

Supporting Information

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Stabilization of a Two-Coordinate $[\text{GeCl}]^+$ Cation by Simultaneous σ and π Donation from a Monodentate Carbodiphosphorane**

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Supporting Information

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General procedure

All reactions were carried out in flame-dried glassware under Ar. All the solvents were purified by distillation over the drying agents [CH_2Cl_2 (CaH_2), pentane, toluene (Na/K)] and were transferred under Ar. MS (EI): Finnigan MAT 8200 (70 Ev), ESIMS: Finnigan MAT 95, accurate mass determinations: Bruker APEX III FT-MS (7 T magnet). NMR: Spectra were recorded on a Bruker DPX 300 or AV 400 spectrometer in the solvents indicated; ^1H and ^{13}C chemical shifts (δ) are given in ppm relative to TMS, coupling constants (J) in Hz. The solvent signals were used as references and the chemical shifts converted to the TMS scale. All commercially available compounds (Acros, Alfa Aesar, Aldrich) were used as received and hexaphenylcarbodiphosphorane (**1**)¹ was prepared according to literature procedures.

Synthesis and characterization of compounds

Compound 2: A solution of **1** (535.0 mg, 1 mmol) in toluene (10 mL) at room temperature was added to solid $\text{GeCl}_2 \cdot \text{dioxane}$ (231.0 mg, 1 mmol) at the same temperature and the resulting suspension stirred overnight. The solvent was then evacuated and the residue washed with pentane (5 mL) to afford **2** as a colourless solid in quantitative yield. Crystals suitable for X-ray analysis were grown by slow diffusion of an ether solution of $\text{GeCl}_2 \cdot \text{dioxane}$ into a toluene solution of **1**.

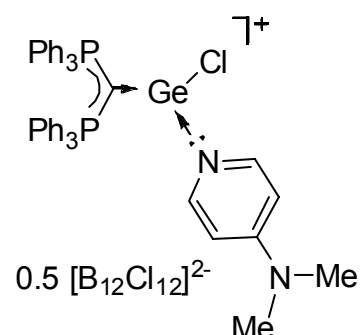
$^{31}\text{P}\{^1\text{H}\}$ NMR (121 MHz, CD_2Cl_2): $\delta = 22.2$ (br) ppm; EI-MS calculated for $\text{C}_{37}\text{H}_{30}\text{Cl}_2\text{GeP}_2$ (680.9): found: 644(M-Cl); Anal. Calcd for $\text{C}_{37}\text{H}_{30}\text{Cl}_2\text{GeP}_2$ (%): C, 65.34; H, 4.45; P, 9.11; Cl, 10.43; found C, 65.31; H, 4.97; P, 9.21; Cl, 10.89. Note: Compound **2** is highly insoluble in most common organic solvents.

Compound 3: A suspension of **2** (227.0 mg, 0.33 mmol) in dichloromethane (10 mL) at room temperature was added to solid $\text{GeCl}_2 \cdot \text{dioxane}$ (77.0 mg, 0.33 mmol). The suspension thus obtained became clear within few minutes affording a pale yellow solution. The solvent was then evacuated and the residue washed with pentane (4 mL) to afford **3** as a colourless solid (165 mg, 60.2%). Crystals suitable for X-ray analysis were grown from $\text{CH}_2\text{Cl}_2/\text{pentane}$ (1:1). ^1H NMR (300 MHz, CD_2Cl_2) $\delta = 7.76\text{--}7.70$ (t, $J = 8.37$ Hz, 12H), $7.57\text{--}7.52$ (t, $J = 7.71$ Hz, 6H), $7.42\text{--}7.37$ (t, $J = 7.31$ Hz, 12H); ^{13}C NMR (75 MHz, CD_2Cl_2): $\delta = 135.4$ (t, $J = 4.89$ Hz), 133.4 (bs), 129.6 (t, $J = 6.26$ Hz), 128.0 (br), 127.0 ppm; $^{31}\text{P}\{^1\text{H}\}$ NMR (121 MHz, CD_2Cl_2): $\delta = 23.3$ ppm; EI-MS calculated for $\text{C}_{37}\text{H}_{30}\text{Cl}_4\text{Ge}_2\text{P}_2$: 823.90; found: 681(M- GeCl_2).

Compound 4: A suspension of **2** (227.0 mg, 0.33 mmol) in dichloromethane (10 mL) at room temperature was added to solid AlCl_3 (45.0 mg, 0.33 mmol). The obtained suspension became clear after stirring the reaction mixture for 30 minutes. In addition it displayed a bright yellow colour. Evacuation of the solvents afforded **4** as a yellow solid. Crystals suitable for X-ray analysis were grown from $\text{CH}_2\text{Cl}_2/\text{pentane}$ (1:1) mixture as pale yellow crystals (184 mg, 67.6%).

^1H NMR (300 MHz, CD_2Cl_2) δ = 7.56-7.33 (m, 30H); ^{13}C NMR (75.5 MHz, CD_2Cl_2): δ 134.8 (m), 134.7 (br), 130.0 (t, J = 6.46 Hz), 124.8(s), 123.6(s); $^{31}\text{P}\{^1\text{H}\}$ NMR (121 MHz, CD_2Cl_2): δ = 23.1 ppm; EI-MS calculated for $[\text{C}_{37}\text{H}_{30}\text{ClGeP}_2]^+$: 644.1; found: 644.

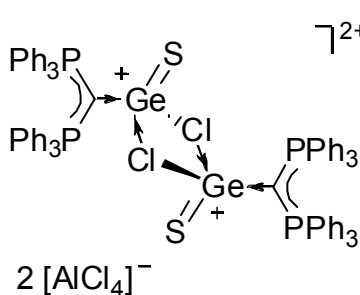
Compound 5: $\text{K}_2\text{B}_{12}\text{Cl}_{12}$ (104.0 mg, 0.165 mmol) and 4-dimethylaminopyridine (40.0 mg, 0.33 mmol) were added



to a suspension of **2** (227.0 mg, 0.33 mmol) in dichloromethane (15 mL) at room temperature. The suspension became clear pale yellow after stirring the reaction mixture for 20 minutes. Filtration to remove the formed KCl and solvent evacuation afforded **5** as a colourless solid. Crystals suitable for X-ray analysis were grown from CH_2Cl_2 /pentane (1:1) mixture (192 mg, 55.6%).

^1H NMR (300 MHz, CD_2Cl_2) δ = 7.72 (br, 2H), 7.62-7.35 (m, 30H), 6.35 (br, 2H), 3.07 (s, 6H); ^{13}C NMR (75.5 MHz, CD_2Cl_2): δ = 156.0 (br), 144.9 (br), 134.5 (t, J = 5.16 Hz), 133.2 (t, J = 5.28 Hz), 132.8 (br), 129.8 (t, J = 6.36 Hz), 129.1 (br), 107.5 (s), 39.9 (s); $^{31}\text{P}\{^1\text{H}\}$ NMR (121 MHz, CD_2Cl_2): δ = 21.69 ppm; ^{11}B NMR (128 MHz, CD_2Cl_2): δ = -12.5 ppm. EI-MS(pos) calculated for $\text{C}_{44}\text{H}_{40}\text{GeN}_2\text{P}_2\text{Cl}$ (767.16): found: 753 $[\text{M}^+(767)\text{-Me}]$, 722.7 $[\text{M}^+(767)\text{-NMe}_2]$.

