Germylene-sulfoxide as potential hemilabile ligands: application in coordination chemistry

Nicolas Lentz,[a] Sonia Mallet-Ladeira,[b] Antoine Baceiredo,[a] Tsuyoshi Kato,[a] David Madec* [a]

[a] *Université de Toulouse, UPS, LHFA, 118 Route de Narbonne, and CNRS, LHFA UMR 5069, F-31062 Toulouse, France*
[b] *Université de Toulouse, UPS, Institut de Chimie de Toulouse, ICT-FR2599, 118 Route de Narbonne, F-31062 Toulouse, France*

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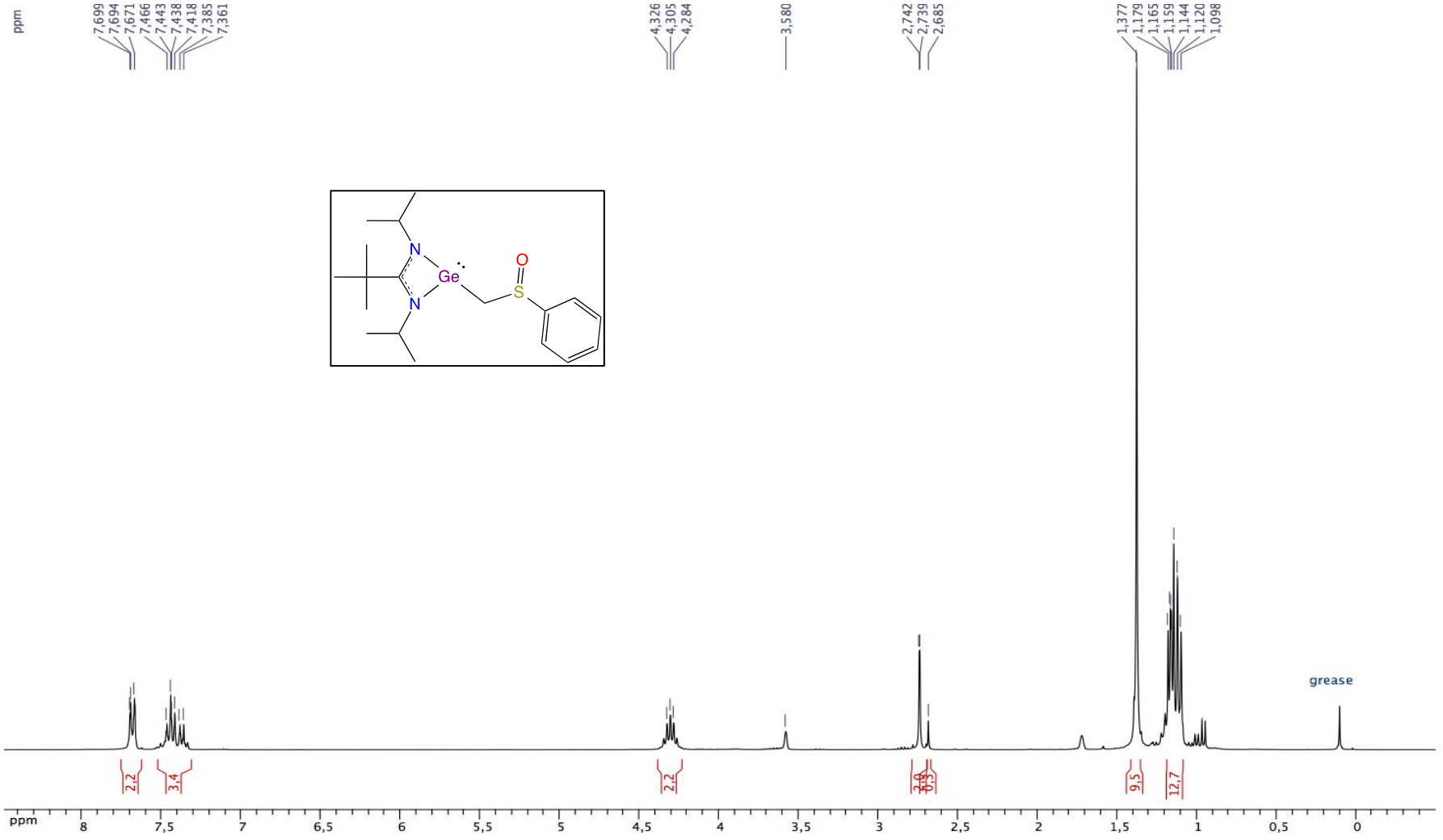
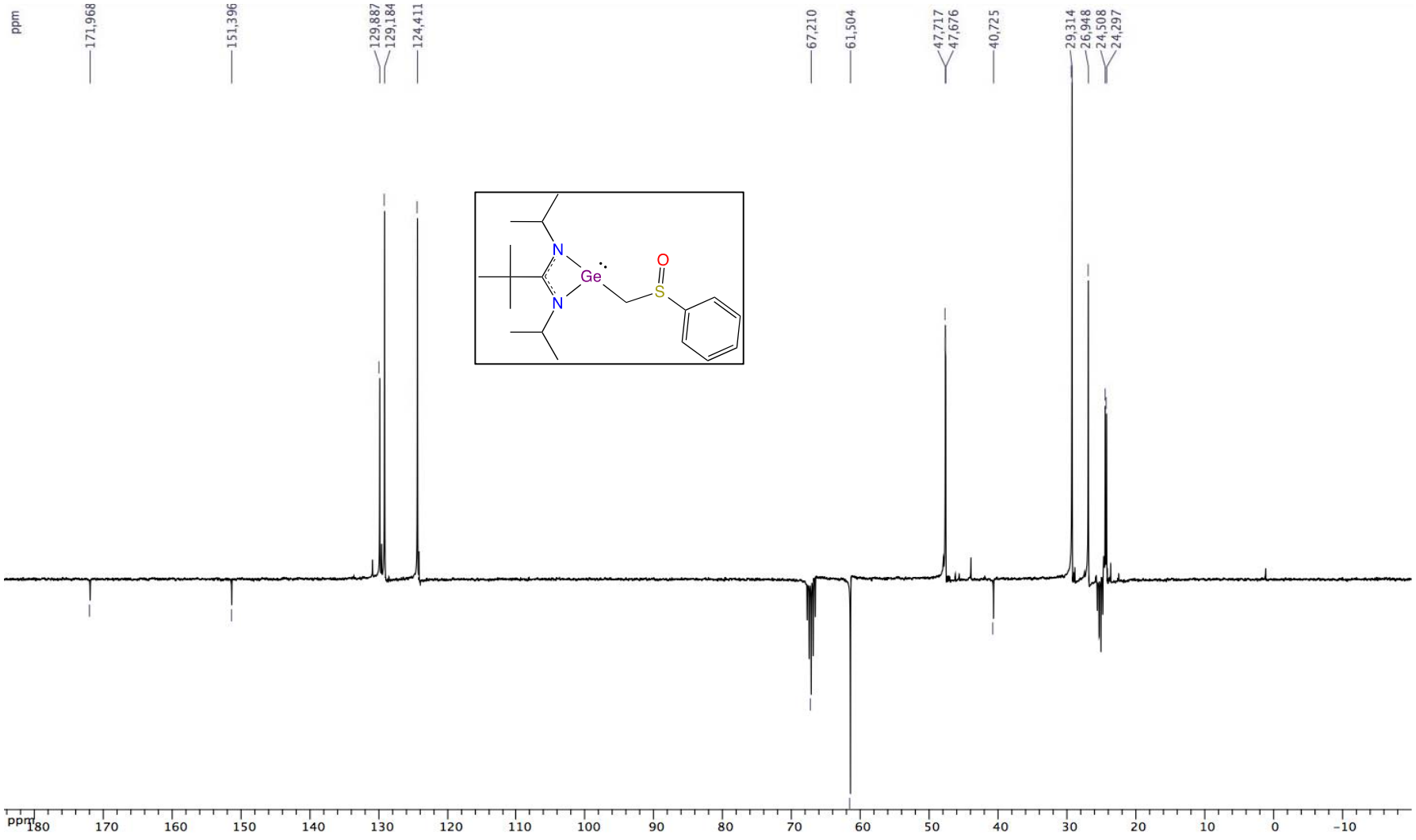
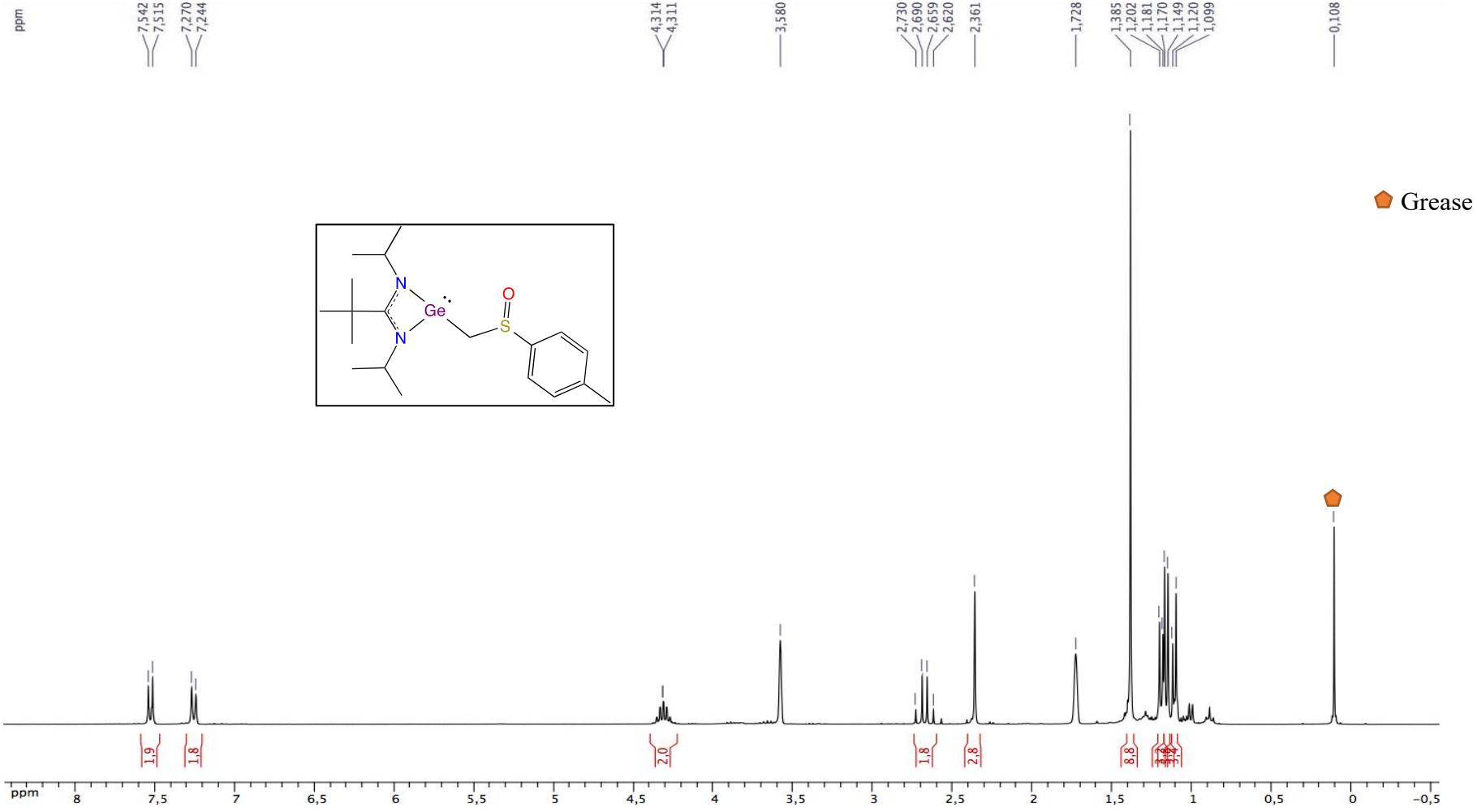


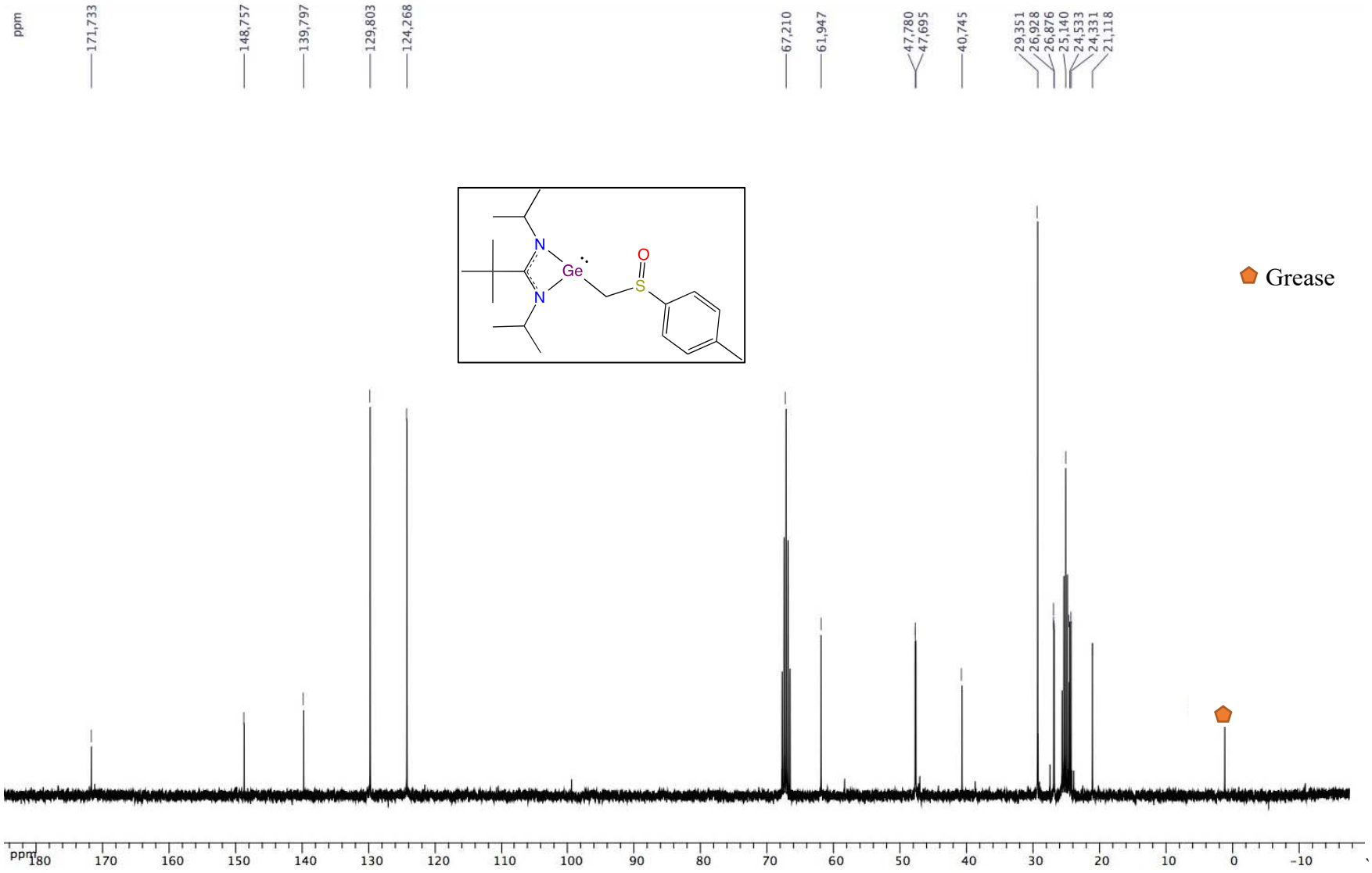
^{1}H NMR spectrum of coumpound **1a** (THF-d_8, 300 MHz)



