(4)-H(4)           119.1
C(4)-C(5)-C(6)           119.1(5)
C(4)-C(5)-C(10)          120.3(4)
C(6)-C(5)-C(10)          120.5(4)
C(7)-C(6)-C(5)           120.8(5)
C(7)-C(6)-H(6)           119.6
C(5)-C(6)-H(6)           119.6
C(6)-C(7)-C(8)           119.9(5)
C(6)-C(7)-H(7)           120.0
C(8)-C(7)-H(7)           120.0
C(9)-C(8)-C(7)           122.0(5)
C(9)-C(8)-H(8)           119.0
C(7)-C(8)-H(8)           119.0
C(8)-C(9)-N(3)           121.3(4)
C(8)-C(9)-C(10)          119.9(4)
N(3)-C(9)-C(10)          118.8(4)
C(5)-C(10)-C(9)          116.7(4)
C(5)-C(10)-C(1)          116.5(4)
C(9)-C(10)-C(1)          126.8(4)
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N(1)-C(11)-N(2)            108.5(4)
N(1)-C(11)-C(12)           128.4(5)
N(2)-C(11)-C(12)           122.9(4)
N(1)-C(11)-Ga(1)            53.5(2)
N(2)-C(11)-Ga(1)            55.0(2)
C(12)-C(11)-Ga(1)          175.4(4)
C(11)-C(12)-H(12A)         109.5
C(11)-C(12)-H(12B)         109.5
H(12A)-C(12)-H(12B)        109.5
C(11)-C(12)-H(12C)         109.5
H(12A)-C(12)-H(12C)        109.5
H(12B)-C(12)-H(12C)        109.5
C(18)-C(13)-C(14)          121.1(5)
C(18)-C(13)-N(2)           118.4(4)
C(14)-C(13)-N(2)           120.3(4)
C(15)-C(14)-C(13)          118.1(5)
C(15)-C(14)-C(19)          120.4(5)
C(13)-C(14)-C(19)          121.6(4)
C(16)-C(15)-C(14)          121.8(5)
C(16)-C(15)-H(15)          119.1
C(14)-C(15)-H(15)          119.1
C(15)-C(16)-C(17)          119.3(5)
C(15)-C(16)-H(16)          120.4
C(17)-C(16)-H(16)          120.4
C(16)-C(17)-C(18)          121.4(5)
C(16)-C(17)-H(17)          119.3
C(18)-C(17)-H(17)          119.3
C(17)-C(18)-C(13)          118.4(5)
C(17)-C(18)-C(20)          120.7(5)
C(13)-C(18)-C(20)          120.9(5)
C(14)-C(19)-H(19A)         109.5
C(14)-C(19)-H(19B)         109.5
H(19A)-C(19)-H(19B)        109.5
C(14)-C(19)-H(19C)         109.5
H(19A)-C(19)-H(19C)        109.5
H(19B)-C(19)-H(19C)        109.5
C(18)-C(20)-H(20A)         109.5
C(18)-C(20)-H(20B)         109.5
H(20A)-C(20)-H(20B)        109.5
C(18)-C(20)-H(20C)         109.5
H(20A)-C(20)-H(20C)        109.5
H(20B)-C(20)-H(20C)        109.5
N(3)-C(21)-N(4)            110.1(4)
N(3)-C(21)-C(22)           126.7(4)
N(4)-C(21)-C(22)           123.2(5)
N(3)-C(21)-Ga(1)            53.5(2)
N(4)-C(21)-Ga(1)            56.6(2)
C(22)-C(21)-Ga(1)          178.5(4)
C(21)-C(22)-H(22A)         109.5
C(21)-C(22)-H(22B)         109.5
H(22A)-C(22)-H(22B)        109.5
C(21)-C(22)-H(22C)         109.5
H(22A)-C(22)-H(22C)        109.5
H(22B)-C(22)-H(22C)        109.5
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C(24)-C(23)-C(28)        120.7(5)
C(24)-C(23)-N(4)         119.4(5)
C(28)-C(23)-N(4)         119.9(5)
C(25)-C(24)-C(23)        118.7(5)
C(25)-C(24)-C(29)        120.5(5)
C(23)-C(24)-C(29)        120.8(5)
C(26)-C(25)-C(24)        121.5(6)
C(26)-C(25)-H(25)        119.3
C(24)-C(25)-H(25)        119.3
C(25)-C(26)-C(27)        119.7(6)
C(25)-C(26)-H(26)        120.2
C(27)-C(26)-H(26)        120.2
C(26)-C(27)-C(28)        121.3(5)
C(26)-C(27)-H(27)        119.4
C(28)-C(27)-H(27)        119.4
C(27)-C(28)-C(23)        117.9(5)
C(27)-C(28)-C(30)        119.3(5)
C(23)-C(28)-C(30)        122.7(5)
C(24)-C(29)-H(29A)       109.5
C(24)-C(29)-H(29B)       109.5
H(29A)-C(29)-H(29B)      109.5
C(24)-C(29)-H(29C)       109.5
H(29A)-C(29)-H(29C)      109.5
H(29B)-C(29)-H(29C)      109.5
C(28)-C(30)-H(30A)       109.5
C(28)-C(30)-H(30B)       109.5
H(30A)-C(30)-H(30B)      109.5
C(28)-C(30)-H(30C)       109.5
H(30A)-C(30)-H(30C)      109.5
H(30B)-C(30)-H(30C)      109.5
C(11)-N(1)-C(1)          131.0(4)
C(11)-N(1)-Ga(1)          94.2(3)
C(1)-N(1)-Ga(1)         133.8(3)
C(11)-N(2)-C(13)        125.6(4)
C(11)-N(2)-Ga(1)         91.9(3)
C(13)-N(2)-Ga(1)        139.9(3)
C(21)-N(3)-C(9)         129.4(4)
C(21)-N(3)-Ga(1)         93.9(3)
C(9)-N(3)-Ga(1)         133.3(3)
C(21)-N(4)-C(23)        124.7(4)
C(21)-N(4)-Ga(1)         90.3(3)
C(23)-N(4)-Ga(1)        144.7(3)
N(3)-Ga(1)-N(1)          85.32(15)
N(3)-Ga(1)-N(2)         139.06(16)
N(1)-Ga(1)-N(2)          65.43(16)
N(3)-Ga(1)-N(4)          65.69(15)
N(1)-Ga(1)-N(4)         130.88(15)
N(2)-Ga(1)-N(4)         112.06(16)
N(3)-Ga(1)-Cl(1)        110.32(12)
N(1)-Ga(1)-Cl(1)        115.30(11)
N(2)-Ga(1)-Cl(1)        107.98(12)
N(4)-Ga(1)-Cl(1)        111.79(12)
N(3)-Ga(1)-C(21)         32.59(15)
N(1)-Ga(1)-C(21)        109.82(16)
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N(2)-Ga(1)-C(21)                    132.52(16)
N(4)-Ga(1)-C(21)                     33.10(15)
Cl(1)-Ga(1)-C(21)                   115.20(12)
N(3)-Ga(1)-C(11)                    113.13(16)
N(1)-Ga(1)-C(11)                     32.32(15)
N(2)-Ga(1)-C(11)                     33.11(15)
N(4)-Ga(1)-C(11)                    127.61(16)
Cl(1)-Ga(1)-C(11)                   116.26(11)
C(21)-Ga(1)-C(11)                   126.69(16)
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Symmetry transformations used to generate equivalent atoms:

