Synthesis and Structures of Homoleptic Germylenes and Stannylenes with Sulfonimidamide Ligands

Nicolas Lentz,[a] Alexandre Sodreau,[a] Alejandra Acuña,[a,b] Sonia Mallet-Ladeira,[c] Eddy Maerten,[a] Jean-Marc Sotiropoulos,[d] René S. Rojas,[b] David Madec* [a]

[a] Université de Toulouse, UPS, LHFA (Laboratoire Hétérochimie Fondamentale et Appliquée), UMR/CNRS 5069, 118 route de Narbonne, 31062 Toulouse Cedex 09, France.

[b] Laboratorio de Química Inorgánica, Facultad de Química y Farmacia, Pontificia, Universidad Católica de Chile, Santiago 6094411, Chile.

[c] Institut de Chimie de Toulouse (ICT, UAR 2599), 118 route de Narbonne, 31062 Toulouse Cedex 09, France.

[d] Université de Pau et des Pays l'Adour et CNRS, IPREM UMR 5254, Hélioparc 2 avenue du Président Angot 64053 Pau, France.

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General Procedures.

All manipulations with air-sensitive materials were performed in a dry and oxygen-free atmosphere of argon by using standard Schlenk-line and glovebox techniques. Solvents were purified with the MBraun SBS-800 purification system. NMR spectra were recorded with the following spectrometers: ^{1}H, Bruker Avance II 300 (300.18 MHz) and Avance III HD 500 MHz; ^{13}C, Bruker Avance II 300 (75.48 MHz) and Avance III HD 500 MHz; ^{31}P, Bruker Avance II 300 (75.48 MHz) and Avance III HD 500 MHz at 298 K; ^{119}Sn, Bruker Avance III HD 500 MHz. Mass spectra were measured on a direct chemical ionization (DCI-CH4) methods, and recorded on a GCT Premier Waters mass spectrometer

Melting points were measured with a capillary electrothermal apparatus. IR spectra were measured on a Varian 640-IR FT-IR spectrometer. All reagents were obtained from commercial suppliers unless otherwise statement.

Single-crystal X-ray data were collected at low temperature (193(2)K) on a Bruker-AXS APEX II Quazar diffractometer equipped with a 30W air-cooled microfocus source (**4** and **6**) or on a Bruker-AXS PHOTON100 D8 VENTURE diffractometer (**1**, **2**, **3** and **5**), using MoK_α radiation (λ= 0.71037 Å). The structures were solved by direct method (SHELXS-97)[1] and by intrinsic phasing method (SHELXT)[2] and refined by full-matrix least-squares method on F2.[3] All the hydrogen atoms were refined isotropically at calculated positions using a riding model and all non-H atoms were refined with anisotropic displacement parameters.

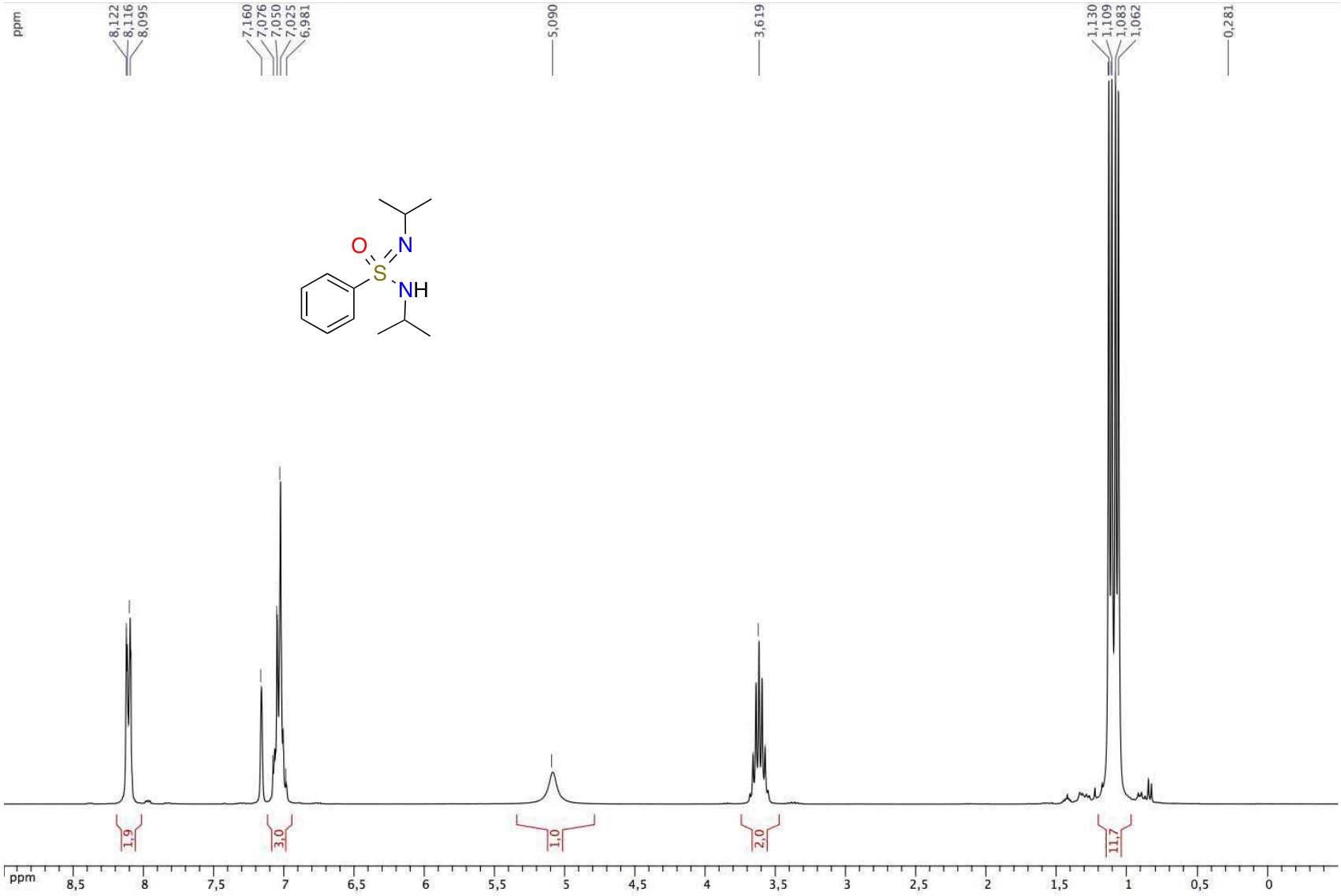
For **3**, some solvent molecules were highly disordered and difficult to model correctly. Therefore the SQUEEZE function of PLATON [4] was used to eliminate the contribution of the electron density of those solvent molecules from the intensity data.

[1] G. M. Sheldrick *Acta Cryst. Sect. A,* **2008**, A64, 112-122

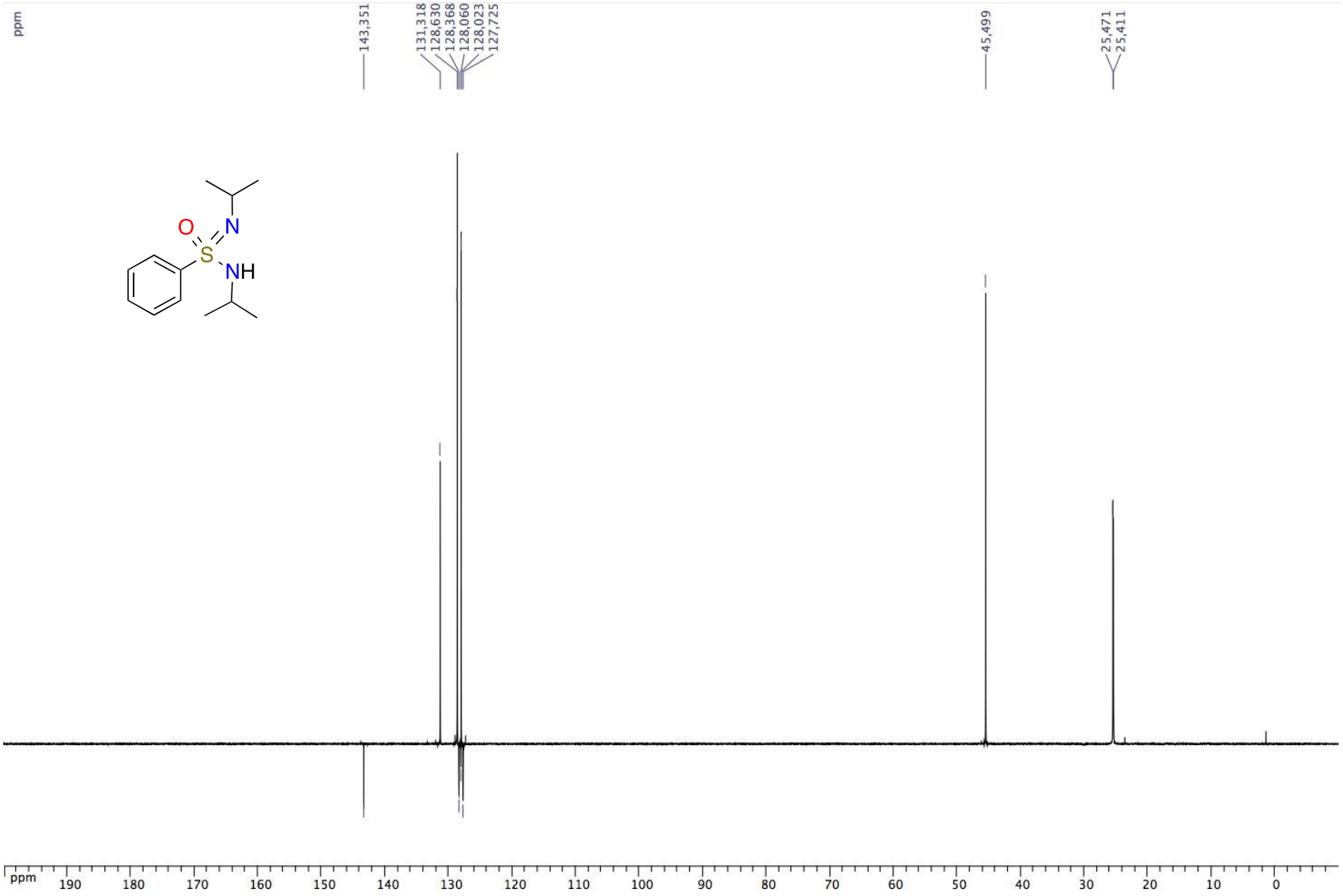
[2] G. M. Sheldrick *Acta Cryst. Sect. A,* **2015**, A71, 3–8.

[3] G. M. Sheldrick *Acta Cryst. Sect. C*, **2015**, C71, 3–8.

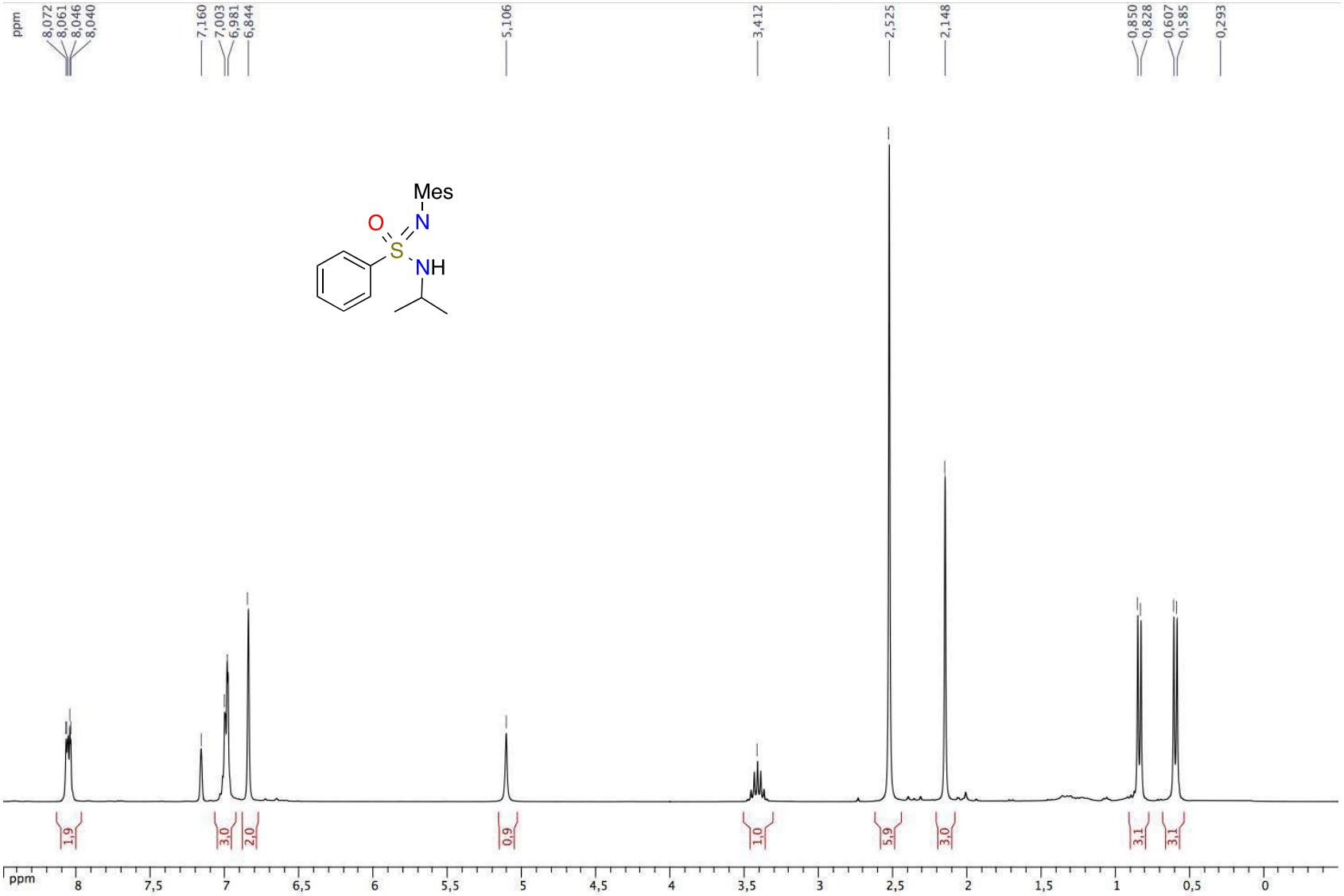
[4] P. v.d. Sluis and A. L. Spek, *Acta Cryst., Sect. A*, **1990**, 46, 194-201.



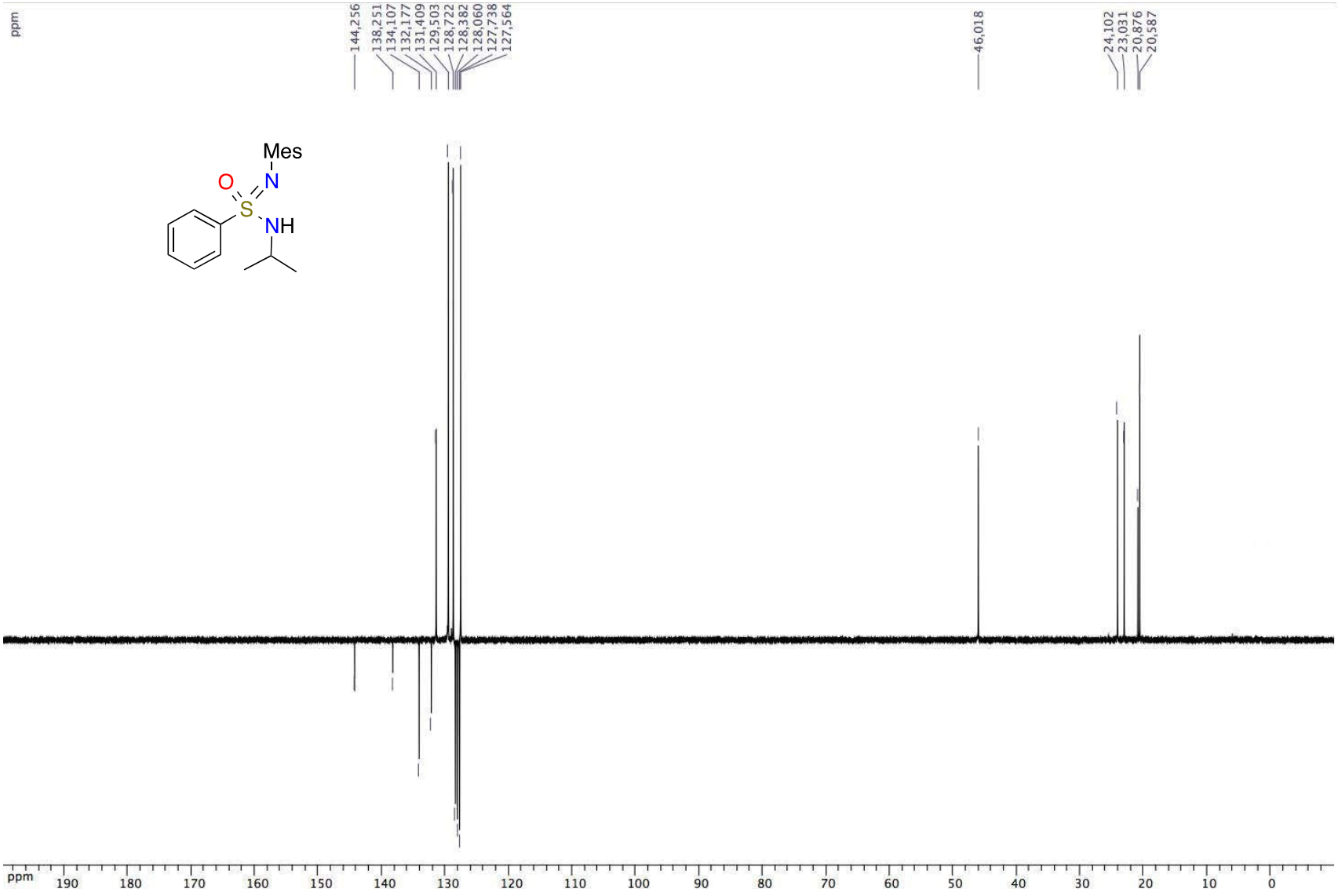
^{1}H NMR spectrum of compound **1** (C_6D_6, 300 MHz)



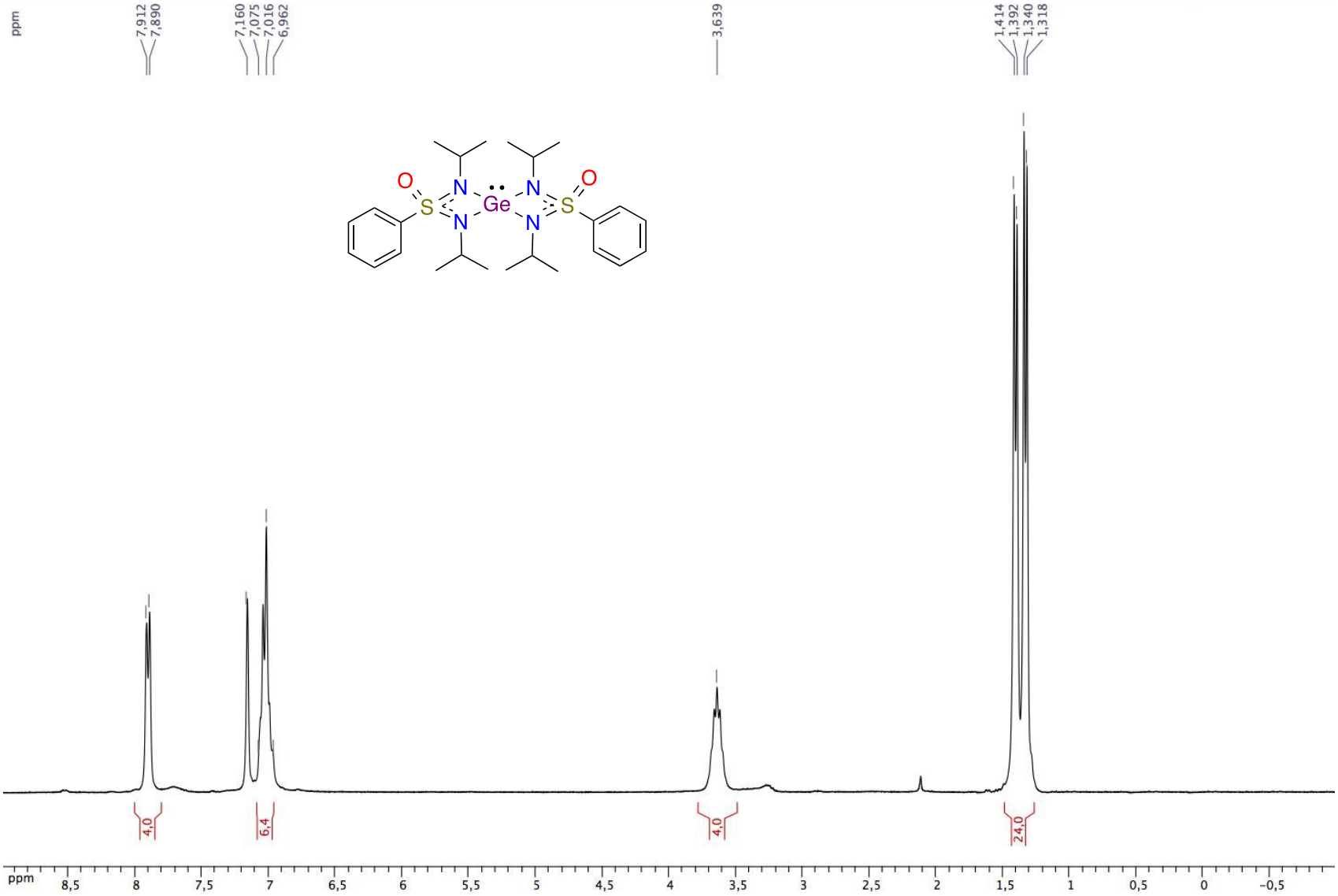
^{13}C NMR spectrum of compound **1** (C_6D_6, 75 MHz)



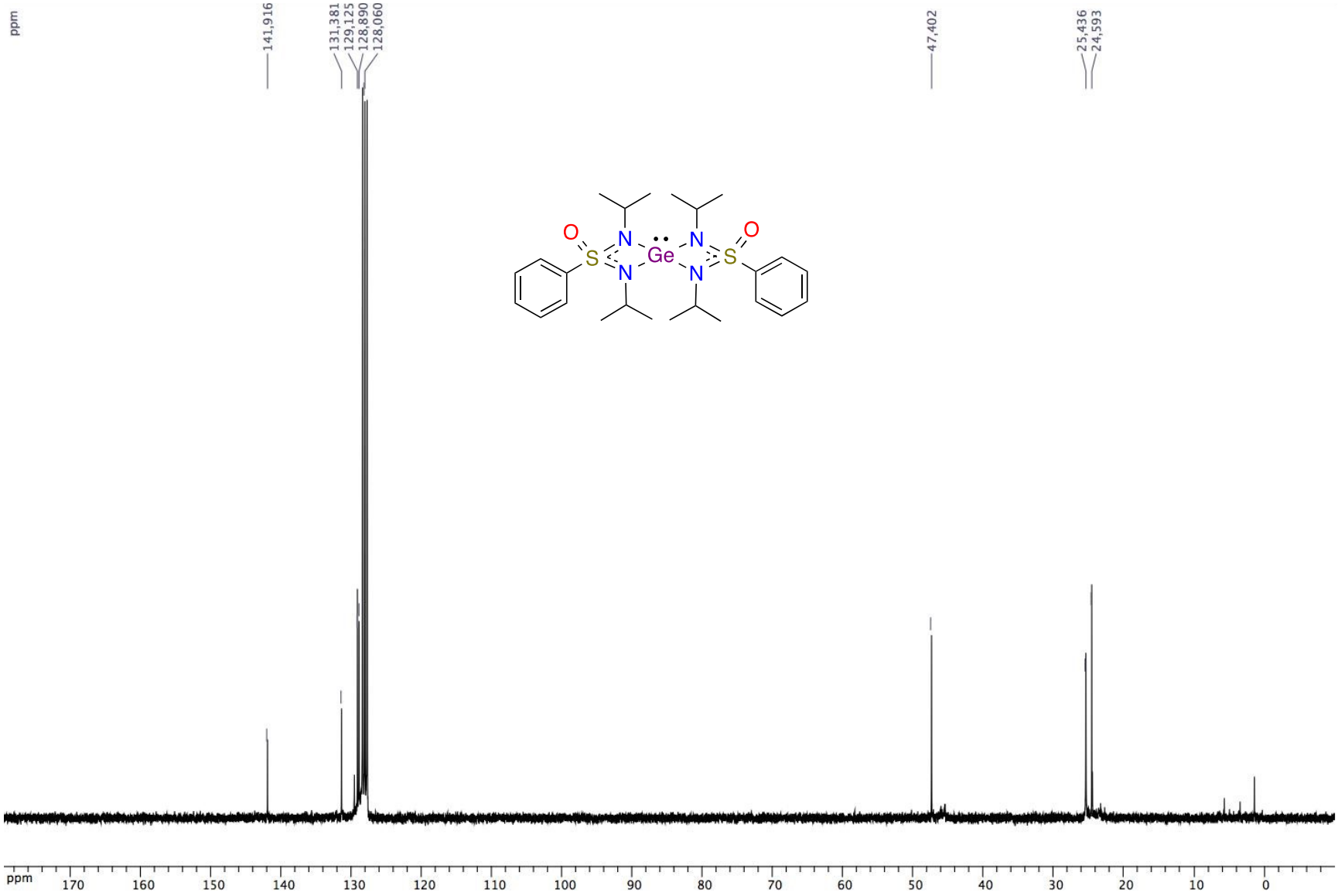
^{1}H NMR spectrum of compound **2** (C_6D_6, 300 MHz)