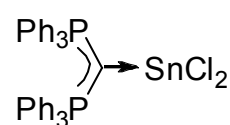
Compound 6: Elemental sulphur (5.3 mg, 0.02 mmol) was added to a solution of **4** (135.0 mg, 0.17 mmol) in



dichloromethane (10 mL) at room temperature causing gradual fading of the yellow colour. The solvents were then evacuated and the residue washed with pentane (1 x 3 mL) to afford **6** as a colourless solid. Crystals suitable for X-ray analysis were grown from CH_2Cl_2 /pentane (1:1) (85 mg, 60.7%).

^1H NMR (300 MHz, CD_2Cl_2) δ = 7.64-7.59 (m, 9H), 7.47-7.38 (m, 21H); ^{13}C NMR (75 MHz, CD_2Cl_2): δ = 134.7 (t, J = 5.11 Hz), 134.4 (bs), 130.0 (t, J = 6.31 Hz), 124.3 (s), 123.1 (s); $^{31}\text{P}\{^1\text{H}\}$ NMR (121 MHz, CD_2Cl_2): δ = 23.42 ppm; ESI-MS(pos) calculated for $\text{C}_{74}\text{H}_{60}\text{Cl}_2\text{Ge}_2\text{P}_4\text{S}_2$: 1354.1, found: 677 1/2(M^+).

Compound 7: To a solution of **1** (535.0 mg, 1 mmol) in toluene (10 mL) at room temperature was added to a

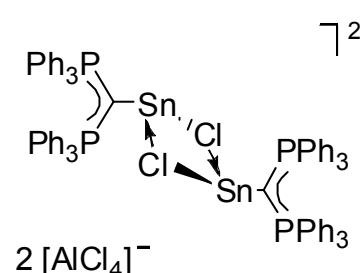


solution of SnCl_2 (190.0 mg, 1 mmol) in THF (2 mL) and the resulting suspension stirred overnight. Solvents were then evacuated and the residue washed with pentane (5 mL) to afford **7** as a colourless solid in quantitative yield.

Elemental Analysis Calcd. for $\text{C}_{37}\text{H}_{30}\text{Cl}_2\text{SnP}_2$ (%): C, 61.19; H, 4.16; Sn, 16.35; P, 8.53; found C, 61.17; H, 4.19; Sn, 16.29; P, 8.50.

Note: Compound **7** is extremely insoluble in most common organic solvents.

Compound 9: Solid AlCl_3 (45.0 mg, 0.33 mmol) was added to a suspension of **7** (242.0 mg, 0.33 mmol) in

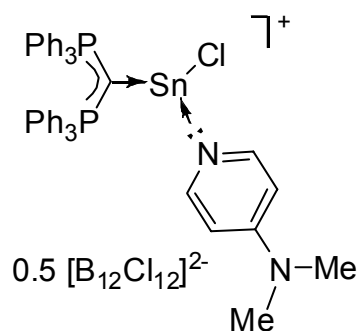


dichloromethane (10 mL) at room temperature. The suspension became clear after stirring the reaction mixture for 1 hr affording a bright yellow solution. Evacuation of the solvents afforded **9** as a yellow solid. Crystals suitable for X-ray analysis were grown from CH_2Cl_2 /pentane (1:1) mixture (193 mg, 67.24%).

^1H NMR (300 MHz, CD_2Cl_2) δ = 7.72-7.66 (m, 6H), 7.61-7.57 (m, 24H); ^{13}C NMR (75. MHz, CD_2Cl_2): δ = 134.8 (s), 133.4 (m), 131.3 (m), 125.1 (br d), 123.9 (br d);

$^{31}\text{P}\{^1\text{H}\}$ NMR (121 MHz, CD_2Cl_2): $\delta = 19.72$ ($^2J_{\text{P-Sn}} = 65.80$ Hz) ppm; $^{119}\text{Sn}\{^1\text{H}\}$ NMR (CD_2Cl_2): $\delta = 249.71$ (br) ppm.

Compound 10: $\text{K}_2\text{B}_{12}\text{Cl}_{12}$ (104.0 mg, 0.165 mmol) and 4-dimethylaminopyridine (40.0 mg, 0.33 mmol) were added



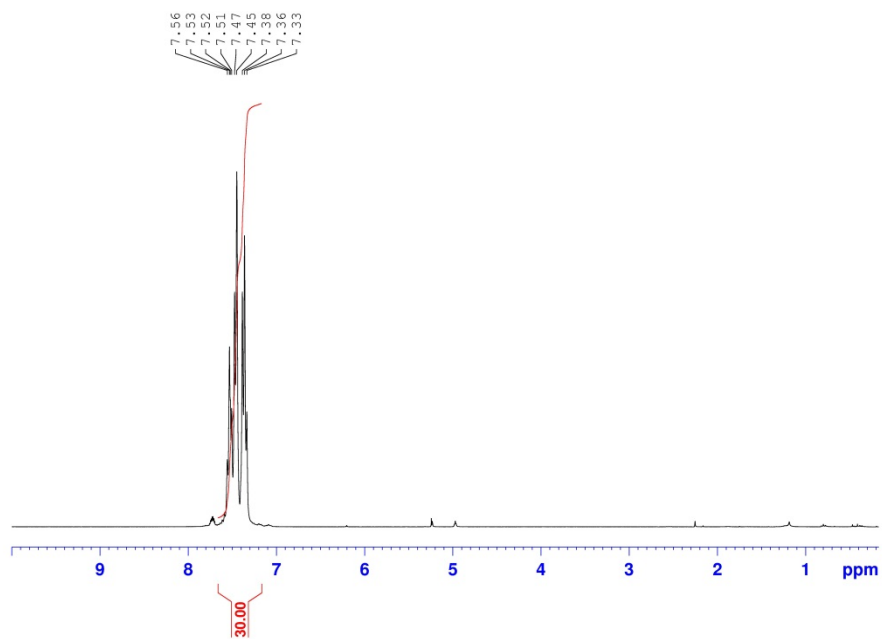
to a suspension of **7** (242.0 mg, 0.33 mmol) in dichloromethane (15 mL) at room temperature. After two hours the suspension became a clear solution. Removal of the generated KCl by filtration and evacuation of the solvents afforded **10** as a colourless solid. Crystals suitable for X-ray analysis were grown from CH_2Cl_2 /pentane (1:1) mixture (192 mg, 53.2%).