Table S36. Anisotropic displacement parameters (A^2 x 10^3) for R229.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	30(3)	21(3)	22(3)	-4(2)	-4(2)	-4(2)
C(2)	20(3)	38(3)	29(3)	-1(3)	1(2)	-4(3)
C(3)	25(3)	32(3)	31(3)	-10(3)	-10(3)	-4(3)
C(4)	34(3)	34(3)	23(3)	-3(3)	-7(3)	5(3)
C(5)	26(3)	26(3)	24(3)	-4(2)	-3(2)	-1(2)
C(6)	40(4)	38(3)	20(3)	2(2)	-1(3)	2(3)
C(7)	41(4)	37(3)	23(3)	3(3)	6(3)	0(3)
C(8)	27(3)	30(3)	24(3)	-1(2)	1(2)	-2(2)
C(9)	23(3)	28(3)	18(3)	0(2)	-4(2)	-2(2)
C(10)	25(3)	18(3)	19(3)	-3(2)	2(2)	0(2)
C(11)	19(3)	27(3)	25(3)	-6(3)	6(3)	-2(2)
C(12)	29(3)	41(3)	33(3)	2(3)	2(3)	-10(3)
C(13)	21(3)	30(3)	26(3)	1(3)	1(2)	-7(3)
C(14)	26(3)	28(3)	25(3)	1(2)	1(3)	-4(3)
C(15)	44(4)	45(4)	20(3)	-1(3)	8(3)	-12(3)
C(16)	57(4)	46(4)	25(3)	7(3)	1(3)	-13(3)
C(17)	47(4)	38(4)	35(3)	16(3)	-7(3)	-6(3)
C(18)	28(3)	30(3)	33(3)	6(3)	0(3)	1(3)
C(19)	35(3)	42(3)	29(3)	-3(3)	7(3)	2(3)
C(20)	42(4)	40(4)	58(4)	15(3)	9(3)	4(3)
C(21)	24(3)	29(3)	25(3)	-3(2)	0(3)	-6(3)
C(22)	25(3)	45(3)	30(3)	-2(3)	7(3)	3(3)
C(23)	19(3)	39(4)	25(3)	11(3)	1(3)	3(3)
C(24)	21(3)	44(4)	29(3)	8(3)	4(3)	1(3)
C(25)	28(3)	57(4)	34(3)	19(3)	-5(3)	-2(3)
C(26)	29(3)	55(4)	46(4)	29(3)	9(3)	8(3)
C(27)	35(4)	42(4)	42(4)	16(3)	14(3)	5(3)
C(28)	25(3)	33(3)	39(3)	4(3)	1(3)	-5(3)
C(29)	54(4)	55(4)	30(3)	0(3)	-15(3)	4(3)
C(30)	47(4)	39(4)	51(4)	1(3)	6(3)	2(3)
N(1)	19(2)	33(3)	20(2)	4(2)	5(2)	1(2)
N(2)	24(2)	32(3)	20(2)	4(2)	1(2)	-1(2)
N(3)	18(2)	33(2)	21(2)	1(2)	-2(2)	4(2)
N(4)	25(3)	30(3)	19(2)	-1(2)	0(2)	3(2)
Cl(1)	33(1)	35(1)	36(1)	-7(1)	-3(1)	3(1)
Ga(1)	19(1)	30(1)	21(1)	0(1)	1(1)	0(1)