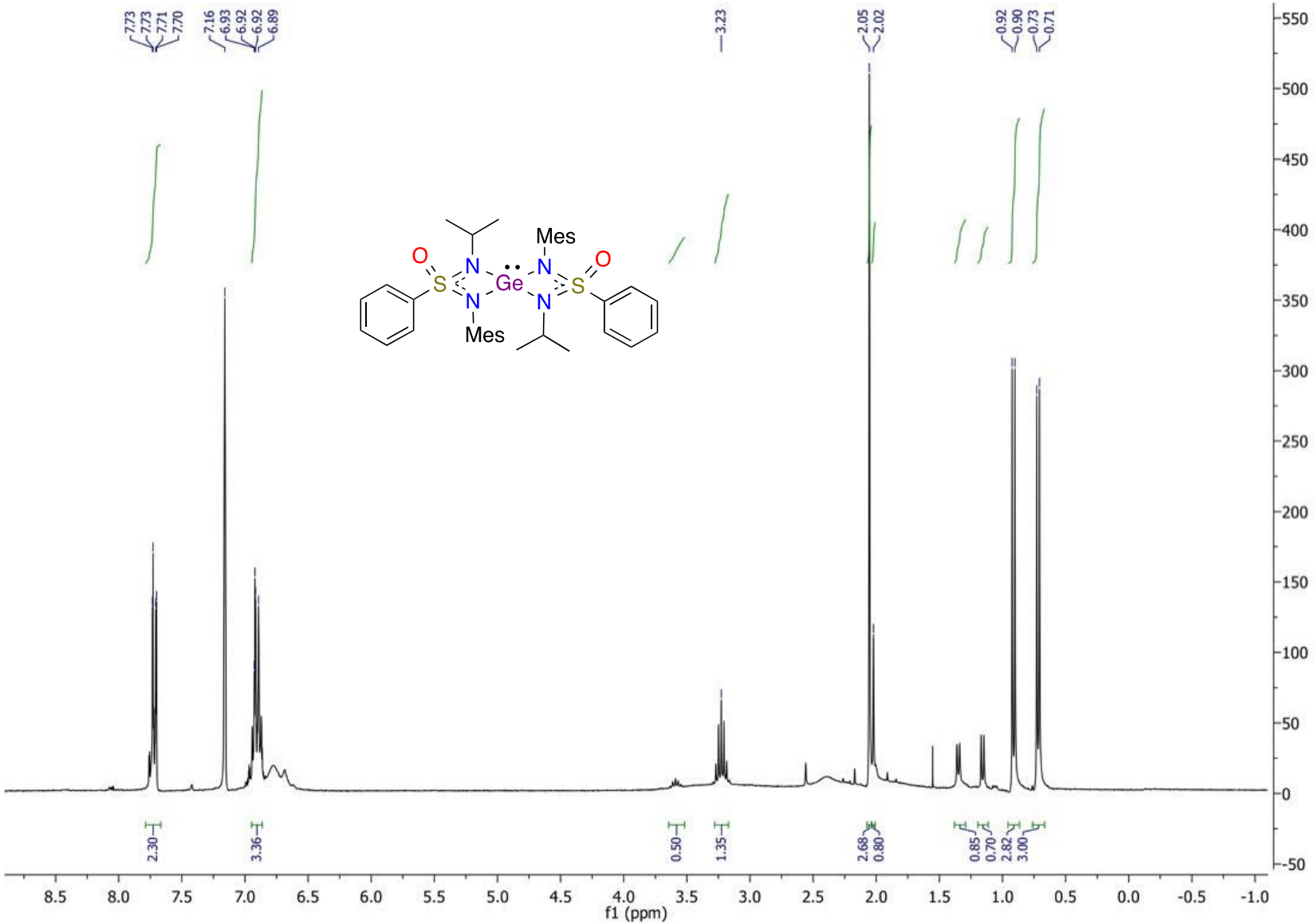
^{13}C NMR spectrum of compound **2** (C_6D_6, 75 MHz)



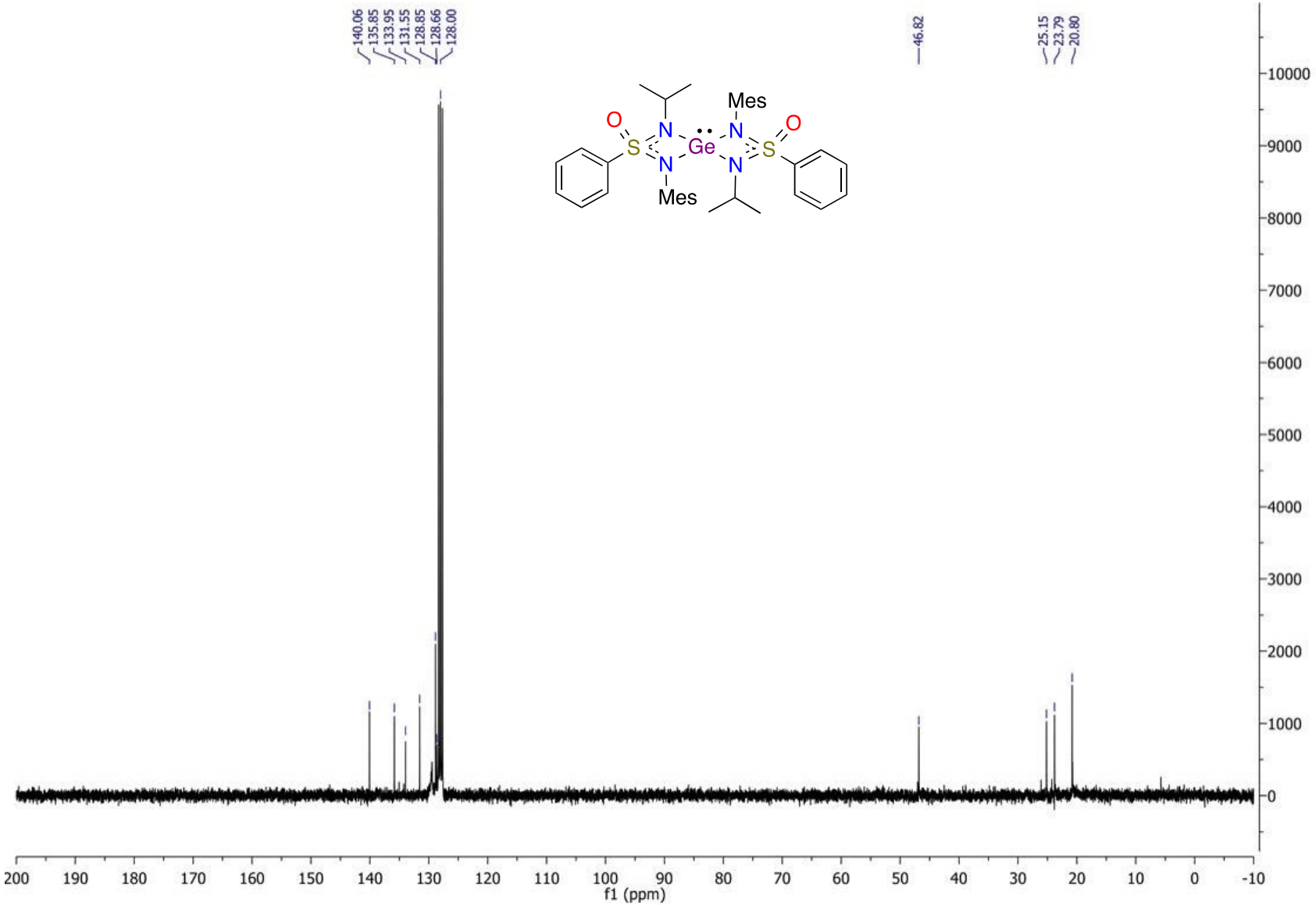
^{1}H NMR spectrum of compound **3** (C_6D_6, 300 MHz)



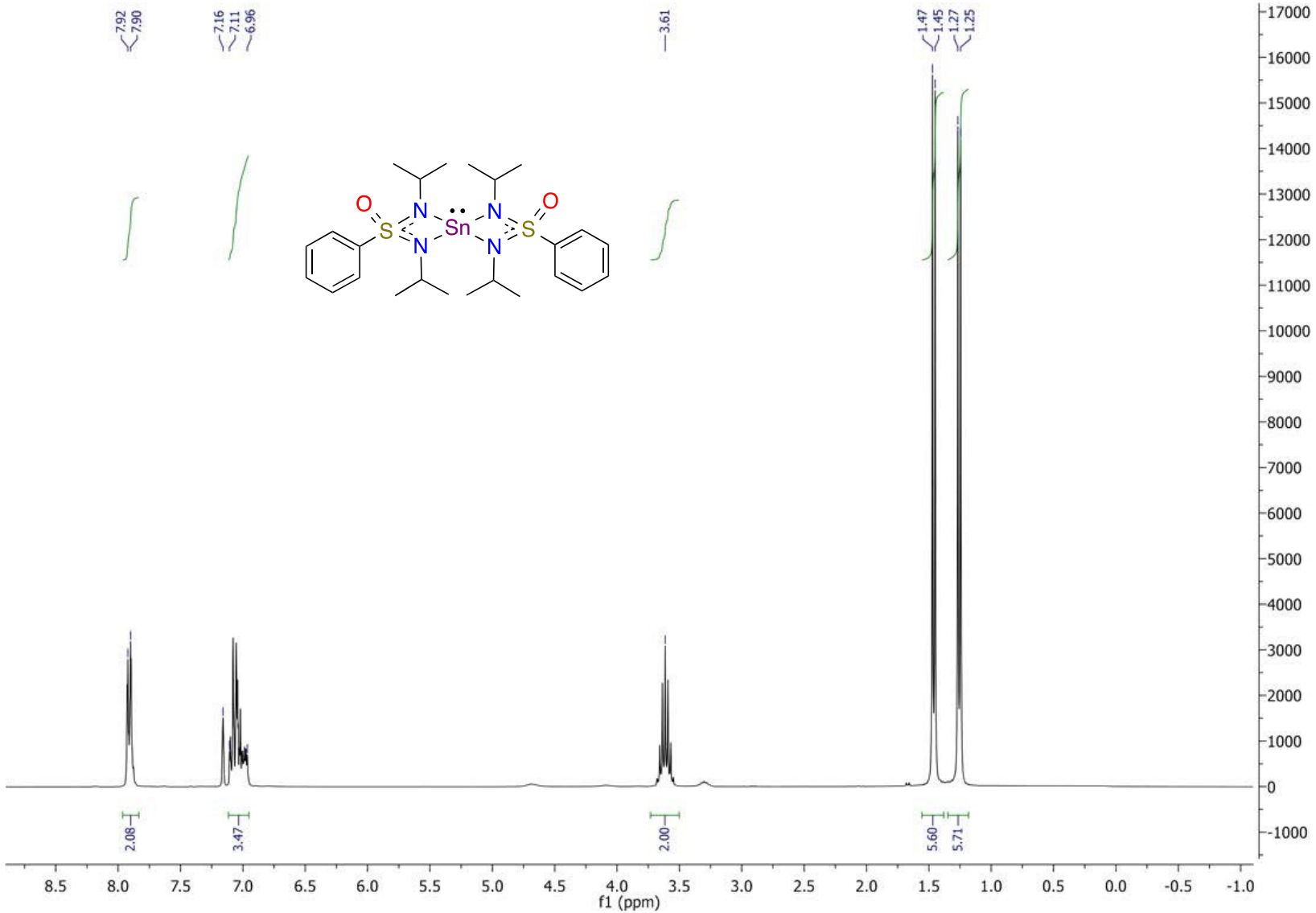
^{13}C NMR spectrum of compound **3** (C_6D_6, 75 MHz)



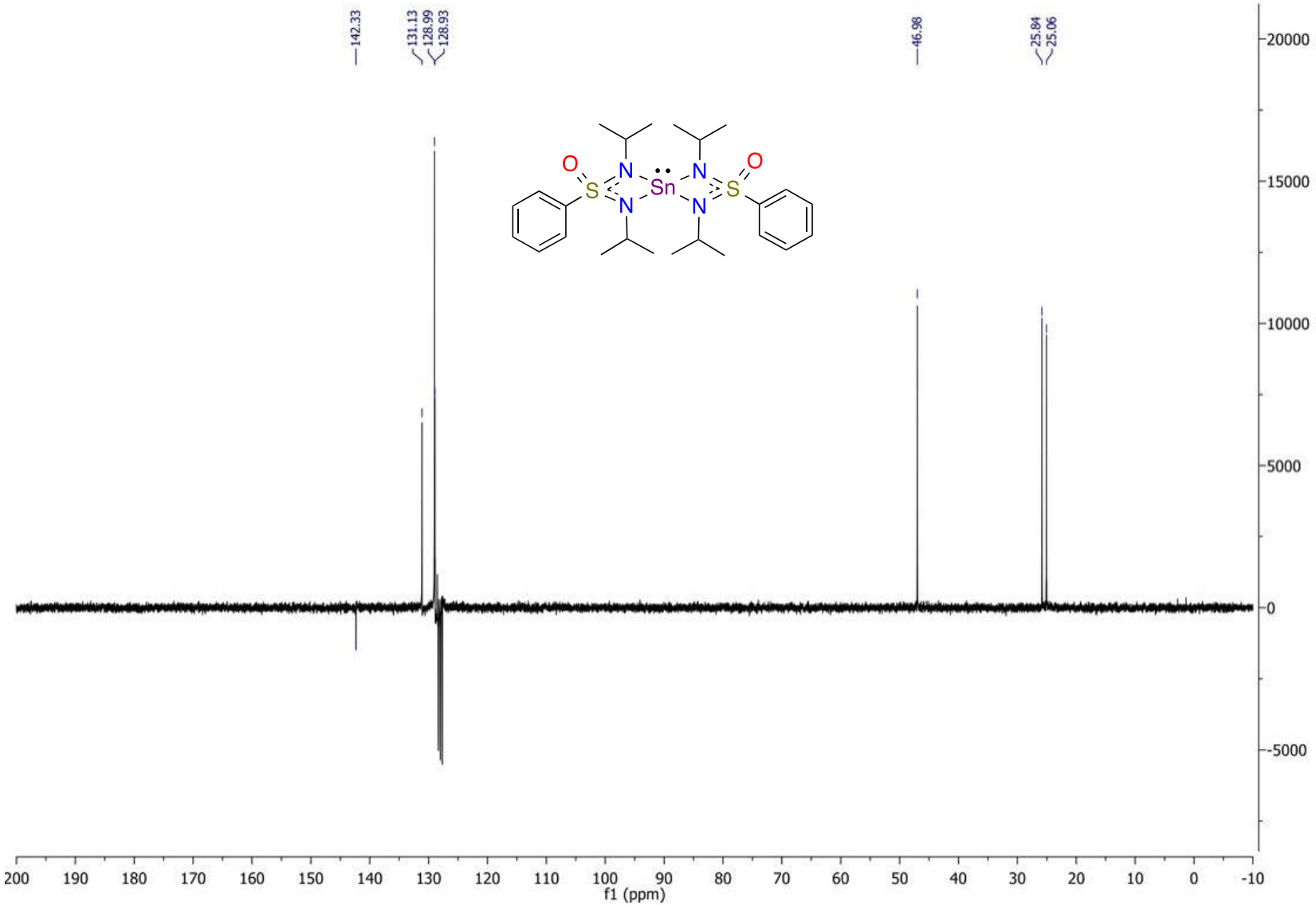
[1]H NMR spectrum of compound **4** (C_6D_6, 300 MHz)



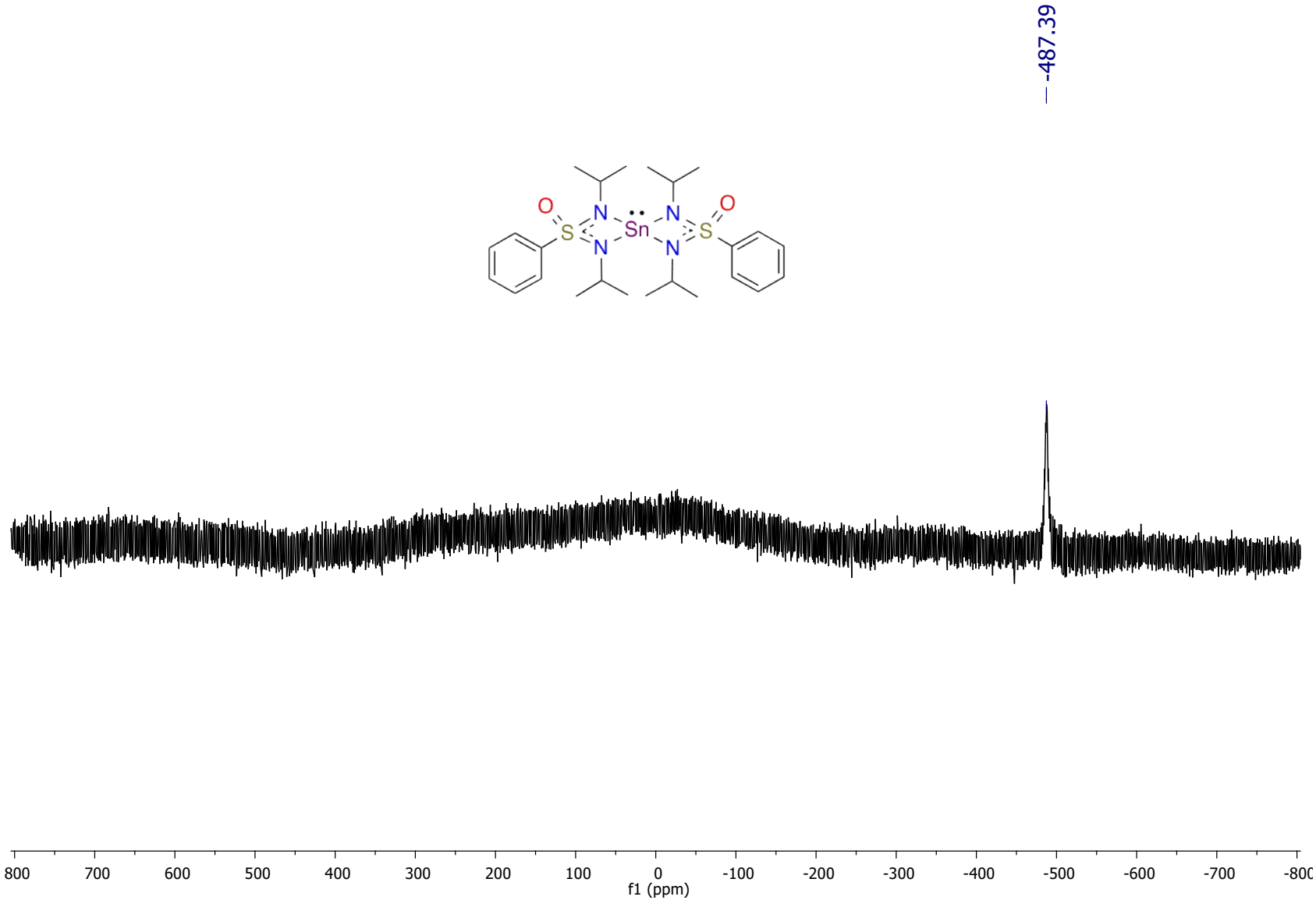
^{13}C NMR spectrum of compound **4** (C_6D_6, 75 MHz)



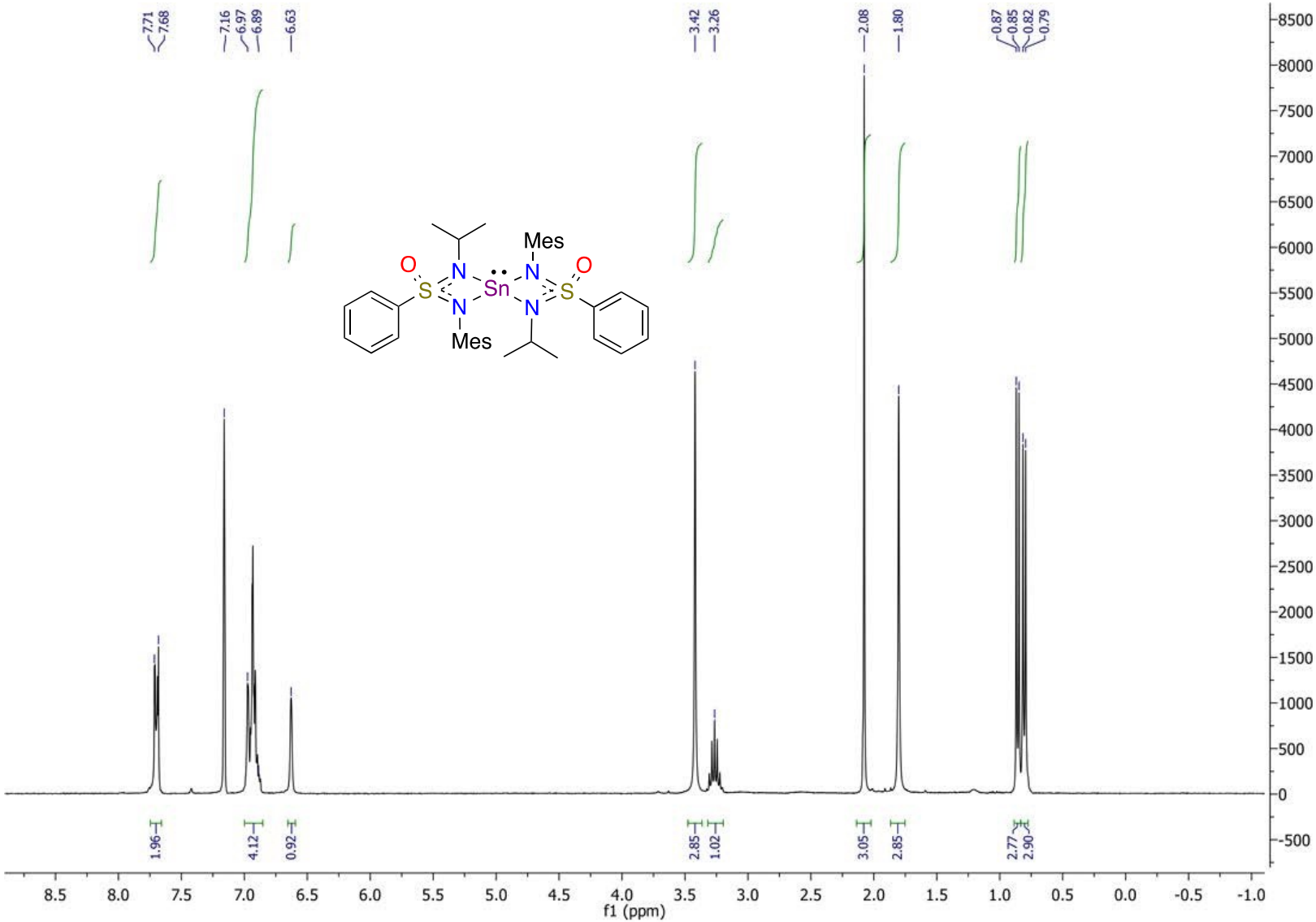
^{1}H NMR spectrum of compound **5** (C_6D_6, 300 MHz)