^1H NMR (300 MHz, CD_2Cl_2) $\delta = 7.63$ - 7.38 (m, 32H), 6.18 (br, 2H), 2.99 (s, 6H); ^{13}C NMR (75 MHz, CD_2Cl_2): $\delta = 155.5$ (br), 146.4 (br), 134.2 (t, $J = 5.10$ Hz), 133.2 (t, $J = 5.35$ Hz), 132.8 (br), 129.8 (t, $J = 6.16$ Hz), 126.0, 107.4 (s), 39.6 (s); $^{31}\text{P}\{^1\text{H}\}$ NMR (121 MHz, CD_2Cl_2): $\delta = 19.71$ ($^2J_{\text{P-Sn}} = 94.47$ Hz) ppm; ^{11}B NMR (128 MHz, CD_2Cl_2): $\delta = -12.5$ ppm. $^{119}\text{Sn}\{^1\text{H}\}$ NMR (CD_2Cl_2): $\delta = 17.28$ (br) ppm.; ES-MS (pos) calculated for $\text{C}_{44}\text{H}_{40}\text{ClN}_2\text{P}_2\text{Sn}$: 813.1; found 813.8; ES-MS (neg): 276.9 ($\text{B}_{12}\text{Cl}_{12}/2$).

Selected NMR Spectra

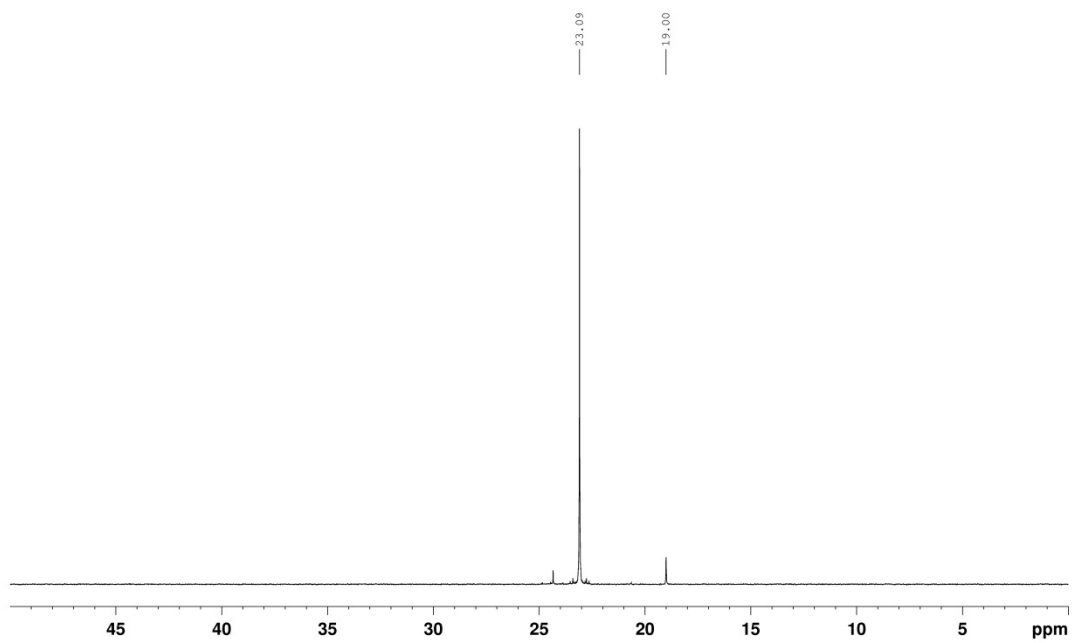
^1H NMR (300 MHz, CD_2Cl_2) **4**

khn-ka-033-01

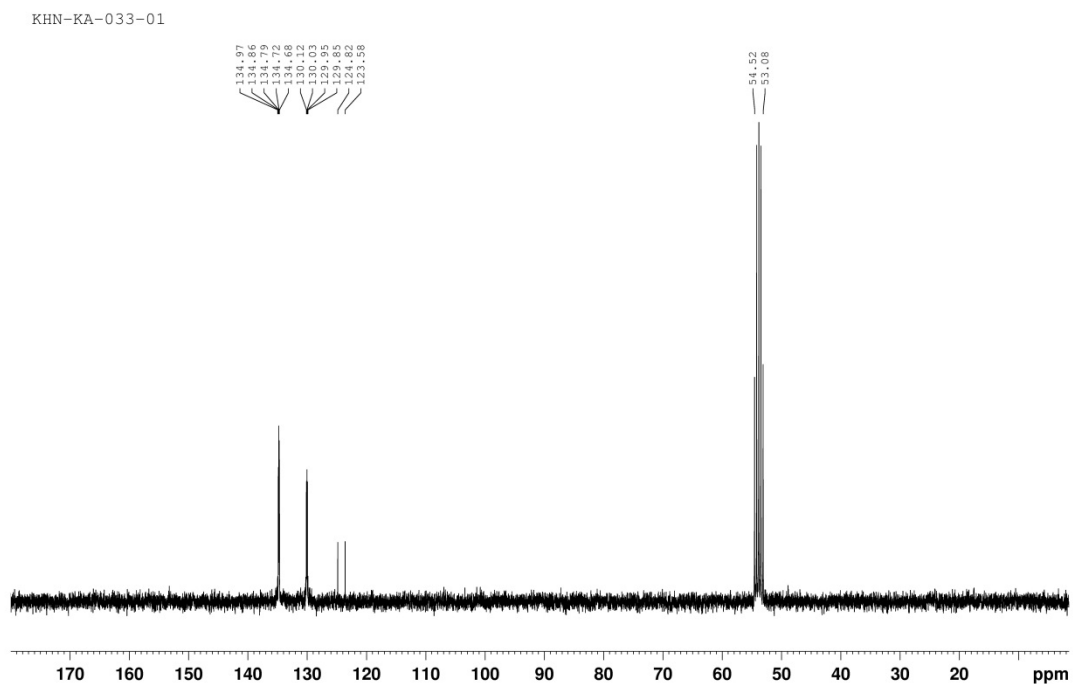


^{31}P NMR (121 MHz, CD_2Cl_2) **4**

khn-ka-033-01

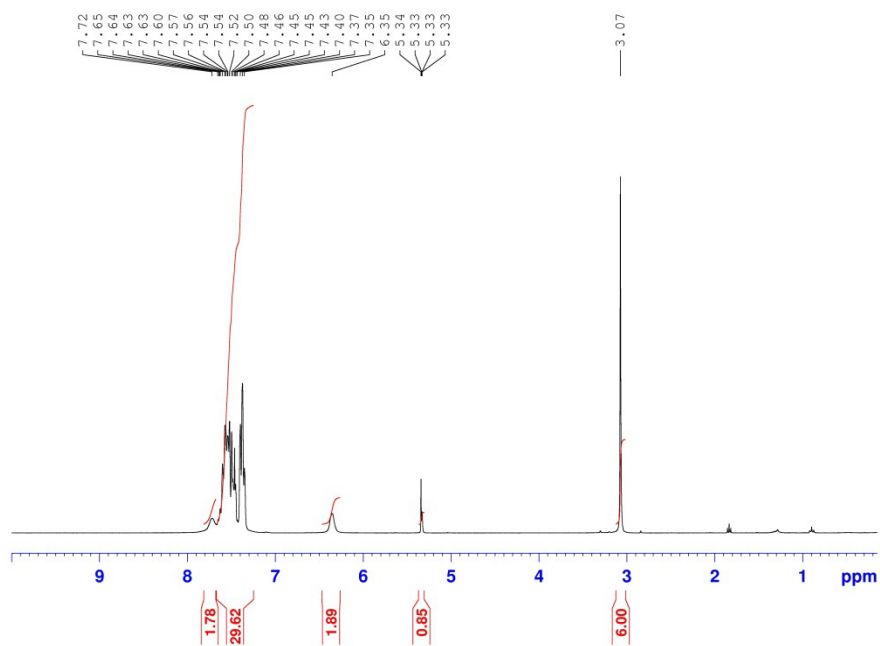


^{13}C NMR (75.5 MHz, CD_2Cl_2) **4**

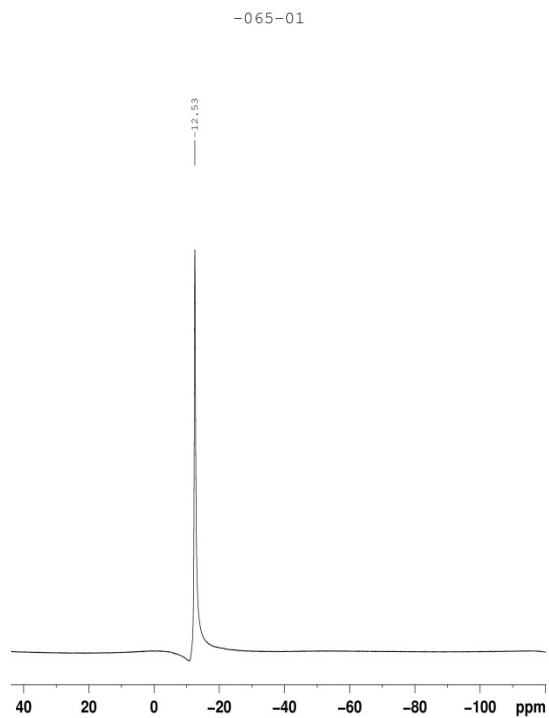


^1H NMR (300 MHz, CD_2Cl_2) **5**

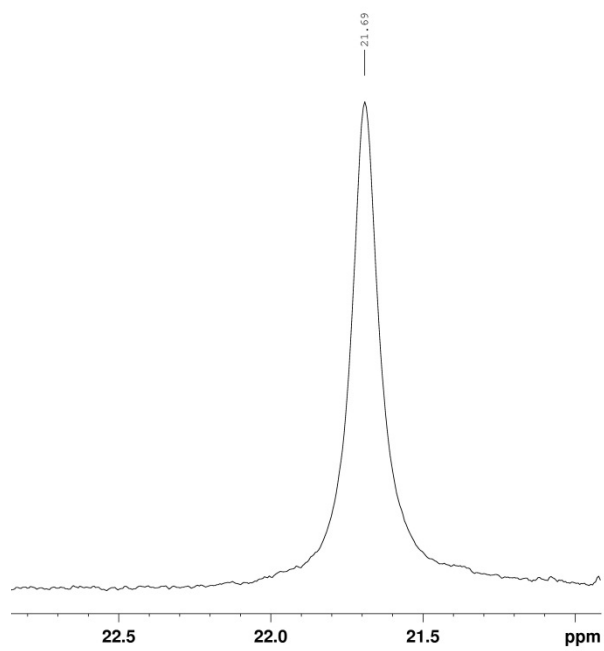
khn-ka-065-01



^{11}B NMR (128 MHz) **(a)** and ^{31}P NMR (121 MHz, CD_2Cl_2) **(b)** 5



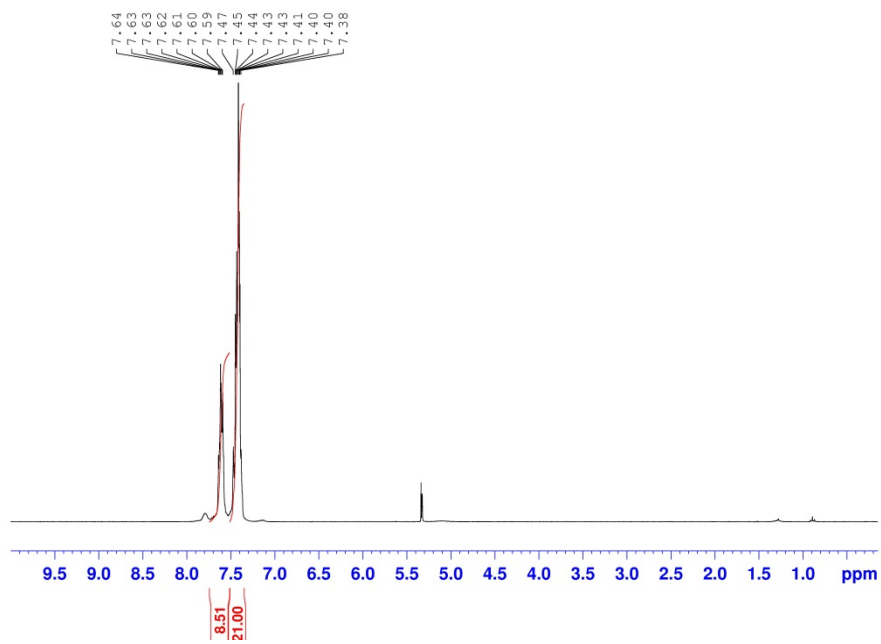
(a)



(b)