Calculations

Calculations were performed with the Gaussian 16 suite of programs [1] using the density functional method B3LYP with dispersion (D3). [2, 3] Tin atom was treated with a Stuttgart-Dresden pseudopotential in combination with its adapted basis set.[4] All other atoms have been described with a 6-31G(d,p) basis set. Geometry optimisations were carried out without any symmetry restrictions. Frequency calculations were undertaken to confirm the nature of the stationary points, yielding one imaginary frequency for transition states (TS) and all of them positive for *minima*. The connectivity of the transition states and their adjacent *minima* was confirmed by intrinsic reaction coordinate (IRC) calculations.[5,6]

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2. a) Becke, A. D. Density-functional exchange-energy approximation with correct asymptotic behavior. *Phys. Rev. A* **1988**, 38, 3098-3100. https://doi.org/10.1103/PhysRevA.38.3098 ; b) Becke, A. D. Density-functional thermochemistry. III. The role of exact exchange. *J. Chem. Phys.* **1993**, *98*, 5648-5652. https://doi.org/10.1063/1.464913 ; c) Lee, C.; Yang, W.; Parr, R. G. Development of the Colle-Salvetti correlation-energy formula into a functional of the electron density. *Phys. Rev. B* **1988**, *37*, 785-789. https://doi.org/10.1103/PhysRevB.37.785

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6. Hratchian, H. P.; Schlegel, H. B. In Theory and Applications of Computational Chemistry: The First 40 Years, Eds D. C. E. Dykstra, G. Frenking, K. S. Kim, G. Scuseria. Elsevier., Amsterdam, 2005.

G (kcal/mol)

1.790
1.633

21.63

0

3.78

39.25

1.759 1.740
2.569

R₂NH

-14.20

2.339
2.317
2.279 2.416

Prototropy

Elimination
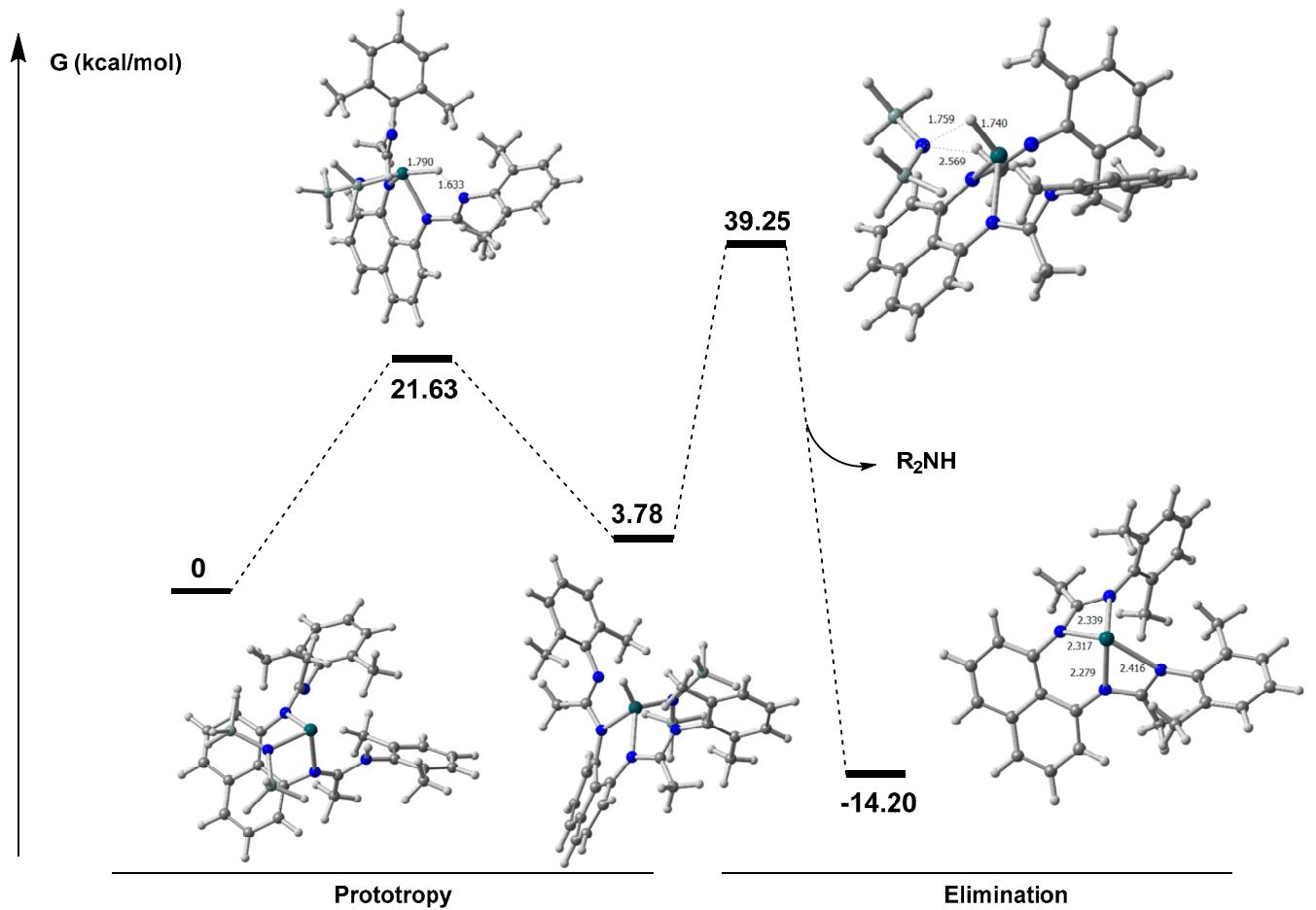
DFT calculations for the formation of **L₁Sn**.