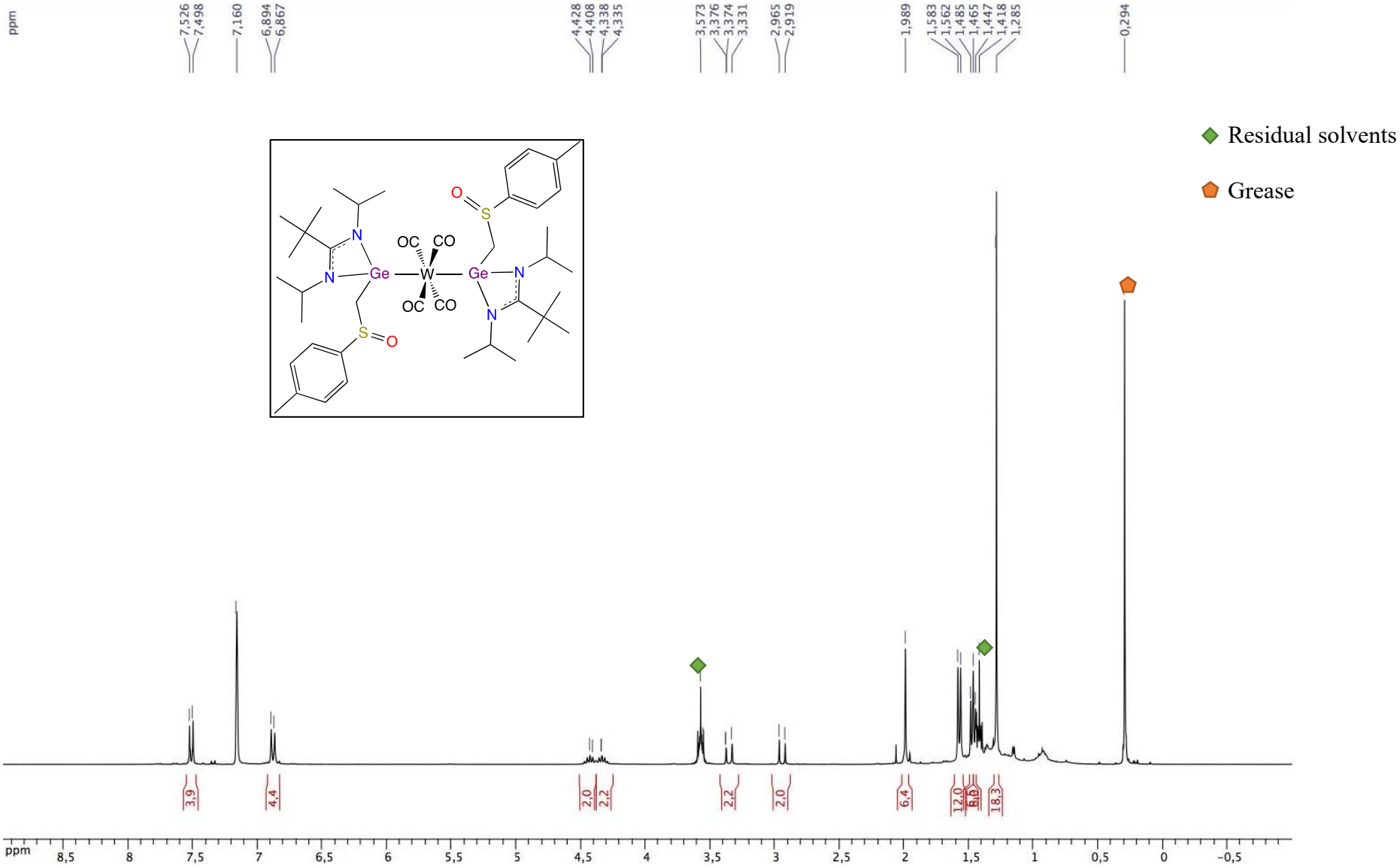
^{13}C NMR spectrum of compound **1a** (THF-d_8, 75 MHz)



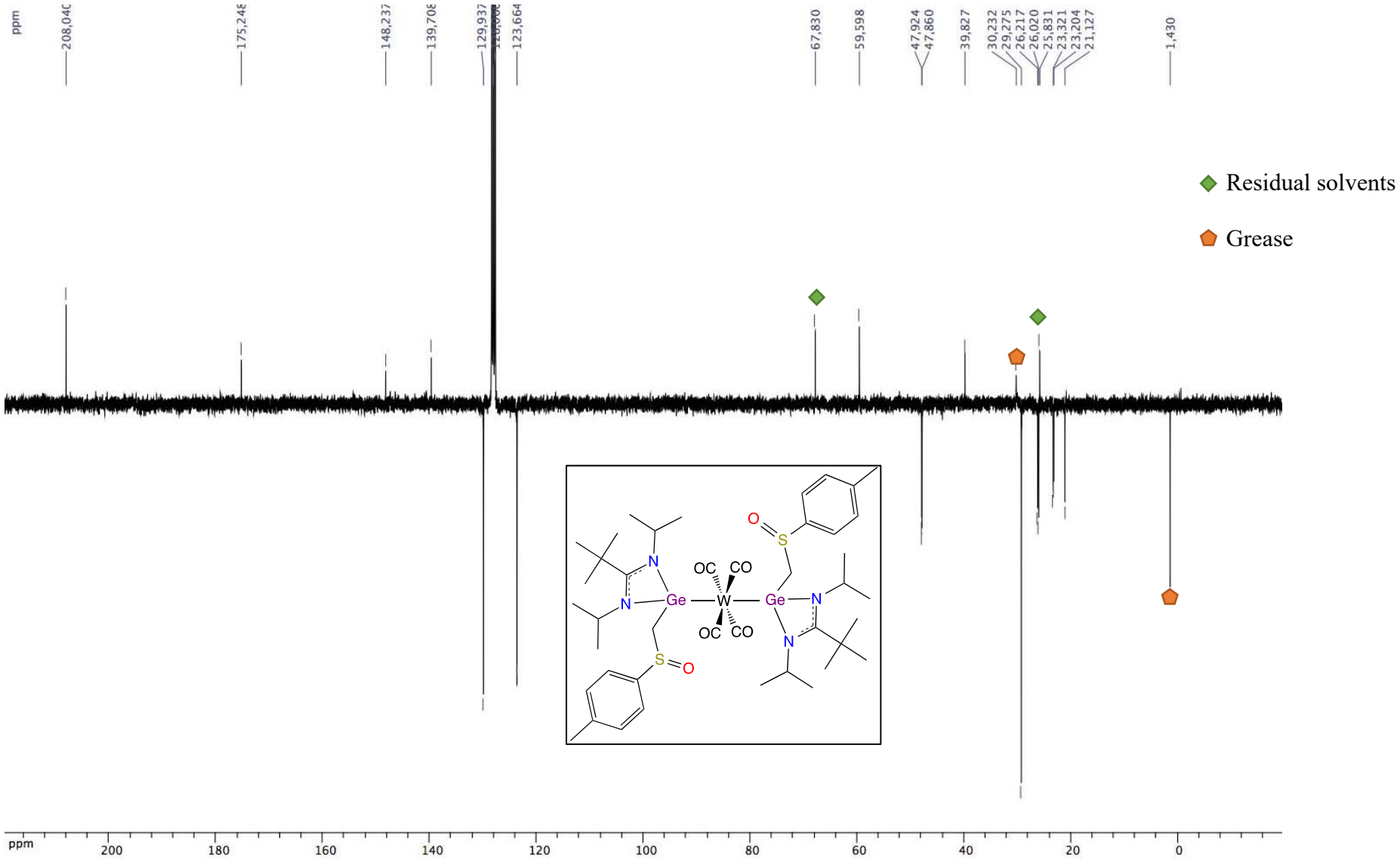
^{1}H NMR spectrum of compound **1b** (THF-d_8, 300 MHz)



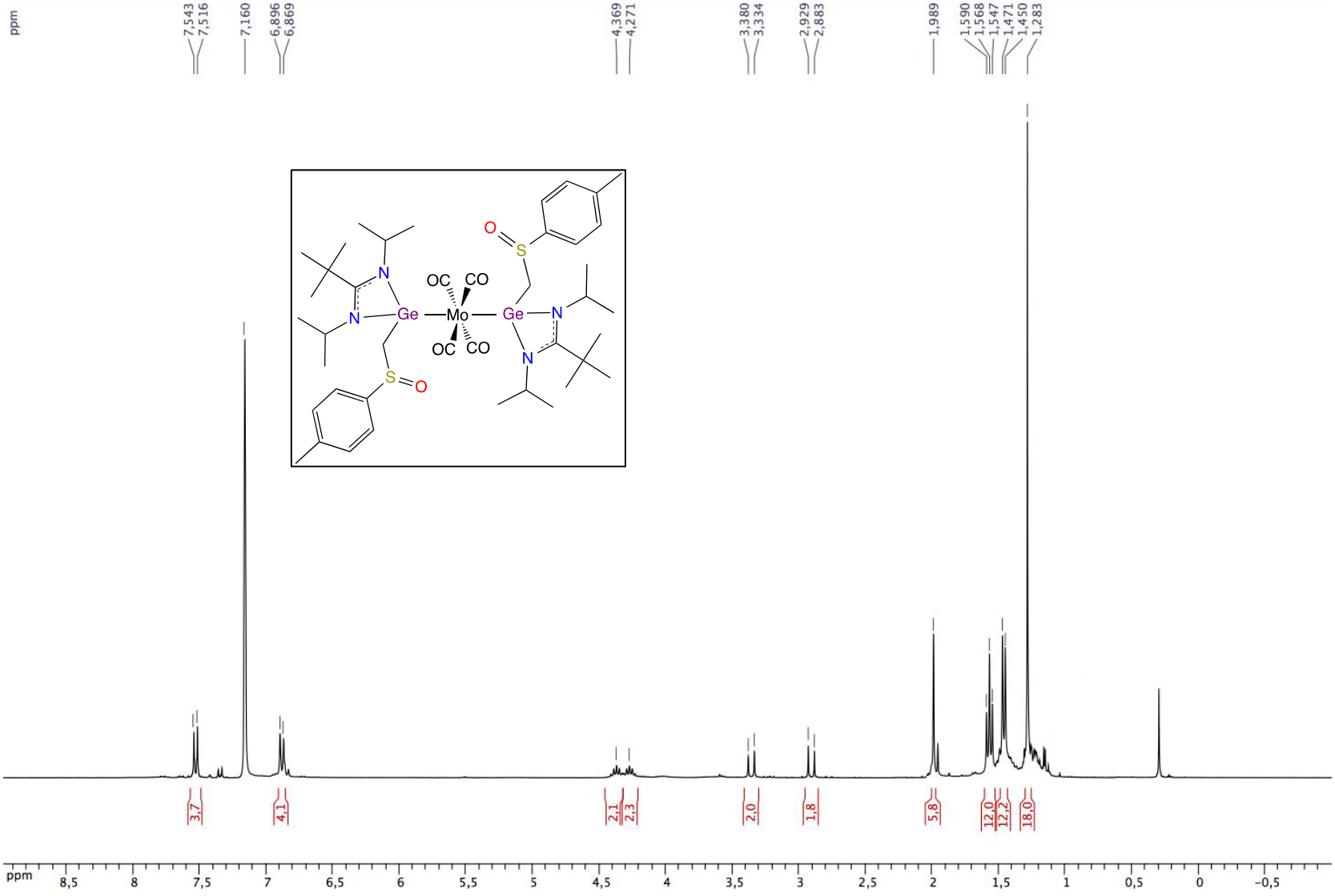
^{13}C NMR spectrum of compound **1b** (THF-d_8, 75 MHz)