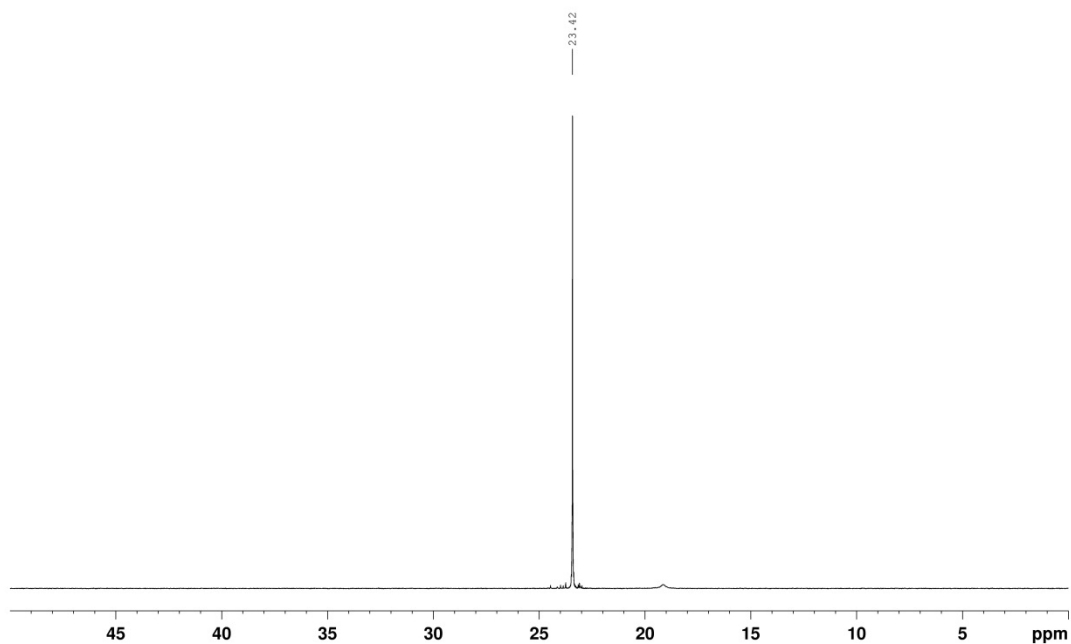
^1H NMR (300 MHz, CD_2Cl_2) 6

khn-ka-094-01



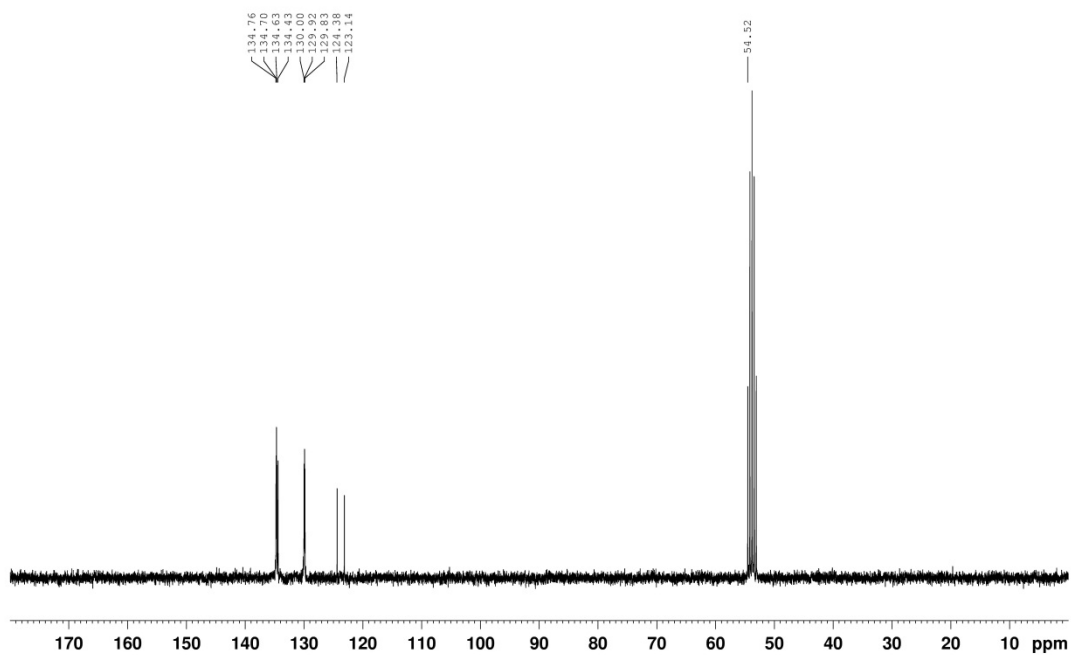
³¹P NMR (121 MHz, CD₂Cl₂) **6**

khn-ka-094-01



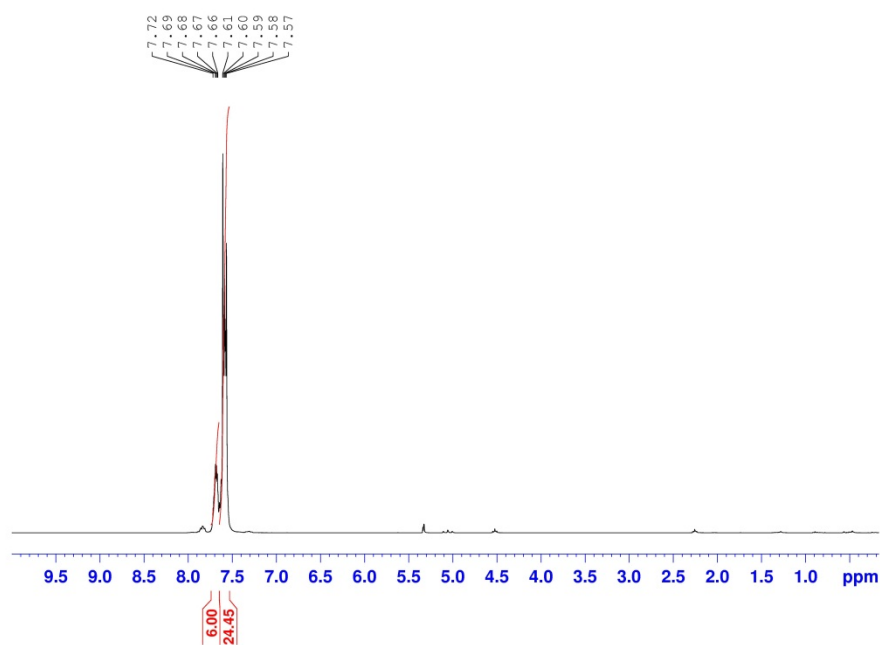
¹³C NMR (75.5 MHz, CD₂Cl₂) **6**

khn-ka-094-01



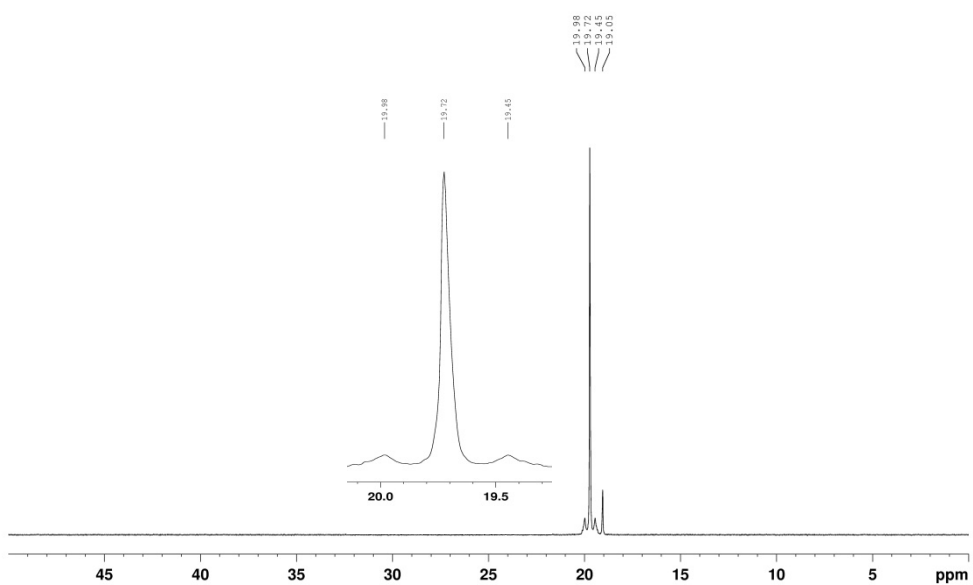
^1H NMR (300 MHz, CD_2Cl_2) **9**

KHN-KA-086-01



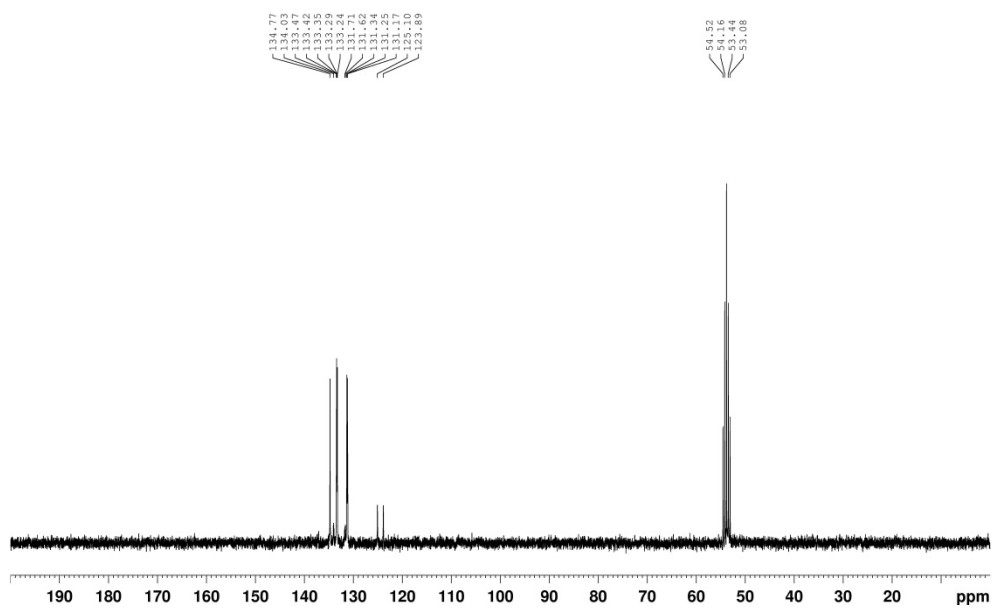
^{31}P NMR (121 MHz, CD_2Cl_2) **9**

KHN-KA-086-01



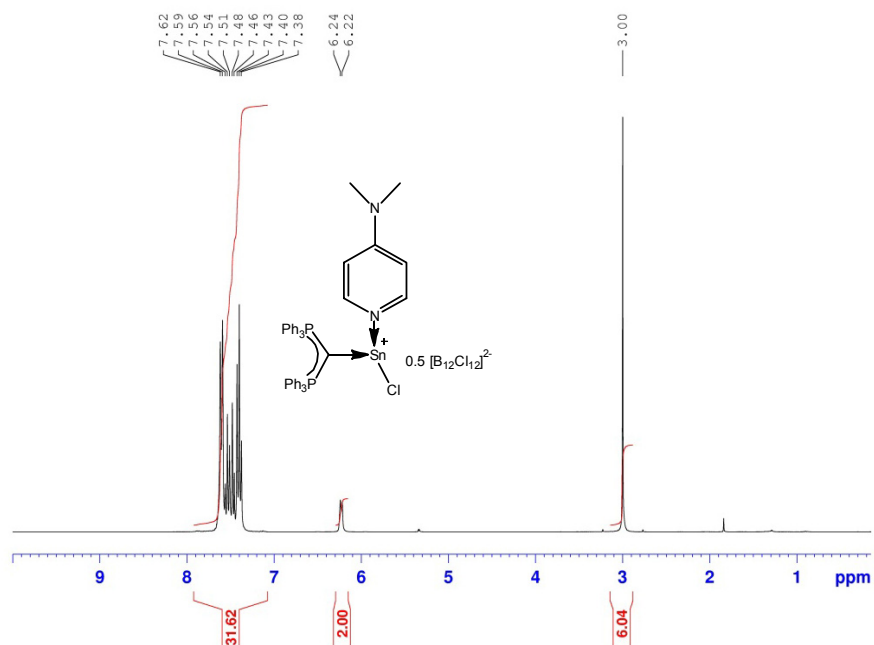
^{13}C NMR (75.5 MHz, CD_2Cl_2) **9**

KHN-KA-086-01



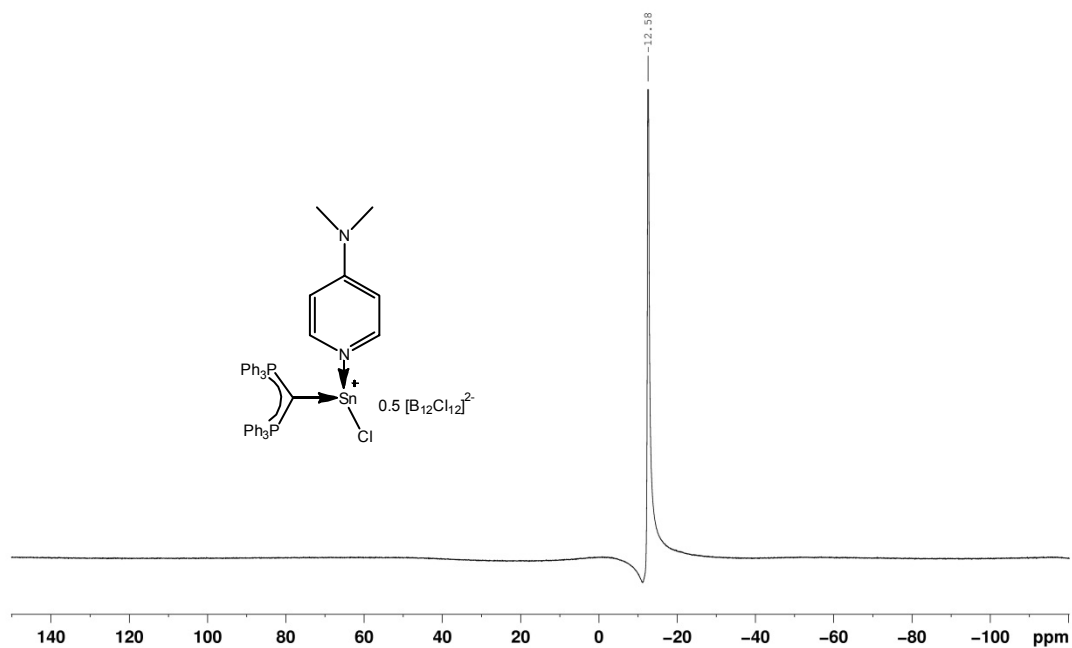
^1H NMR (300 MHz, CD_2Cl_2) **10**

khn-ka-087-01



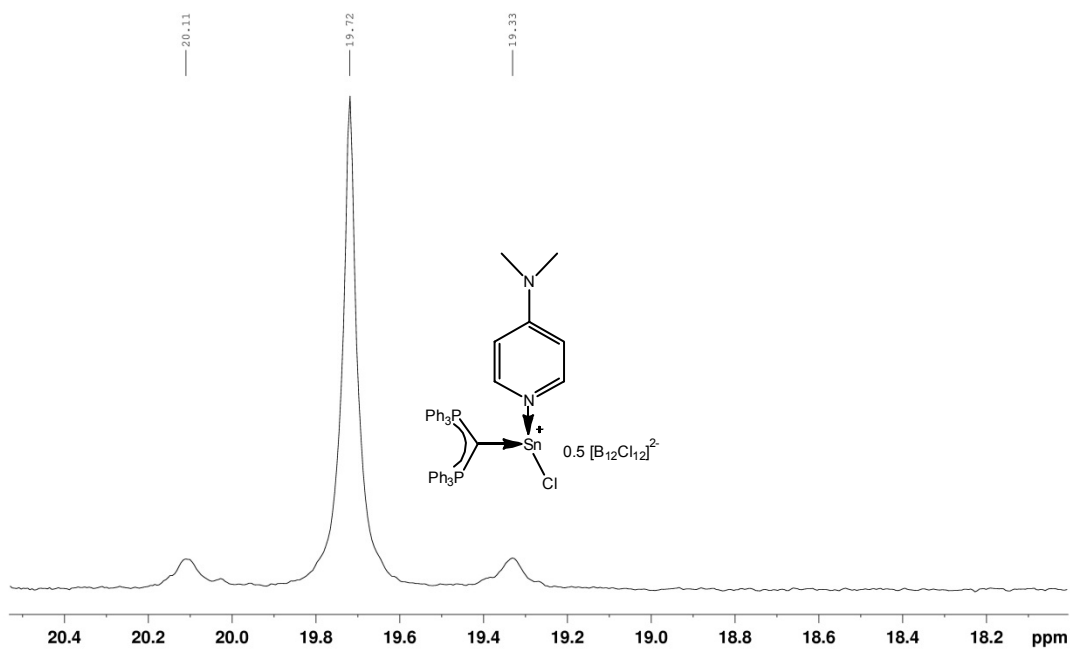