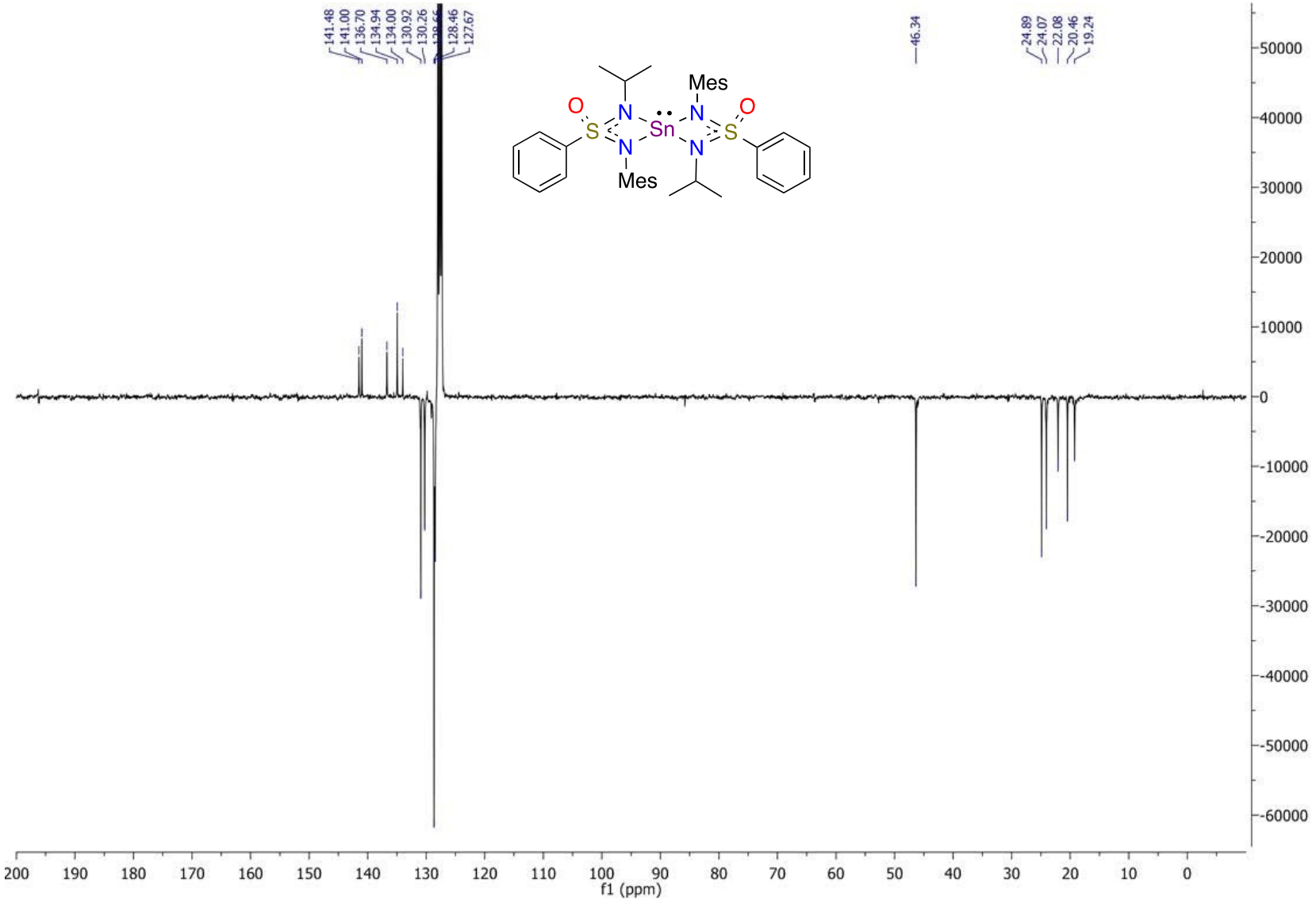
^{13}C NMR spectrum of compound **5** (C_6D_6, 75 MHz)



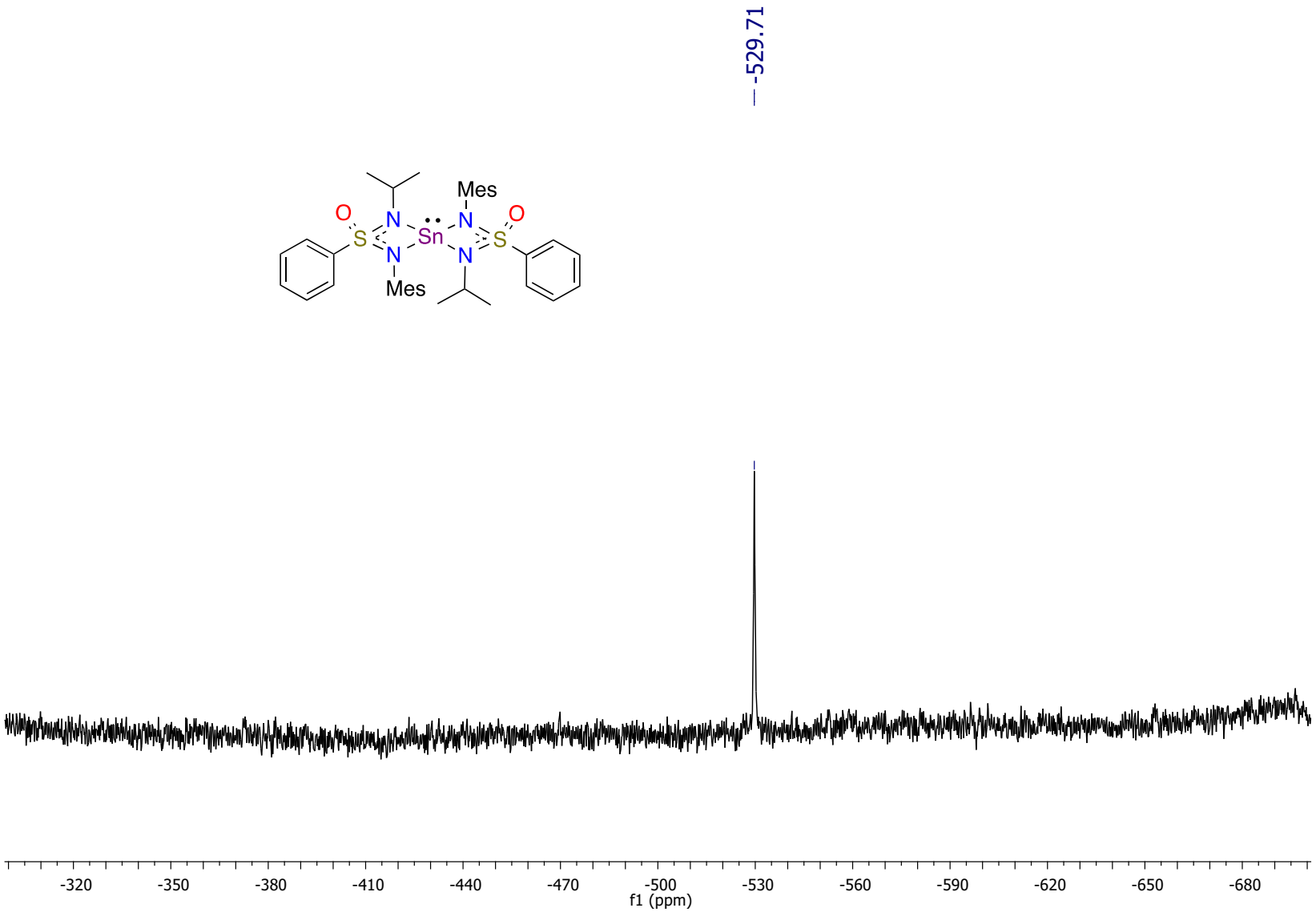
^{119}Sn NMR spectrum of compound **5** (C_6D_6, 186 MHz)



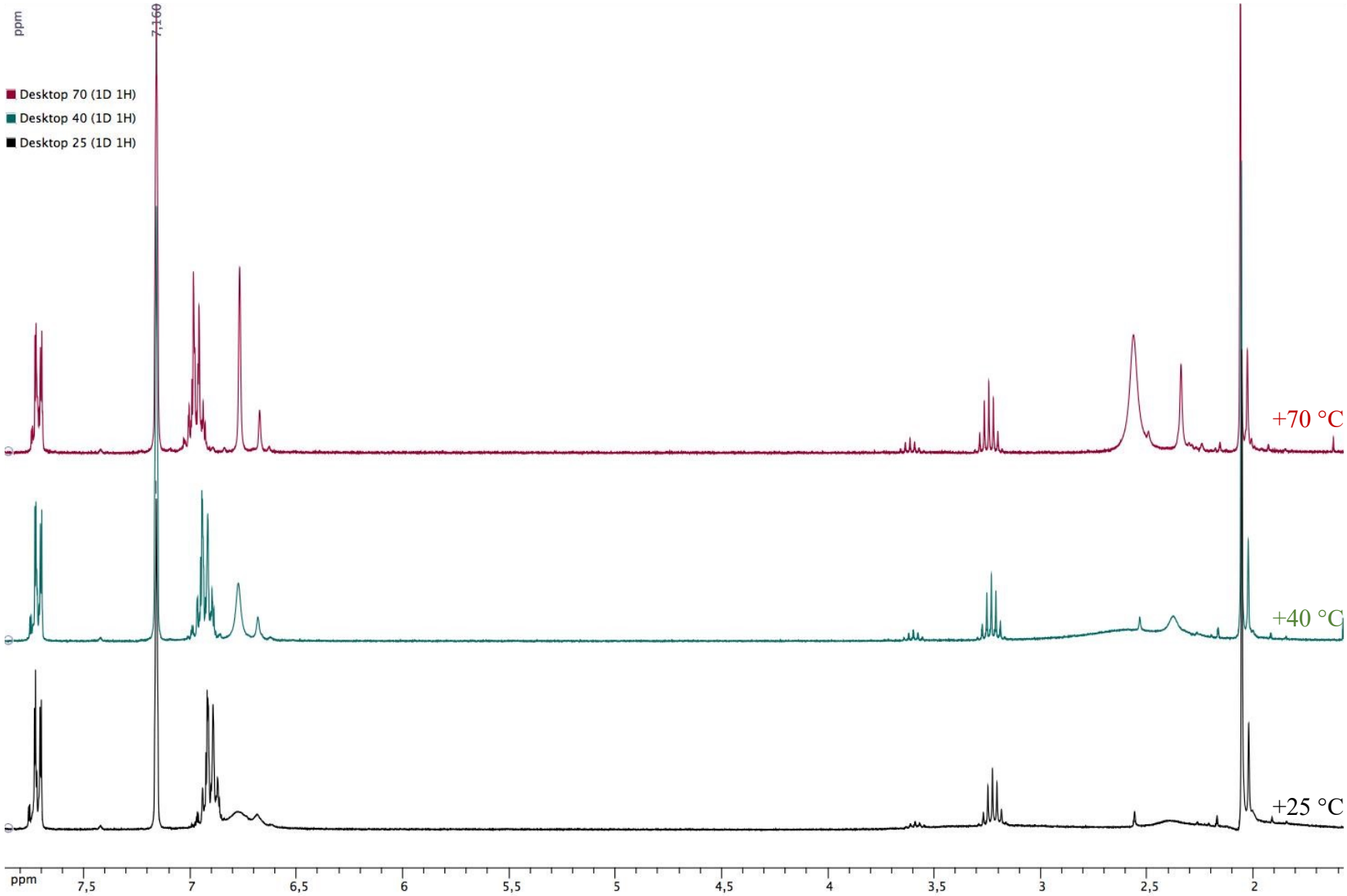
^{1}H NMR spectrum of compound **6** (C_6D_6, 300 MHz)



^{13}C NMR spectrum of compound **6** (C_6D_6, 75 MHz)



^{119}Sn NMR spectrum of compound **6** (C_6D_6, 186 MHz)



VT ^{1}H NMR spectrum of compound **4** from +20 °C to +70 °C (C_6D_6, 300 MHz)

Crystal data and structure refinement of compound 1

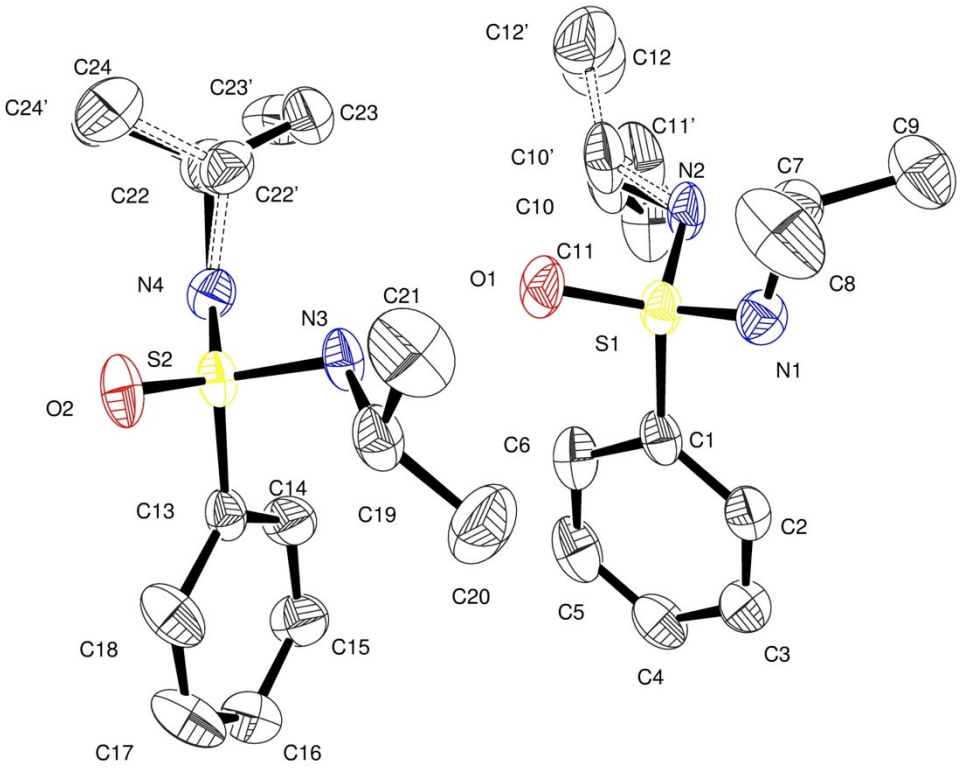


Figure 1 : Asymmetric Unit

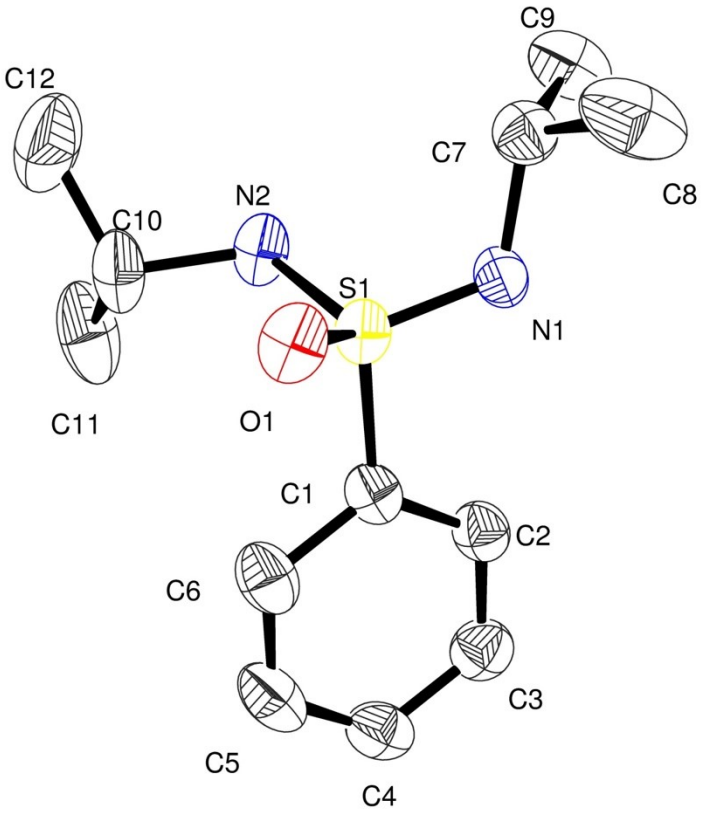


Figure 2 : Molecule

Table 1. Crystal data and structure refinement for NL265ligand.

Identification code	NL265ligand
Empirical formula	C12 H20 N2 O S
Formula weight	240.36
Temperature	193(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P -1
Unit cell dimensions	a = 10.5404(7) A alpha = 76.984(2) deg. b = 10.5595(7) A beta = 88.549(2) deg. c = 12.5470(9) A gamma = 89.718(2) deg.
Volume	1360.18(16) A^3
Z, Calculated density	4, 1.174 Mg/m^3
Absorption coefficient	0.222 mm^-1
Max. and min. transmission	0.7451 and 0.6565
F(000)	520
Crystal size	0.140 x 0.100 x 0.040 mm
Theta range for data collection	3.017 to 24.763 deg.
Limiting indices	-12<=h<=12, -12<=k<=12, -14<=l<=14
Reflections collected / unique	34528 / 4527 [R(int) = 0.0616]
Completeness to theta = 24.763	96.8 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4527 / 164 / 361
Goodness-of-fit on F^2	1.028
Final R indices [I>2sigma(I)]	R1 = 0.0433, wR2 = 0.0961
R indices (all data)	R1 = 0.0714, wR2 = 0.1095
Largest diff. peak and hole	0.179 and -0.334 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for nl265ligand_a. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	1859(2)	7727(2)	5731(2)	34(1)
C(2)	1310(2)	8838(3)	5130(2)	39(1)
C(3)	1307(2)	9048(3)	3999(2)	45(1)
C(4)	1849(2)	8159(3)	3481(2)	46(1)
C(5)	2400(2)	7053(3)	4082(2)	53(1)
C(6)	2412(2)	6835(3)	5206(2)	49(1)
C(7)	1144(2)	8616(3)	8637(2)	43(1)
C(8)	2031(3)	9588(4)	8947(3)	80(1)
C(9)	-218(3)	8946(4)	8840(2)	61(1)
N(2)	832(2)	6216(2)	7642(2)	38(1)
C(10)	1050(16)	4854(9)	7578(12)	52(2)
C(11)	171(10)	4512(13)	6750(14)	74(3)
C(12)	872(14)	3986(12)	8698(13)	82(3)
C(10')	1110(20)	4819(11)	7846(15)	55(3)
C(11')	163(13)	4112(14)	7315(18)	76(3)
C(12')	1179(16)	4248(16)	9072(14)	77(4)
C(13)	6876(2)	6787(2)	5821(2)	31(1)
C(14)	5918(2)	6392(3)	5238(2)	43(1)
C(15)	5940(2)	6750(3)	4111(2)	47(1)
C(16)	6903(2)	7526(3)	3564(2)	47(1)
C(17)	7844(3)	7931(3)	4139(2)	60(1)
C(18)	7852(2)	7557(3)	5267(2)	50(1)
C(19)	6101(2)	8809(2)	7476(2)	42(1)
C(20)	5268(3)	9587(3)	6610(3)	72(1)
C(21)	5993(3)	9216(4)	8558(3)	72(1)
N(1)	1361(2)	8615(2)	7458(2)	38(1)
N(3)	5813(2)	7413(2)	7655(2)	34(1)
N(4)	6275(2)	5057(2)	7558(2)	35(1)
C(22)	6014(16)	4400(20)	8729(14)	44(3)
C(23)	4624(14)	4026(19)	8864(17)	50(4)
C(24)	6824(12)	3159(19)	9027(15)	72(4)
C(22')	5844(8)	4515(11)	8714(7)	41(2)
C(23')	4760(10)	3595(12)	8701(9)	67(3)
C(24')	6930(6)	3828(13)	9372(6)	79(3)
O(1)	3063(1)	6806(2)	7519(1)	44(1)
O(2)	8031(1)	6754(2)	7622(1)	43(1)
S(1)	1837(1)	7382(1)	7184(1)	34(1)
S(2)	6806(1)	6411(1)	7266(1)	32(1)

Table 3. Bond lengths [A] and angles [deg] for nl265ligand_a.