Coordinates, energies

L1

Sum of electronic and thermal Free Energies=   -2021.440506 au

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N    1.342588000000   -1.965339000000   -0.026149000000
C   -3.098596000000   -2.529756000000    2.590868000000
H   -3.776410000000   -2.909169000000    3.349073000000
C    2.395962000000    2.673886000000    0.475996000000
C    3.336214000000    1.868689000000    1.145782000000
C   -3.027583000000   -1.134078000000    2.373977000000
N   -1.036840000000    1.400586000000    0.462289000000
C    0.342767000000    1.823397000000    2.467140000000
C    4.611217000000    2.409666000000    1.364445000000
H    5.348785000000    1.801756000000    1.880219000000
C   -2.319885000000   -3.382585000000    1.841651000000
H   -2.367337000000   -4.455123000000    2.003962000000
C    0.720171000000   -1.934788000000   -2.434087000000
N   -0.738039000000   -1.130530000000   -0.641957000000
C   -3.846485000000   -0.252274000000    3.131048000000
H   -4.533974000000   -0.684026000000    3.852302000000
C    4.949178000000    3.682003000000    0.919935000000
H    5.946881000000    4.072001000000    1.095384000000
C   -2.122670000000   -0.603394000000    1.388612000000
C    4.233185000000   -4.230868000000    0.206254000000
H    4.465287000000   -5.193420000000    0.654534000000
C    2.721194000000    3.965717000000    0.013208000000
C    2.938069000000   -3.728882000000    0.316338000000
C   -1.401673000000   -1.520094000000    0.543460000000
C    0.495175000000   -1.682876000000   -0.955231000000
C    3.048587000000    0.470642000000    1.632050000000
H    2.893655000000    0.460279000000    2.716951000000
H    3.899555000000   -0.181669000000    1.423458000000
H    2.174510000000    0.014159000000    1.167035000000
C    1.859548000000   -4.493053000000    1.037188000000
H    1.136130000000   -4.922210000000    0.332501000000
H    1.289909000000   -3.830189000000    1.695362000000
H    2.280695000000   -5.314658000000    1.622911000000
C    0.094771000000    1.795014000000    0.983498000000
C    4.007063000000    4.454057000000    0.241740000000
H    4.266382000000    5.448135000000   -0.109852000000
C   -1.504572000000   -2.881575000000    0.816436000000
H   -0.964282000000   -3.572187000000    0.180866000000
C   -3.785761000000    1.106467000000    2.951647000000
H   -4.432051000000    1.770088000000    3.516775000000
C    3.626431000000   -1.742087000000   -0.941820000000
C    5.228012000000   -3.511948000000   -0.457475000000
H    6.236411000000   -3.908027000000   -0.527736000000
C   -2.854022000000    1.646819000000    2.039692000000
H   -2.766126000000    2.720451000000    1.909343000000
C    2.622679000000   -2.480038000000   -0.270957000000
C   -2.021821000000    0.823184000000    1.311924000000
C    4.918757000000   -2.277581000000   -1.017496000000
H    5.690851000000   -1.705104000000   -1.525934000000
C    1.696976000000    4.796850000000   -0.717824000000
H    0.756846000000    4.858842000000   -0.160478000000
H    1.455275000000    4.377129000000   -1.703051000000
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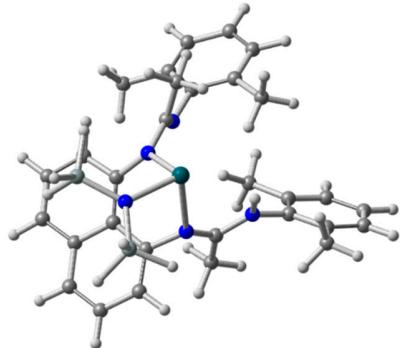
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H    3.197277000000     -0.468430000000     -2.643579000000
H    4.207948000000      0.281372000000     -1.408631000000
N    1.090804000000      2.192498000000      0.153217000000
H    0.834329000000      2.234783000000     -0.827035000000
N   -3.415153000000      0.352186000000     -1.456907000000
Si  -4.104156000000     -1.241852000000     -1.528045000000
H   -4.410959000000     -1.836196000000     -0.200785000000
H   -5.388116000000     -1.207430000000     -2.290899000000
H   -3.173443000000     -2.156366000000     -2.244989000000
Si  -4.433477000000      1.725096000000     -1.185908000000
H   -5.303955000000      1.586441000000      0.013989000000
H   -3.562134000000      2.923103000000     -0.989887000000
H   -5.337622000000      2.027294000000     -2.334849000000
H   -0.493411000000      2.308850000000      2.968553000000
H    0.396371000000      0.798409000000      2.842745000000
H    1.266692000000      2.345789000000      2.705392000000
H    0.813202000000     -0.997923000000     -2.994882000000
H   -0.138389000000     -2.475512000000     -2.841196000000
H    1.629973000000     -2.513317000000     -2.596844000000
```

TS1 (Prototropy from NH → SnH)

Sum of electronic and thermal Free Energies=   -2021.406023 au