¹¹B NMR (128 MHz) **10**

khn-ka-087-01



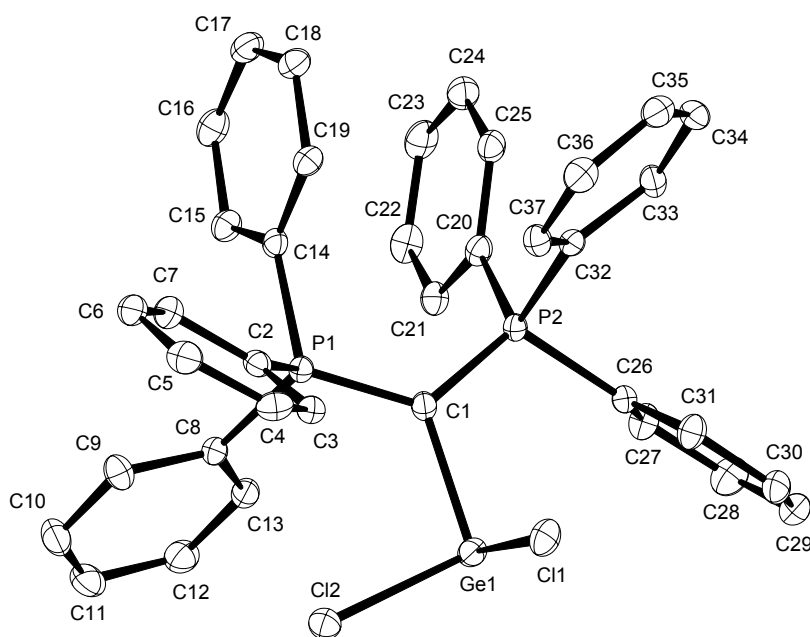
³¹P NMR (121 MHz, CD₂Cl₂) **9**

khn-ka-087-01



X-ray structures

Compound 2



Empirical formula	$C_{37}H_{30}Cl_2GeP_2$
Color	colorless
Formula weight	680.04 $g \cdot mol^{-1}$
Temperature	100 K
Wavelength	0.71073 Å
Crystal system	MONOCLINIC
Space group	P2₁/c, (no. 14)
Unit cell dimensions	$a = 15.6999(9)$ Å $\alpha = 90^\circ$. $b = 11.6983(8)$ Å $\beta = 111.382(5)^\circ$. $c = 17.7864(10)$ Å $\gamma = 90^\circ$.
Volume	3041.8(3) Å ³
Z	4
Density (calculated)	1.485 $Mg \cdot m^{-3}$
Absorption coefficient	1.315 mm^{-1}
F(000)	1392 e
Crystal size	0.12 x 0.09 x 0.05 mm^3