C(1)-C(2)	1.377(3)
C(1)-C(6)	1.384(4)
C(1)-S(1)	1.776(2)
C(2)-C(3)	1.386(4)
C(2)-H(2)	0.9500
C(3)-C(4)	1.372(4)
C(3)-H(3)	0.9500
C(4)-C(5)	1.374(4)
C(4)-H(4)	0.9500
C(5)-C(6)	1.377(4)
C(5)-H(5)	0.9500
C(6)-H(6)	0.9500
C(7)-N(1)	1.491(3)
C(7)-C(9)	1.505(4)
C(7)-C(8)	1.512(4)
C(7)-H(7)	1.0000
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
N(2)-C(10')	1.467(12)
N(2)-C(10)	1.475(10)
N(2)-S(1)	1.6226(19)
N(2)-H(2A)	0.870(10)
C(10)-C(12)	1.503(10)
C(10)-C(11)	1.513(10)
C(10)-H(10)	1.0000
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(10')-C(11')	1.501(12)
C(10')-C(12')	1.524(12)
C(10')-H(10')	1.0000
C(11')-H(11D)	0.9800
C(11')-H(11E)	0.9800
C(11')-H(11F)	0.9800
C(12')-H(12D)	0.9800
C(12')-H(12E)	0.9800
C(12')-H(12F)	0.9800
C(13)-C(14)	1.380(3)
C(13)-C(18)	1.385(3)
C(13)-S(2)	1.767(2)
C(14)-C(15)	1.379(4)
C(14)-H(14)	0.9500
C(15)-C(16)	1.376(3)
C(15)-H(15)	0.9500
C(16)-C(17)	1.366(4)
C(16)-H(16)	0.9500

C(17)-C(18)	1.382(4)
C(17)-H(17)	0.9500
C(18)-H(18)	0.9500
C(19)-N(3)	1.472(3)
C(19)-C(20)	1.505(4)
C(19)-C(21)	1.515(4)
C(19)-H(19)	1.0000
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
N(1)-S(1)	1.501(2)
N(3)-S(2)	1.628(2)
N(3)-H(3A)	0.868(10)
N(4)-C(22')	1.494(7)
N(4)-C(22)	1.497(14)
N(4)-S(2)	1.501(2)
C(22)-C(23)	1.513(14)
C(22)-C(24)	1.536(16)
C(22)-H(22)	1.0000
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800
C(22')-C(23')	1.506(10)
C(22')-C(24')	1.512(8)
C(22')-H(22')	1.0000
C(23')-H(23D)	0.9800
C(23')-H(23E)	0.9800
C(23')-H(23F)	0.9800
C(24')-H(24D)	0.9800
C(24')-H(24E)	0.9800
C(24')-H(24F)	0.9800
O(1)-S(1)	1.4562(15)
O(2)-S(2)	1.4506(15)

C(2)-C(1)-C(6)	120.1(2)
C(2)-C(1)-S(1)	121.3(2)
C(6)-C(1)-S(1)	118.61(19)
C(1)-C(2)-C(3)	119.5(3)
C(1)-C(2)-H(2)	120.3
C(3)-C(2)-H(2)	120.3
C(4)-C(3)-C(2)	120.4(3)
C(4)-C(3)-H(3)	119.8
C(2)-C(3)-H(3)	119.8
C(3)-C(4)-C(5)	120.1(3)
C(3)-C(4)-H(4)	120.0
C(5)-C(4)-H(4)	120.0
C(4)-C(5)-C(6)	120.1(3)
C(4)-C(5)-H(5)	119.9
C(6)-C(5)-H(5)	119.9
C(5)-C(6)-C(1)	119.9(3)
C(5)-C(6)-H(6)	120.1
C(1)-C(6)-H(6)	120.1

N(1)-C(7)-C(9)	110.0(2)
N(1)-C(7)-C(8)	109.1(2)
C(9)-C(7)-C(8)	110.9(3)
N(1)-C(7)-H(7)	109.0
C(9)-C(7)-H(7)	109.0
C(8)-C(7)-H(7)	109.0
C(7)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(7)-C(9)-H(9A)	109.5
C(7)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(7)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(10')-N(2)-S(1)	126.0(9)
C(10)-N(2)-S(1)	123.7(7)
C(10')-N(2)-H(2A)	119(2)
C(10)-N(2)-H(2A)	114.6(19)
S(1)-N(2)-H(2A)	112.5(17)
N(2)-C(10)-C(12)	109.3(9)
N(2)-C(10)-C(11)	109.2(9)
C(12)-C(10)-C(11)	112.7(9)
N(2)-C(10)-H(10)	108.5
C(12)-C(10)-H(10)	108.5
C(11)-C(10)-H(10)	108.5
C(10)-C(11)-H(11A)	109.5
C(10)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(10)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(10)-C(12)-H(12A)	109.5
C(10)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(10)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
N(2)-C(10')-C(11')	111.8(11)
N(2)-C(10')-C(12')	110.1(11)
C(11')-C(10')-C(12')	112.0(11)
N(2)-C(10')-H(10')	107.6
C(11')-C(10')-H(10')	107.6
C(12')-C(10')-H(10')	107.6
C(10')-C(11')-H(11D)	109.5
C(10')-C(11')-H(11E)	109.5
H(11D)-C(11')-H(11E)	109.5
C(10')-C(11')-H(11F)	109.5
H(11D)-C(11')-H(11F)	109.5
H(11E)-C(11')-H(11F)	109.5
C(10')-C(12')-H(12D)	109.5
C(10')-C(12')-H(12E)	109.5
H(12D)-C(12')-H(12E)	109.5
C(10')-C(12')-H(12F)	109.5
H(12D)-C(12')-H(12F)	109.5

H(12E)-C(12')-H(12F)	109.5
C(14)-C(13)-C(18)	119.6(2)
C(14)-C(13)-S(2)	120.38(17)
C(18)-C(13)-S(2)	119.84(19)
C(15)-C(14)-C(13)	120.2(2)
C(15)-C(14)-H(14)	119.9
C(13)-C(14)-H(14)	119.9
C(16)-C(15)-C(14)	120.0(2)
C(16)-C(15)-H(15)	120.0
C(14)-C(15)-H(15)	120.0
C(17)-C(16)-C(15)	119.9(3)
C(17)-C(16)-H(16)	120.0
C(15)-C(16)-H(16)	120.0
C(16)-C(17)-C(18)	120.8(2)
C(16)-C(17)-H(17)	119.6
C(18)-C(17)-H(17)	119.6
C(17)-C(18)-C(13)	119.4(2)
C(17)-C(18)-H(18)	120.3
C(13)-C(18)-H(18)	120.3
N(3)-C(19)-C(20)	110.6(2)
N(3)-C(19)-C(21)	109.2(2)
C(20)-C(19)-C(21)	113.4(3)
N(3)-C(19)-H(19)	107.8
C(20)-C(19)-H(19)	107.8
C(21)-C(19)-H(19)	107.8
C(19)-C(20)-H(20A)	109.5
C(19)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(19)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(19)-C(21)-H(21A)	109.5
C(19)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(19)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(7)-N(1)-S(1)	117.61(17)
C(19)-N(3)-S(2)	121.24(15)
C(19)-N(3)-H(3A)	116.8(17)
S(2)-N(3)-H(3A)	111.0(18)
C(22')-N(4)-S(2)	118.5(5)
C(22)-N(4)-S(2)	120.4(11)
N(4)-C(22)-C(23)	108.5(14)
N(4)-C(22)-C(24)	109.4(13)
C(23)-C(22)-C(24)	109.1(15)
N(4)-C(22)-H(22)	110.0
C(23)-C(22)-H(22)	110.0
C(24)-C(22)-H(22)	109.9
C(22)-C(23)-H(23A)	109.5
C(22)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(22)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(22)-C(24)-H(24A)	109.5
C(22)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5

C(22)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
N(4)-C(22')-C(23')	108.1(8)
N(4)-C(22')-C(24')	110.2(6)
C(23')-C(22')-C(24')	111.1(8)
N(4)-C(22')-H(22')	109.1
C(23')-C(22')-H(22')	109.1
C(24')-C(22')-H(22')	109.1
C(22')-C(23')-H(23D)	109.5
C(22')-C(23')-H(23E)	109.5
H(23D)-C(23')-H(23E)	109.5
C(22')-C(23')-H(23F)	109.5
H(23D)-C(23')-H(23F)	109.5
H(23E)-C(23')-H(23F)	109.5
C(22')-C(24')-H(24D)	109.5
C(22')-C(24')-H(24E)	109.5
H(24D)-C(24')-H(24E)	109.5
C(22')-C(24')-H(24F)	109.5
H(24D)-C(24')-H(24F)	109.5
H(24E)-C(24')-H(24F)	109.5
O(1)-S(1)-N(1)	123.44(11)
O(1)-S(1)-N(2)	103.97(10)
N(1)-S(1)-N(2)	109.70(11)
O(1)-S(1)-C(1)	106.41(11)
N(1)-S(1)-C(1)	104.08(11)
N(2)-S(1)-C(1)	108.64(11)
O(2)-S(2)-N(4)	123.29(10)
O(2)-S(2)-N(3)	104.62(10)
N(4)-S(2)-N(3)	109.86(11)
O(2)-S(2)-C(13)	106.65(10)
N(4)-S(2)-C(13)	103.78(11)
N(3)-S(2)-C(13)	107.90(11)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for nl265ligand_a.
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)	21(1)	39(2)	47(1)	-16(1)	0(1)	-2(1)
C(2)	32(1)	40(2)	47(2)	-13(1)	2(1)	2(1)
C(3)	39(1)	47(2)	49(2)	-7(1)	1(1)	-1(1)
C(4)	38(1)	56(2)	47(2)	-21(1)	6(1)	-11(1)
C(5)	42(2)	60(2)	67(2)	-35(2)	7(1)	1(1)
C(6)	39(1)	49(2)	62(2)	-20(2)	-1(1)	10(1)
C(7)	44(1)	45(2)	41(1)	-10(1)	-4(1)	2(1)
C(8)	55(2)	123(4)	76(2)	-56(2)	9(2)	-25(2)
C(9)	49(2)	82(2)	59(2)	-32(2)	1(1)	-1(2)
N(2)	17(1)	33(1)	62(1)	-6(1)	-2(1)	1(1)
C(10)	30(4)	31(4)	96(6)	-16(3)	13(4)	-2(3)
C(11)	47(3)	52(5)	135(8)	-47(5)	-11(5)	-5(4)
C(12)	71(6)	44(5)	121(7)	1(5)	17(5)	-7(4)
C(10')	27(4)	36(4)	101(7)	-17(4)	7(5)	1(3)
C(11')	48(4)	54(6)	133(9)	-39(6)	9(6)	-6(4)
C(12')	66(7)	45(7)	104(7)	18(5)	8(5)	2(5)
C(13)	25(1)	25(1)	45(1)	-11(1)	2(1)	2(1)
C(14)	33(1)	47(2)	45(2)	-1(1)	-4(1)	-11(1)
C(15)	43(1)	50(2)	47(2)	-5(1)	-7(1)	-11(1)
C(16)	52(2)	45(2)	44(2)	-10(1)	7(1)	-7(1)
C(17)	53(2)	70(2)	58(2)	-19(2)	22(1)	-29(2)
C(18)	37(1)	62(2)	56(2)	-25(2)	10(1)	-19(1)

C(19)	29(1)	34(2)	63(2)	-15(1)	5(1)	-2(1)
C(20)	65(2)	41(2)	103(3)	2(2)	-14(2)	6(2)
C(21)	79(2)	61(2)	87(2)	-40(2)	12(2)	-13(2)
N(1)	41(1)	33(1)	40(1)	-12(1)	-1(1)	2(1)
N(3)	19(1)	33(1)	52(1)	-17(1)	-1(1)	0(1)
N(4)	35(1)	31(1)	38(1)	-8(1)	-4(1)	2(1)
C(22)	42(5)	49(6)	40(5)	-6(5)	-5(4)	-2(4)
C(23)	37(4)	64(9)	47(6)	-11(6)	2(4)	5(5)
C(24)	43(5)	78(8)	72(7)	28(6)	8(5)	19(5)
C(22')	45(3)	42(3)	35(3)	-9(2)	-6(2)	5(2)
C(23')	71(4)	76(6)	45(4)	5(4)	1(3)	-22(4)
C(24')	66(3)	107(7)	54(4)	6(4)	-14(3)	13(4)
O(1)	20(1)	46(1)	63(1)	-5(1)	-10(1)	0(1)
O(2)	19(1)	57(1)	59(1)	-25(1)	-8(1)	3(1)
S(1)	21(1)	34(1)	47(1)	-9(1)	-4(1)	0(1)
S(2)	20(1)	35(1)	44(1)	-14(1)	-3(1)	2(1)

Crystal data and structure refinement of compound 2

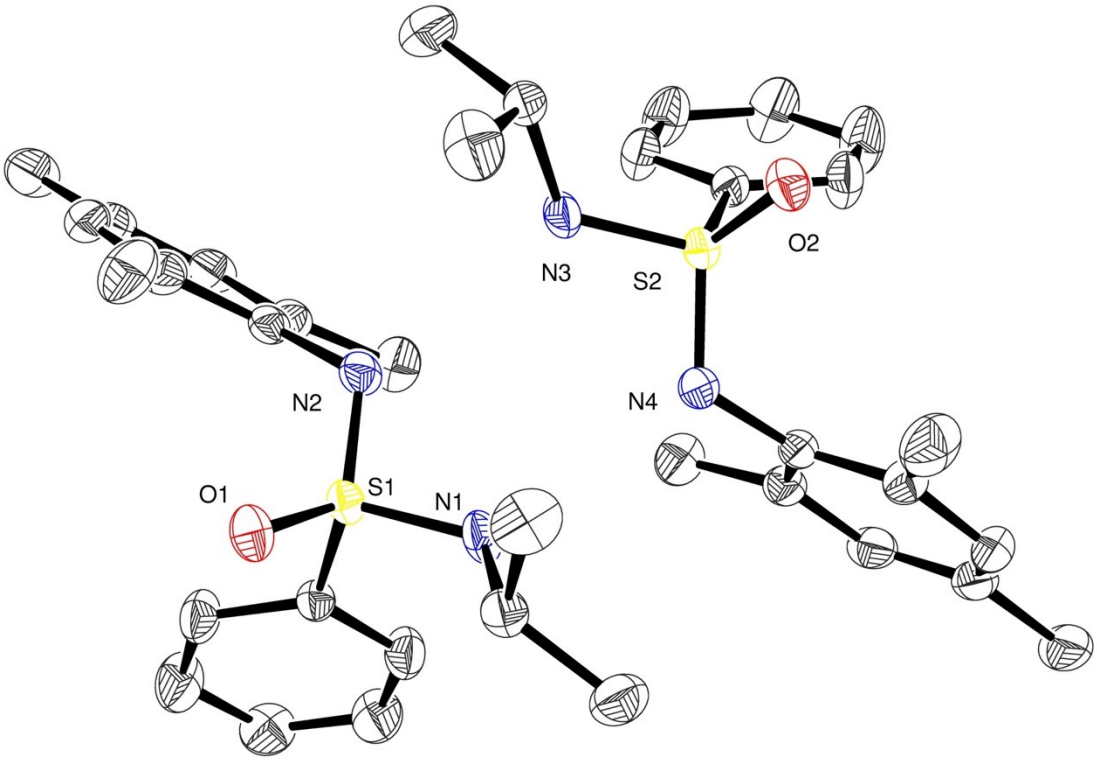


Figure 2 : Asymmetric Unit

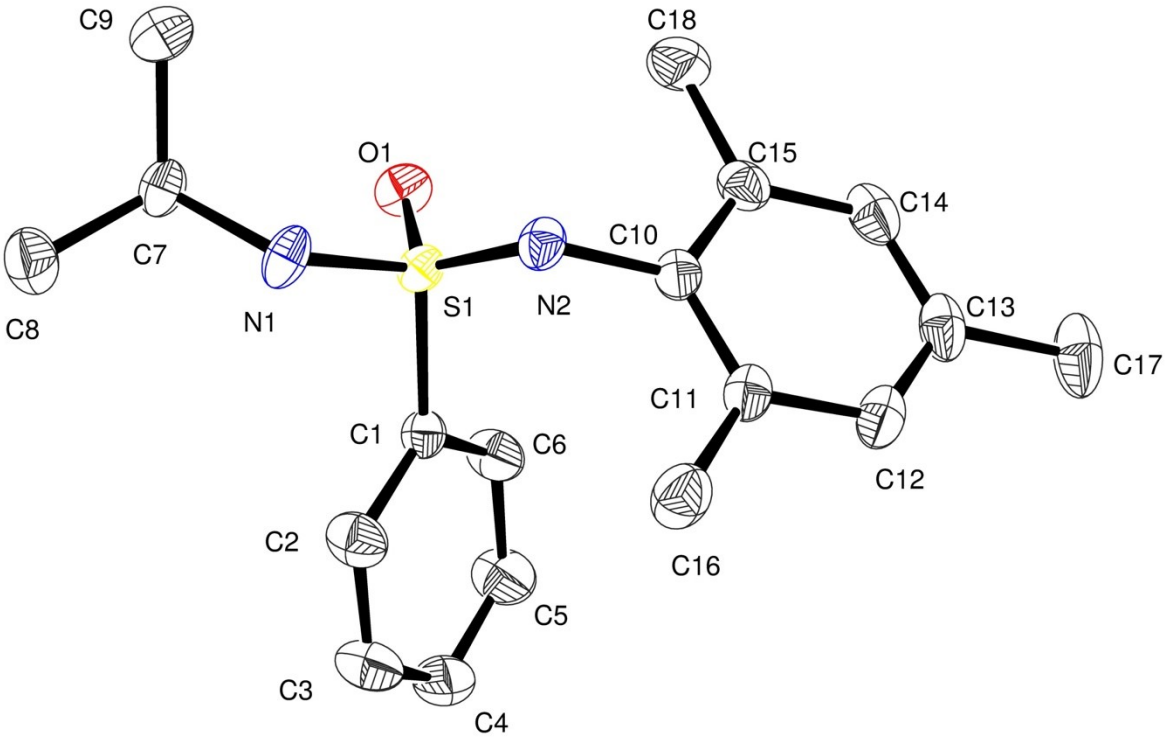


Figure 2 : Molecule

Table 1. Crystal data and structure refinement for NL267.

Identification code	NL267
Empirical formula	C18 H24 N2 O S
Formula weight	316.45
Temperature	193(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P -1

Unit cell dimensions a = 11.989(3) A alpha = 64.437(9) deg.

b = 12.149(3) A beta = 88.604(8) deg.

c = 13.386(3) A gamma = 83.874(13) deg.

Volume	1748.5(8) A^3
Z, Calculated density	4, 1.202 Mg/m^3
Absorption coefficient	0.189 mm^-1
Max. and min. transmission	0.7461 and 0.7248
F(000)	680
Crystal size	0.480 x 0.460 x 0.120 mm
Theta range for data collection	3.072 to 30.511 deg.
Limiting indices	-17<=h<=17, -17<=k<=17, -19<=l<=19
Reflections collected / unique	81609 / 10619 [R(int) = 0.0259]
Completeness to theta = 25.242	99.6 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10619 / 0 / 415
Goodness-of-fit on F^2	1.042
Final R indices [I>2sigma(I)]	R1 = 0.0375, wR2 = 0.0989
R indices (all data)	R1 = 0.0466, wR2 = 0.1061
Largest diff. peak and hole	0.370 and -0.383 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for nl267_a. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	1189(1)	4852(1)	8107(1)	23(1)
C(2)	1366(1)	5645(1)	7015(1)	34(1)
C(3)	1488(1)	6866(1)	6749(1)	41(1)
C(4)	1426(1)	7293(1)	7555(1)	40(1)
C(5)	1228(1)	6502(1)	8639(1)	44(1)
C(6)	1109(1)	5274(1)	8922(1)	34(1)
C(7)	-371(1)	2946(1)	7214(1)	26(1)
C(8)	-648(1)	3620(1)	5983(1)	38(1)
C(9)	-484(1)	1581(1)	7660(1)	41(1)
C(10)	2950(1)	2660(1)	9668(1)	24(1)
C(11)	3874(1)	3350(1)	9324(1)	27(1)
C(12)	4569(1)	3401(1)	10124(1)	32(1)
C(13)	4393(1)	2766(1)	11250(1)	34(1)
C(14)	3497(1)	2062(1)	11572(1)	35(1)
C(15)	2760(1)	2000(1)	10807(1)	29(1)
C(16)	4138(1)	4010(1)	8120(1)	38(1)
C(17)	5146(1)	2842(2)	12105(1)	49(1)
C(18)	1799(1)	1225(1)	11233(1)	43(1)
C(19)	4498(1)	1129(1)	6526(1)	23(1)
C(20)	5171(1)	1370(1)	7222(1)	32(1)
C(21)	6269(1)	1613(2)	6933(1)	42(1)
C(22)	6689(1)	1605(2)	5967(1)	48(1)
C(23)	6016(1)	1372(2)	5267(1)	48(1)
C(25)	4912(1)	1136(1)	5543(1)	34(1)
C(26)	2960(1)	-671(1)	8997(1)	27(1)
C(27)	1785(1)	-953(1)	9416(1)	42(1)
C(28)	3766(1)	-803(1)	9914(1)	45(1)
C(29)	2384(1)	2798(1)	5049(1)	24(1)
C(30)	2944(1)	3861(1)	4635(1)	27(1)
C(31)	2939(1)	4585(1)	3491(1)	33(1)
C(32)	2382(1)	4297(1)	2754(1)	36(1)
C(33)	1813(1)	3260(1)	3182(1)	37(1)
C(34)	1801(1)	2492(1)	4317(1)	30(1)
C(35)	3528(1)	4248(1)	5394(1)	38(1)
C(36)	2379(1)	5101(2)	1520(1)	50(1)
C(37)	1163(1)	1377(1)	4720(1)	44(1)
N(1)	784(1)	3141(1)	7412(1)	27(1)
N(2)	2275(1)	2546(1)	8845(1)	25(1)
N(3)	2908(1)	592(1)	8108(1)	27(1)
N(4)	2318(1)	2098(1)	6229(1)	24(1)
O(1)	187(1)	2959(1)	9278(1)	30(1)
O(2)	2909(1)	-186(1)	6665(1)	29(1)
S(1)	1106(1)	3261(1)	8514(1)	22(1)
S(2)	3064(1)	889(1)	6834(1)	21(1)

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Table 3. Bond lengths [A] and angles [deg] for nl267_a.

C(1)-C(2)	1.3870(16)
C(1)-C(6)	1.3897(15)
C(1)-S(1)	1.7810(12)
C(2)-C(3)	1.3910(19)
C(2)-H(2)	0.9500
C(3)-C(4)	1.383(2)
C(3)-H(3)	0.9500
C(4)-C(5)	1.383(2)
C(4)-H(4)	0.9500
C(5)-C(6)	1.3948(18)
C(5)-H(5)	0.9500
C(6)-H(6)	0.9500
C(7)-N(1)	1.4790(14)
C(7)-C(8)	1.5171(17)
C(7)-C(9)	1.5213(18)
C(7)-H(7)	1.0000
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-C(11)	1.4077(16)
C(10)-C(15)	1.4089(16)
C(10)-N(2)	1.4444(13)
C(11)-C(12)	1.3999(15)
C(11)-C(16)	1.5016(18)
C(12)-C(13)	1.3875(19)
C(12)-H(12)	0.9500
C(13)-C(14)	1.388(2)
C(13)-C(17)	1.5145(17)
C(14)-C(15)	1.3996(17)
C(14)-H(14)	0.9500
C(15)-C(18)	1.5090(19)
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-C(20)	1.3883(15)
C(19)-C(25)	1.3920(15)
C(19)-S(2)	1.7829(12)
C(20)-C(21)	1.3896(18)
C(20)-H(20)	0.9500
C(21)-C(22)	1.381(2)
C(21)-H(21)	0.9500
C(22)-C(23)	1.387(2)
C(22)-H(22)	0.9500
C(23)-C(25)	1.3904(18)
C(23)-H(23)	0.9500

C(25)-H(25)	0.9500
C(26)-N(3)	1.4773(14)
C(26)-C(27)	1.5211(18)
C(26)-C(28)	1.5224(18)
C(26)-H(26)	1.0000
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(30)	1.4059(16)
C(29)-C(34)	1.4113(16)
C(29)-N(4)	1.4400(13)
C(30)-C(31)	1.3984(16)
C(30)-C(35)	1.5030(17)
C(31)-C(32)	1.386(2)
C(31)-H(31)	0.9500
C(32)-C(33)	1.388(2)
C(32)-C(36)	1.5132(17)
C(33)-C(34)	1.3989(17)
C(33)-H(33)	0.9500
C(34)-C(37)	1.5099(19)
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
C(37)-H(37A)	0.9800
C(37)-H(37B)	0.9800
C(37)-H(37C)	0.9800
N(1)-S(1)	1.6032(10)
N(1)-H(1A)	0.855(18)
N(2)-S(1)	1.5343(10)
N(3)-S(2)	1.5938(10)
N(3)-H(3A)	0.877(17)
N(4)-S(2)	1.5311(10)
O(1)-S(1)	1.4486(9)
O(2)-S(2)	1.4492(9)

C(2)-C(1)-C(6)	120.53(11)
C(2)-C(1)-S(1)	121.31(8)
C(6)-C(1)-S(1)	118.12(9)
C(1)-C(2)-C(3)	119.16(11)
C(1)-C(2)-H(2)	120.4
C(3)-C(2)-H(2)	120.4
C(4)-C(3)-C(2)	120.82(12)
C(4)-C(3)-H(3)	119.6
C(2)-C(3)-H(3)	119.6
C(5)-C(4)-C(3)	119.71(12)
C(5)-C(4)-H(4)	120.1
C(3)-C(4)-H(4)	120.1
C(4)-C(5)-C(6)	120.25(12)
C(4)-C(5)-H(5)	119.9
C(6)-C(5)-H(5)	119.9
C(1)-C(6)-C(5)	119.49(11)
C(1)-C(6)-H(6)	120.3

C(5)-C(6)-H(6)	120.3
N(1)-C(7)-C(8)	108.80(10)
N(1)-C(7)-C(9)	110.28(10)
C(8)-C(7)-C(9)	111.84(10)
N(1)-C(7)-H(7)	108.6
C(8)-C(7)-H(7)	108.6
C(9)-C(7)-H(7)	108.6
C(7)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(7)-C(9)-H(9A)	109.5
C(7)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(7)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(11)-C(10)-C(15)	119.87(10)
C(11)-C(10)-N(2)	118.97(10)
C(15)-C(10)-N(2)	120.90(10)
C(12)-C(11)-C(10)	119.09(11)
C(12)-C(11)-C(16)	119.57(11)
C(10)-C(11)-C(16)	121.33(10)
C(13)-C(12)-C(11)	121.99(12)
C(13)-C(12)-H(12)	119.0
C(11)-C(12)-H(12)	119.0
C(12)-C(13)-C(14)	117.94(11)
C(12)-C(13)-C(17)	121.34(13)
C(14)-C(13)-C(17)	120.71(13)
C(13)-C(14)-C(15)	122.46(12)
C(13)-C(14)-H(14)	118.8
C(15)-C(14)-H(14)	118.8
C(14)-C(15)-C(10)	118.61(11)
C(14)-C(15)-C(18)	118.79(11)
C(10)-C(15)-C(18)	122.60(11)
C(11)-C(16)-H(16A)	109.5
C(11)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(11)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(13)-C(17)-H(17A)	109.5
C(13)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(13)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(15)-C(18)-H(18A)	109.5
C(15)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(15)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(20)-C(19)-C(25)	120.59(10)
C(20)-C(19)-S(2)	120.67(8)
C(25)-C(19)-S(2)	118.65(8)