```
Sn   0.279203000000     -0.193096000000      0.752522000000
N    2.165799000000     -1.074855000000     -0.301388000000
C    1.299949000000      5.034334000000     -1.795186000000
H    1.260993000000      6.088254000000     -2.052031000000
C   -3.762050000000     -1.526349000000     -0.008655000000
C   -3.575846000000     -2.633616000000     -0.861065000000
C    0.113422000000      4.409373000000     -1.330439000000
N   -1.301745000000      1.108401000000     -0.142472000000
C   -3.336414000000      0.798933000000     -1.582044000000
C   -4.649364000000     -3.497779000000     -1.088806000000
H   -4.510628000000     -4.348264000000     -1.750957000000
C    2.473010000000      4.331561000000     -1.876653000000
H    3.391138000000      4.817371000000     -2.192133000000
C    3.364074000000      0.090488000000     -2.132933000000
N    1.420588000000      0.949698000000     -0.740795000000
C   -1.053530000000      5.201980000000     -1.190384000000
H   -1.002527000000      6.250629000000     -1.465755000000
C   -5.883569000000     -3.284760000000     -0.477532000000
H   -6.707830000000     -3.967128000000     -0.660368000000
C    0.103968000000      3.007635000000     -0.989702000000
C    3.195440000000     -4.425961000000     -1.516374000000
H    2.932095000000     -5.136973000000     -2.294472000000
C   -5.001522000000     -1.308670000000      0.626837000000
C    2.513054000000     -3.207023000000     -1.451805000000
C    1.354299000000      2.292755000000     -1.120974000000
C    2.323982000000      0.003850000000     -1.053815000000
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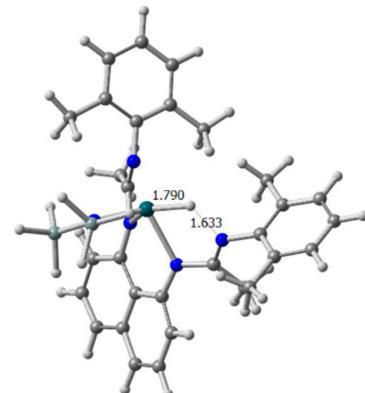
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H    1.722241000000   -2.133027000000   -3.169647000000
H    0.537156000000   -2.477832000000   -1.920169000000
H    1.107664000000   -3.776312000000   -2.980978000000
C   -2.440414000000    0.417432000000   -0.417359000000
C   -6.050444000000   -2.197457000000    0.377537000000
H   -7.007400000000   -2.032413000000    0.865345000000
C   -2.205275000000    4.657977000000   -0.681275000000
H   -3.090961000000    5.268526000000   -0.534488000000
C    3.853928000000   -2.605954000000    0.514543000000
C    4.189613000000   -4.740067000000   -0.593182000000
H    4.706034000000   -5.693036000000   -0.653731000000
C   -2.233702000000    3.301340000000   -0.327750000000
H   -3.130560000000    2.887097000000    0.118383000000
C    2.865423000000   -2.292902000000   -0.438810000000
C   -1.142939000000    2.452932000000   -0.509794000000
C    4.509283000000   -3.835585000000    0.418036000000
H    5.275449000000   -4.084079000000    1.146952000000
C   -5.173837000000   -0.137546000000    1.559169000000
H   -5.166779000000    0.817994000000    1.020358000000
H   -4.354662000000   -0.091094000000    2.283124000000
H   -6.121028000000   -0.204092000000    2.100423000000
C    4.185183000000   -1.623546000000    1.607760000000
H    4.903465000000   -2.050092000000    2.311969000000
H    3.289643000000   -1.324204000000    2.161816000000
H    4.613347000000   -0.700539000000    1.202051000000
N   -2.685288000000   -0.666836000000    0.286026000000
H   -1.215445000000   -1.178115000000    0.779199000000
N    1.025681000000    0.772738000000    2.427710000000
Si   2.279509000000    1.975387000000    2.286246000000
H    2.843064000000    2.212169000000    3.646099000000
H    3.381440000000    1.512353000000    1.404320000000
H    1.793337000000    3.275552000000    1.758540000000
Si   0.232076000000    0.512661000000    3.953370000000
H   -0.418082000000    1.743281000000    4.485856000000
H   -0.822373000000   -0.518724000000    3.752924000000
H    1.172753000000    0.027964000000    5.001369000000
H    3.583157000000   -0.907413000000   -2.513545000000
H    4.296329000000    0.494372000000   -1.725512000000
H    3.034920000000    0.743062000000   -2.942957000000
H   -4.311657000000    1.149519000000   -1.233413000000
H   -3.520829000000   -0.094929000000   -2.183165000000
H   -2.889143000000    1.576032000000   -2.199057000000
C    2.500480000000    2.973953000000   -1.516224000000
H    3.451420000000    2.462692000000   -1.501545000000
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SnH derivative