θ range for data collection	2.79 to 33.15°.
Index ranges	-24 ≤ h ≤ 24, -18 ≤ k ≤ 18, -27 ≤ l ≤ 27
Reflections collected	61538
Independent reflections	11576 [$R_{int} = 0.1056$]
Reflections with $I > 2\sigma(I)$	7193

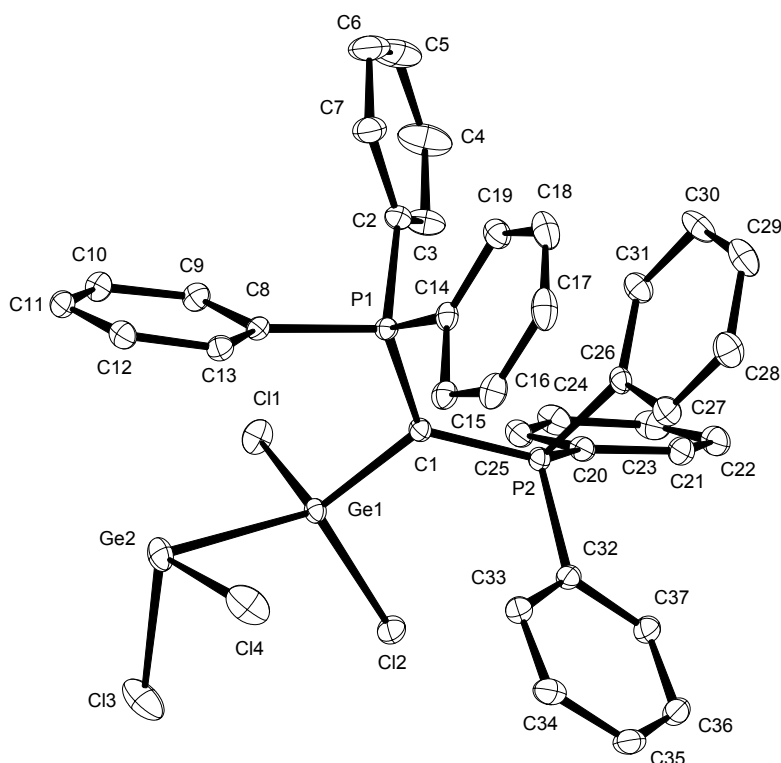
Completeness to $\theta = 27.50^\circ$	99.9 %	
Absorption correction	Gaussian	
Max. and min. transmission	0.94 and 0.85	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	11576 / 0 / 379	
Goodness-of-fit on F^2	1.075	
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0627$	$wR^2 = 0.1325$
R indices (all data)	$R_1 = 0.1257$	$wR^2 = 0.1616$
Largest diff. peak and hole	1.534 and -1.068 e · Å ⁻³	

Bond lengths [Å] and angles [°].