C(19)-C(20)-C(21)	119.43(11)
C(19)-C(20)-H(20)	120.3
C(21)-C(20)-H(20)	120.3
C(22)-C(21)-C(20)	120.20(12)
C(22)-C(21)-H(21)	119.9
C(20)-C(21)-H(21)	119.9
C(21)-C(22)-C(23)	120.42(12)
C(21)-C(22)-H(22)	119.8
C(23)-C(22)-H(22)	119.8
C(22)-C(23)-C(25)	119.90(12)
C(22)-C(23)-H(23)	120.1
C(25)-C(23)-H(23)	120.1
C(23)-C(25)-C(19)	119.45(11)
C(23)-C(25)-H(25)	120.3
C(19)-C(25)-H(25)	120.3
N(3)-C(26)-C(27)	109.43(10)
N(3)-C(26)-C(28)	109.29(10)
C(27)-C(26)-C(28)	112.32(11)
N(3)-C(26)-H(26)	108.6
C(27)-C(26)-H(26)	108.6
C(28)-C(26)-H(26)	108.6
C(26)-C(27)-H(27A)	109.5
C(26)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(26)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(26)-C(28)-H(28A)	109.5
C(26)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(26)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(30)-C(29)-C(34)	120.07(10)
C(30)-C(29)-N(4)	119.18(10)
C(34)-C(29)-N(4)	120.45(10)
C(31)-C(30)-C(29)	119.01(11)
C(31)-C(30)-C(35)	119.43(11)
C(29)-C(30)-C(35)	121.55(10)
C(32)-C(31)-C(30)	122.02(12)
C(32)-C(31)-H(31)	119.0
C(30)-C(31)-H(31)	119.0
C(31)-C(32)-C(33)	118.00(11)
C(31)-C(32)-C(36)	121.10(14)
C(33)-C(32)-C(36)	120.90(13)
C(32)-C(33)-C(34)	122.55(12)
C(32)-C(33)-H(33)	118.7
C(34)-C(33)-H(33)	118.7
C(33)-C(34)-C(29)	118.32(12)
C(33)-C(34)-C(37)	119.48(11)
C(29)-C(34)-C(37)	122.19(11)
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(32)-C(36)-H(36A)	109.5

C(32)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36B)	109.5
C(32)-C(36)-H(36C)	109.5
H(36A)-C(36)-H(36C)	109.5
H(36B)-C(36)-H(36C)	109.5
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(7)-N(1)-S(1)	120.73(8)
C(7)-N(1)-H(1A)	117.7(11)
S(1)-N(1)-H(1A)	114.6(11)
C(10)-N(2)-S(1)	120.03(7)
C(26)-N(3)-S(2)	123.04(8)
C(26)-N(3)-H(3A)	119.4(11)
S(2)-N(3)-H(3A)	117.3(11)
C(29)-N(4)-S(2)	120.61(7)
O(1)-S(1)-N(2)	121.31(6)
O(1)-S(1)-N(1)	110.08(5)
N(2)-S(1)-N(1)	103.75(5)
O(1)-S(1)-C(1)	104.62(5)
N(2)-S(1)-C(1)	110.21(5)
N(1)-S(1)-C(1)	106.06(5)
O(2)-S(2)-N(4)	121.32(5)
O(2)-S(2)-N(3)	109.71(5)
N(4)-S(2)-N(3)	103.39(5)
O(2)-S(2)-C(19)	104.71(5)
N(4)-S(2)-C(19)	109.73(5)
N(3)-S(2)-C(19)	107.40(5)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for nl267_a.
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)	23(1)	24(1)	22(1)	-12(1)	0(1)	-2(1)
C(2)	44(1)	34(1)	24(1)	-13(1)	6(1)	-5(1)
C(3)	51(1)	31(1)	32(1)	-6(1)	8(1)	-8(1)
C(4)	50(1)	26(1)	44(1)	-13(1)	-2(1)	-8(1)
C(5)	72(1)	31(1)	37(1)	-20(1)	-3(1)	-8(1)
C(6)	54(1)	28(1)	24(1)	-14(1)	0(1)	-5(1)
C(7)	18(1)	35(1)	31(1)	-18(1)	0(1)	-3(1)
C(8)	33(1)	42(1)	35(1)	-13(1)	-7(1)	1(1)
C(9)	37(1)	39(1)	45(1)	-12(1)	0(1)	-16(1)
C(10)	26(1)	22(1)	27(1)	-14(1)	-4(1)	2(1)
C(11)	24(1)	29(1)	31(1)	-17(1)	-3(1)	1(1)
C(12)	26(1)	35(1)	43(1)	-24(1)	-7(1)	2(1)
C(13)	35(1)	35(1)	39(1)	-25(1)	-14(1)	12(1)
C(14)	44(1)	32(1)	27(1)	-14(1)	-9(1)	8(1)
C(15)	37(1)	22(1)	28(1)	-11(1)	-3(1)	1(1)
C(16)	32(1)	49(1)	36(1)	-19(1)	4(1)	-11(1)
C(17)	46(1)	59(1)	53(1)	-39(1)	-24(1)	16(1)
C(18)	55(1)	37(1)	31(1)	-6(1)	1(1)	-15(1)
C(19)	22(1)	26(1)	21(1)	-11(1)	1(1)	0(1)
C(20)	29(1)	45(1)	24(1)	-18(1)	1(1)	-6(1)
C(21)	30(1)	65(1)	34(1)	-23(1)	-2(1)	-12(1)
C(22)	26(1)	81(1)	40(1)	-26(1)	7(1)	-14(1)

C(23)	31(1)	84(1)	37(1)	-34(1)	12(1)	-12(1)
C(25)	28(1)	55(1)	28(1)	-26(1)	4(1)	-5(1)
C(26)	38(1)	21(1)	21(1)	-8(1)	3(1)	0(1)
C(27)	49(1)	38(1)	42(1)	-18(1)	15(1)	-18(1)
C(28)	53(1)	41(1)	35(1)	-14(1)	-14(1)	8(1)
C(29)	21(1)	28(1)	21(1)	-11(1)	1(1)	3(1)
C(30)	26(1)	28(1)	25(1)	-10(1)	2(1)	2(1)
C(31)	32(1)	31(1)	27(1)	-6(1)	6(1)	4(1)
C(32)	36(1)	42(1)	21(1)	-9(1)	1(1)	15(1)
C(33)	37(1)	47(1)	26(1)	-19(1)	-7(1)	10(1)
C(34)	27(1)	37(1)	28(1)	-16(1)	-4(1)	3(1)
C(35)	43(1)	34(1)	35(1)	-14(1)	-1(1)	-9(1)
C(36)	57(1)	54(1)	22(1)	-8(1)	1(1)	20(1)
C(37)	44(1)	47(1)	45(1)	-22(1)	-12(1)	-8(1)
N(1)	20(1)	41(1)	32(1)	-26(1)	2(1)	-5(1)
N(2)	25(1)	26(1)	29(1)	-16(1)	-2(1)	-1(1)
N(3)	40(1)	21(1)	19(1)	-9(1)	7(1)	-1(1)
N(4)	23(1)	28(1)	21(1)	-10(1)	3(1)	1(1)
O(1)	30(1)	35(1)	28(1)	-16(1)	9(1)	-8(1)
O(2)	33(1)	28(1)	30(1)	-18(1)	3(1)	-5(1)
S(1)	22(1)	25(1)	23(1)	-14(1)	2(1)	-4(1)
S(2)	22(1)	23(1)	19(1)	-11(1)	3(1)	-2(1)

Crystal data and structure refinement of compound 3

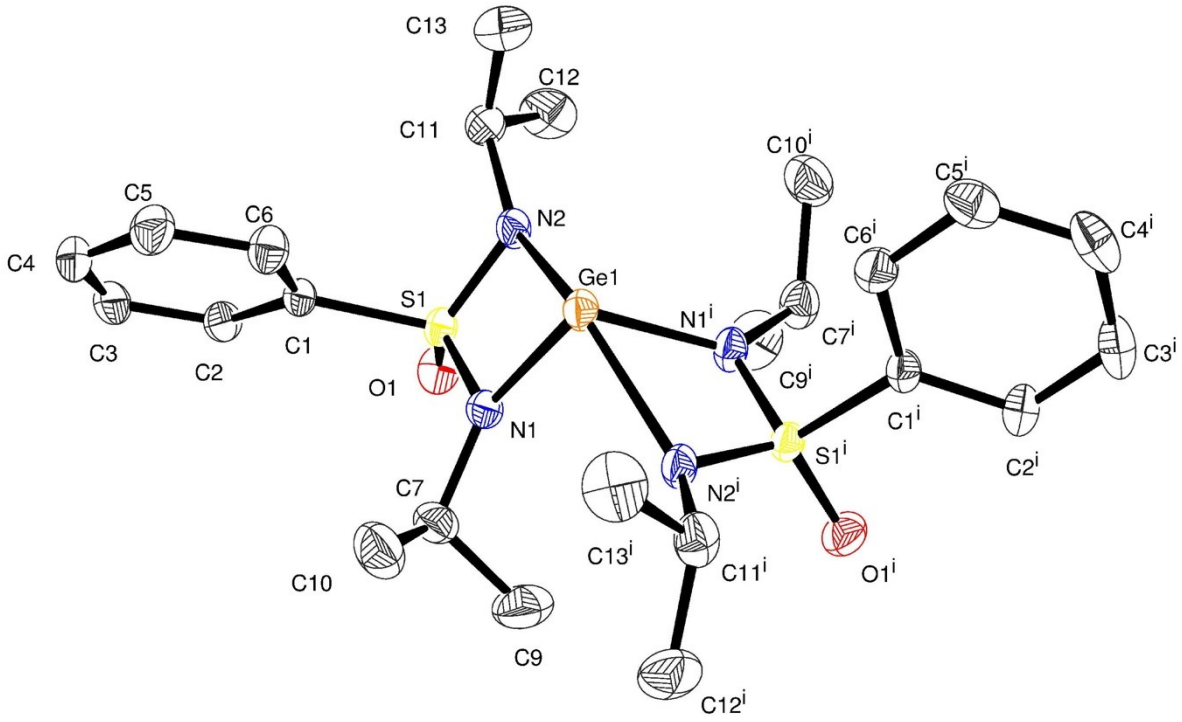

Figure 1 : Asymmetric Unit [Symmetry Code : 1-x,1-y,z]

Table 1. Crystal data and structure refinement for NL265.

Identification code	NL265	
Empirical formula	C24 H38 Ge N4 O2 S2	
Formula weight	551.31	
Temperature	193(2) K	
Wavelength	0.71073 Å	
Crystal system	Tetragonal	
Space group	$I4_1$	
Unit cell dimensions	a = 21.9417(7) Å	α= 90°.
	b = 21.9417(7) Å	β= 90°.
	c = 6.6868(2) Å	γ = 90°.
Volume	3219.3(2) $Å^3$	
Z	4	
Density (calculated)	1.137 Mg/m^3	

Absorption coefficient	1.104 mm^{-1}
Max. and min. transmission	0.7463 and 0.6494
F(000)	1160
Crystal size	0.300 x 0.200 x 0.160 mm^3
Theta range for data collection	2.936 to 31.886°.
Index ranges	-21<=h<=32, -32<=k<=32, -9<=l<=9
Reflections collected	38402
Independent reflections	5530 [R(int) = 0.0265]
Completeness to theta = 25.242°	99.2 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5530 / 1 / 154
Goodness-of-fit on F^2	1.023
Final R indices [I>2sigma(I)]	R1 = 0.0198, wR2 = 0.0483
R indices (all data)	R1 = 0.0236, wR2 = 0.0503
Absolute structure parameter	-0.0079(18)
Largest diff. peak and hole	0.204 and -0.209 $e.Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for NL265. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	4008(1)	6442(1)	4491(2)	21(1)
C(2)	3717(1)	6936(1)	5370(2)	27(1)
C(3)	3616(1)	7458(1)	4242(3)	34(1)
C(4)	3805(1)	7486(1)	2273(3)	36(1)
C(5)	4083(1)	6984(1)	1395(3)	34(1)
C(6)	4184(1)	6460(1)	2497(2)	28(1)
C(7)	5286(1)	6144(1)	6803(3)	31(1)
C(9)	5616(1)	5869(1)	8575(3)	47(1)
C(10)	5711(1)	6426(1)	5281(3)	44(1)
C(11)	3358(1)	5150(1)	4097(3)	31(1)
C(12)	2975(1)	4793(1)	5594(3)	45(1)
C(13)	3342(1)	4870(1)	2028(3)	47(1)
Ge(1)	5000	5000	3860(1)	22(1)
N(1)	4896(1)	5682(1)	5832(2)	24(1)
N(2)	3998(1)	5199(1)	4772(2)	24(1)
O(1)	3938(1)	5905(1)	7895(2)	31(1)
S(1)	4185(1)	5779(1)	5929(1)	21(1)

Table 3. Bond lengths [Å] and angles [°] for NL265.

C(1)-C(2)	1.3874(19)
C(1)-C(6)	1.389(2)
C(1)-S(1)	1.7881(14)
C(2)-C(3)	1.390(2)
C(2)-H(2)	0.9500
C(3)-C(4)	1.382(3)
C(3)-H(3)	0.9500
C(4)-C(5)	1.389(3)
C(4)-H(4)	0.9500
C(5)-C(6)	1.384(2)
C(5)-H(5)	0.9500
C(6)-H(6)	0.9500
C(7)-N(1)	1.4761(19)
C(7)-C(10)	1.512(3)
C(7)-C(9)	1.513(3)
C(7)-H(7)	1.0000
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-N(2)	1.4786(19)
C(11)-C(13)	1.515(3)
C(11)-C(12)	1.524(3)
C(11)-H(11)	1.0000
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
Ge(1)-N(1)#1	2.0085(12)
Ge(1)-N(1)	2.0085(12)
Ge(1)-N(2)	2.3241(12)
Ge(1)-N(2)#1	2.3241(12)

N(1)-S(1)	1.5757(12)
N(2)-S(1)	1.5445(13)
O(1)-S(1)	1.4484(11)

C(2)-C(1)-C(6)	120.91(14)
C(2)-C(1)-S(1)	120.51(12)
C(6)-C(1)-S(1)	118.56(11)
C(1)-C(2)-C(3)	119.12(15)
C(1)-C(2)-H(2)	120.4
C(3)-C(2)-H(2)	120.4
C(4)-C(3)-C(2)	120.37(15)
C(4)-C(3)-H(3)	119.8
C(2)-C(3)-H(3)	119.8
C(3)-C(4)-C(5)	119.98(15)
C(3)-C(4)-H(4)	120.0
C(5)-C(4)-H(4)	120.0
C(6)-C(5)-C(4)	120.29(17)
C(6)-C(5)-H(5)	119.9
C(4)-C(5)-H(5)	119.9
C(5)-C(6)-C(1)	119.30(15)
C(5)-C(6)-H(6)	120.3
C(1)-C(6)-H(6)	120.3
N(1)-C(7)-C(10)	110.01(14)
N(1)-C(7)-C(9)	110.39(14)
C(10)-C(7)-C(9)	113.29(16)
N(1)-C(7)-H(7)	107.6
C(10)-C(7)-H(7)	107.6
C(9)-C(7)-H(7)	107.6
C(7)-C(9)-H(9A)	109.5
C(7)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(7)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(7)-C(10)-H(10A)	109.5
C(7)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(7)-C(10)-H(10C)	109.5

H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
N(2)-C(11)-C(13)	109.22(15)
N(2)-C(11)-C(12)	111.14(14)
C(13)-C(11)-C(12)	112.24(16)
N(2)-C(11)-H(11)	108.0
C(13)-C(11)-H(11)	108.0
C(12)-C(11)-H(11)	108.0
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(11)-C(13)-H(13A)	109.5
C(11)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(11)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
N(1)#1-Ge(1)-N(1)	97.90(7)
N(1)#1-Ge(1)-N(2)	94.31(5)
N(1)-Ge(1)-N(2)	65.17(5)
N(1)#1-Ge(1)-N(2)#1	65.17(5)
N(1)-Ge(1)-N(2)#1	94.31(5)
N(2)-Ge(1)-N(2)#1	149.57(7)
C(7)-N(1)-S(1)	117.66(10)
C(7)-N(1)-Ge(1)	137.25(10)
S(1)-N(1)-Ge(1)	103.84(6)
C(11)-N(2)-S(1)	117.78(10)
C(11)-N(2)-Ge(1)	143.60(10)
S(1)-N(2)-Ge(1)	91.95(6)
O(1)-S(1)-N(2)	120.81(7)
O(1)-S(1)-N(1)	115.67(7)
N(2)-S(1)-N(1)	97.64(6)
O(1)-S(1)-C(1)	104.55(7)
N(2)-S(1)-C(1)	110.05(7)
N(1)-S(1)-C(1)	107.64(7)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,z+0

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for NL265. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	21(1)	18(1)	25(1)	0(1)	-1(1)	3(1)
C(2)	28(1)	22(1)	30(1)	-6(1)	-3(1)	6(1)
C(3)	38(1)	18(1)	46(1)	-5(1)	-11(1)	6(1)
C(4)	40(1)	22(1)	46(1)	10(1)	-14(1)	-3(1)
C(5)	37(1)	34(1)	31(1)	9(1)	-1(1)	-2(1)
C(6)	31(1)	26(1)	27(1)	2(1)	4(1)	5(1)
C(7)	28(1)	26(1)	39(1)	-8(1)	-3(1)	0(1)
C(9)	44(1)	57(1)	40(1)	-10(1)	-14(1)	1(1)
C(10)	38(1)	31(1)	62(1)	2(1)	3(1)	-6(1)
C(11)	23(1)	27(1)	43(1)	-2(1)	-8(1)	4(1)
C(12)	24(1)	54(1)	58(1)	-4(1)	5(1)	-5(1)
C(13)	49(1)	51(1)	40(1)	-4(1)	-13(1)	-1(1)
Ge(1)	26(1)	19(1)	22(1)	0	0	3(1)
N(1)	20(1)	20(1)	31(1)	-4(1)	-2(1)	4(1)
N(2)	20(1)	19(1)	31(1)	-2(1)	0(1)	4(1)
O(1)	36(1)	33(1)	25(1)	1(1)	7(1)	6(1)
S(1)	21(1)	19(1)	22(1)	1(1)	2(1)	5(1)

Crystal data and structure refinement of compound 4

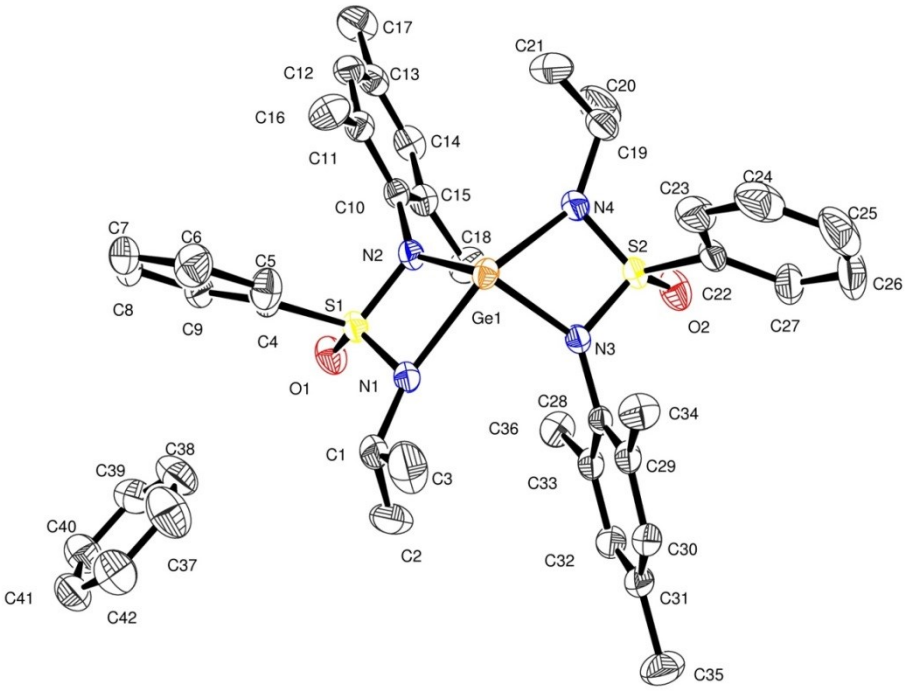

Figure 1 : Asymmetric Unit

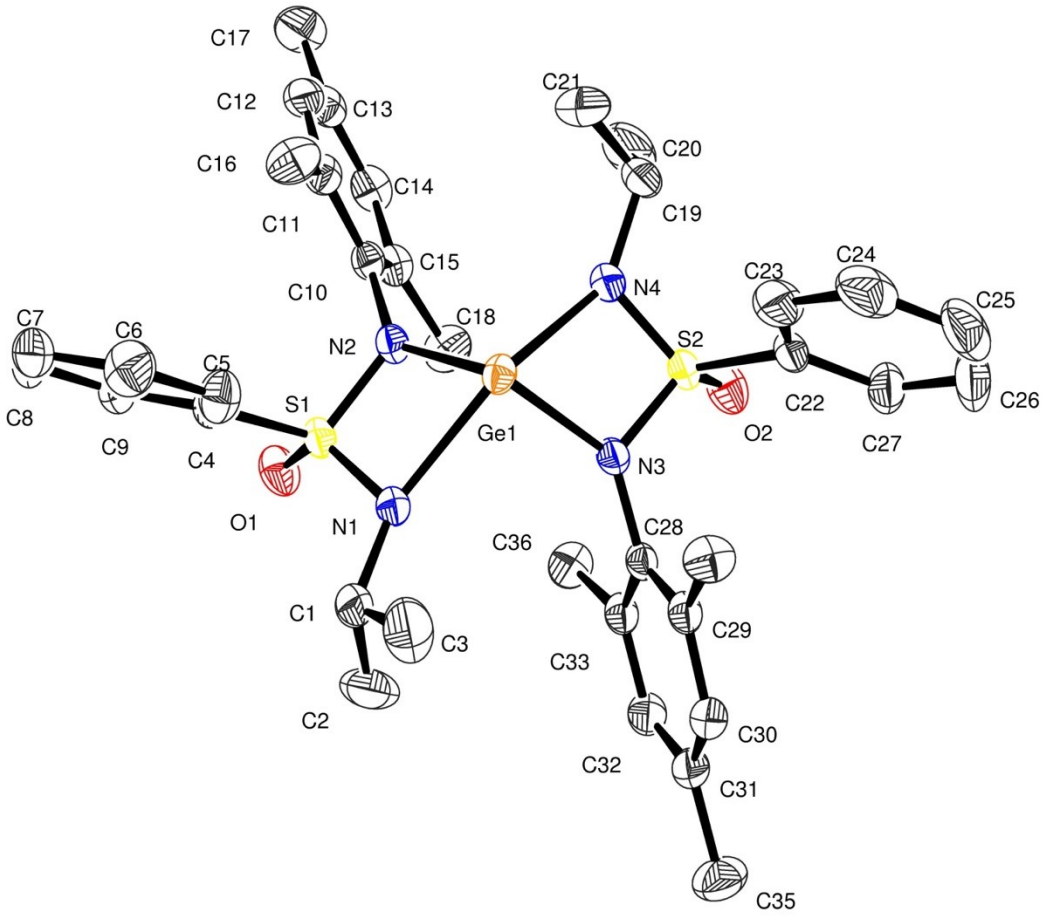

Figure 2 : Molecule

Table 1. Crystal data and structure refinement for 4.