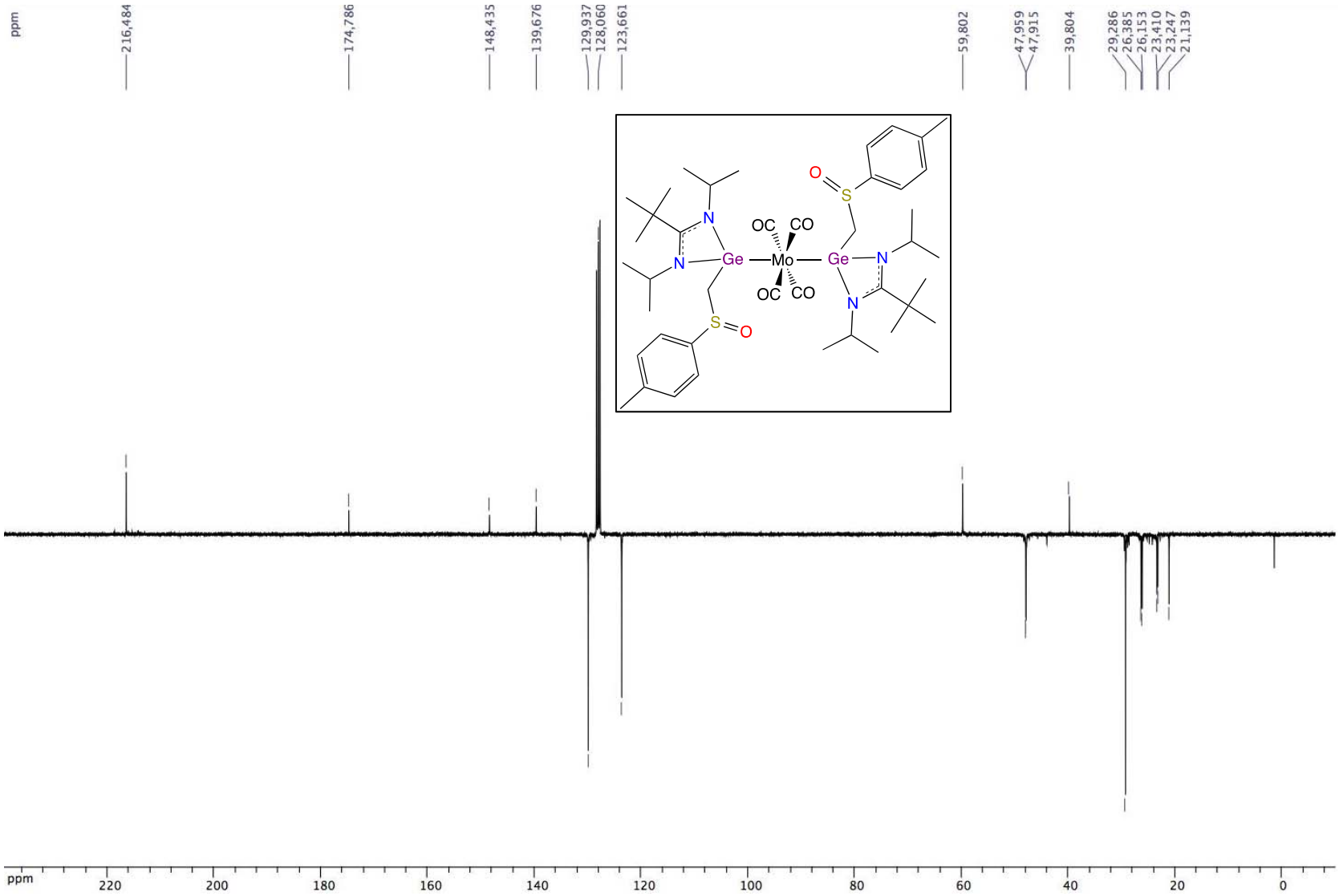
^{1}H NMR spectrum of compound **2a** (C_6D_6, 300 MHz)



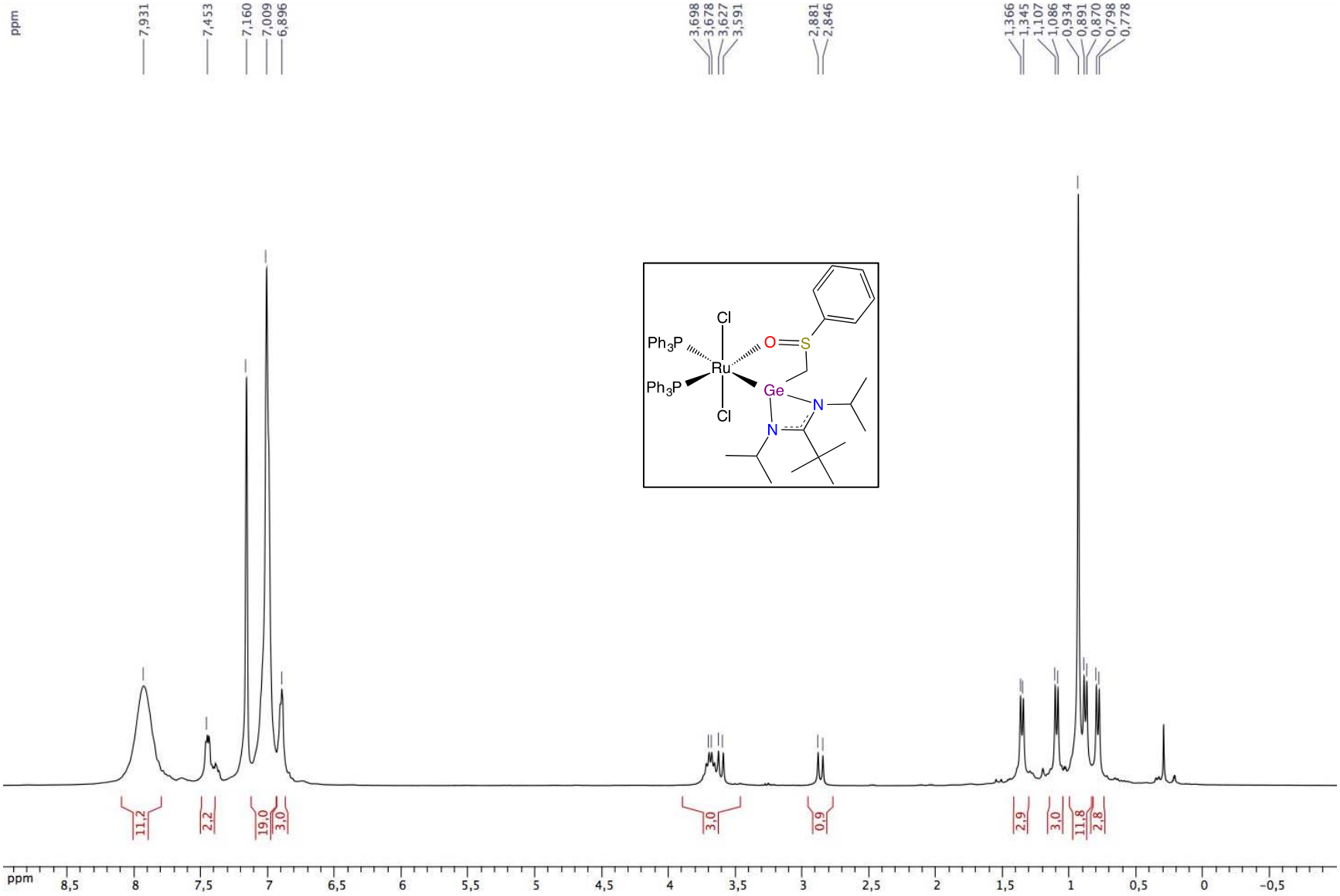
^{13}C NMR spectrum of compound **2a** (C_6D_6, 75 MHz)



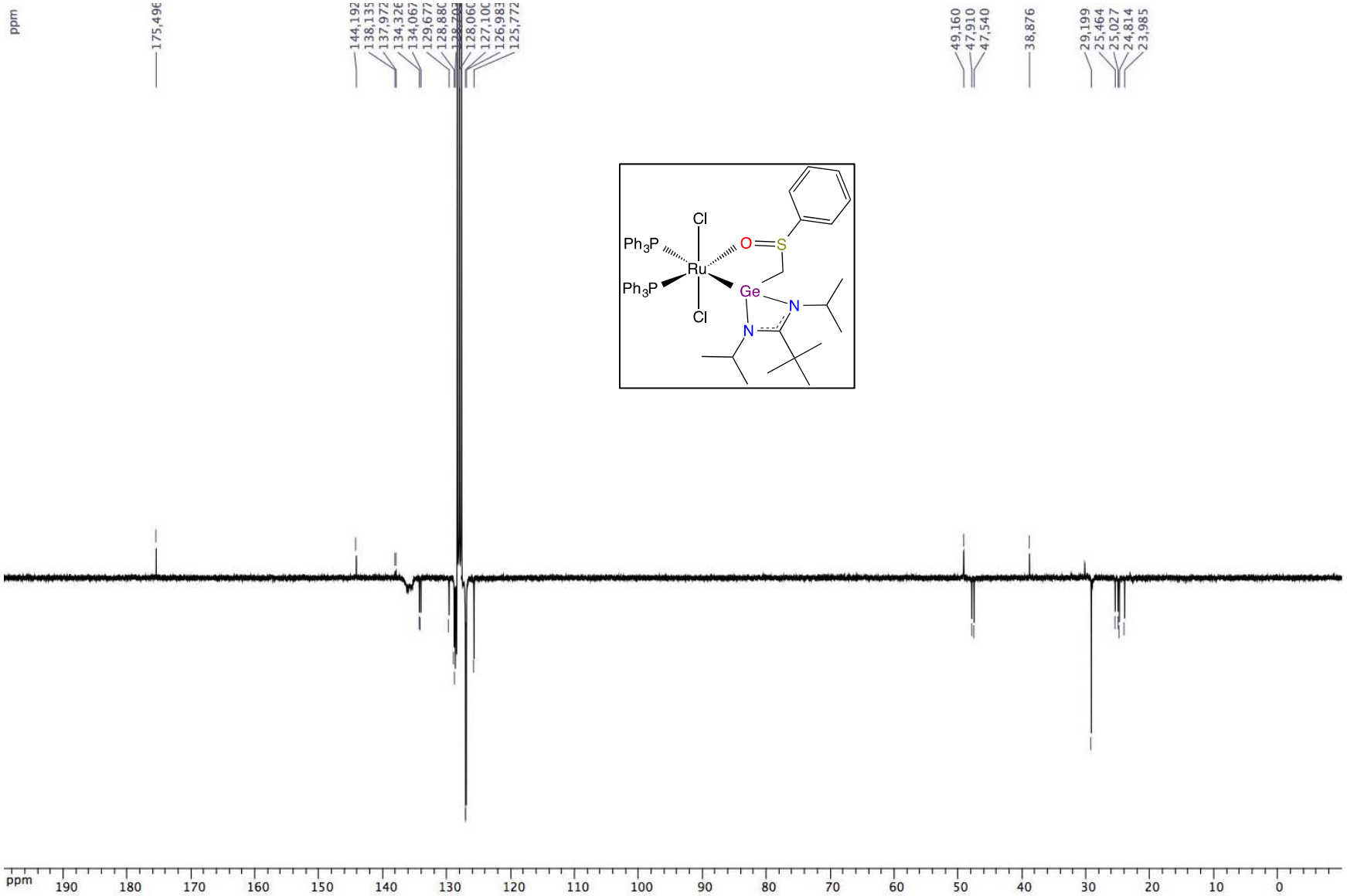
^{1}H NMR spectrum of compound **2b** (C_6D_6, 300 MHz)



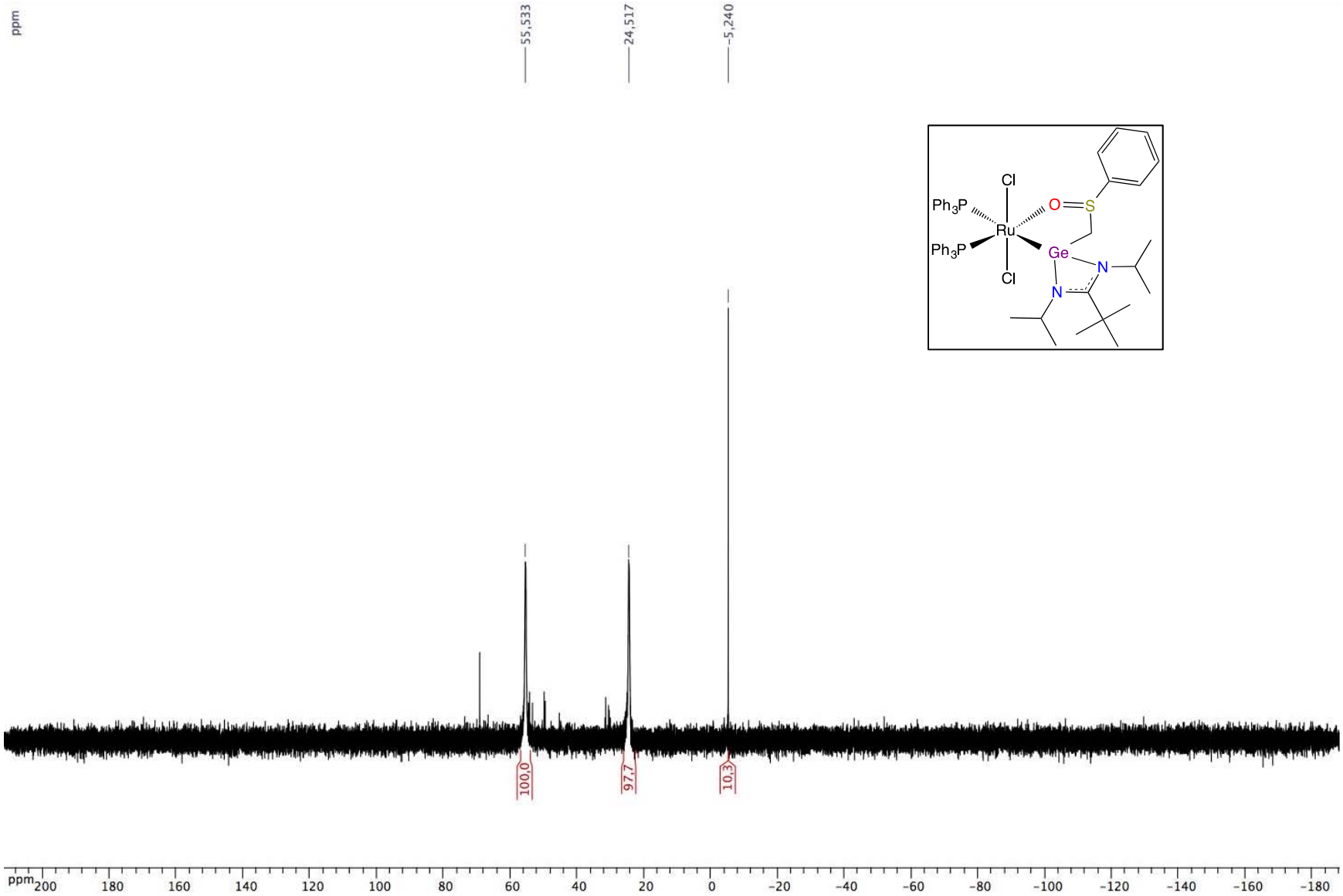
^{13}C NMR spectrum of compound **2b** (C_6D_6, 75 MHz)