Sum of electronic and thermal Free Energies=   -2021.434479 au

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Sn   0.006770000000   -0.355066000000   -0.371221000000
N    2.394203000000   -0.471119000000   -0.595504000000
```

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C    0.704582000000    5.573690000000   -0.721809000000
H    0.643253000000    6.651064000000   -0.603780000000
C   -3.515866000000   -1.515846000000   -0.470199000000
C   -4.040295000000   -1.548692000000   -1.778071000000
C   -0.142870000000    4.754843000000    0.070380000000
N   -1.352905000000    1.227589000000    0.246820000000
C   -3.892946000000    1.287281000000    0.324097000000
C   -5.063416000000   -2.455685000000   -2.067913000000
H   -5.473823000000   -2.484280000000   -3.073601000000
C    1.565216000000    5.009568000000   -1.629953000000
H    2.180646000000    5.634357000000   -2.269932000000
C    3.777662000000    1.562959000000   -0.917666000000
N    1.245065000000    1.402286000000   -0.791822000000
C   -1.026985000000    5.351482000000    1.007662000000
H   -1.021850000000    6.432153000000    1.110286000000
C   -5.550791000000   -3.321317000000   -1.091078000000
H   -6.341527000000   -4.025001000000   -1.332431000000
C   -0.105321000000    3.326333000000   -0.076426000000
C    4.834991000000   -3.195629000000   -1.101811000000
H    5.091453000000   -3.926775000000   -1.863395000000
C   -3.992634000000   -2.391142000000    0.523923000000
C    3.807077000000   -2.285913000000   -1.353487000000
C    0.945759000000    2.766009000000   -0.890969000000
C    2.474305000000    0.827238000000   -0.778477000000
C   -3.498553000000   -0.621833000000   -2.837216000000
H   -3.708403000000    0.429789000000   -2.608976000000
H   -3.939854000000   -0.844037000000   -3.811881000000
H   -2.411342000000   -0.713285000000   -2.922556000000
C    3.038298000000   -2.311369000000   -2.648575000000
H    3.078047000000   -1.343406000000   -3.159602000000
H    1.979063000000   -2.526229000000   -2.472745000000
H    3.434335000000   -3.073180000000   -3.324586000000
C   -2.563196000000    0.606772000000    0.150573000000
C   -5.013023000000   -3.287213000000    0.193715000000
H   -5.385019000000   -3.965540000000    0.956645000000
C   -1.850071000000    4.571124000000    1.780940000000
H   -2.491070000000    5.020370000000    2.533208000000
C    4.158143000000   -1.319479000000    0.874107000000
C    5.525194000000   -3.178409000000    0.109606000000
H    6.319035000000   -3.895488000000    0.294489000000
C   -1.898031000000    3.179677000000    1.575691000000
H   -2.572479000000    2.575095000000    2.167771000000
C    3.482966000000   -1.336565000000   -0.364141000000
C   -1.119816000000    2.560402000000    0.604274000000
C    5.182436000000   -2.248775000000    1.086780000000
H    5.703826000000   -2.245471000000    2.039916000000
C   -3.407607000000   -2.347619000000    1.910879000000
H   -3.668061000000   -1.416862000000    2.427776000000
H   -2.316006000000   -2.386027000000    1.877201000000
H   -3.772006000000   -3.181108000000    2.516407000000
C    3.768364000000   -0.344877000000    1.956605000000
H    4.152684000000   -0.672361000000    2.925466000000
H    2.682108000000   -0.258546000000    2.024371000000
H    4.161275000000    0.662001000000    1.771931000000
N   -2.439463000000   -0.652344000000   -0.177416000000
H   -0.170068000000   -1.189565000000   -1.835965000000
N    0.242128000000   -1.221606000000    1.492141000000
Si  -0.173104000000   -0.276804000000    2.888139000000
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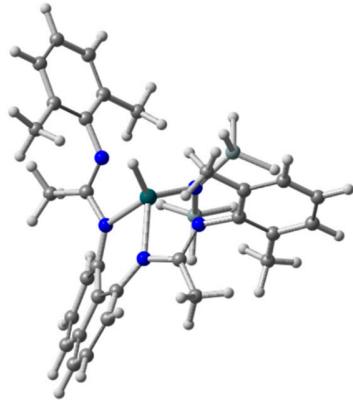
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Si   0.823333000000   -2.854311000000    1.603919000000
H   -0.186475000000   -3.766785000000    2.214205000000
H    1.096498000000   -3.337366000000    0.224413000000
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H    4.585241000000    0.960050000000   -0.503530000000
H    3.733384000000    2.532915000000   -0.418993000000
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H   -4.220464000000    1.225748000000    1.366307000000
H   -4.639147000000    0.774407000000   -0.284664000000
H   -3.838479000000    2.341485000000    0.050340000000
C    1.688558000000    3.609440000000   -1.709056000000
H    2.397165000000    3.178545000000   -2.403734000000
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Amine elimination

Sum of electronic and thermal Free Energies=   -2021.377957 au