Identification code	4
Empirical formula	C36 H46 Ge N4 O2 S2, C6 H6
Formula weight	781.61
Temperature	193(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P 21/c
Unit cell dimensions	a = 15.4414(5) A alpha = 90 deg. b = 7.9913(3) A beta = 94.717(2) deg. c = 33.5748(10) A gamma = 90 deg.
Volume	4129.0(2) A^3

Z, Calculated density	4, 1.257 Mg/m^3
Absorption coefficient	0.882 mm^-1
F(000)	1648
Crystal size	0.160 x 0.140 x 0.080 mm
Theta range for data collection	1.323 to 38.427 deg.
Limiting indices	-26<=h<=27, -13<=k<=13, -58<=l<=44
Reflections collected / unique	113581 / 22870 [R(int) = 0.0451]
Completeness to theta = 25.242	99.6 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	22870 / 0 / 470
Goodness-of-fit on F^2	1.018
Final R indices [I>2sigma(I)]	R1 = 0.0466, wR2 = 0.1014
R indices (all data)	R1 = 0.0940, wR2 = 0.1174
Largest diff. peak and hole	0.449 and -0.531 e.A^-3

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

	x	y	z	U(eq)
C(1)	5419(1)	3796(3)	3276(1)	44(1)
C(2)	5132(1)	5288(4)	3017(1)	75(1)
C(3)	5640(1)	2271(4)	3032(1)	71(1)
C(4)	5404(1)	3480(2)	4223(1)	29(1)
C(5)	5497(1)	1779(2)	4148(1)	37(1)
C(6)	5026(1)	623(2)	4349(1)	45(1)
C(7)	4467(1)	1172(3)	4624(1)	45(1)
C(8)	4380(1)	2851(3)	4700(1)	44(1)
C(9)	4845(1)	4025(2)	4498(1)	35(1)
C(10)	7310(1)	5531(2)	4524(1)	25(1)
C(11)	7393(1)	4516(2)	4865(1)	29(1)
C(12)	7691(1)	5236(2)	5231(1)	33(1)
C(13)	7899(1)	6920(2)	5266(1)	34(1)
C(14)	7833(1)	7881(2)	4922(1)	35(1)
C(15)	7550(1)	7225(2)	4549(1)	30(1)
C(16)	7176(1)	2678(2)	4854(1)	41(1)
C(17)	8169(1)	7679(3)	5668(1)	50(1)
C(18)	7542(1)	8314(2)	4183(1)	41(1)
C(19)	9595(1)	4334(3)	4180(1)	47(1)
C(20)	9793(1)	5971(4)	4394(1)	71(1)
C(21)	9440(1)	2911(4)	4468(1)	71(1)
C(22)	9654(1)	3603(2)	3243(1)	32(1)
C(23)	9667(1)	1945(2)	3365(1)	45(1)
C(24)	10203(1)	825(3)	3187(1)	58(1)
C(25)	10712(1)	1370(3)	2893(1)	66(1)
C(26)	10686(1)	3005(3)	2771(1)	63(1)
C(27)	10164(1)	4148(3)	2947(1)	44(1)
C(28)	7649(1)	5010(2)	2885(1)	24(1)
C(29)	7624(1)	3764(2)	2591(1)	27(1)
C(30)	7276(1)	4158(2)	2205(1)	31(1)
C(31)	6970(1)	5746(2)	2105(1)	34(1)
C(32)	6989(1)	6951(2)	2403(1)	33(1)
C(33)	7315(1)	6613(2)	2794(1)	28(1)
C(34)	7950(1)	2014(2)	2671(1)	37(1)
C(35)	6627(1)	6148(3)	1682(1)	54(1)
C(36)	7262(1)	7923(2)	3112(1)	37(1)
C(37)	3098(1)	5694(3)	3674(1)	68(1)
C(38)	3344(1)	7029(3)	3913(1)	58(1)
C(39)	2733(1)	8163(2)	4010(1)	50(1)
C(40)	1876(1)	7960(2)	3867(1)	50(1)
C(41)	1629(1)	6625(2)	3628(1)	49(1)
C(42)	2239(1)	5480(3)	3531(1)	56(1)
N(1)	6183(1)	4234(2)	3551(1)	31(1)
N(2)	7022(1)	4837(1)	4141(1)	26(1)

N(3)	7969(1)	4644(1)	3289(1)	25(1)
N(4)	8822(1)	4486(2)	3892(1)	33(1)
O(1)	5615(1)	6535(1)	4015(1)	39(1)
O(2)	9266(1)	6668(1)	3367(1)	42(1)
S(1)	6036(1)	4945(1)	3970(1)	26(1)
S(2)	8938(1)	5031(1)	3456(1)	27(1)
Ge(1)	7535(1)	3287(1)	3742(1)	24(1)

Table 3. Bond lengths [A] and angles [deg] for 4.

C(1)-N(1)	1.4786(18)
C(1)-C(2)	1.519(3)
C(1)-C(3)	1.523(3)
C(1)-H(1)	1.0000
C(2)-H(2A)	0.9800
C(2)-H(2B)	0.9800
C(2)-H(2C)	0.9800
C(3)-H(3A)	0.9800
C(3)-H(3B)	0.9800
C(3)-H(3C)	0.9800
C(4)-C(9)	1.3859(18)
C(4)-C(5)	1.392(2)
C(4)-S(1)	1.7841(13)
C(5)-C(6)	1.386(2)
C(5)-H(5)	0.9500
C(6)-C(7)	1.384(3)
C(6)-H(6)	0.9500
C(7)-C(8)	1.374(3)
C(7)-H(7)	0.9500
C(8)-C(9)	1.390(2)
C(8)-H(8)	0.9500
C(9)-H(9)	0.9500
C(10)-C(11)	1.4005(18)
C(10)-C(15)	1.4043(19)
C(10)-N(2)	1.4359(16)
C(11)-C(12)	1.3985(19)
C(11)-C(16)	1.506(2)
C(12)-C(13)	1.386(2)
C(12)-H(12)	0.9500
C(13)-C(14)	1.383(2)
C(13)-C(17)	1.509(2)
C(14)-C(15)	1.395(2)
C(14)-H(14)	0.9500
C(15)-C(18)	1.504(2)
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-N(4)	1.4779(18)
C(19)-C(20)	1.513(3)
C(19)-C(21)	1.525(3)
C(19)-H(19)	1.0000
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-C(23)	1.387(2)

C(22)-C(27)	1.388(2)
C(22)-S(2)	1.7778(14)
C(23)-C(24)	1.387(2)
C(23)-H(23)	0.9500
C(24)-C(25)	1.383(3)
C(24)-H(24)	0.9500
C(25)-C(26)	1.369(4)
C(25)-H(25)	0.9500
C(26)-C(27)	1.384(3)
C(26)-H(26)	0.9500
C(27)-H(27)	0.9500
C(28)-C(29)	1.4014(18)
C(28)-C(33)	1.4049(18)
C(28)-N(3)	1.4342(16)
C(29)-C(30)	1.3958(19)
C(29)-C(34)	1.5034(19)
C(30)-C(31)	1.386(2)
C(30)-H(30)	0.9500
C(31)-C(32)	1.385(2)
C(31)-C(35)	1.510(2)
C(32)-C(33)	1.3954(19)
C(32)-H(32)	0.9500
C(33)-C(36)	1.502(2)
C(34)-H(34A)	0.9800
C(34)-H(34B)	0.9800
C(34)-H(34C)	0.9800
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
C(37)-C(38)	1.370(3)
C(37)-C(42)	1.384(3)
C(37)-H(37)	0.9500
C(38)-C(39)	1.366(3)
C(38)-H(38)	0.9500
C(39)-C(40)	1.381(2)
C(39)-H(39)	0.9500
C(40)-C(41)	1.370(3)
C(40)-H(40)	0.9500
C(41)-C(42)	1.372(3)
C(41)-H(41)	0.9500
C(42)-H(42)	0.9500
N(1)-S(1)	1.5505(12)
N(1)-Ge(1)	2.2635(11)
N(2)-S(1)	1.5845(11)
N(2)-Ge(1)	2.0328(10)
N(3)-S(2)	1.5842(11)
N(3)-Ge(1)	2.0273(10)
N(4)-S(2)	1.5512(12)
N(4)-Ge(1)	2.2257(12)
O(1)-S(1)	1.4415(11)
O(2)-S(2)	1.4419(11)

N(1)-C(1)-C(2)	110.56(15)
N(1)-C(1)-C(3)	108.79(14)
C(2)-C(1)-C(3)	112.82(18)

N(1)-C(1)-H(1)	108.2
C(2)-C(1)-H(1)	108.2
C(3)-C(1)-H(1)	108.2
C(1)-C(2)-H(2A)	109.5
C(1)-C(2)-H(2B)	109.5
H(2A)-C(2)-H(2B)	109.5
C(1)-C(2)-H(2C)	109.5
H(2A)-C(2)-H(2C)	109.5
H(2B)-C(2)-H(2C)	109.5
C(1)-C(3)-H(3A)	109.5
C(1)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	109.5
C(1)-C(3)-H(3C)	109.5
H(3A)-C(3)-H(3C)	109.5
H(3B)-C(3)-H(3C)	109.5
C(9)-C(4)-C(5)	120.44(13)
C(9)-C(4)-S(1)	120.48(12)
C(5)-C(4)-S(1)	119.06(10)
C(6)-C(5)-C(4)	119.75(14)
C(6)-C(5)-H(5)	120.1
C(4)-C(5)-H(5)	120.1
C(7)-C(6)-C(5)	119.62(17)
C(7)-C(6)-H(6)	120.2
C(5)-C(6)-H(6)	120.2
C(8)-C(7)-C(6)	120.60(15)
C(8)-C(7)-H(7)	119.7
C(6)-C(7)-H(7)	119.7
C(7)-C(8)-C(9)	120.39(15)
C(7)-C(8)-H(8)	119.8
C(9)-C(8)-H(8)	119.8
C(4)-C(9)-C(8)	119.18(16)
C(4)-C(9)-H(9)	120.4
C(8)-C(9)-H(9)	120.4
C(11)-C(10)-C(15)	120.23(12)
C(11)-C(10)-N(2)	120.61(12)
C(15)-C(10)-N(2)	119.08(12)
C(12)-C(11)-C(10)	118.73(13)
C(12)-C(11)-C(16)	118.61(13)
C(10)-C(11)-C(16)	122.66(12)
C(13)-C(12)-C(11)	122.07(14)
C(13)-C(12)-H(12)	119.0
C(11)-C(12)-H(12)	119.0
C(14)-C(13)-C(12)	117.91(13)
C(14)-C(13)-C(17)	121.37(15)
C(12)-C(13)-C(17)	120.71(15)
C(13)-C(14)-C(15)	122.43(14)
C(13)-C(14)-H(14)	118.8
C(15)-C(14)-H(14)	118.8
C(14)-C(15)-C(10)	118.54(13)
C(14)-C(15)-C(18)	119.74(13)
C(10)-C(15)-C(18)	121.67(12)
C(11)-C(16)-H(16A)	109.5
C(11)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(11)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(13)-C(17)-H(17A)	109.5

C(13)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(13)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(15)-C(18)-H(18A)	109.5
C(15)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(15)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
N(4)-C(19)-C(20)	111.20(16)
N(4)-C(19)-C(21)	108.49(15)
C(20)-C(19)-C(21)	112.23(17)
N(4)-C(19)-H(19)	108.3
C(20)-C(19)-H(19)	108.3
C(21)-C(19)-H(19)	108.3
C(19)-C(20)-H(20A)	109.5
C(19)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(19)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(19)-C(21)-H(21A)	109.5
C(19)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(19)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(23)-C(22)-C(27)	121.09(15)
C(23)-C(22)-S(2)	119.27(11)
C(27)-C(22)-S(2)	119.59(13)
C(22)-C(23)-C(24)	118.90(18)
C(22)-C(23)-H(23)	120.6
C(24)-C(23)-H(23)	120.6
C(25)-C(24)-C(23)	120.0(2)
C(25)-C(24)-H(24)	120.0
C(23)-C(24)-H(24)	120.0
C(26)-C(25)-C(24)	120.71(18)
C(26)-C(25)-H(25)	119.6
C(24)-C(25)-H(25)	119.6
C(25)-C(26)-C(27)	120.35(19)
C(25)-C(26)-H(26)	119.8
C(27)-C(26)-H(26)	119.8
C(26)-C(27)-C(22)	119.0(2)
C(26)-C(27)-H(27)	120.5
C(22)-C(27)-H(27)	120.5
C(29)-C(28)-C(33)	120.41(12)
C(29)-C(28)-N(3)	120.61(11)
C(33)-C(28)-N(3)	118.88(12)
C(30)-C(29)-C(28)	118.69(12)
C(30)-C(29)-C(34)	118.29(13)
C(28)-C(29)-C(34)	123.01(12)
C(31)-C(30)-C(29)	121.89(13)
C(31)-C(30)-H(30)	119.1
C(29)-C(30)-H(30)	119.1
C(32)-C(31)-C(30)	118.42(13)
C(32)-C(31)-C(35)	121.02(14)

C(30)-C(31)-C(35)	120.56(15)
C(31)-C(32)-C(33)	121.92(13)
C(31)-C(32)-H(32)	119.0
C(33)-C(32)-H(32)	119.0
C(32)-C(33)-C(28)	118.61(13)
C(32)-C(33)-C(36)	119.87(12)
C(28)-C(33)-C(36)	121.45(12)
C(29)-C(34)-H(34A)	109.5
C(29)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
C(29)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
C(31)-C(35)-H(35A)	109.5
C(31)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5
C(31)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5
C(33)-C(36)-H(36A)	109.5
C(33)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36B)	109.5
C(33)-C(36)-H(36C)	109.5
H(36A)-C(36)-H(36C)	109.5
H(36B)-C(36)-H(36C)	109.5
C(38)-C(37)-C(42)	120.84(19)
C(38)-C(37)-H(37)	119.6
C(42)-C(37)-H(37)	119.6
C(39)-C(38)-C(37)	119.47(18)
C(39)-C(38)-H(38)	120.3
C(37)-C(38)-H(38)	120.3
C(38)-C(39)-C(40)	120.05(19)
C(38)-C(39)-H(39)	120.0
C(40)-C(39)-H(39)	120.0
C(41)-C(40)-C(39)	120.52(18)
C(41)-C(40)-H(40)	119.7
C(39)-C(40)-H(40)	119.7
C(40)-C(41)-C(42)	119.67(17)
C(40)-C(41)-H(41)	120.2
C(42)-C(41)-H(41)	120.2
C(41)-C(42)-C(37)	119.4(2)
C(41)-C(42)-H(42)	120.3
C(37)-C(42)-H(42)	120.3
C(1)-N(1)-S(1)	118.94(10)
C(1)-N(1)-Ge(1)	140.20(11)
S(1)-N(1)-Ge(1)	93.71(5)
C(10)-N(2)-S(1)	121.47(8)
C(10)-N(2)-Ge(1)	135.75(8)
S(1)-N(2)-Ge(1)	102.00(5)
C(28)-N(3)-S(2)	122.46(8)
C(28)-N(3)-Ge(1)	135.13(8)
S(2)-N(3)-Ge(1)	101.54(5)
C(19)-N(4)-S(2)	119.37(10)
C(19)-N(4)-Ge(1)	140.34(11)
S(2)-N(4)-Ge(1)	94.53(5)
O(1)-S(1)-N(1)	121.34(7)
O(1)-S(1)-N(2)	115.98(6)
N(1)-S(1)-N(2)	95.90(6)

O(1)-S(1)-C(4)	104.96(6)
N(1)-S(1)-C(4)	108.55(7)
N(2)-S(1)-C(4)	109.72(6)
O(2)-S(2)-N(4)	121.24(8)
O(2)-S(2)-N(3)	116.15(6)
N(4)-S(2)-N(3)	95.70(6)
O(2)-S(2)-C(22)	105.06(7)
N(4)-S(2)-C(22)	108.82(7)
N(3)-S(2)-C(22)	109.44(6)
N(3)-Ge(1)-N(2)	109.87(5)
N(3)-Ge(1)-N(4)	66.08(4)
N(2)-Ge(1)-N(4)	88.77(4)
N(3)-Ge(1)-N(1)	87.85(4)
N(2)-Ge(1)-N(1)	65.37(4)
N(4)-Ge(1)-N(1)	134.89(5)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for 4. 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(1)	73(1)	31(1)	-1(1)	4(1)	-14(1)
C(2)	44(1)	121(2)	58(1)	42(1)	-19(1)	-23(1)
C(3)	46(1)	114(2)	54(1)	-44(1)	12(1)	-23(1)
C(4)	23(1)	34(1)	29(1)	1(1)	6(1)	-1(1)
C(5)	39(1)	34(1)	40(1)	-4(1)	13(1)	-8(1)
C(6)	47(1)	38(1)	50(1)	2(1)	6(1)	-13(1)
C(7)	32(1)	60(1)	45(1)	16(1)	5(1)	-13(1)
C(8)	27(1)	66(1)	40(1)	12(1)	13(1)	5(1)
C(9)	26(1)	45(1)	36(1)	4(1)	10(1)	8(1)
C(10)	23(1)	25(1)	28(1)	-3(1)	5(1)	2(1)
C(11)	29(1)	26(1)	31(1)	-1(1)	6(1)	5(1)
C(12)	32(1)	37(1)	30(1)	-1(1)	3(1)	8(1)
C(13)	29(1)	39(1)	35(1)	-10(1)	2(1)	7(1)
C(14)	34(1)	28(1)	44(1)	-10(1)	5(1)	0(1)
C(15)	30(1)	25(1)	35(1)	-2(1)	5(1)	1(1)
C(16)	56(1)	28(1)	38(1)	4(1)	3(1)	2(1)
C(17)	50(1)	57(1)	41(1)	-19(1)	-3(1)	9(1)
C(18)	53(1)	28(1)	43(1)	3(1)	6(1)	-6(1)
C(19)	26(1)	84(1)	32(1)	-6(1)	0(1)	15(1)
C(20)	39(1)	115(2)	56(1)	-36(1)	-9(1)	3(1)
C(21)	54(1)	118(2)	39(1)	20(1)	-1(1)	28(1)
C(22)	21(1)	45(1)	31(1)	-4(1)	4(1)	5(1)
C(23)	43(1)	48(1)	43(1)	0(1)	3(1)	19(1)

C(24)	53(1)	62(1)	58(1)	-14(1)	-8(1)	30(1)
C(25)	35(1)	97(2)	67(1)	-39(1)	1(1)	23(1)
C(26)	33(1)	100(2)	57(1)	-28(1)	21(1)	-3(1)
C(27)	28(1)	65(1)	38(1)	-11(1)	11(1)	-8(1)
C(28)	19(1)	26(1)	27(1)	5(1)	6(1)	0(1)
C(29)	23(1)	26(1)	31(1)	3(1)	7(1)	1(1)
C(30)	28(1)	37(1)	28(1)	0(1)	5(1)	2(1)
C(31)	29(1)	45(1)	30(1)	8(1)	5(1)	8(1)
C(32)	32(1)	33(1)	35(1)	11(1)	7(1)	8(1)
C(33)	25(1)	26(1)	33(1)	5(1)	7(1)	2(1)
C(34)	45(1)	28(1)	39(1)	0(1)	1(1)	4(1)
C(35)	62(1)	66(1)	33(1)	9(1)	0(1)	24(1)
C(36)	45(1)	28(1)	40(1)	2(1)	7(1)	7(1)
C(37)	46(1)	57(1)	100(2)	-3(1)	9(1)	13(1)
C(38)	36(1)	55(1)	81(1)	11(1)	-9(1)	1(1)
C(39)	48(1)	44(1)	56(1)	7(1)	-9(1)	-4(1)
C(40)	39(1)	49(1)	61(1)	0(1)	1(1)	5(1)
C(41)	34(1)	55(1)	57(1)	3(1)	-3(1)	-5(1)
C(42)	53(1)	49(1)	67(1)	-7(1)	4(1)	-2(1)
N(1)	22(1)	43(1)	27(1)	0(1)	4(1)	-3(1)
N(2)	21(1)	27(1)	28(1)	-3(1)	5(1)	1(1)
N(3)	19(1)	29(1)	28(1)	5(1)	4(1)	0(1)
N(4)	23(1)	49(1)	27(1)	-2(1)	3(1)	5(1)
O(1)	30(1)	31(1)	56(1)	4(1)	9(1)	8(1)
O(2)	29(1)	37(1)	60(1)	1(1)	8(1)	-7(1)
S(1)	21(1)	27(1)	31(1)	1(1)	6(1)	1(1)
S(2)	19(1)	32(1)	31(1)	0(1)	5(1)	1(1)
Ge(1)	27(1)	22(1)	25(1)	2(1)	8(1)	3(1)

Crystal data and structure refinement of compound 5

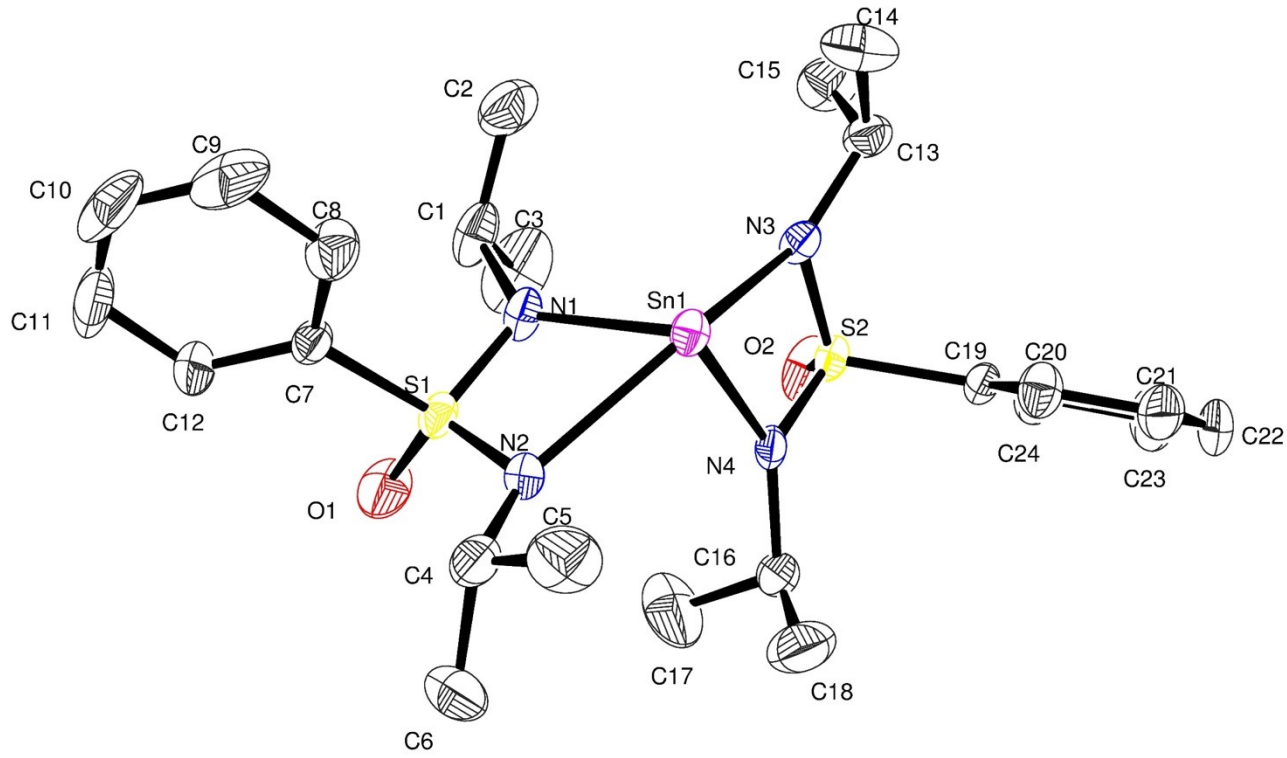

Figure 2 : Asymmetric Unit

Table 1. Crystal data and structure refinement for 5.