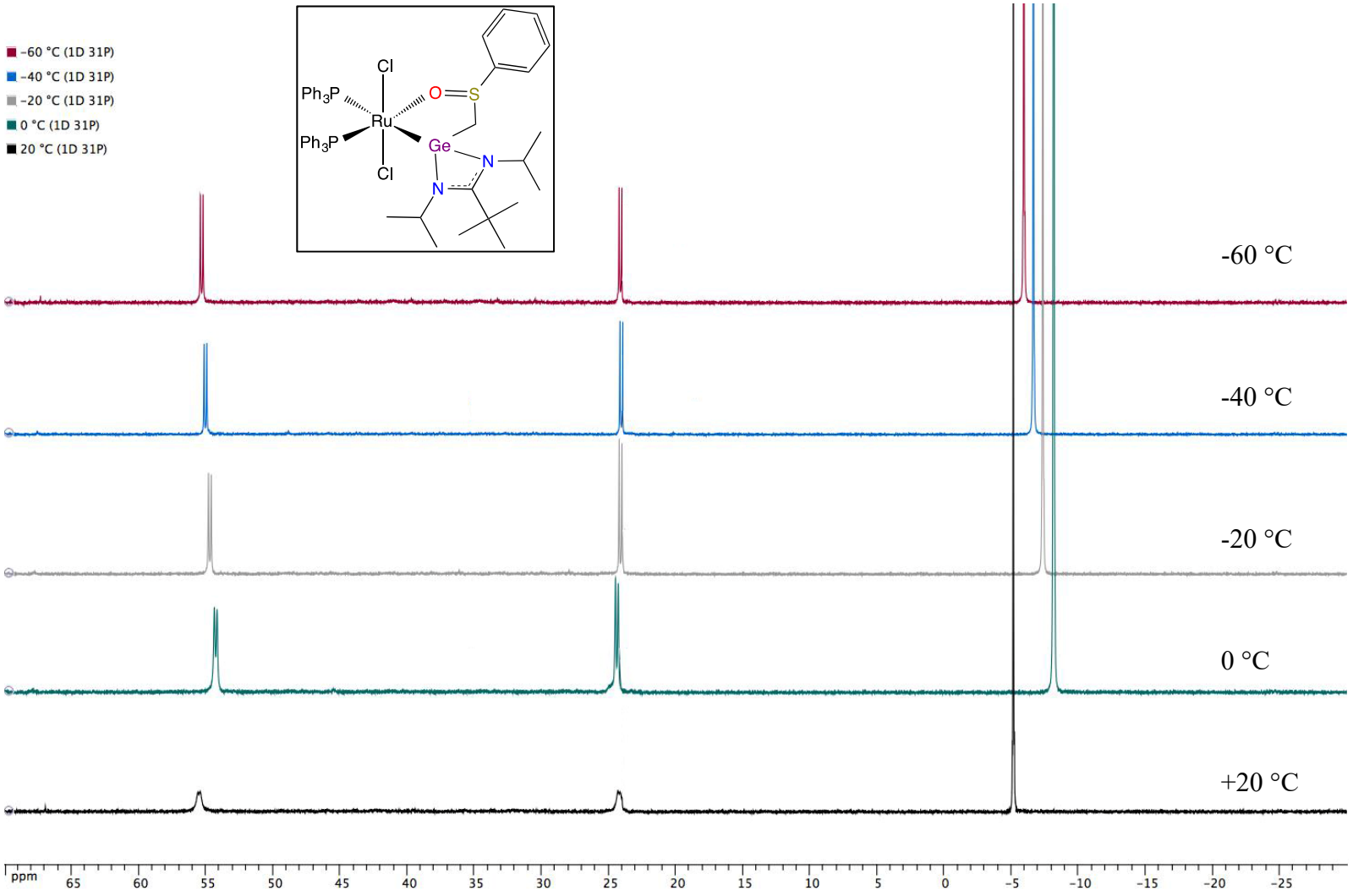
^{1}H NMR spectrum of compound **3a** (C_6D_6, 300 MHz)



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



^{31}P NMR spectrum of compound **3a** (C_6D_6, 121.49 MHz)



VT ^{31}P NMR spectrum of compound **3a** from +20 °C to -60 °C (THF-d_8, 121.49 MHz)

Crystal data and structure refinement of compound 2a

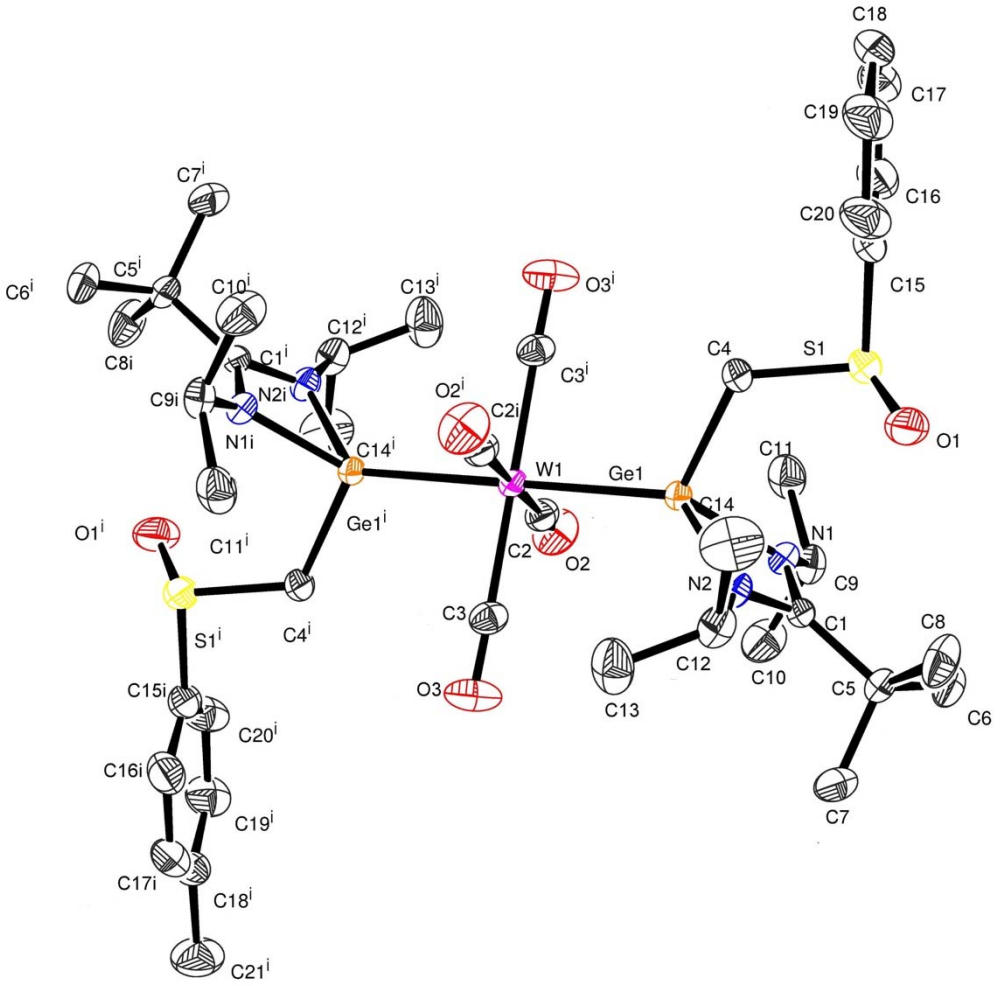


Figure S 2 : Molecule 2a

Table 1 : Crystal data and structure refinement for 2a

Empirical formula	C42 H64 Ge2 N4 O6 S2 W, 2(C4 H8 O)
Formula weight	1258.36
Temperature	193(2) K
Wavelength	0.71073 A
Crystal system, space group	triclinic, P -1
Unit cell dimensions	a = 9.9512(4) A alpha = 79.8470(10) deg.
	b = 11.6654(5) A beta = 77.244(2) deg.
	c = 13.3526(6) A gamma = 70.587(2) deg.
Volume	1416.88(11) A^3
Z, Calculated density	1, 1.475 Mg/m^3
Absorption coefficient	3.203 mm^-1

F(000)	642
Crystal size	0.16 x 0.12 x 0.04 mm
Theta range for data collection	3.15 to 31.91 deg.
Limiting indices	-14<=h<=14, -17<=k<=17, -19<=l<=19
Reflections collected / unique	36625 / 9692 [R(int) = 0.0346]
Completeness to theta = 31.91	99.5 %
Max. and min. transmission	0.7463 and 0.6343
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9692 / 37 / 332
Goodness-of-fit on F^2	1.114
Final R indices [I>2sigma(I)]	R1 = 0.0301, wR2 = 0.0544
R indices (all data)	R1 = 0.0396, wR2 = 0.0576
Largest diff. peak and hole	0.751 and -0.764 e.A^-3

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

	x	y	z	U(eq)
C(1)	1143(2)	7232(2)	3305(2)	21(1)
C(2)	3596(2)	5307(2)	6348(2)	27(1)
C(3)	4071(2)	3784(2)	4787(2)	28(1)
C(5)	-253(2)	7585(2)	2859(2)	27(1)
C(6)	-1535(3)	8509(2)	3445(2)	36(1)
C(7)	-672(3)	6421(2)	2889(2)	41(1)
C(8)	8(3)	8203(3)	1746(2)	44(1)
C(9)	365(2)	8028(2)	5087(2)	29(1)
C(10)	-231(3)	7047(3)	5748(2)	44(1)
C(11)	1200(3)	8476(2)	5681(2)	39(1)
C(12)	2901(3)	5938(2)	1924(2)	30(1)
C(13)	3589(4)	4580(3)	2201(2)	48(1)
C(14)	3952(4)	6491(3)	1161(2)	55(1)
C(16)	4638(3)	10939(2)	2948(2)	42(1)
C(17)	5720(3)	11491(2)	2619(2)	42(1)
C(18)	6592(3)	11347(2)	1665(2)	39(1)
C(19)	6367(3)	10639(3)	1027(2)	45(1)
C(20)	5294(4)	10072(3)	1345(2)	47(1)
C(21)	7783(4)	11933(3)	1330(3)	59(1)
C(22)	1015(6)	3288(5)	1317(3)	98(2)
C(23)	1457(5)	2471(5)	539(4)	90(1)
C(24)	2591(5)	2923(4)	-192(4)	82(1)
C(25)	2084(4)	4252(4)	-106(3)	72(1)
N(1)	1346(2)	7564(2)	4160(1)	23(1)
N(2)	2436(2)	6551(2)	2863(1)	24(1)
O(2)	2826(2)	5454(2)	7123(2)	46(1)
O(3)	3561(2)	3074(2)	4681(2)	47(1)
O(4)	1215(3)	4437(3)	872(2)	74(1)
C(4)	4229(2)	8064(2)	3287(2)	29(1)
C(15)	4442(3)	10221(2)	2310(2)	38(1)
S(1)	3030(6)	9510(5)	2842(4)	39(1)
O(1)	2512(4)	9369(3)	1926(3)	55(1)
S(1')	3170(9)	9362(7)	2592(6)	44(1)
O(1')	2007(5)	10073(4)	3336(5)	67(2)
Ge(1)	3416(1)	6698(1)	3936(1)	20(1)
W(1)	5000	5000	5000	20(1)

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

C(1)-N(2)	1.335(3)
C(1)-N(1)	1.344(3)
C(1)-C(5)	1.534(3)
C(1)-Ge(1)	2.436(2)
C(2)-O(2)	1.145(3)
C(2)-W(1)	2.026(2)
C(3)-O(3)	1.147(3)
C(3)-W(1)	2.020(2)
C(5)-C(6)	1.531(3)
C(5)-C(8)	1.539(3)
C(5)-C(7)	1.540(3)
C(6)-H(6A)	0.9800
C(6)-H(6B)	0.9800
C(6)-H(6C)	0.9800
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)	1.459(3)
C(9)-C(10)	1.518(3)
C(9)-C(11)	1.523(3)
C(9)-H(9)	1.0000
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-N(2)	1.462(3)
C(12)-C(14)	1.515(4)
C(12)-C(13)	1.517(4)
C(12)-H(12)	1.0000
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(16)-C(15)	1.377(4)
C(16)-C(17)	1.385(4)
C(16)-H(16)	0.9500
C(17)-C(18)	1.377(4)
C(17)-H(17)	0.9500
C(18)-C(19)	1.383(4)
C(18)-C(21)	1.506(4)
C(19)-C(20)	1.389(4)
C(19)-H(19)	0.9500
C(20)-C(15)	1.382(4)
C(20)-H(20)	0.9500
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800

C(22)-O(4)	1.426(5)
C(22)-C(23)	1.432(6)
C(22)-H(22A)	0.9900
C(22)-H(22B)	0.9900
C(23)-C(24)	1.494(5)
C(23)-H(23A)	0.9900
C(23)-H(23B)	0.9900
C(24)-C(25)	1.480(6)
C(24)-H(24A)	0.9900
C(24)-H(24B)	0.9900
C(25)-O(4)	1.406(4)
C(25)-H(25A)	0.9900
C(25)-H(25B)	0.9900
N(1)-Ge(1)	1.9506(18)
N(2)-Ge(1)	1.9609(17)
C(4)-S(1')	1.772(8)
C(4)-S(1)	1.801(6)
C(4)-Ge(1)	2.002(2)
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
C(15)-S(1')	1.803(9)
C(15)-S(1)	1.815(6)
S(1)-O(1)	1.481(6)
S(1')-O(1')	1.470(8)
Ge(1)-W(1)	2.5195(2)
W(1)-C(3)#1	2.019(2)
W(1)-C(2)#1	2.026(2)
W(1)-Ge(1)#1	2.5195(2)

N(2)-C(1)-N(1)	106.56(17)
N(2)-C(1)-C(5)	124.78(19)
N(1)-C(1)-C(5)	128.60(19)
N(2)-C(1)-Ge(1)	53.49(10)
N(1)-C(1)-Ge(1)	53.07(10)
C(5)-C(1)-Ge(1)	177.40(15)
O(2)-C(2)-W(1)	178.2(2)
O(3)-C(3)-W(1)	178.4(2)
C(6)-C(5)-C(1)	113.87(19)
C(6)-C(5)-C(8)	106.0(2)
C(1)-C(5)-C(8)	108.85(19)
C(6)-C(5)-C(7)	108.2(2)
C(1)-C(5)-C(7)	108.59(19)
C(8)-C(5)-C(7)	111.4(2)
C(5)-C(6)-H(6A)	109.5
C(5)-C(6)-H(6B)	109.5
H(6A)-C(6)-H(6B)	109.5
C(5)-C(6)-H(6C)	109.5
H(6A)-C(6)-H(6C)	109.5
H(6B)-C(6)-H(6C)	109.5
C(5)-C(7)-H(7A)	109.5
C(5)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(5)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
C(5)-C(8)-H(8A)	109.5
C(5)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5