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Sn  -0.015271000000    0.027585000000    0.923622000000
N   -1.014386000000   -1.889642000000    0.061604000000
C    5.090374000000   -1.390345000000   -1.602219000000
H    6.111352000000   -1.349545000000   -1.968873000000
C   -2.296066000000    2.497909000000   -0.227936000000
C   -3.528207000000    2.091286000000   -0.773984000000
C    4.320354000000   -0.198096000000   -1.622063000000
N    0.935411000000    1.136177000000   -0.706496000000
C   -4.633805000000    2.936189000000   -0.643036000000
H   -5.584896000000    2.628597000000   -1.068380000000
C    4.565834000000   -2.559232000000   -1.113070000000
H    5.165455000000   -3.463156000000   -1.076527000000
N    1.139115000000   -1.506609000000   -0.146031000000
C    4.911818000000    0.994699000000   -2.112459000000
H    5.939741000000    0.957166000000   -2.459176000000
C   -4.528099000000    4.155548000000    0.021134000000
H   -5.395481000000    4.801552000000    0.115816000000
C    2.960861000000   -0.200595000000   -1.151145000000
C   -4.160778000000   -3.203588000000   -1.409624000000
H   -4.643762000000   -3.290906000000   -2.378996000000
C   -2.180825000000    3.719514000000    0.470017000000
C   -2.887758000000   -2.626525000000   -1.338479000000
C    2.441193000000   -1.454269000000   -0.656761000000
C    0.145998000000   -2.350497000000   -0.408887000000
C   -3.639974000000    0.769887000000   -1.481370000000
H   -2.959698000000    0.715207000000   -2.336969000000
H   -4.657246000000    0.600589000000   -1.842609000000
H   -3.375234000000   -0.059324000000   -0.819645000000
C   -2.220146000000   -2.119967000000   -2.593591000000
H   -1.609065000000   -2.890859000000   -3.077137000000
H   -1.564456000000   -1.273100000000   -2.380638000000
H   -2.969850000000   -1.800922000000   -3.321994000000
C   -0.101110000000    1.896268000000   -1.064366000000
C   -3.308725000000    4.537911000000    0.575794000000
H   -3.227255000000    5.479910000000    1.110716000000
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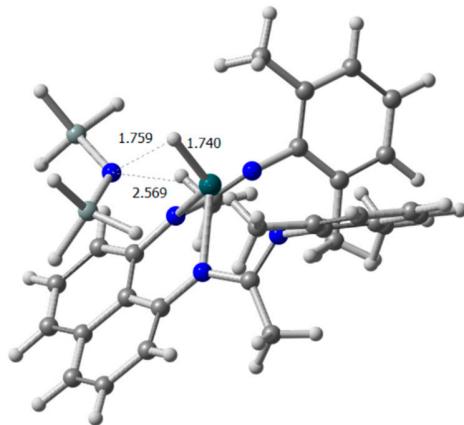
H	2.856659000000	-3.486567000000	-0.178739000000
C	4.207331000000	2.171013000000	-2.122761000000
H	4.669390000000	3.090405000000	-2.468100000000
C	-2.931811000000	-2.944832000000	1.096359000000
C	-4.815403000000	-3.646232000000	-0.264777000000
H	-5.804738000000	-4.086764000000	-0.339171000000
C	2.882223000000	2.198022000000	-1.655625000000
H	2.364261000000	3.145814000000	-1.596482000000
C	-2.270069000000	-2.514520000000	-0.073367000000
C	2.238283000000	1.052440000000	-1.206330000000
C	-4.202059000000	-3.510755000000	0.980046000000
H	-4.712958000000	-3.849323000000	1.876843000000
C	-0.880801000000	4.120057000000	1.119635000000
H	-0.492068000000	3.325002000000	1.762655000000
H	-1.013880000000	5.015938000000	1.730312000000
H	-0.092058000000	4.335093000000	0.390418000000
C	-2.270960000000	-2.787382000000	2.441124000000
H	-2.176732000000	-1.731375000000	2.720012000000
H	-1.256746000000	-3.198525000000	2.445027000000
H	-2.850590000000	-3.286317000000	3.221395000000
N	-1.175384000000	1.638373000000	-0.317753000000
H	0.354394000000	0.416615000000	2.578398000000
N	2.096925000000	0.367399000000	2.345447000000
Si	2.925147000000	1.860822000000	2.242793000000
H	2.000090000000	2.882337000000	1.657557000000
H	3.372848000000	2.413396000000	3.560426000000
H	4.134194000000	1.845844000000	1.364677000000
Si	2.605448000000	-1.109567000000	3.036842000000
H	3.000114000000	-1.031817000000	4.477826000000
H	1.439087000000	-2.057297000000	2.971166000000
H	3.729352000000	-1.794710000000	2.332061000000
C	0.307075000000	-3.670636000000	-1.102976000000
H	-0.655407000000	-4.073803000000	-1.411349000000
H	0.971996000000	-3.568317000000	-1.963952000000
H	0.768671000000	-4.383695000000	-0.413671000000
C	-0.124662000000	2.873098000000	-2.203715000000
H	0.201448000000	3.863870000000	-1.872963000000
H	0.549802000000	2.546326000000	-2.997412000000
H	-1.142625000000	2.968339000000	-2.584678000000

L1Sn

Sum of electronic and thermal Free Energies=   -1383.498096 au

|			
Sn	-0.073500000000	0.048241000000	-1.607961000000
N	0.305976000000	-1.891444000000	-0.357900000000
C	-5.752003000000	-0.343197000000	0.362869000000
H	-6.774774000000	-0.100632000000	0.635195000000
N	1.150883000000	1.381768000000	-0.008333000000
C	2.350574000000	2.126564000000	0.062408000000
C	2.408389000000	3.414621000000	-0.518380000000
C	-4.753632000000	0.650330000000	0.544536000000