Identification code	5
Empirical formula	C24 H38 N4 O2 S2 Sn
Formula weight	597.41
Temperature	193(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P 21/c
Unit cell dimensions	a = 8.3489(8) A alpha = 90 deg. b = 43.317(4) A beta = 107.199(2) deg. c = 8.2449(8) A gamma = 90 deg.
Volume	2848.4(5) A^3
Z, Calculated density	4, 1.393 Mg/m^3
Absorption coefficient	1.070 mm^-1
F(000)	1232

Crystal size	0.38 x 0.2 x 0.04 mm
Theta range for data collection	2.821 to 25.367 deg.
Limiting indices	-10<=h<=10, -52<=k<=52, -9<=l<=9
Reflections collected / unique	49056 / 5176 [R(int) = 0.0378]
Completeness to theta = 25.242	99.6 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5176 / 0 / 306
Goodness-of-fit on F^2	1.487
Final R indices [I>2sigma(I)]	R1 = 0.0611, wR2 = 0.1395
R indices (all data)	R1 = 0.0615, wR2 = 0.1396
Largest diff. peak and hole	0.916 and -2.284 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 5. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	9070(9)	3722(2)	4841(10)	41(2)
C(2)	9463(12)	3547(3)	3425(13)	71(3)
C(3)	9076(11)	3517(2)	6331(11)	53(2)
C(4)	4848(9)	4604(2)	3339(9)	38(2)
C(5)	3164(11)	4589(2)	3668(12)	54(2)
C(6)	4758(12)	4775(2)	1704(13)	60(3)
C(7)	8430(8)	4423(2)	5805(8)	26(1)
C(8)	9758(9)	4620(2)	5927(10)	37(2)
C(9)	10577(11)	4746(2)	7513(13)	58(3)
C(10)	10070(13)	4676(2)	8894(12)	62(3)
C(11)	8756(13)	4487(2)	8762(10)	56(2)
C(12)	7916(10)	4358(2)	7201(9)	40(2)
C(13)	5111(9)	2928(2)	4023(9)	32(2)
C(14)	6677(11)	2741(2)	4151(11)	48(2)
C(15)	4836(13)	2972(2)	5735(11)	55(2)
C(16)	3850(10)	3764(2)	-561(8)	39(2)
C(17)	2419(14)	3985(2)	-612(12)	69(3)
C(18)	5312(16)	3919(3)	-885(11)	78(4)
C(19)	2807(7)	3068(1)	306(8)	23(1)
C(20)	1396(8)	3146(2)	751(9)	32(2)
C(21)	-102(9)	2998(2)	-33(10)	42(2)
C(22)	-177(11)	2777(2)	-1251(11)	51(2)
C(23)	1242(12)	2700(2)	-1672(11)	51(2)
C(24)	2770(9)	2843(2)	-886(9)	37(2)
N(4)	4351(7)	3619(1)	1161(6)	26(1)
O(1)	8353(7)	4331(1)	2725(6)	47(1)
O(2)	5868(6)	3149(1)	429(6)	40(1)
N(1)	7429(7)	3878(1)	4222(7)	29(1)
N(2)	5514(7)	4291(1)	3336(7)	30(1)
N(3)	5179(7)	3234(1)	3269(7)	26(1)
S(1)	7419(2)	4234(1)	3853(2)	26(1)
S(2)	4726(2)	3265(1)	1302(2)	23(1)
Sn(1)	4769(1)	3765(1)	3820(1)	24(1)

Table 3. Bond lengths [A] and angles [deg] for 5.

C(1)-N(1)	1.477(9)
C(1)-C(2)	1.507(11)
C(1)-C(3)	1.513(12)
C(1)-H(1)	1.0000
C(2)-H(2A)	0.9800
C(2)-H(2B)	0.9800
C(2)-H(2C)	0.9800
C(3)-H(3A)	0.9800
C(3)-H(3B)	0.9800
C(3)-H(3C)	0.9800
C(4)-N(2)	1.469(9)
C(4)-C(5)	1.510(11)
C(4)-C(6)	1.519(11)
C(4)-H(4)	1.0000
C(5)-H(5A)	0.9800
C(5)-H(5B)	0.9800
C(5)-H(5C)	0.9800
C(6)-H(6A)	0.9800
C(6)-H(6B)	0.9800
C(6)-H(6C)	0.9800
C(7)-C(12)	1.371(10)
C(7)-C(8)	1.379(9)
C(7)-S(1)	1.779(6)
C(8)-C(9)	1.396(11)
C(8)-H(8)	0.9500
C(9)-C(10)	1.361(15)
C(9)-H(9)	0.9500
C(10)-C(11)	1.347(14)
C(10)-H(10)	0.9500
C(11)-C(12)	1.387(11)
C(11)-H(11)	0.9500
C(12)-H(12)	0.9500
C(13)-N(3)	1.473(9)
C(13)-C(15)	1.507(11)
C(13)-C(14)	1.513(10)
C(13)-H(13)	1.0000
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(18)	1.485(12)
C(16)-N(4)	1.495(8)
C(16)-C(17)	1.521(13)
C(16)-H(16)	1.0000
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-C(20)	1.376(9)
C(19)-C(24)	1.378(9)

C(19)-S(2)	1.786(6)
C(20)-C(21)	1.384(10)
C(20)-H(20)	0.9500
C(21)-C(22)	1.375(12)
C(21)-H(21)	0.9500
C(22)-C(23)	1.371(13)
C(22)-H(22)	0.9500
C(23)-C(24)	1.395(11)
C(23)-H(23)	0.9500
C(24)-H(24)	0.9500
N(4)-S(2)	1.563(6)
N(4)-Sn(1)	2.208(5)
O(1)-S(1)	1.442(5)
O(2)-S(2)	1.445(5)
N(1)-S(1)	1.572(6)
N(1)-Sn(1)	2.202(5)
N(2)-S(1)	1.539(6)
N(2)-Sn(1)	2.426(5)
N(3)-S(2)	1.558(5)
N(3)-Sn(1)	2.389(5)

N(1)-C(1)-C(2)	110.8(6)
N(1)-C(1)-C(3)	109.2(6)
C(2)-C(1)-C(3)	112.6(8)
N(1)-C(1)-H(1)	108.0
C(2)-C(1)-H(1)	108.0
C(3)-C(1)-H(1)	108.0
C(1)-C(2)-H(2A)	109.5
C(1)-C(2)-H(2B)	109.5
H(2A)-C(2)-H(2B)	109.5
C(1)-C(2)-H(2C)	109.5
H(2A)-C(2)-H(2C)	109.5
H(2B)-C(2)-H(2C)	109.5
C(1)-C(3)-H(3A)	109.5
C(1)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	109.5
C(1)-C(3)-H(3C)	109.5
H(3A)-C(3)-H(3C)	109.5
H(3B)-C(3)-H(3C)	109.5
N(2)-C(4)-C(5)	109.4(6)
N(2)-C(4)-C(6)	111.5(7)
C(5)-C(4)-C(6)	112.2(7)
N(2)-C(4)-H(4)	107.9
C(5)-C(4)-H(4)	107.9
C(6)-C(4)-H(4)	107.9
C(4)-C(5)-H(5A)	109.5
C(4)-C(5)-H(5B)	109.5
H(5A)-C(5)-H(5B)	109.5
C(4)-C(5)-H(5C)	109.5
H(5A)-C(5)-H(5C)	109.5
H(5B)-C(5)-H(5C)	109.5
C(4)-C(6)-H(6A)	109.5
C(4)-C(6)-H(6B)	109.5
H(6A)-C(6)-H(6B)	109.5
C(4)-C(6)-H(6C)	109.5
H(6A)-C(6)-H(6C)	109.5
H(6B)-C(6)-H(6C)	109.5
C(12)-C(7)-C(8)	120.6(6)

C(12)-C(7)-S(1)	118.9(5)
C(8)-C(7)-S(1)	120.4(5)
C(7)-C(8)-C(9)	118.1(8)
C(7)-C(8)-H(8)	120.9
C(9)-C(8)-H(8)	120.9
C(10)-C(9)-C(8)	120.6(8)
C(10)-C(9)-H(9)	119.7
C(8)-C(9)-H(9)	119.7
C(11)-C(10)-C(9)	121.1(8)
C(11)-C(10)-H(10)	119.5
C(9)-C(10)-H(10)	119.5
C(10)-C(11)-C(12)	119.6(9)
C(10)-C(11)-H(11)	120.2
C(12)-C(11)-H(11)	120.2
C(7)-C(12)-C(11)	120.0(8)
C(7)-C(12)-H(12)	120.0
C(11)-C(12)-H(12)	120.0
N(3)-C(13)-C(15)	108.5(6)
N(3)-C(13)-C(14)	111.6(6)
C(15)-C(13)-C(14)	111.7(6)
N(3)-C(13)-H(13)	108.3
C(15)-C(13)-H(13)	108.3
C(14)-C(13)-H(13)	108.3
C(13)-C(14)-H(14A)	109.5
C(13)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(13)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(13)-C(15)-H(15A)	109.5
C(13)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(13)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(18)-C(16)-N(4)	110.3(6)
C(18)-C(16)-C(17)	113.1(8)
N(4)-C(16)-C(17)	106.7(7)
C(18)-C(16)-H(16)	108.9
N(4)-C(16)-H(16)	108.9
C(17)-C(16)-H(16)	108.9
C(16)-C(17)-H(17A)	109.5
C(16)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(16)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(16)-C(18)-H(18A)	109.5
C(16)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(16)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(20)-C(19)-C(24)	121.6(6)
C(20)-C(19)-S(2)	118.9(5)
C(24)-C(19)-S(2)	119.6(5)
C(19)-C(20)-C(21)	119.2(7)
C(19)-C(20)-H(20)	120.4

C(21)-C(20)-H(20)	120.4
C(22)-C(21)-C(20)	120.2(7)
C(22)-C(21)-H(21)	119.9
C(20)-C(21)-H(21)	119.9
C(23)-C(22)-C(21)	120.0(7)
C(23)-C(22)-H(22)	120.0
C(21)-C(22)-H(22)	120.0
C(22)-C(23)-C(24)	120.8(8)
C(22)-C(23)-H(23)	119.6
C(24)-C(23)-H(23)	119.6
C(19)-C(24)-C(23)	118.2(7)
C(19)-C(24)-H(24)	120.9
C(23)-C(24)-H(24)	120.9
C(16)-N(4)-S(2)	118.5(5)
C(16)-N(4)-Sn(1)	137.8(5)
S(2)-N(4)-Sn(1)	103.7(3)
C(1)-N(1)-S(1)	117.9(5)
C(1)-N(1)-Sn(1)	137.8(5)
S(1)-N(1)-Sn(1)	104.0(3)
C(4)-N(2)-S(1)	120.5(5)
C(4)-N(2)-Sn(1)	138.9(5)
S(1)-N(2)-Sn(1)	95.7(3)
C(13)-N(3)-S(2)	119.4(4)
C(13)-N(3)-Sn(1)	139.5(4)
S(2)-N(3)-Sn(1)	96.3(3)
O(1)-S(1)-N(2)	119.1(3)
O(1)-S(1)-N(1)	116.0(3)
N(2)-S(1)-N(1)	99.0(3)
O(1)-S(1)-C(7)	104.3(3)
N(2)-S(1)-C(7)	110.6(3)
N(1)-S(1)-C(7)	107.6(3)
O(2)-S(2)-N(3)	119.7(3)
O(2)-S(2)-N(4)	116.9(3)
N(3)-S(2)-N(4)	98.3(3)
O(2)-S(2)-C(19)	103.8(3)
N(3)-S(2)-C(19)	110.2(3)
N(4)-S(2)-C(19)	107.6(3)
N(1)-Sn(1)-N(4)	94.0(2)
N(1)-Sn(1)-N(3)	92.78(19)
N(4)-Sn(1)-N(3)	61.69(19)
N(1)-Sn(1)-N(2)	61.2(2)
N(4)-Sn(1)-N(2)	94.42(19)
N(3)-Sn(1)-N(2)	144.57(19)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for 5. 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)	26(4)	46(5)	46(4)	-18(4)	3(3)	0(3)
C(2)	46(5)	96(8)	73(7)	-34(6)	22(5)	18(5)
C(3)	44(5)	51(5)	50(5)	7(4)	-8(4)	8(4)
C(4)	38(4)	32(4)	33(4)	-4(3)	-5(3)	0(3)
C(5)	49(5)	45(5)	67(6)	4(4)	17(4)	17(4)
C(6)	53(5)	44(5)	73(6)	24(5)	6(5)	-5(4)
C(7)	26(3)	29(3)	21(3)	-4(3)	3(3)	-3(3)
C(8)	29(4)	34(4)	42(4)	3(3)	1(3)	-10(3)
C(9)	44(5)	37(5)	68(6)	-17(4)	-19(4)	-9(4)
C(10)	67(6)	53(5)	42(5)	-25(4)	-22(5)	19(5)
C(11)	79(7)	64(6)	20(4)	-10(4)	7(4)	18(5)
C(12)	46(4)	44(4)	29(4)	-12(3)	12(3)	-9(4)
C(13)	35(4)	27(3)	30(4)	0(3)	1(3)	4(3)
C(14)	53(5)	38(4)	51(5)	2(4)	9(4)	13(4)
C(15)	72(6)	58(6)	40(5)	21(4)	24(4)	12(5)
C(16)	50(4)	37(4)	20(3)	-1(3)	-5(3)	-16(3)
C(17)	90(8)	42(5)	47(5)	1(4)	-23(5)	4(5)
C(18)	129(10)	78(7)	34(5)	-9(5)	36(6)	-55(7)
C(19)	19(3)	26(3)	20(3)	-1(2)	2(2)	-2(2)
C(20)	27(3)	38(4)	33(4)	-9(3)	11(3)	-6(3)
C(21)	25(4)	58(5)	44(4)	12(4)	9(3)	-4(3)
C(22)	40(4)	52(5)	48(5)	5(4)	-7(4)	-30(4)
C(23)	59(6)	43(5)	47(5)	-16(4)	7(4)	-18(4)

C(24)	37(4)	37(4)	34(4)	-12(3)	6(3)	-2(3)
N(4)	25(3)	33(3)	18(3)	-2(2)	3(2)	-14(2)
O(1)	46(3)	74(4)	22(3)	-1(3)	12(2)	-18(3)
O(2)	25(2)	63(4)	36(3)	-25(3)	16(2)	1(2)
N(1)	22(3)	28(3)	34(3)	-10(2)	4(2)	-3(2)
N(2)	27(3)	30(3)	29(3)	2(2)	3(2)	-6(2)
N(3)	24(3)	29(3)	20(3)	-3(2)	0(2)	1(2)
S(1)	26(1)	37(1)	15(1)	-4(1)	4(1)	-8(1)
S(2)	16(1)	31(1)	21(1)	-6(1)	6(1)	-3(1)
Sn(1)	23(1)	26(1)	22(1)	-4(1)	6(1)	-2(1)

Crystal data and structure refinement of compound 6

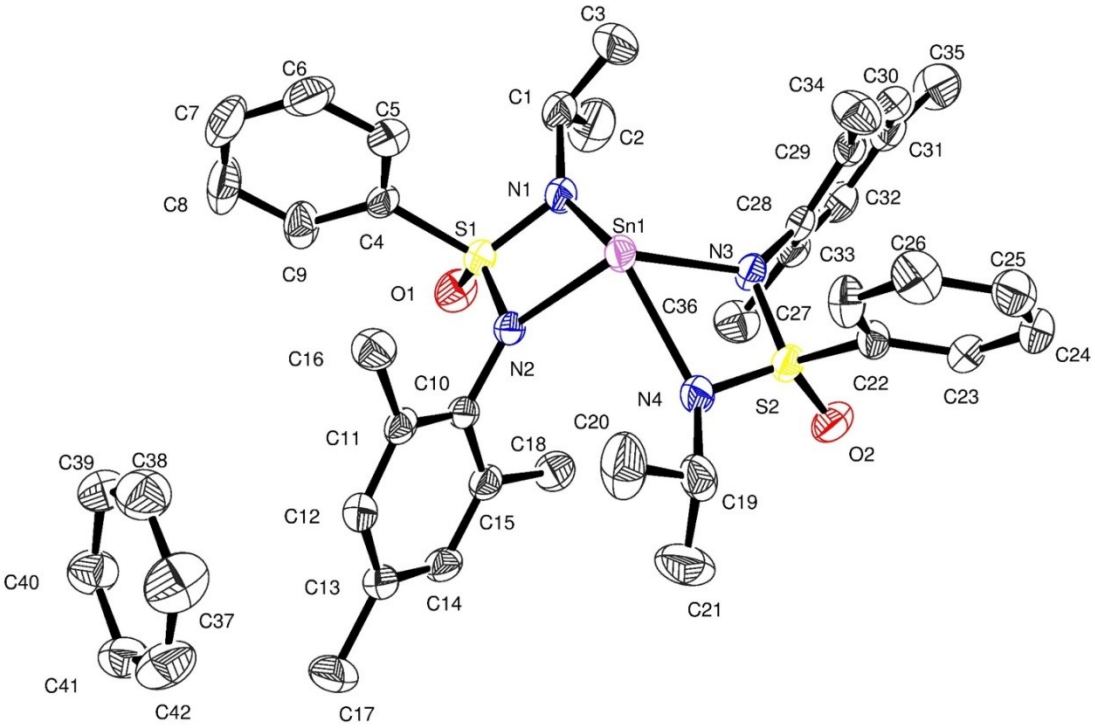

Figure 1 : Asymmetric Unit

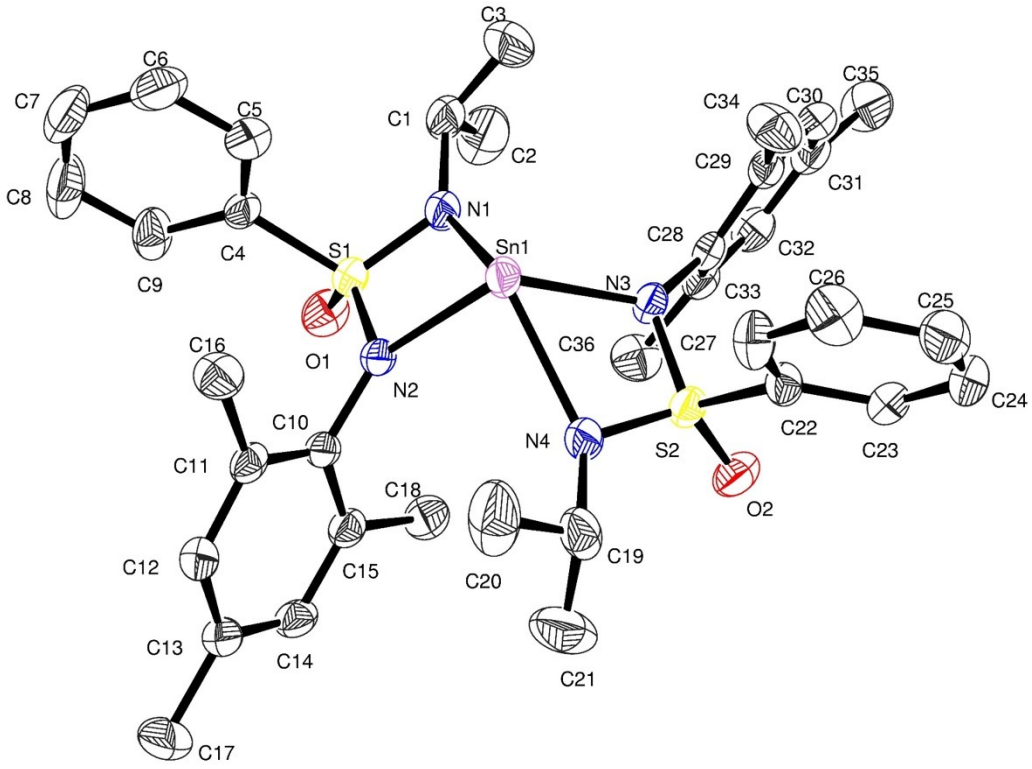

Figure 2 : Molecule

Table 1. Crystal data and structure refinement for 6.

Identification code	6
Empirical formula	C36 H46 N4 O2 S2 Sn, C6 H6
Formula weight	827.71
Temperature	193(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P 21/c
Unit cell dimensions	a = 15.5421(8) A alpha = 90 deg. b = 8.0005(4) A beta = 96.144(2) deg. c = 33.9053(16) A gamma = 90 deg.
Volume	4191.7(4) A^3
Z, Calculated density	4, 1.312 Mg/m^3
Absorption coefficient	0.747 mm^-1
F(000)	1720
Crystal size	0.200 x 0.080 x 0.060 mm
Theta range for data collection	1.318 to 26.196 deg.
Limiting indices	-19<=h<=19, -9<=k<=9, -42<=l<=42
Reflections collected / unique	93393 / 8354 [R(int) = 0.0739]
Completeness to theta = 25.242	99.7 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8354 / 0 / 470
Goodness-of-fit on F^2	1.032
Final R indices [I>2sigma(I)]	R1 = 0.0346, wR2 = 0.0723
R indices (all data)	R1 = 0.0558, wR2 = 0.0813
Largest diff. peak and hole	0.671 and -0.434 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 6. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	4664(2)	5284(5)	4161(1)	50(1)
C(2)	4819(2)	3541(6)	4337(1)	71(1)
C(3)	4552(2)	6563(6)	4481(1)	73(1)
C(4)	4711(2)	6272(4)	3236(1)	32(1)
C(5)	4765(2)	7899(4)	3371(1)	47(1)
C(6)	5298(2)	9022(5)	3201(1)	60(1)
C(7)	5761(2)	8495(6)	2897(1)	62(1)
C(8)	5696(2)	6885(6)	2764(1)	59(1)
C(9)	5175(2)	5743(4)	2931(1)	42(1)
C(10)	2683(2)	4969(3)	2857(1)	26(1)
C(11)	2643(2)	6209(3)	2566(1)	28(1)
C(12)	2257(2)	5828(4)	2186(1)	34(1)
C(13)	1924(2)	4262(4)	2091(1)	37(1)
C(14)	1963(2)	3064(4)	2386(1)	36(1)
C(15)	2326(2)	3387(3)	2773(1)	30(1)
C(16)	3001(2)	7948(4)	2645(1)	39(1)
C(17)	1534(3)	3882(5)	1673(1)	61(1)
C(18)	2293(2)	2078(4)	3091(1)	42(1)
C(19)	444(2)	6069(5)	3300(1)	46(1)
C(20)	659(2)	7520(6)	3037(1)	76(1)
C(21)	156(2)	4505(6)	3064(1)	76(1)
C(22)	412(2)	6531(4)	4237(1)	31(1)
C(23)	-144(2)	5997(4)	4503(1)	38(1)
C(24)	-617(2)	7159(5)	4692(1)	46(1)
C(25)	-538(2)	8832(5)	4616(1)	47(1)
C(26)	25(2)	9381(4)	4352(1)	48(1)
C(27)	499(2)	8224(4)	4162(1)	40(1)
C(28)	2317(2)	4465(3)	4571(1)	26(1)
C(29)	2422(2)	5445(3)	4915(1)	30(1)
C(30)	2724(2)	4699(4)	5274(1)	35(1)
C(31)	2922(2)	3017(4)	5300(1)	37(1)
C(32)	2840(2)	2083(4)	4955(1)	38(1)
C(33)	2549(2)	2765(3)	4587(1)	31(1)
C(34)	2221(2)	7301(4)	4906(1)	46(1)
C(35)	3205(2)	2212(5)	5697(1)	54(1)
C(36)	2519(2)	1712(4)	4219(1)	46(1)
C(37)	1878(2)	9386(5)	1321(1)	66(1)
C(38)	2732(2)	9572(5)	1469(1)	57(1)
C(39)	3330(2)	8393(4)	1391(1)	48(1)
C(40)	3073(2)	7043(4)	1159(1)	47(1)
C(41)	2224(2)	6855(4)	1010(1)	47(1)
C(42)	1628(2)	8023(5)	1090(1)	59(1)
N(1)	3882(2)	5330(3)	3868(1)	34(1)
N(2)	3026(1)	5351(3)	3257(1)	27(1)

N(3)	2033(1)	5209(3)	4196(1)	28(1)
N(4)	1207(1)	5725(3)	3587(1)	34(1)
O(1)	4272(1)	3216(3)	3333(1)	42(1)
O(2)	645(1)	3468(2)	4049(1)	41(1)
S(1)	3973(1)	4859(1)	3431(1)	30(1)
S(2)	1066(1)	5057(1)	4006(1)	30(1)
Sn(1)	2593(1)	6853(1)	3753(1)	29(1)

Table 3. Bond lengths [A] and angles [deg] for 6.