C(5)-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)-C(10)	111.2(2)
N(1)-C(9)-C(11)	107.75(19)
C(10)-C(9)-C(11)	111.0(2)
N(1)-C(9)-H(9)	109.0
C(10)-C(9)-H(9)	109.0
C(11)-C(9)-H(9)	109.0
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(9)-C(11)-H(11A)	109.5
C(9)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(9)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
N(2)-C(12)-C(14)	109.6(2)
N(2)-C(12)-C(13)	109.3(2)
C(14)-C(12)-C(13)	111.2(2)
N(2)-C(12)-H(12)	108.9
C(14)-C(12)-H(12)	108.9
C(13)-C(12)-H(12)	108.9
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(15)-C(16)-C(17)	119.2(3)
C(15)-C(16)-H(16)	120.4
C(17)-C(16)-H(16)	120.4
C(18)-C(17)-C(16)	121.4(3)
C(18)-C(17)-H(17)	119.3
C(16)-C(17)-H(17)	119.3
C(17)-C(18)-C(19)	118.7(2)
C(17)-C(18)-C(21)	120.6(3)
C(19)-C(18)-C(21)	120.7(3)
C(18)-C(19)-C(20)	120.8(3)
C(18)-C(19)-H(19)	119.6
C(20)-C(19)-H(19)	119.6
C(15)-C(20)-C(19)	119.4(3)
C(15)-C(20)-H(20)	120.3
C(19)-C(20)-H(20)	120.3
C(18)-C(21)-H(21A)	109.5
C(18)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(18)-C(21)-H(21C)	109.5

H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
O(4)-C(22)-C(23)	109.7(3)
O(4)-C(22)-H(22A)	109.7
C(23)-C(22)-H(22A)	109.7
O(4)-C(22)-H(22B)	109.7
C(23)-C(22)-H(22B)	109.7
H(22A)-C(22)-H(22B)	108.2
C(22)-C(23)-C(24)	101.9(4)
C(22)-C(23)-H(23A)	111.4
C(24)-C(23)-H(23A)	111.4
C(22)-C(23)-H(23B)	111.4
C(24)-C(23)-H(23B)	111.4
H(23A)-C(23)-H(23B)	109.3
C(25)-C(24)-C(23)	103.4(3)
C(25)-C(24)-H(24A)	111.1
C(23)-C(24)-H(24A)	111.1
C(25)-C(24)-H(24B)	111.1
C(23)-C(24)-H(24B)	111.1
H(24A)-C(24)-H(24B)	109.1
O(4)-C(25)-C(24)	107.7(3)
O(4)-C(25)-H(25A)	110.2
C(24)-C(25)-H(25A)	110.2
O(4)-C(25)-H(25B)	110.2
C(24)-C(25)-H(25B)	110.2
H(25A)-C(25)-H(25B)	108.5
C(1)-N(1)-C(9)	133.08(18)
C(1)-N(1)-Ge(1)	93.51(13)
C(9)-N(1)-Ge(1)	130.62(14)
C(1)-N(2)-C(12)	132.06(18)
C(1)-N(2)-Ge(1)	93.32(13)
C(12)-N(2)-Ge(1)	134.62(15)
C(25)-O(4)-C(22)	106.6(3)
S(1')-C(4)-S(1)	12.2(4)
S(1')-C(4)-Ge(1)	119.7(3)
S(1)-C(4)-Ge(1)	119.2(2)
S(1')-C(4)-H(4A)	116.9
S(1)-C(4)-H(4A)	107.5
Ge(1)-C(4)-H(4A)	107.5
S(1')-C(4)-H(4B)	96.6
S(1)-C(4)-H(4B)	107.5
Ge(1)-C(4)-H(4B)	107.5
H(4A)-C(4)-H(4B)	107.0
C(16)-C(15)-C(20)	120.5(2)
C(16)-C(15)-S(1')	127.1(3)
C(20)-C(15)-S(1')	112.3(3)
C(16)-C(15)-S(1)	115.1(3)
C(20)-C(15)-S(1)	124.4(3)
S(1')-C(15)-S(1)	12.0(4)
O(1)-S(1)-C(4)	109.4(4)
O(1)-S(1)-C(15)	104.4(3)
C(4)-S(1)-C(15)	95.4(3)
O(1')-S(1')-C(4)	108.3(5)
O(1')-S(1')-C(15)	102.0(5)
C(4)-S(1')-C(15)	96.9(4)
N(1)-Ge(1)-N(2)	66.61(7)
N(1)-Ge(1)-C(4)	101.18(8)
N(2)-Ge(1)-C(4)	102.18(9)

N(1)-Ge(1)-C(1)	33.42(7)
N(2)-Ge(1)-C(1)	33.19(7)
C(4)-Ge(1)-C(1)	104.10(8)
N(1)-Ge(1)-W(1)	132.68(5)
N(2)-Ge(1)-W(1)	127.82(5)
C(4)-Ge(1)-W(1)	115.30(6)
C(1)-Ge(1)-W(1)	140.48(5)
C(3)#1-W(1)-C(3)	180.000(1)
C(3)#1-W(1)-C(2)	91.01(9)
C(3)-W(1)-C(2)	88.99(9)
C(3)#1-W(1)-C(2)#1	88.99(9)
C(3)-W(1)-C(2)#1	91.01(9)
C(2)-W(1)-C(2)#1	180.0
C(3)#1-W(1)-Ge(1)	88.12(7)
C(3)-W(1)-Ge(1)	91.88(7)
C(2)-W(1)-Ge(1)	94.54(6)
C(2)#1-W(1)-Ge(1)	85.46(6)
C(3)#1-W(1)-Ge(1)#1	91.88(7)
C(3)-W(1)-Ge(1)#1	88.12(7)
C(2)-W(1)-Ge(1)#1	85.46(6)
C(2)#1-W(1)-Ge(1)#1	94.54(6)
Ge(1)-W(1)-Ge(1)#1	179.999(9)

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

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for ?.
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)	19(1)	26(1)	4(1)	-8(1)	-8(1)
C(2)	25(1)	30(1)	27(1)	1(1)	-6(1)	-10(1)
C(3)	26(1)	34(1)	24(1)	1(1)	-4(1)	-14(1)
C(5)	21(1)	28(1)	34(1)	1(1)	-12(1)	-6(1)
C(6)	24(1)	34(1)	45(2)	-3(1)	-14(1)	-1(1)
C(7)	31(1)	40(1)	58(2)	-10(1)	-16(1)	-14(1)
C(8)	34(1)	55(2)	36(1)	7(1)	-16(1)	-4(1)
C(9)	25(1)	27(1)	28(1)	-5(1)	-6(1)	0(1)
C(10)	37(2)	61(2)	33(1)	9(1)	-5(1)	-21(1)
C(11)	48(2)	31(1)	38(1)	-12(1)	-14(1)	-4(1)
C(12)	27(1)	35(1)	26(1)	-9(1)	-6(1)	-4(1)
C(13)	58(2)	37(1)	46(2)	-16(1)	-20(1)	2(1)
C(14)	53(2)	76(2)	35(2)	-14(2)	9(1)	-26(2)
C(16)	39(2)	30(1)	53(2)	-2(1)	-1(1)	-9(1)
C(17)	44(2)	28(1)	55(2)	-6(1)	-7(1)	-13(1)
C(18)	39(1)	31(1)	48(2)	11(1)	-14(1)	-18(1)
C(19)	57(2)	45(2)	35(1)	9(1)	-9(1)	-26(1)
C(20)	68(2)	46(2)	39(1)	12(1)	-24(1)	-35(2)
C(21)	59(2)	64(2)	64(2)	10(2)	-12(2)	-40(2)
C(22)	116(4)	128(4)	51(2)	-16(3)	18(2)	-58(4)
C(23)	88(3)	92(3)	100(4)	-18(3)	-1(3)	-47(3)
C(24)	67(3)	91(3)	89(3)	-37(3)	19(2)	-34(2)
C(25)	55(2)	88(3)	69(2)	-8(2)	2(2)	-25(2)
N(1)	19(1)	24(1)	26(1)	-2(1)	-6(1)	-5(1)
N(2)	22(1)	27(1)	22(1)	-2(1)	-7(1)	-5(1)
O(2)	36(1)	61(1)	35(1)	-7(1)	3(1)	-13(1)
O(3)	57(1)	56(1)	46(1)	-6(1)	-7(1)	-40(1)
O(4)	66(2)	91(2)	69(2)	-34(2)	0(1)	-28(2)
C(4)	26(1)	22(1)	38(1)	8(1)	-12(1)	-9(1)
C(15)	35(1)	27(1)	54(2)	17(1)	-20(1)	-15(1)
S(1)	33(1)	28(1)	57(2)	14(1)	-20(1)	-14(1)
O(1)	64(2)	48(2)	69(3)	28(2)	-46(2)	-35(2)
S(1')	30(2)	32(2)	65(3)	22(2)	-19(2)	-12(1)
O(1')	32(3)	33(3)	105(5)	12(3)	19(3)	1(2)
Ge(1)	18(1)	18(1)	23(1)	2(1)	-6(1)	-6(1)
W(1)	18(1)	20(1)	24(1)	2(1)	-7(1)	-7(1)

Crystal data and structure refinement of compound 2b

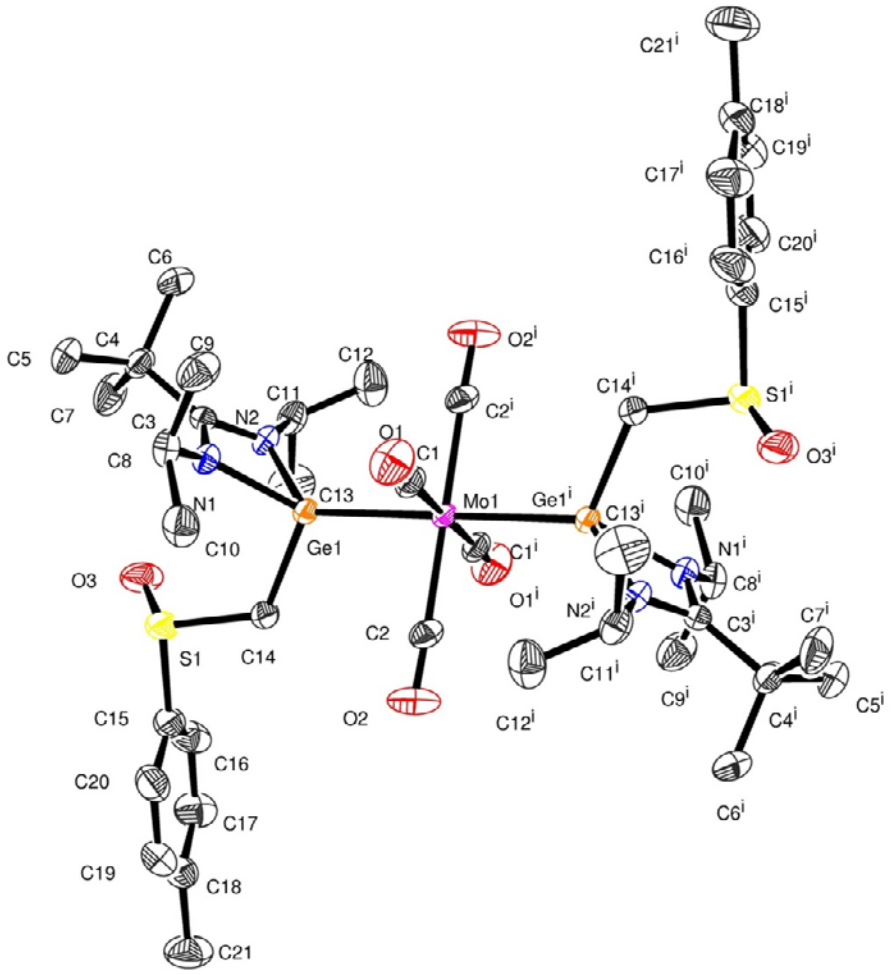


Table 5. Crystal data and structure refinement for 2b.

Identification code	2b
Empirical formula	C42 H64 Ge2 Mo N4 O6 S2,2(C4 H8 O)
Formula weight	1170.42
Temperature	193(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P -1
Unit cell dimensions	a = 9.9669(5) A alpha = 79.929(3) deg. b = 11.7085(8) A beta = 77.221(2) deg. c = 13.3702(10) A gamma = 70.656(2) deg.
Volume	1426.94(16) A^3

Z, Calculated density	1, 1.362 Mg/m^3
Absorption coefficient	1.387 mm^-1
F(000)	610
Crystal size	0.220 x 0.180 x 0.080 mm
Theta range for data collection	3.144 to 25.684 deg.
Limiting indices	-11<=h<=12, -14<=k<=14, -16<=l<=16
Reflections collected / unique	21442 / 5306 [R(int) = 0.0717]
Completeness to theta = 25.242	98.6 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5306 / 37 / 332
Goodness-of-fit on F^2	1.123
Final R indices [I>2sigma(I)]	R1 = 0.0658, wR2 = 0.0867
R indices (all data)	R1 = 0.0947, wR2 = 0.0939
Largest diff. peak and hole	0.804 and -0.946 e.A^-3

Table 6. Atomic coordinates (x 10^4) and equivalent isotropic
displacement parameters (A^2 x 10^3) for nl336b_a.
U(eq) is defined as one third of the trace of the orthogonalized
Uij tensor.

	x	y	z	U(eq)
C(1)	6397(5)	4701(4)	3648(4)	30(1)
C(2)	4066(5)	3784(4)	4785(3)	29(1)
C(3)	8856(5)	2765(4)	6697(3)	23(1)
C(4)	10247(5)	2410(4)	7144(4)	30(1)
C(5)	11531(5)	1490(4)	6557(4)	39(1)
C(6)	10668(6)	3572(5)	7119(4)	44(1)
C(7)	9990(6)	1788(5)	8255(4)	46(1)
C(8)	9631(5)	1973(4)	4912(3)	30(1)
C(9)	10230(6)	2953(5)	4249(4)	47(1)
C(10)	8804(6)	1520(5)	4319(4)	42(1)
C(11)	7095(5)	4056(4)	8079(3)	31(1)
C(12)	6426(6)	5410(5)	7808(4)	49(2)
C(13)	6040(6)	3509(6)	8844(4)	56(2)
C(14)	5770(5)	1940(4)	6709(4)	30(1)
C(15)	5554(6)	-215(4)	7693(4)	39(1)
S(1)	6962(9)	503(8)	7157(10)	41(2)
O(3)	7475(8)	644(6)	8077(6)	57(3)
S(1')	6835(12)	634(11)	7405(13)	46(4)
O(3')	7999(10)	-73(8)	6649(9)	75(4)
C(16)	4703(7)	-72(5)	8657(4)	48(2)
C(17)	3637(6)	-635(5)	8976(4)	46(1)
C(18)	3408(6)	-1341(4)	8336(4)	40(1)
C(19)	4292(6)	-1487(5)	7386(4)	44(1)
C(20)	5363(6)	-934(5)	7058(4)	44(1)
C(21)	2236(7)	-1941(6)	8668(5)	61(2)
C(22)	9005(12)	6721(10)	8691(7)	121(4)
C(23)	8519(10)	7558(8)	9459(7)	102(3)
C(24)	7409(9)	7103(8)	10168(7)	95(3)
C(25)	7919(8)	5756(8)	10111(6)	83(2)
Mo(1)	5000	5000	5000	20(1)
Ge(1)	6586(1)	3305(1)	6062(1)	22(1)
N(1)	8654(4)	2434(3)	5843(3)	25(1)
N(2)	7563(4)	3440(3)	7141(3)	25(1)
O(1)	7169(4)	4554(4)	2871(3)	48(1)
O(2)	3564(4)	3074(4)	4679(3)	50(1)
O(4)	8787(6)	5576(5)	9128(4)	87(2)

Table 7. Bond lengths [A] and angles [deg] for nl336b_a.