N	-1.063143000000	1.224820000000	0.073674000000

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C    0.076486000000    2.637833000000    1.839911000000
H    1.030864000000    2.493445000000    2.348991000000
H   -0.748045000000    2.385605000000    2.509355000000
H   -0.007114000000    3.699698000000    1.590735000000
C    3.611867000000    4.123447000000   -0.472613000000
H    3.656838000000    5.113636000000   -0.917992000000
C   -5.436551000000   -1.573351000000   -0.157378000000
H   -6.206993000000   -2.323493000000   -0.307818000000
C   -1.492382000000   -3.296251000000    0.682735000000
H   -2.225014000000   -2.954481000000    1.418377000000
H   -0.677742000000   -3.819265000000    1.180854000000
H   -2.003497000000   -4.001511000000    0.021719000000
N   -1.776297000000   -1.237228000000   -0.705584000000
C   -5.123577000000    1.918636000000    1.061718000000
H   -6.165060000000    2.094616000000    1.312615000000
C    4.748186000000    3.572888000000    0.114956000000
H    5.676883000000    4.134746000000    0.139752000000
C   -3.383645000000    0.372308000000    0.203206000000
C    3.332037000000   -4.005586000000   -0.141848000000
H    3.994507000000   -4.550455000000   -0.808679000000
C    3.503917000000    1.550674000000    0.631598000000
C    2.235075000000   -3.328686000000   -0.679009000000
C   -3.089748000000   -0.935132000000   -0.331438000000
C   -0.985702000000   -2.130515000000   -0.124626000000
C    1.211345000000    4.004611000000   -1.223005000000
H    0.777112000000    3.290104000000   -1.929506000000
H    1.496760000000    4.901381000000   -1.778246000000
H    0.409088000000    4.290746000000   -0.533622000000
C    1.965612000000   -3.338880000000   -2.161363000000
H    2.080443000000   -2.339529000000   -2.597239000000
H    0.941187000000   -3.656882000000   -2.379479000000
H    2.654908000000   -4.010081000000   -2.679669000000
C    0.036053000000    1.769202000000    0.608338000000
C    4.689680000000    2.290236000000    0.653484000000
H    5.575500000000    1.847553000000    1.100639000000
C   -4.106095000000   -1.859979000000   -0.515111000000
H   -3.856985000000   -2.815010000000   -0.963856000000
C   -4.182814000000    2.905311000000    1.213705000000
H   -4.466927000000    3.887783000000    1.578589000000
C    1.631340000000   -2.582851000000    1.578057000000
C    3.580555000000   -3.992260000000    1.229467000000
H    4.437080000000   -4.523002000000    1.633478000000
C   -2.839870000000    2.659682000000    0.877856000000
H   -2.129702000000    3.472718000000    0.944623000000
C    1.374300000000   -2.627237000000    0.189756000000
C   -2.403554000000    1.419679000000    0.418370000000
C    2.734280000000   -3.282854000000    2.077121000000
H    2.939157000000   -3.249018000000    3.143698000000
C    3.450746000000    0.163986000000    1.207305000000
H    3.118086000000   -0.566336000000    0.465550000000
H    2.739696000000    0.103322000000    2.035674000000
H    4.430345000000   -0.149322000000    1.576229000000
C    0.775662000000   -1.752151000000    2.502015000000
H   -0.137703000000   -2.272846000000    2.810340000000
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H    1.327202000000   -1.503603000000    3.412429000000
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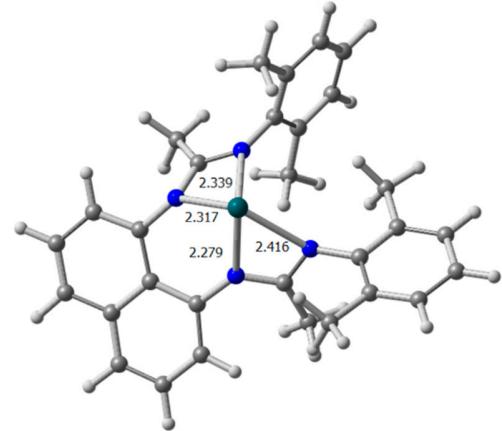
Dimethylamine

Sum of electronic and thermal Free Energies=   -637.965039 au

N   0.000013000000   0.619231000000   0.013062000000
Si -1.568800000000   -0.134296000000   -0.001379000000
Si   1.568801000000   -0.134298000000   -0.001374000000
H   -0.000056000000   1.627612000000   -0.100148000000
H   2.501052000000   0.609543000000   0.888029000000
H   2.199845000000   -0.185867000000   -1.350864000000
H   1.398947000000   -1.524682000000   0.486474000000
H   -1.399201000000   -1.524548000000   0.486909000000
H   -2.501148000000   0.609826000000   0.887694000000
H   -2.199551000000   -0.186184000000   -1.350986000000
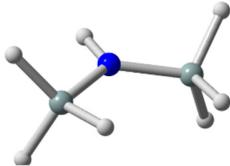
SnCl$_2$

Sum of electronic and thermal Free Energies=   -923.922288 au

Sn   0.000000000000   0.000000000000   0.639572000000
Cl   0.000000000000   1.823507000000   -0.940547000000
Cl   0.000000000000   -1.823507000000   -0.940547000000

GeCl$_2$

Sum of electronic and thermal Free Energies=   -2995.495709 au

Cl   0.000000000000   -1.702742000000   -0.688640000000
Cl   0.000000000000   1.702742000000   -0.688640000000
Ge   0.000000000000   0.000000000000   0.731680000000