C(1)-N(1)	1.485(4)
C(1)-C(3)	1.515(5)
C(1)-C(2)	1.526(5)
C(1)-H(1)	1.0000
C(2)-H(2A)	0.9800
C(2)-H(2B)	0.9800
C(2)-H(2C)	0.9800
C(3)-H(3A)	0.9800
C(3)-H(3B)	0.9800
C(3)-H(3C)	0.9800
C(4)-C(5)	1.379(4)
C(4)-C(9)	1.388(4)
C(4)-S(1)	1.786(3)
C(5)-C(6)	1.388(5)
C(5)-H(5)	0.9500
C(6)-C(7)	1.383(5)
C(6)-H(6)	0.9500
C(7)-C(8)	1.364(5)
C(7)-H(7)	0.9500
C(8)-C(9)	1.382(5)
C(8)-H(8)	0.9500
C(9)-H(9)	0.9500
C(10)-C(11)	1.398(4)
C(10)-C(15)	1.399(4)
C(10)-N(2)	1.435(3)
C(11)-C(12)	1.394(4)
C(11)-C(16)	1.512(4)
C(12)-C(13)	1.381(4)
C(12)-H(12)	0.9500
C(13)-C(14)	1.382(4)
C(13)-C(17)	1.513(4)
C(14)-C(15)	1.396(4)
C(14)-H(14)	0.9500
C(15)-C(18)	1.507(4)
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-N(4)	1.477(4)
C(19)-C(20)	1.522(5)
C(19)-C(21)	1.525(5)
C(19)-H(19)	1.0000
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-C(23)	1.380(4)

C(22)-C(27)	1.387(4)
C(22)-S(2)	1.791(3)
C(23)-C(24)	1.385(4)
C(23)-H(23)	0.9500
C(24)-C(25)	1.371(5)
C(24)-H(24)	0.9500
C(25)-C(26)	1.390(5)
C(25)-H(25)	0.9500
C(26)-C(27)	1.384(4)
C(26)-H(26)	0.9500
C(27)-H(27)	0.9500
C(28)-C(29)	1.401(4)
C(28)-C(33)	1.407(4)
C(28)-N(3)	1.431(3)
C(29)-C(30)	1.391(4)
C(29)-C(34)	1.517(4)
C(30)-C(31)	1.381(4)
C(30)-H(30)	0.9500
C(31)-C(32)	1.383(4)
C(31)-C(35)	1.514(4)
C(32)-C(33)	1.393(4)
C(32)-H(32)	0.9500
C(33)-C(36)	1.503(4)
C(34)-H(34A)	0.9800
C(34)-H(34B)	0.9800
C(34)-H(34C)	0.9800
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
C(37)-C(42)	1.373(5)
C(37)-C(38)	1.376(5)
C(37)-H(37)	0.9500
C(38)-C(39)	1.370(5)
C(38)-H(38)	0.9500
C(39)-C(40)	1.370(4)
C(39)-H(39)	0.9500
C(40)-C(41)	1.369(4)
C(40)-H(40)	0.9500
C(41)-C(42)	1.362(5)
C(41)-H(41)	0.9500
C(42)-H(42)	0.9500
N(1)-S(1)	1.553(2)
N(1)-Sn(1)	2.342(2)
N(2)-S(1)	1.576(2)
N(2)-Sn(1)	2.229(2)
N(3)-S(2)	1.576(2)
N(3)-Sn(1)	2.240(2)
N(4)-S(2)	1.558(2)
N(4)-Sn(1)	2.347(2)
O(1)-S(1)	1.444(2)
O(2)-S(2)	1.443(2)

N(1)-C(1)-C(3)	108.2(3)
N(1)-C(1)-C(2)	111.5(3)
C(3)-C(1)-C(2)	111.3(3)

N(1)-C(1)-H(1)	108.6
C(3)-C(1)-H(1)	108.6
C(2)-C(1)-H(1)	108.6
C(1)-C(2)-H(2A)	109.5
C(1)-C(2)-H(2B)	109.5
H(2A)-C(2)-H(2B)	109.5
C(1)-C(2)-H(2C)	109.5
H(2A)-C(2)-H(2C)	109.5
H(2B)-C(2)-H(2C)	109.5
C(1)-C(3)-H(3A)	109.5
C(1)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	109.5
C(1)-C(3)-H(3C)	109.5
H(3A)-C(3)-H(3C)	109.5
H(3B)-C(3)-H(3C)	109.5
C(5)-C(4)-C(9)	121.0(3)
C(5)-C(4)-S(1)	119.6(2)
C(9)-C(4)-S(1)	119.2(2)
C(4)-C(5)-C(6)	119.5(3)
C(4)-C(5)-H(5)	120.3
C(6)-C(5)-H(5)	120.3
C(7)-C(6)-C(5)	119.5(4)
C(7)-C(6)-H(6)	120.3
C(5)-C(6)-H(6)	120.3
C(8)-C(7)-C(6)	120.5(3)
C(8)-C(7)-H(7)	119.7
C(6)-C(7)-H(7)	119.7
C(7)-C(8)-C(9)	121.0(4)
C(7)-C(8)-H(8)	119.5
C(9)-C(8)-H(8)	119.5
C(8)-C(9)-C(4)	118.6(3)
C(8)-C(9)-H(9)	120.7
C(4)-C(9)-H(9)	120.7
C(11)-C(10)-C(15)	120.7(2)
C(11)-C(10)-N(2)	120.1(2)
C(15)-C(10)-N(2)	119.0(2)
C(12)-C(11)-C(10)	118.7(3)
C(12)-C(11)-C(16)	118.7(3)
C(10)-C(11)-C(16)	122.6(2)
C(13)-C(12)-C(11)	121.8(3)
C(13)-C(12)-H(12)	119.1
C(11)-C(12)-H(12)	119.1
C(12)-C(13)-C(14)	118.3(3)
C(12)-C(13)-C(17)	120.2(3)
C(14)-C(13)-C(17)	121.4(3)
C(13)-C(14)-C(15)	122.3(3)
C(13)-C(14)-H(14)	118.9
C(15)-C(14)-H(14)	118.9
C(14)-C(15)-C(10)	118.1(3)
C(14)-C(15)-C(18)	120.1(3)
C(10)-C(15)-C(18)	121.7(2)
C(11)-C(16)-H(16A)	109.5
C(11)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(11)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(13)-C(17)-H(17A)	109.5

C(13)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(13)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(15)-C(18)-H(18A)	109.5
C(15)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(15)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
N(4)-C(19)-C(20)	108.4(3)
N(4)-C(19)-C(21)	111.2(3)
C(20)-C(19)-C(21)	113.0(3)
N(4)-C(19)-H(19)	108.0
C(20)-C(19)-H(19)	108.0
C(21)-C(19)-H(19)	108.0
C(19)-C(20)-H(20A)	109.5
C(19)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(19)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(19)-C(21)-H(21A)	109.5
C(19)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(19)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(23)-C(22)-C(27)	120.1(3)
C(23)-C(22)-S(2)	120.3(2)
C(27)-C(22)-S(2)	119.4(2)
C(22)-C(23)-C(24)	119.6(3)
C(22)-C(23)-H(23)	120.2
C(24)-C(23)-H(23)	120.2
C(25)-C(24)-C(23)	120.5(3)
C(25)-C(24)-H(24)	119.8
C(23)-C(24)-H(24)	119.8
C(24)-C(25)-C(26)	120.3(3)
C(24)-C(25)-H(25)	119.9
C(26)-C(25)-H(25)	119.9
C(27)-C(26)-C(25)	119.5(3)
C(27)-C(26)-H(26)	120.3
C(25)-C(26)-H(26)	120.3
C(26)-C(27)-C(22)	120.0(3)
C(26)-C(27)-H(27)	120.0
C(22)-C(27)-H(27)	120.0
C(29)-C(28)-C(33)	120.2(3)
C(29)-C(28)-N(3)	120.4(2)
C(33)-C(28)-N(3)	119.3(2)
C(30)-C(29)-C(28)	119.1(3)
C(30)-C(29)-C(34)	119.2(3)
C(28)-C(29)-C(34)	121.7(3)
C(31)-C(30)-C(29)	121.8(3)
C(31)-C(30)-H(30)	119.1
C(29)-C(30)-H(30)	119.1
C(30)-C(31)-C(32)	118.2(3)
C(30)-C(31)-C(35)	120.9(3)

C(32)-C(31)-C(35)	120.9(3)
C(31)-C(32)-C(33)	122.6(3)
C(31)-C(32)-H(32)	118.7
C(33)-C(32)-H(32)	118.7
C(32)-C(33)-C(28)	118.1(3)
C(32)-C(33)-C(36)	120.2(3)
C(28)-C(33)-C(36)	121.7(3)
C(29)-C(34)-H(34A)	109.5
C(29)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
C(29)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
C(31)-C(35)-H(35A)	109.5
C(31)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5
C(31)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5
C(33)-C(36)-H(36A)	109.5
C(33)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36B)	109.5
C(33)-C(36)-H(36C)	109.5
H(36A)-C(36)-H(36C)	109.5
H(36B)-C(36)-H(36C)	109.5
C(42)-C(37)-C(38)	119.8(4)
C(42)-C(37)-H(37)	120.1
C(38)-C(37)-H(37)	120.1
C(39)-C(38)-C(37)	120.1(3)
C(39)-C(38)-H(38)	119.9
C(37)-C(38)-H(38)	119.9
C(38)-C(39)-C(40)	119.4(3)
C(38)-C(39)-H(39)	120.3
C(40)-C(39)-H(39)	120.3
C(41)-C(40)-C(39)	120.6(3)
C(41)-C(40)-H(40)	119.7
C(39)-C(40)-H(40)	119.7
C(42)-C(41)-C(40)	120.0(3)
C(42)-C(41)-H(41)	120.0
C(40)-C(41)-H(41)	120.0
C(41)-C(42)-C(37)	120.0(3)
C(41)-C(42)-H(42)	120.0
C(37)-C(42)-H(42)	120.0
C(1)-N(1)-S(1)	118.7(2)
C(1)-N(1)-Sn(1)	138.5(2)
S(1)-N(1)-Sn(1)	97.52(11)
C(10)-N(2)-S(1)	122.49(17)
C(10)-N(2)-Sn(1)	135.72(17)
S(1)-N(2)-Sn(1)	101.43(10)
C(28)-N(3)-S(2)	121.33(18)
C(28)-N(3)-Sn(1)	137.33(17)
S(2)-N(3)-Sn(1)	101.20(11)
C(19)-N(4)-S(2)	118.9(2)
C(19)-N(4)-Sn(1)	137.6(2)
S(2)-N(4)-Sn(1)	97.36(11)
O(1)-S(1)-N(1)	120.28(13)
O(1)-S(1)-N(2)	116.90(12)
N(1)-S(1)-N(2)	96.85(12)

O(1)-S(1)-C(4)	104.88(14)
N(1)-S(1)-C(4)	109.11(14)
N(2)-S(1)-C(4)	108.34(13)
O(2)-S(2)-N(4)	120.18(13)
O(2)-S(2)-N(3)	116.75(12)
N(4)-S(2)-N(3)	97.10(12)
O(2)-S(2)-C(22)	104.64(13)
N(4)-S(2)-C(22)	108.40(13)
N(3)-S(2)-C(22)	109.42(13)
N(2)-Sn(1)-N(3)	111.06(8)
N(2)-Sn(1)-N(1)	61.54(8)
N(3)-Sn(1)-N(1)	88.24(8)
N(2)-Sn(1)-N(4)	87.40(8)
N(3)-Sn(1)-N(4)	61.55(8)
N(1)-Sn(1)-N(4)	125.94(9)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for 6. 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)	28(2)	88(3)	34(2)	2(2)	3(1)	-13(2)
C(2)	45(2)	109(4)	57(2)	33(2)	-6(2)	-1(2)
C(3)	50(2)	131(4)	39(2)	-21(2)	2(2)	-20(2)
C(4)	20(2)	48(2)	27(2)	5(1)	-1(1)	-7(1)
C(5)	44(2)	58(2)	39(2)	-2(2)	4(2)	-19(2)
C(6)	55(2)	66(3)	53(2)	10(2)	-10(2)	-31(2)
C(7)	34(2)	95(3)	57(2)	33(2)	1(2)	-21(2)
C(8)	33(2)	96(3)	52(2)	27(2)	17(2)	6(2)
C(9)	27(2)	63(2)	39(2)	10(2)	9(1)	10(2)
C(10)	19(1)	33(2)	27(2)	-7(1)	5(1)	0(1)
C(11)	21(1)	29(2)	36(2)	-6(1)	10(1)	0(1)
C(12)	30(2)	42(2)	30(2)	0(1)	7(1)	-2(1)
C(13)	31(2)	47(2)	32(2)	-9(1)	7(1)	-9(1)
C(14)	31(2)	36(2)	41(2)	-14(2)	8(1)	-10(1)
C(15)	25(2)	31(2)	35(2)	-4(1)	8(1)	-2(1)
C(16)	47(2)	31(2)	40(2)	0(1)	3(2)	-4(1)
C(17)	71(3)	71(3)	38(2)	-11(2)	-3(2)	-33(2)
C(18)	45(2)	34(2)	45(2)	-1(2)	7(2)	-10(1)
C(19)	31(2)	78(3)	30(2)	0(2)	5(1)	14(2)
C(20)	50(2)	125(4)	52(2)	37(2)	10(2)	20(2)
C(21)	44(2)	124(4)	57(2)	-37(3)	-13(2)	16(2)
C(22)	26(2)	40(2)	29(2)	-2(1)	7(1)	3(1)
C(23)	28(2)	48(2)	39(2)	-5(2)	7(1)	-8(1)

C(24)	30(2)	68(3)	43(2)	-9(2)	14(2)	-5(2)
C(25)	33(2)	62(2)	46(2)	-13(2)	5(2)	13(2)
C(26)	50(2)	44(2)	49(2)	2(2)	4(2)	15(2)
C(27)	40(2)	42(2)	40(2)	6(2)	15(1)	9(2)
C(28)	21(1)	28(1)	31(2)	4(1)	8(1)	-3(1)
C(29)	30(2)	28(2)	33(2)	-2(1)	10(1)	-6(1)
C(30)	32(2)	38(2)	34(2)	-2(1)	5(1)	-9(1)
C(31)	30(2)	41(2)	39(2)	11(2)	4(1)	-7(1)
C(32)	35(2)	27(2)	51(2)	6(2)	7(2)	-2(1)
C(33)	28(2)	25(2)	40(2)	-2(1)	9(1)	-3(1)
C(34)	68(2)	28(2)	41(2)	-7(1)	6(2)	-1(2)
C(35)	57(2)	56(2)	47(2)	20(2)	-2(2)	-6(2)
C(36)	51(2)	33(2)	54(2)	-10(2)	6(2)	5(2)
C(37)	48(2)	59(2)	93(3)	-6(2)	9(2)	15(2)
C(38)	59(3)	52(2)	60(2)	-12(2)	7(2)	-4(2)
C(39)	33(2)	60(2)	48(2)	0(2)	-1(2)	-5(2)
C(40)	39(2)	50(2)	50(2)	-2(2)	-1(2)	5(2)
C(41)	46(2)	47(2)	44(2)	3(2)	-8(2)	-5(2)
C(42)	35(2)	63(3)	76(3)	8(2)	-8(2)	-2(2)
N(1)	24(1)	52(2)	27(1)	0(1)	5(1)	-3(1)
N(2)	21(1)	32(1)	27(1)	-6(1)	6(1)	0(1)
N(3)	22(1)	33(1)	31(1)	3(1)	7(1)	-1(1)
N(4)	25(1)	49(2)	29(1)	-3(1)	5(1)	2(1)
O(1)	32(1)	41(1)	54(1)	-2(1)	7(1)	7(1)
O(2)	31(1)	38(1)	55(1)	-5(1)	9(1)	-8(1)
S(1)	23(1)	37(1)	31(1)	-1(1)	6(1)	-2(1)
S(2)	25(1)	33(1)	34(1)	-3(1)	8(1)	-2(1)
Sn(1)	32(1)	28(1)	28(1)	-4(1)	10(1)	-3(1)

Calculations

Calculations were performed with the Gaussian 09 suite of programs [5] using the density functional method B3LYP with dispersion (D3). [6, 7] Tin atom was treated with a Stuttgart-Dresden pseudopotential in combination with its adapted basis set.[8]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.[9,10]
The electron density of the optimized structures was subjected to an Atoms-In Molecules analysis (QTAIM analysis) [11,12,13] using AIMAll software. [14]

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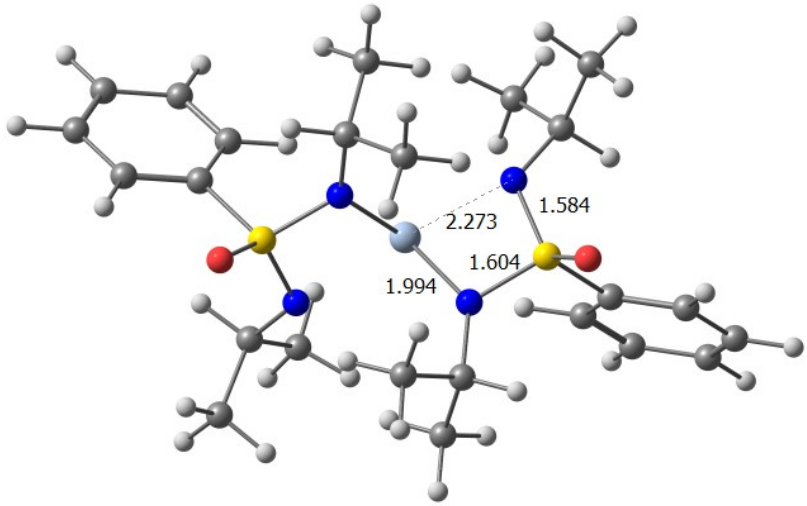
Coordinates:

Compound 3



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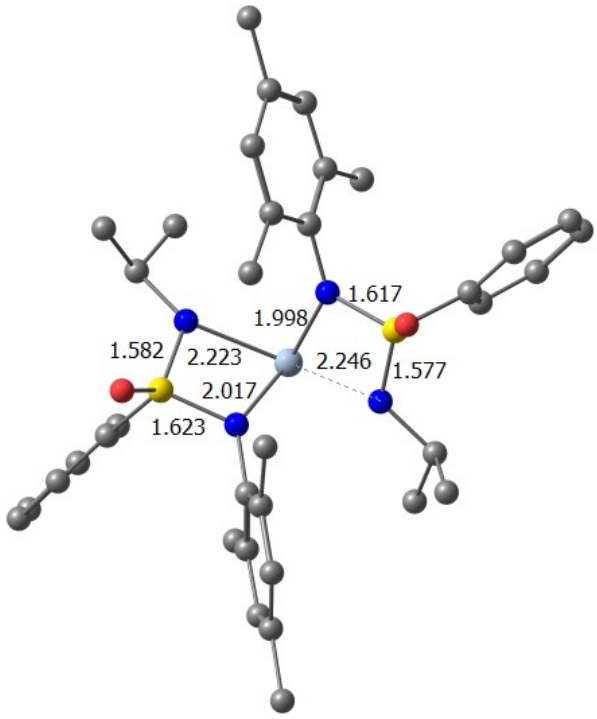
Compound 4 (Hydrogen atoms are removed for clarity)



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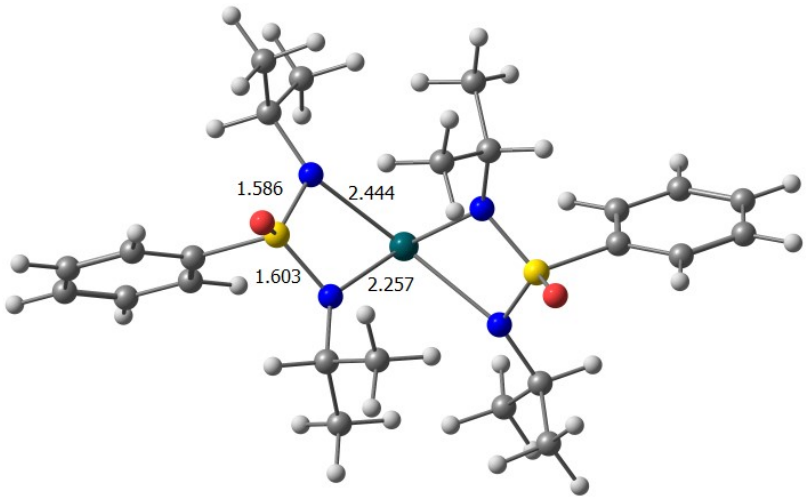
Compound 5



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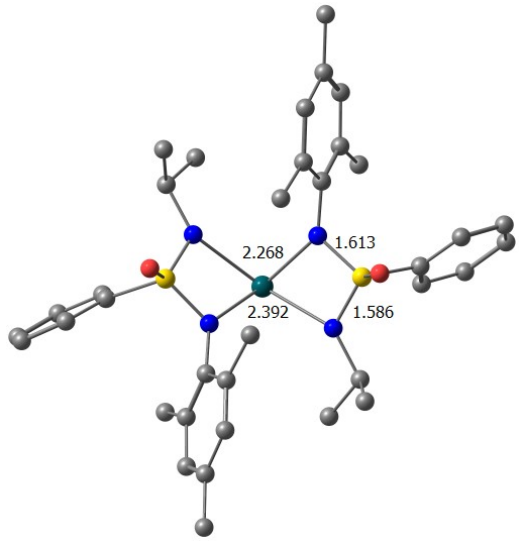
S	-2.492798000000	0.254210000000	0.725059000000
S	2.492771000000	-0.254056000000	0.725047000000
Sn	0.000016000000	-0.000026000000	-1.035240000000

Compound 6 (H atoms removed for clarity)



C	0.409087000000	-3.488219000000	-0.355639000000
C	0.033198000000	-4.122270000000	0.987652000000
C	-0.705801000000	-3.667289000000	-1.385902000000
C	3.417517000000	-2.129495000000	-0.445215000000
C	3.298678000000	-2.387905000000	-1.811560000000
C	4.429703000000	-2.763691000000	-2.531887000000
C	5.666852000000	-2.861362000000	-1.889684000000
C	5.772365000000	-2.599788000000	-0.522381000000
C	4.642179000000	-2.238986000000	0.211204000000
C	2.684760000000	1.042216000000	0.573556000000
C	3.690110000000	1.538974000000	-0.280042000000
C	4.508586000000	2.579539000000	0.174539000000
C	4.362673000000	3.131960000000	1.446005000000
C	3.349283000000	2.630284000000	2.268716000000
C	2.498794000000	1.603277000000	1.856603000000
C	3.910262000000	0.990540000000	-1.667768000000
C	5.271203000000	4.235534000000	1.927276000000
C	1.383265000000	1.139605000000	2.752762000000
C	-0.408941000000	3.487956000000	-0.356653000000
C	-0.032914000000	4.122386000000	0.986421000000
C	0.705841000000	3.666717000000	-1.387092000000
C	-3.417355000000	2.129326000000	-0.445968000000
C	-3.298369000000	2.387503000000	-1.812341000000
C	-4.429322000000	2.763123000000	-2.532869000000
C	-5.666549000000	2.860878000000	-1.890830000000
C	-5.772212000000	2.599548000000	-0.523493000000
C	-4.642103000000	2.238892000000	0.210282000000
C	-2.684791000000	-1.042086000000	0.573726000000
C	-3.690413000000	-1.538650000000	-0.279715000000

C	-4.509012000000	-2.579000000000	0.174997000000
C	-4.363016000000	-3.131427000000	1.446504000000
C	-3.349392000000	-2.629984000000	2.268998000000
C	-2.498753000000	-1.603106000000	1.856729000000
C	-3.910596000000	-0.990130000000	-1.667403000000
C	-5.272232000000	-4.234349000000	1.927982000000
C	-1.383026000000	-1.139613000000	2.752732000000
N	0.669288000000	-2.042396000000	-0.242995000000
N	1.785015000000	0.040978000000	0.105926000000
N	-1.784990000000	-0.041022000000	0.105866000000
N	-0.669165000000	2.042184000000	-0.243568000000
O	2.269947000000	-1.845617000000	1.879829000000
O	-2.269937000000	1.846066000000	1.879243000000
S	1.987911000000	-1.518093000000	0.465489000000
S	-1.987826000000	1.518126000000	0.465020000000
Sn	0.000051000000	-0.000214000000	-1.293277000000