C(1)-O(1)	1.150(6)
C(1)-Mo(1)	2.028(5)
C(2)-O(2)	1.144(5)
C(2)-Mo(1)	2.029(5)
C(3)-N(2)	1.338(5)
C(3)-N(1)	1.343(5)
C(3)-C(4)	1.533(6)
C(4)-C(5)	1.533(7)
C(4)-C(7)	1.543(7)
C(4)-C(6)	1.545(6)
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)-H(7A)	0.9800
C(7)-H(7B)	0.9800
C(7)-H(7C)	0.9800
C(8)-N(1)	1.463(6)
C(8)-C(10)	1.522(6)
C(8)-C(9)	1.524(7)
C(8)-H(8)	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)	1.465(6)
C(11)-C(12)	1.515(7)
C(11)-C(13)	1.517(7)
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
C(14)-S(1')	1.787(11)
C(14)-S(1)	1.799(9)
C(14)-Ge(1)	2.008(4)
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(15)-C(20)	1.377(7)
C(15)-C(16)	1.380(8)
C(15)-S(1')	1.804(12)
C(15)-S(1)	1.821(9)
S(1)-O(3)	1.485(13)
S(1')-O(3')	1.480(17)
C(16)-C(17)	1.382(7)
C(16)-H(16)	0.9500
C(17)-C(18)	1.388(7)
C(17)-H(17)	0.9500

C(18)-C(19)	1.378(7)
C(18)-C(21)	1.504(7)
C(19)-C(20)	1.380(7)
C(19)-H(19)	0.9500
C(20)-H(20)	0.9500
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-O(4)	1.431(10)
C(22)-C(23)	1.438(11)
C(22)-H(22A)	0.9900
C(22)-H(22B)	0.9900
C(23)-C(24)	1.468(10)
C(23)-H(23A)	0.9900
C(23)-H(23B)	0.9900
C(24)-C(25)	1.498(10)
C(24)-H(24A)	0.9900
C(24)-H(24B)	0.9900
C(25)-O(4)	1.412(8)
C(25)-H(25A)	0.9900
C(25)-H(25B)	0.9900
Mo(1)-C(1)#1	2.028(5)
Mo(1)-C(2)#1	2.029(5)
Mo(1)-Ge(1)	2.5261(4)
Mo(1)-Ge(1)#1	2.5261(5)
Ge(1)-N(1)	1.955(4)
Ge(1)-N(2)	1.964(4)

O(1)-C(1)-Mo(1)	178.4(4)
O(2)-C(2)-Mo(1)	178.2(4)
N(2)-C(3)-N(1)	106.5(4)
N(2)-C(3)-C(4)	124.8(4)
N(1)-C(3)-C(4)	128.6(4)
C(3)-C(4)-C(5)	114.0(4)
C(3)-C(4)-C(7)	109.1(4)
C(5)-C(4)-C(7)	105.8(4)
C(3)-C(4)-C(6)	108.5(4)
C(5)-C(4)-C(6)	108.2(4)
C(7)-C(4)-C(6)	111.3(4)
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(4)-C(7)-H(7A)	109.5
C(4)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(4)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
N(1)-C(8)-C(10)	108.2(4)

N(1)-C(8)-C(9)	111.3(4)
C(10)-C(8)-C(9)	111.1(4)
N(1)-C(8)-H(8)	108.7
C(10)-C(8)-H(8)	108.7
C(9)-C(8)-H(8)	108.7
C(8)-C(9)-H(9A)	109.5
C(8)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(8)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(8)-C(10)-H(10A)	109.5
C(8)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(8)-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(12)	109.7(4)
N(2)-C(11)-C(13)	109.7(4)
C(12)-C(11)-C(13)	111.4(4)
N(2)-C(11)-H(11)	108.7
C(12)-C(11)-H(11)	108.7
C(13)-C(11)-H(11)	108.7
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
S(1')-C(14)-Ge(1)	119.8(4)
S(1)-C(14)-Ge(1)	119.2(3)
S(1)-C(14)-H(14A)	107.5
Ge(1)-C(14)-H(14A)	107.5
S(1)-C(14)-H(14B)	107.5
Ge(1)-C(14)-H(14B)	107.5
H(14A)-C(14)-H(14B)	107.0
C(20)-C(15)-C(16)	120.3(5)
C(20)-C(15)-S(1')	126.7(7)
C(16)-C(15)-S(1')	113.0(7)
C(20)-C(15)-S(1)	115.1(6)
C(16)-C(15)-S(1)	124.7(6)
O(3)-S(1)-C(14)	109.5(7)
O(3)-S(1)-C(15)	104.0(7)
C(14)-S(1)-C(15)	95.8(4)
O(3')-S(1')-C(14)	107.9(10)
O(3')-S(1')-C(15)	102.5(10)
C(14)-S(1')-C(15)	96.8(6)
C(15)-C(16)-C(17)	119.8(5)
C(15)-C(16)-H(16)	120.1
C(17)-C(16)-H(16)	120.1
C(16)-C(17)-C(18)	120.7(5)
C(16)-C(17)-H(17)	119.7

C(18)-C(17)-H(17)	119.7
C(19)-C(18)-C(17)	118.3(5)
C(19)-C(18)-C(21)	120.5(5)
C(17)-C(18)-C(21)	121.2(5)
C(18)-C(19)-C(20)	121.6(5)
C(18)-C(19)-H(19)	119.2
C(20)-C(19)-H(19)	119.2
C(15)-C(20)-C(19)	119.3(5)
C(15)-C(20)-H(20)	120.4
C(19)-C(20)-H(20)	120.4
C(18)-C(21)-H(21A)	109.5
C(18)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(18)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
O(4)-C(22)-C(23)	110.4(7)
O(4)-C(22)-H(22A)	109.6
C(23)-C(22)-H(22A)	109.6
O(4)-C(22)-H(22B)	109.6
C(23)-C(22)-H(22B)	109.6
H(22A)-C(22)-H(22B)	108.1
C(22)-C(23)-C(24)	101.7(7)
C(22)-C(23)-H(23A)	111.4
C(24)-C(23)-H(23A)	111.4
C(22)-C(23)-H(23B)	111.4
C(24)-C(23)-H(23B)	111.4
H(23A)-C(23)-H(23B)	109.3
C(23)-C(24)-C(25)	104.9(7)
C(23)-C(24)-H(24A)	110.8
C(25)-C(24)-H(24A)	110.8
C(23)-C(24)-H(24B)	110.8
C(25)-C(24)-H(24B)	110.8
H(24A)-C(24)-H(24B)	108.8
O(4)-C(25)-C(24)	106.1(6)
O(4)-C(25)-H(25A)	110.5
C(24)-C(25)-H(25A)	110.5
O(4)-C(25)-H(25B)	110.5
C(24)-C(25)-H(25B)	110.5
H(25A)-C(25)-H(25B)	108.7
C(1)#1-Mo(1)-C(1)	180.0(3)
C(1)#1-Mo(1)-C(2)	88.96(18)
C(1)-Mo(1)-C(2)	91.04(18)
C(1)#1-Mo(1)-C(2)#1	91.04(18)
C(1)-Mo(1)-C(2)#1	88.96(18)
C(2)-Mo(1)-C(2)#1	180.0
C(1)#1-Mo(1)-Ge(1)	85.27(12)
C(1)-Mo(1)-Ge(1)	94.73(12)
C(2)-Mo(1)-Ge(1)	88.14(13)
C(2)#1-Mo(1)-Ge(1)	91.86(13)
C(1)#1-Mo(1)-Ge(1)#1	94.73(12)
C(1)-Mo(1)-Ge(1)#1	85.27(12)
C(2)-Mo(1)-Ge(1)#1	91.86(13)
C(2)#1-Mo(1)-Ge(1)#1	88.14(13)
Ge(1)-Mo(1)-Ge(1)#1	180.0
N(1)-Ge(1)-N(2)	66.47(15)
N(1)-Ge(1)-C(14)	100.89(17)
N(2)-Ge(1)-C(14)	101.79(17)

N(1)-Ge(1)-Mo(1)	133.06(11)
N(2)-Ge(1)-Mo(1)	128.14(11)
C(14)-Ge(1)-Mo(1)	115.26(13)
C(3)-N(1)-C(8)	133.3(4)
C(3)-N(1)-Ge(1)	93.6(3)
C(8)-N(1)-Ge(1)	130.1(3)
C(3)-N(2)-C(11)	132.1(4)
C(3)-N(2)-Ge(1)	93.4(3)
C(11)-N(2)-Ge(1)	134.5(3)
C(25)-O(4)-C(22)	106.7(6)

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

Table 8. Anisotropic displacement parameters (A^2 x 10^3) for nl336b_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)	22(3)	33(3)	34(3)	6(2)	-11(2)	-9(2)
C(2)	22(3)	37(3)	29(3)	-1(2)	-2(2)	-13(2)
C(3)	22(2)	20(2)	29(2)	2(2)	-6(2)	-9(2)
C(4)	22(3)	34(3)	34(3)	0(2)	-10(2)	-8(2)
C(5)	26(3)	38(3)	50(3)	-2(2)	-16(2)	-4(2)
C(6)	32(3)	43(3)	65(4)	-9(3)	-18(3)	-16(2)
C(7)	36(3)	54(4)	41(3)	11(3)	-18(2)	-5(3)
C(8)	26(3)	29(3)	29(3)	-4(2)	-7(2)	1(2)
C(9)	36(3)	64(4)	40(3)	8(3)	-7(2)	-20(3)
C(10)	47(3)	38(3)	41(3)	-16(2)	-14(3)	-4(2)
C(11)	28(3)	39(3)	26(3)	-6(2)	-9(2)	-5(2)
C(12)	59(4)	39(3)	45(3)	-15(3)	-21(3)	0(3)
C(13)	54(4)	77(5)	35(3)	-14(3)	10(3)	-24(3)
C(14)	25(3)	26(3)	40(3)	6(2)	-11(2)	-10(2)
C(15)	36(3)	30(3)	53(3)	16(2)	-18(3)	-16(2)
S(1)	40(3)	30(2)	59(5)	17(3)	-24(3)	-19(2)
O(3)	65(5)	51(5)	73(5)	29(4)	-49(4)	-37(4)
S(1')	32(3)	41(4)	62(7)	21(4)	-18(3)	-12(2)
O(3')	32(6)	35(6)	120(10)	14(5)	24(6)	5(4)
C(16)	70(4)	43(3)	44(3)	14(3)	-27(3)	-32(3)
C(17)	59(4)	52(4)	34(3)	11(3)	-11(3)	-30(3)
C(18)	44(3)	31(3)	48(3)	9(2)	-16(3)	-16(2)
C(19)	48(4)	29(3)	58(4)	-5(3)	-11(3)	-13(2)
C(20)	41(3)	30(3)	55(4)	-3(3)	-1(3)	-10(2)
C(21)	65(5)	64(4)	67(4)	9(3)	-14(3)	-44(4)
C(22)	156(10)	153(10)	69(6)	-22(6)	31(6)	-95(8)
C(23)	98(7)	108(7)	110(7)	-26(6)	-1(6)	-50(6)
C(24)	74(6)	105(7)	109(7)	-49(5)	26(5)	-42(5)
C(25)	61(5)	109(7)	73(5)	-13(5)	9(4)	-32(4)
Mo(1)	17(1)	21(1)	23(1)	2(1)	-6(1)	-7(1)
Ge(1)	19(1)	22(1)	25(1)	2(1)	-7(1)	-7(1)
N(1)	22(2)	27(2)	26(2)	-1(2)	-7(2)	-5(2)
N(2)	18(2)	29(2)	27(2)	-3(2)	-6(2)	-5(2)
O(1)	37(2)	63(3)	36(2)	-5(2)	5(2)	-13(2)
O(2)	60(3)	62(3)	48(2)	-10(2)	-7(2)	-45(2)
O(4)	73(4)	111(5)	85(4)	-40(3)	2(3)	-34(3)

Crystal data and structure refinement of compound 3a

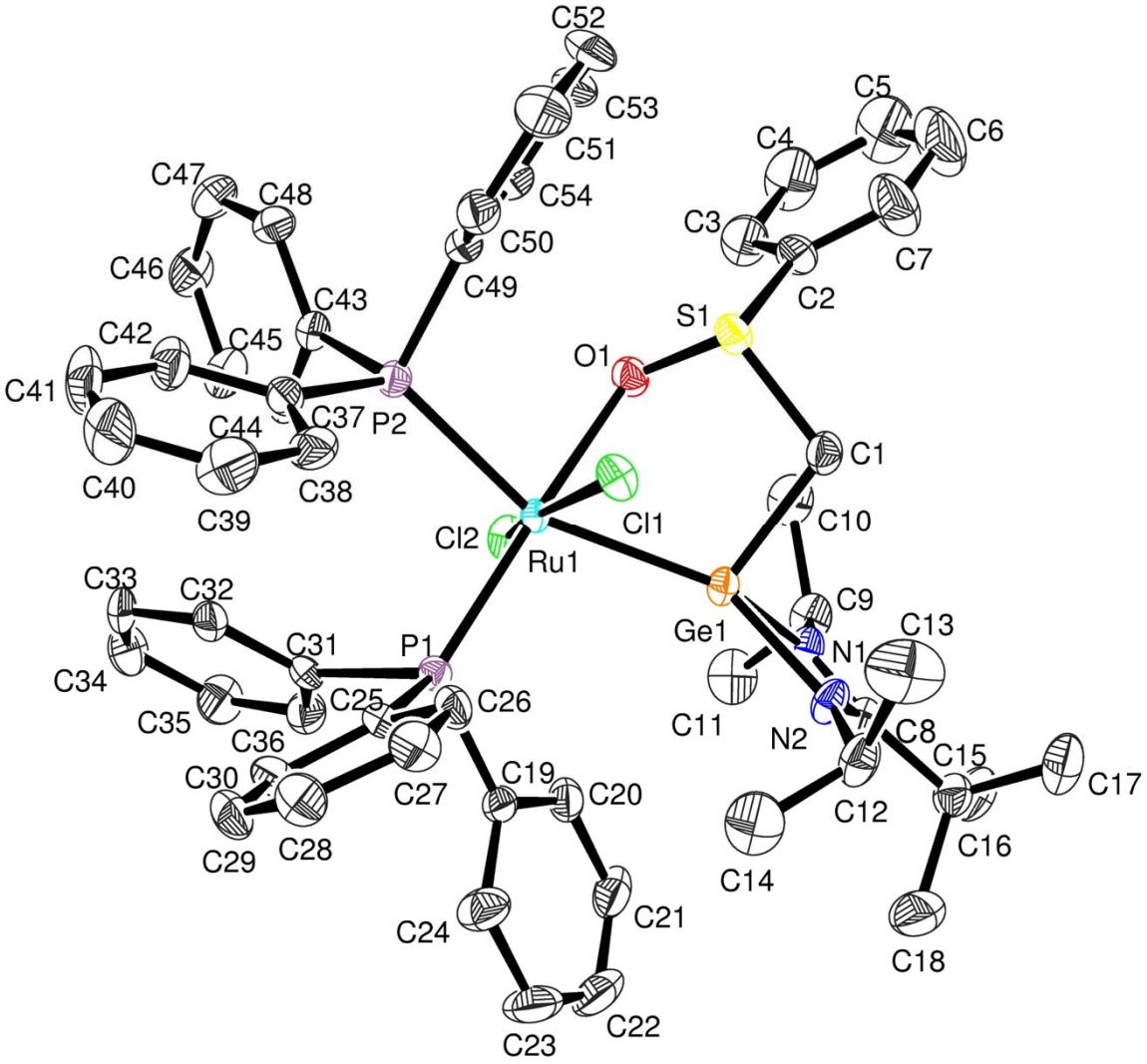


Table 9. Crystal data and structure refinement for 3a.

Identification code	3a
Empirical formula	C54 H60 Cl2 Ge N2 O P2 Ru S
Formula weight	1091.62
Temperature	193(2) K
Wavelength	0.71073 A
Crystal system, space group	monoclinic, P 21/c
Unit cell dimensions	a = 12.5612(6) A alpha = 90 deg. b = 24.1634(10) A beta = 96.627(2) deg.

	c = 16.9752(9) A gamma = 90 deg.
Volume	5117.9(4) A^3
Z, Calculated density	4, 1.417 Mg/m^3
Absorption coefficient	1.130 mm^-1
F(000)	2248
Crystal size	0.04 x 0.04 x 0.02 mm
Theta range for data collection	3.45 to 25.35 deg.
Limiting indices	-15<=h<=14, -29<=k<=29, -20<=l<=19
Reflections collected / unique	58061 / 9335 [R(int) = 0.1056]
Completeness to theta = 25.35	99.6 %
Max. and min. transmission	0.7454 and 0.6817
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9335 / 0 / 584
Goodness-of-fit on F^2	1.032
Final R indices [I>2sigma(I)]	R1 = 0.0446, wR2 = 0.0996
R indices (all data)	R1 = 0.0866, wR2 = 0.1195
Largest diff. peak and hole	0.428 and -0.558 e.A^-3

Table 10. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for nicolas2_a. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	3574(4)	5847(2)	7583(3)	25(1)
C(2)	3396(4)	4698(2)	7515(3)	29(1)
C(3)	3677(5)	4351(2)	6938(4)	39(2)
C(4)	2990(5)	3929(2)	6678(4)	55(2)
C(5)	2062(6)	3854(3)	7013(5)	68(2)
C(6)	1775(5)	4203(3)	7583(5)	70(2)
C(7)	2463(5)	4625(2)	7841(4)	54(2)
C(8)	3291(4)	6891(2)	6225(3)	23(1)
C(9)	3292(4)	6032(2)	5288(3)	29(1)
C(10)	3340(4)	5432(2)	5598(3)	34(1)
C(11)	4007(5)	6104(2)	4637(3)	40(1)
C(12)	3838(4)	7455(2)	7475(3)	32(1)
C(13)	3523(6)	7268(2)	8270(4)	60(2)
C(14)	4937(5)	7713(2)	7570(4)	48(2)
C(15)	2456(4)	7279(2)	5801(3)	29(1)
C(16)	1950(4)	7085(2)	5001(4)	43(2)
C(17)	1531(4)	7344(2)	6317(4)	45(2)
C(18)	3003(5)	7837(2)	5667(4)	52(2)
C(19)	6971(4)	7088(2)	6405(3)	22(1)
C(20)	6201(4)	6956(2)	5786(3)	28(1)
C(21)	5791(4)	7352(2)	5247(3)	37(1)
C(22)	6124(5)	7889(2)	5319(4)	45(2)
C(23)	6893(5)	8036(2)	5935(4)	47(2)
C(24)	7308(4)	7635(2)	6469(3)	36(1)
C(25)	8211(4)	6973(2)	7893(3)	21(1)
C(26)	7663(4)	7148(2)	8518(3)	24(1)
C(27)	8164(4)	7480(2)	9117(3)	30(1)
C(28)	9212(4)	7643(2)	9108(3)	32(1)
C(29)	9756(4)	7487(2)	8483(3)	33(1)
C(30)	9258(4)	7164(2)	7876(3)	28(1)
C(31)	8643(4)	6276(2)	6605(3)	21(1)
C(32)	9542(4)	6052(2)	7056(3)	25(1)
C(33)	10331(4)	5800(2)	6691(4)	35(1)
C(34)	10258(4)	5765(2)	5875(4)	39(2)
C(35)	9372(4)	5988(2)	5418(3)	36(1)
C(36)	8585(4)	6246(2)	5784(3)	30(1)
C(37)	8738(4)	5460(2)	8688(3)	24(1)
C(38)	8630(4)	5922(2)	9161(3)	31(1)
C(39)	9478(5)	6118(2)	9663(4)	46(2)
C(40)	10464(5)	5864(3)	9706(4)	49(2)
C(41)	10591(4)	5411(3)	9252(4)	44(2)
C(42)	9745(4)	5206(2)	8738(3)	34(1)
C(43)	8181(4)	4672(2)	7453(3)	23(1)
C(44)	8441(4)	4786(2)	6702(3)	23(1)

C(45)	8929(4)	4395(2)	6271(3)	32(1)
C(46)	9161(4)	3881(2)	6579(3)	35(1)
C(47)	8913(4)	3760(2)	7329(4)	40(2)
C(48)	8441(4)	4151(2)	7767(3)	32(1)
C(49)	6855(4)	4795(2)	8679(3)	23(1)
C(50)	6846(4)	4937(2)	9473(3)	29(1)
C(51)	6216(5)	4643(2)	9945(4)	43(2)
C(52)	5590(5)	4219(2)	9633(4)	48(2)
C(53)	5586(4)	4078(2)	8852(4)	37(2)
C(54)	6212(4)	4358(2)	8380(3)	30(1)
N(1)	3627(3)	6402(2)	5981(2)	24(1)
N(2)	3816(3)	6983(2)	6941(3)	24(1)
O(1)	5198(2)	5187(1)	7381(2)	23(1)
P(1)	7508(1)	6542(1)	7105(1)	18(1)
P(2)	7584(1)	5216(1)	8013(1)	19(1)
S(1)	4296(1)	5232(1)	7911(1)	23(1)
Cl(1)	5851(1)	6152(1)	8644(1)	23(1)
Cl(2)	6369(1)	5526(1)	6030(1)	25(1)
Ge(1)	4603(1)	6286(1)	6968(1)	19(1)
Ru(1)	6350(1)	5863(1)	7358(1)	15(1)

Table 11. Bond lengths [A] and angles [deg] for nicolas2_a.

C(1)-S(1)	1.797(5)
C(1)-Ge(1)	2.050(5)
C(1)-H(1A)	0.9900
C(1)-H(1B)	0.9900
C(2)-C(7)	1.364(7)
C(2)-C(3)	1.366(7)
C(2)-S(1)	1.794(5)
C(3)-C(4)	1.375(7)
C(3)-H(3)	0.9500
C(4)-C(5)	1.366(9)
C(4)-H(4)	0.9500
C(5)-C(6)	1.364(10)
C(5)-H(5)	0.9500
C(6)-C(7)	1.375(8)
C(6)-H(6)	0.9500
C(7)-H(7)	0.9500
C(8)-N(2)	1.333(6)
C(8)-N(1)	1.338(6)
C(8)-C(15)	1.524(7)
C(9)-N(1)	1.499(6)
C(9)-C(11)	1.513(7)
C(9)-C(10)	1.540(7)
C(9)-H(9)	1.0000
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-N(2)	1.454(6)
C(12)-C(14)	1.506(7)
C(12)-C(13)	1.518(8)
C(12)-H(12)	1.0000
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)-C(16)	1.507(7)
C(15)-C(17)	1.542(7)
C(15)-C(18)	1.542(7)
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)	1.380(7)
C(19)-C(24)	1.388(6)
C(19)-P(1)	1.852(5)

C(20)-C(21)	1.383(7)
C(20)-H(20)	0.9500
C(21)-C(22)	1.364(8)
C(21)-H(21)	0.9500
C(22)-C(23)	1.385(8)
C(22)-H(22)	0.9500
C(23)-C(24)	1.387(7)
C(23)-H(23)	0.9500
C(24)-H(24)	0.9500
C(25)-C(26)	1.394(7)
C(25)-C(30)	1.397(7)
C(25)-P(1)	1.840(5)
C(26)-C(27)	1.389(7)
C(26)-H(26)	0.9500
C(27)-C(28)	1.375(7)
C(27)-H(27)	0.9500
C(28)-C(29)	1.379(7)
C(28)-H(28)	0.9500
C(29)-C(30)	1.385(7)
C(29)-H(29)	0.9500
C(30)-H(30)	0.9500
C(31)-C(36)	1.389(7)
C(31)-C(32)	1.398(7)
C(31)-P(1)	1.855(5)
C(32)-C(33)	1.372(7)
C(32)-H(32)	0.9500
C(33)-C(34)	1.381(8)
C(33)-H(33)	0.9500
C(34)-C(35)	1.389(8)
C(34)-H(34)	0.9500
C(35)-C(36)	1.376(7)
C(35)-H(35)	0.9500
C(36)-H(36)	0.9500
C(37)-C(38)	1.389(7)
C(37)-C(42)	1.401(7)
C(37)-P(2)	1.839(5)
C(38)-C(39)	1.370(7)
C(38)-H(38)	0.9500
C(39)-C(40)	1.377(8)
C(39)-H(39)	0.9500
C(40)-C(41)	1.357(8)
C(40)-H(40)	0.9500
C(41)-C(42)	1.387(7)
C(41)-H(41)	0.9500
C(42)-H(42)	0.9500
C(43)-C(44)	1.380(7)
C(43)-C(48)	1.390(6)
C(43)-P(2)	1.833(5)
C(44)-C(45)	1.380(7)
C(44)-H(44)	0.9500
C(45)-C(46)	1.366(7)
C(45)-H(45)	0.9500
C(46)-C(47)	1.377(8)
C(46)-H(46)	0.9500
C(47)-C(48)	1.378(7)
C(47)-H(47)	0.9500
C(48)-H(48)	0.9500
C(49)-C(54)	1.389(7)

C(49)-C(50)	1.392(7)
C(49)-P(2)	1.841(5)
C(50)-C(51)	1.386(7)
C(50)-H(50)	0.9500
C(51)-C(52)	1.361(8)
C(51)-H(51)	0.9500
C(52)-C(53)	1.369(8)
C(52)-H(52)	0.9500
C(53)-C(54)	1.365(7)
C(53)-H(53)	0.9500
C(54)-H(54)	0.9500
N(1)-Ge(1)	1.979(4)
N(2)-Ge(1)	1.951(4)
O(1)-S(1)	1.530(3)
O(1)-Ru(1)	2.185(3)
P(1)-Ru(1)	2.2661(12)
P(2)-Ru(1)	2.3832(12)
Cl(1)-Ru(1)	2.4410(12)
Cl(2)-Ru(1)	2.3995(12)
Ge(1)-Ru(1)	2.4429(6)

S(1)-C(1)-Ge(1)	105.1(2)
S(1)-C(1)-H(1A)	110.7
Ge(1)-C(1)-H(1A)	110.7
S(1)-C(1)-H(1B)	110.7
Ge(1)-C(1)-H(1B)	110.7
H(1A)-C(1)-H(1B)	108.8
C(7)-C(2)-C(3)	121.1(5)
C(7)-C(2)-S(1)	118.4(4)
C(3)-C(2)-S(1)	120.4(4)
C(2)-C(3)-C(4)	118.7(6)
C(2)-C(3)-H(3)	120.6
C(4)-C(3)-H(3)	120.6
C(5)-C(4)-C(3)	119.9(6)
C(5)-C(4)-H(4)	120.0
C(3)-C(4)-H(4)	120.0
C(6)-C(5)-C(4)	121.4(6)
C(6)-C(5)-H(5)	119.3
C(4)-C(5)-H(5)	119.3
C(5)-C(6)-C(7)	118.5(6)
C(5)-C(6)-H(6)	120.8
C(7)-C(6)-H(6)	120.8
C(2)-C(7)-C(6)	120.3(6)
C(2)-C(7)-H(7)	119.9
C(6)-C(7)-H(7)	119.9
N(2)-C(8)-N(1)	106.8(4)
N(2)-C(8)-C(15)	124.7(4)
N(1)-C(8)-C(15)	128.4(5)
N(1)-C(9)-C(11)	111.6(4)
N(1)-C(9)-C(10)	107.3(4)
C(11)-C(9)-C(10)	110.8(4)
N(1)-C(9)-H(9)	109.0
C(11)-C(9)-H(9)	109.0
C(10)-C(9)-H(9)	109.0
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(9)-C(11)-H(11A)	109.5
C(9)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(9)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
N(2)-C(12)-C(14)	109.9(4)
N(2)-C(12)-C(13)	109.4(4)
C(14)-C(12)-C(13)	111.0(5)
N(2)-C(12)-H(12)	108.8
C(14)-C(12)-H(12)	108.8
C(13)-C(12)-H(12)	108.8
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(16)-C(15)-C(8)	115.5(4)
C(16)-C(15)-C(17)	106.1(4)
C(8)-C(15)-C(17)	108.5(4)
C(16)-C(15)-C(18)	106.8(5)
C(8)-C(15)-C(18)	108.2(4)
C(17)-C(15)-C(18)	111.9(4)
C(15)-C(16)-H(16A)	109.5
C(15)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(15)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(15)-C(17)-H(17A)	109.5
C(15)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(15)-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(24)	117.5(5)
C(20)-C(19)-P(1)	119.6(4)
C(24)-C(19)-P(1)	122.9(4)
C(19)-C(20)-C(21)	121.2(5)
C(19)-C(20)-H(20)	119.4
C(21)-C(20)-H(20)	119.4
C(22)-C(21)-C(20)	120.8(6)
C(22)-C(21)-H(21)	119.6

C(20)-C(21)-H(21)	119.6
C(21)-C(22)-C(23)	119.5(5)
C(21)-C(22)-H(22)	120.3
C(23)-C(22)-H(22)	120.3
C(22)-C(23)-C(24)	119.4(5)
C(22)-C(23)-H(23)	120.3
C(24)-C(23)-H(23)	120.3
C(19)-C(24)-C(23)	121.7(5)
C(19)-C(24)-H(24)	119.1
C(23)-C(24)-H(24)	119.1
C(26)-C(25)-C(30)	117.8(4)
C(26)-C(25)-P(1)	119.1(3)
C(30)-C(25)-P(1)	123.0(4)
C(27)-C(26)-C(25)	120.6(4)
C(27)-C(26)-H(26)	119.7
C(25)-C(26)-H(26)	119.7
C(28)-C(27)-C(26)	120.8(5)
C(28)-C(27)-H(27)	119.6
C(26)-C(27)-H(27)	119.6
C(27)-C(28)-C(29)	119.3(5)
C(27)-C(28)-H(28)	120.3
C(29)-C(28)-H(28)	120.3
C(28)-C(29)-C(30)	120.3(5)
C(28)-C(29)-H(29)	119.8
C(30)-C(29)-H(29)	119.8
C(29)-C(30)-C(25)	121.0(5)
C(29)-C(30)-H(30)	119.5
C(25)-C(30)-H(30)	119.5
C(36)-C(31)-C(32)	118.3(4)
C(36)-C(31)-P(1)	121.6(4)
C(32)-C(31)-P(1)	119.8(4)
C(33)-C(32)-C(31)	120.3(5)
C(33)-C(32)-H(32)	119.8
C(31)-C(32)-H(32)	119.8
C(32)-C(33)-C(34)	120.8(5)
C(32)-C(33)-H(33)	119.6
C(34)-C(33)-H(33)	119.6
C(33)-C(34)-C(35)	119.6(5)
C(33)-C(34)-H(34)	120.2
C(35)-C(34)-H(34)	120.2
C(36)-C(35)-C(34)	119.6(5)
C(36)-C(35)-H(35)	120.2
C(34)-C(35)-H(35)	120.2
C(35)-C(36)-C(31)	121.4(5)
C(35)-C(36)-H(36)	119.3
C(31)-C(36)-H(36)	119.3
C(38)-C(37)-C(42)	117.7(5)
C(38)-C(37)-P(2)	119.7(4)
C(42)-C(37)-P(2)	122.6(4)
C(39)-C(38)-C(37)	121.2(5)
C(39)-C(38)-H(38)	119.4
C(37)-C(38)-H(38)	119.4
C(38)-C(39)-C(40)	120.5(6)
C(38)-C(39)-H(39)	119.8
C(40)-C(39)-H(39)	119.8
C(41)-C(40)-C(39)	119.6(5)
C(41)-C(40)-H(40)	120.2
C(39)-C(40)-H(40)	120.2

C(40)-C(41)-C(42)	120.9(5)
C(40)-C(41)-H(41)	119.5
C(42)-C(41)-H(41)	119.5
C(41)-C(42)-C(37)	120.1(5)
C(41)-C(42)-H(42)	119.9
C(37)-C(42)-H(42)	119.9
C(44)-C(43)-C(48)	117.7(4)
C(44)-C(43)-P(2)	119.3(3)
C(48)-C(43)-P(2)	122.8(4)
C(45)-C(44)-C(43)	121.3(5)
C(45)-C(44)-H(44)	119.4
C(43)-C(44)-H(44)	119.4
C(46)-C(45)-C(44)	120.5(5)
C(46)-C(45)-H(45)	119.7
C(44)-C(45)-H(45)	119.7
C(45)-C(46)-C(47)	119.1(5)
C(45)-C(46)-H(46)	120.5
C(47)-C(46)-H(46)	120.5
C(46)-C(47)-C(48)	120.7(5)
C(46)-C(47)-H(47)	119.7
C(48)-C(47)-H(47)	119.7
C(47)-C(48)-C(43)	120.7(5)
C(47)-C(48)-H(48)	119.7
C(43)-C(48)-H(48)	119.7
C(54)-C(49)-C(50)	118.1(5)
C(54)-C(49)-P(2)	120.4(4)
C(50)-C(49)-P(2)	121.2(4)
C(51)-C(50)-C(49)	120.2(5)
C(51)-C(50)-H(50)	119.9
C(49)-C(50)-H(50)	119.9
C(52)-C(51)-C(50)	120.2(6)
C(52)-C(51)-H(51)	119.9
C(50)-C(51)-H(51)	119.9
C(51)-C(52)-C(53)	120.1(5)
C(51)-C(52)-H(52)	119.9
C(53)-C(52)-H(52)	119.9
C(54)-C(53)-C(52)	120.4(5)
C(54)-C(53)-H(53)	119.8
C(52)-C(53)-H(53)	119.8
C(53)-C(54)-C(49)	120.9(6)
C(53)-C(54)-H(54)	119.5
C(49)-C(54)-H(54)	119.5
C(8)-N(1)-C(9)	134.5(4)
C(8)-N(1)-Ge(1)	92.8(3)
C(9)-N(1)-Ge(1)	132.1(3)
C(8)-N(2)-C(12)	132.1(4)
C(8)-N(2)-Ge(1)	94.2(3)
C(12)-N(2)-Ge(1)	133.5(3)
S(1)-O(1)-Ru(1)	119.64(17)
C(25)-P(1)-C(19)	99.8(2)
C(25)-P(1)-C(31)	101.5(2)
C(19)-P(1)-C(31)	101.3(2)
C(25)-P(1)-Ru(1)	122.47(16)
C(19)-P(1)-Ru(1)	116.37(16)
C(31)-P(1)-Ru(1)	112.36(14)
C(43)-P(2)-C(37)	102.3(2)
C(43)-P(2)-C(49)	100.6(2)
C(37)-P(2)-C(49)	101.9(2)

C(43)-P(2)-Ru(1)	120.78(17)
C(37)-P(2)-Ru(1)	120.23(15)
C(49)-P(2)-Ru(1)	107.80(15)
O(1)-S(1)-C(2)	101.9(2)
O(1)-S(1)-C(1)	105.0(2)
C(2)-S(1)-C(1)	101.9(2)
N(2)-Ge(1)-N(1)	66.13(16)
N(2)-Ge(1)-C(1)	96.38(17)
N(1)-Ge(1)-C(1)	97.96(19)
N(2)-Ge(1)-Ru(1)	143.65(12)
N(1)-Ge(1)-Ru(1)	137.58(11)
C(1)-Ge(1)-Ru(1)	104.16(13)
O(1)-Ru(1)-P(1)	170.10(9)
O(1)-Ru(1)-P(2)	84.15(9)
P(1)-Ru(1)-P(2)	99.56(4)
O(1)-Ru(1)-Cl(2)	80.86(9)
P(1)-Ru(1)-Cl(2)	89.50(4)
P(2)-Ru(1)-Cl(2)	98.00(4)
O(1)-Ru(1)-Cl(1)	87.65(9)
P(1)-Ru(1)-Cl(1)	101.50(4)
P(2)-Ru(1)-Cl(1)	89.49(4)
Cl(2)-Ru(1)-Cl(1)	165.53(4)
O(1)-Ru(1)-Ge(1)	75.06(8)
P(1)-Ru(1)-Ge(1)	102.77(3)
P(2)-Ru(1)-Ge(1)	156.45(4)
Cl(2)-Ru(1)-Ge(1)	89.61(3)
Cl(1)-Ru(1)-Ge(1)	78.87(3)

Symmetry transformations used to generate equivalent atoms:

Table 12. Anisotropic displacement parameters (A^2 x 10^3) for nicolas2_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(3)	26(2)	28(3)	-2(2)	6(2)	3(2)
C(2)	23(3)	24(3)	38(4)	1(2)	-1(3)	8(2)
C(3)	34(3)	31(3)	52(4)	-9(3)	0(3)	-4(3)
C(4)	44(4)	36(3)	81(6)	-24(3)	-5(4)	-6(3)
C(5)	44(4)	41(4)	114(7)	-20(4)	-10(4)	-17(3)
C(6)	36(4)	61(4)	115(7)	-11(5)	17(4)	-22(4)
C(7)	39(4)	45(3)	80(5)	-15(3)	20(4)	-17(3)
C(8)	19(3)	21(2)	30(3)	1(2)	4(2)	2(2)
C(9)	27(3)	35(3)	21(3)	-9(2)	-9(2)	-1(2)
C(10)	35(3)	35(3)	32(4)	-14(3)	-3(3)	0(3)
C(11)	42(4)	50(3)	27(3)	-10(3)	0(3)	0(3)
C(12)	28(3)	31(3)	37(4)	-9(3)	1(3)	9(2)
C(13)	93(5)	45(4)	45(4)	-18(3)	21(4)	-5(4)
C(14)	45(4)	38(3)	59(5)	-22(3)	-3(3)	-5(3)
C(15)	22(3)	30(3)	33(3)	2(2)	-3(2)	1(2)
C(16)	34(3)	48(3)	43(4)	5(3)	-8(3)	12(3)
C(17)	29(3)	49(3)	55(4)	-6(3)	1(3)	11(3)
C(18)	45(4)	38(3)	70(5)	19(3)	-5(3)	1(3)
C(19)	21(3)	23(2)	24(3)	4(2)	8(2)	4(2)
C(20)	19(3)	36(3)	28(3)	6(2)	3(2)	2(2)
C(21)	28(3)	50(4)	32(4)	11(3)	5(3)	14(3)
C(22)	53(4)	39(3)	45(4)	20(3)	18(3)	25(3)
C(23)	61(4)	26(3)	55(5)	16(3)	18(4)	6(3)
C(24)	42(4)	31(3)	34(4)	8(3)	-5(3)	2(3)
C(25)	20(3)	19(2)	25(3)	2(2)	4(2)	-3(2)
C(26)	17(3)	23(2)	31(3)	-2(2)	1(2)	-4(2)
C(27)	35(3)	28(3)	28(3)	-7(2)	10(3)	-1(2)
C(28)	32(3)	30(3)	32(4)	-7(2)	-3(3)	-6(2)
C(29)	21(3)	30(3)	47(4)	-2(3)	3(3)	-9(2)
C(30)	29(3)	25(2)	31(3)	0(2)	8(3)	-7(2)
C(31)	18(3)	22(2)	24(3)	5(2)	8(2)	-2(2)
C(32)	18(3)	29(3)	27(3)	4(2)	0(2)	-2(2)
C(33)	14(3)	40(3)	51(4)	12(3)	8(3)	7(2)
C(34)	28(3)	47(3)	46(4)	3(3)	24(3)	7(3)
C(35)	37(3)	48(3)	26(3)	6(3)	16(3)	8(3)
C(36)	26(3)	35(3)	30(3)	5(2)	5(3)	3(2)
C(37)	19(3)	29(3)	23(3)	8(2)	0(2)	-2(2)
C(38)	32(3)	30(3)	28(3)	7(2)	-5(3)	0(2)
C(39)	48(4)	37(3)	47(4)	-3(3)	-17(3)	-5(3)
C(40)	32(4)	67(4)	41(4)	6(3)	-19(3)	-10(3)
C(41)	19(3)	69(4)	43(4)	2(3)	-7(3)	5(3)
C(42)	24(3)	47(3)	30(3)	4(3)	-1(3)	4(3)
C(43)	19(3)	24(2)	26(3)	1(2)	4(2)	3(2)
C(44)	19(3)	24(2)	26(3)	1(2)	3(2)	5(2)
C(45)	33(3)	40(3)	22(3)	-5(2)	-1(3)	8(3)
C(46)	36(3)	34(3)	36(4)	-7(3)	11(3)	11(3)

C(47)	37(3)	23(3)	60(4)	4(3)	10(3)	12(2)
C(48)	31(3)	28(3)	40(4)	11(3)	11(3)	7(2)
C(49)	22(3)	21(2)	26(3)	5(2)	5(2)	3(2)
C(50)	26(3)	33(3)	27(3)	5(2)	3(2)	2(2)
C(51)	47(4)	57(4)	26(4)	13(3)	15(3)	6(3)
C(52)	42(4)	41(3)	67(5)	23(3)	30(4)	-1(3)
C(53)	32(3)	22(3)	59(5)	8(3)	16(3)	-4(2)
C(54)	28(3)	24(3)	38(4)	6(2)	6(3)	5(2)
N(1)	21(2)	28(2)	23(3)	-5(2)	-1(2)	3(2)
N(2)	23(2)	20(2)	28(3)	-8(2)	-2(2)	6(2)
O(1)	20(2)	21(2)	29(2)	-3(2)	4(2)	-3(1)
P(1)	17(1)	19(1)	17(1)	1(1)	3(1)	0(1)
P(2)	18(1)	21(1)	19(1)	1(1)	3(1)	2(1)
S(1)	20(1)	24(1)	27(1)	-2(1)	4(1)	-4(1)
Cl(1)	23(1)	29(1)	19(1)	-6(1)	6(1)	-4(1)
Cl(2)	24(1)	31(1)	20(1)	-6(1)	1(1)	4(1)
Ge(1)	16(1)	20(1)	21(1)	-2(1)	0(1)	2(1)
Ru(1)	13(1)	17(1)	14(1)	-2(1)	1(1)	0(1)