Ge(1)-C(1)	2.063(3)	Ge(1)-Cl(2)	2.3231(9)
Ge(1)-Cl(1)	2.3855(9)	P(1)-C(1)	1.721(3) P(1)-
C(8)	1.816(3)	P(1)-C(14)	1.817(3) P(1)-
C(2)	1.828(3)	P(2)-C(1)	1.711(3) P(2)-
C(20)	1.815(3)	P(2)-C(26)	1.823(3) P(2)-
C(32)	1.826(3)	C(2)-C(3)	1.395(4) C(2)-
C(7)	1.400(4)	C(3)-C(4)	1.396(5) C(4)-
C(5)	1.387(5)	C(5)-C(6)	1.384(5) C(6)-
C(7)	1.377(5)	C(8)-C(9)	1.393(4) C(8)-
C(13)	1.402(4)	C(9)-C(10)	1.394(5) C(10)-
C(11)	1.383(6)	C(11)-C(12)	1.387(5) C(12)-
C(13)	1.386(4)	C(14)-C(19)	1.401(4) C(14)-
C(15)	1.403(4)	C(15)-C(16)	1.394(5) C(16)-
C(17)	1.381(5)	C(17)-C(18)	1.390(5) C(18)-
C(19)	1.391(5)	C(20)-C(25)	1.395(5) C(20)-
C(21)	1.406(4)	C(21)-C(22)	1.385(5) C(22)-
C(23)	1.394(5)	C(23)-C(24)	1.367(5) C(24)-
C(25)	1.391(5)	C(26)-C(27)	1.388(5) C(26)-
C(31)	1.395(4)	C(27)-C(28)	1.397(5) C(28)-
C(29)	1.387(5)	C(29)-C(30)	1.370(5) C(30)-
C(31)	1.390(5)	C(32)-C(37)	1.384(4) C(32)-
C(33)	1.401(4)	C(33)-C(34)	1.388(4) C(34)-
C(35)	1.388(5)	C(35)-C(36)	1.382(5) C(36)-
C(37)	1.401(4)		
C(1)-Ge(1)-Cl(2)	99.49(9)	C(1)-Ge(1)-Cl(1)	98.97(9) Cl(2)-
Ge(1)-Cl(1)	93.61(3)	C(1)-P(1)-C(8)	111.88(15)
C(1)-P(1)-C(14)	113.95(15)	C(8)-P(1)-C(14)	105.93(14)
C(1)-P(1)-C(2)	115.39(15)	C(8)-P(1)-C(2)	106.56(14)
C(14)-P(1)-C(2)	102.19(14)	C(1)-P(2)-C(20)	115.33(15)
C(1)-P(2)-C(26)	110.36(15)	C(20)-P(2)-C(26)	106.19(15)
C(1)-P(2)-C(32)	116.05(15)	C(20)-P(2)-C(32)	106.43(15)
C(26)-P(2)-C(32)	101.13(14)	P(2)-C(1)-P(1)	122.84(19)
P(2)-C(1)-Ge(1)	113.47(16)	P(1)-C(1)-Ge(1)	123.36(17)
C(3)-C(2)-C(7)	119.0(3)	C(3)-C(2)-P(1)	121.2(2) C(7)-
C(2)-P(1)	119.9(2)	C(2)-C(3)-C(4)	119.8(3) C(5)-
C(4)-C(3)	120.4(3)	C(6)-C(5)-C(4)	119.8(3) C(7)-
C(6)-C(5)	120.3(3)	C(6)-C(7)-C(2)	120.7(3) C(9)-

C(8)-C(13)	119.3(3)	C(9)-C(8)-P(1)	122.1(3) C(13)-
C(8)-P(1)	118.7(2)	C(8)-C(9)-C(10)	119.9(3) C(11)-
C(10)-C(9)	120.5(3)	C(10)-C(11)-C(12)	119.9(3) C(13)-
C(12)-C(11)	120.1(3)	C(12)-C(13)-C(8)	120.3(3) C(19)-
C(14)-C(15)	119.4(3)	C(19)-C(14)-P(1)	118.9(2) C(15)-
C(14)-P(1)	121.7(2)	C(16)-C(15)-C(14)	119.7(3) C(17)-
C(16)-C(15)	120.2(3)	C(16)-C(17)-C(18)	120.7(3) C(17)-
C(18)-C(19)	119.6(3)	C(18)-C(19)-C(14)	120.4(3) C(25)-
C(20)-C(21)	118.9(3)	C(25)-C(20)-P(2)	123.2(2) C(21)-
C(20)-P(2)	117.9(2)	C(22)-C(21)-C(20)	120.3(3) C(21)-
C(22)-C(23)	120.3(3)	C(24)-C(23)-C(22)	119.2(3) C(23)-
C(24)-C(25)	121.8(3)	C(24)-C(25)-C(20)	119.5(3) C(27)-
C(26)-C(31)	119.1(3)	C(27)-C(26)-P(2)	123.1(2) C(31)-
C(26)-P(2)	117.9(2)	C(26)-C(27)-C(28)	120.0(3) C(29)-
C(28)-C(27)	120.0(3)	C(30)-C(29)-C(28)	120.4(3) C(29)-
C(30)-C(31)	119.8(3)	C(30)-C(31)-C(26)	120.8(3) C(37)-
C(32)-C(33)	118.9(3)	C(37)-C(32)-P(2)	120.4(2) C(33)-
C(32)-P(2)	120.6(2)	C(34)-C(33)-C(32)	120.6(3) C(35)-
C(34)-C(33)	119.9(3)	C(36)-C(35)-C(34)	120.1(3) C(35)-
C(36)-C(37)	119.9(3)	C(32)-C(37)-C(36)	120.5(3)

Compound 3:



Empirical formula	$C_{37}H_{30}Cl_4Ge_2P_2$	
Color	colourless	
Formula weight	823.53 $g \cdot mol^{-1}$	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	MONOCLINIC	
Space group	$P2_1/n$, (no. 14)	
Unit cell dimensions	$a = 11.7376(10)$ Å	$\alpha = 90^\circ$.
	$b = 15.8495(7)$ Å	$\beta = 96.713(6)^\circ$.
	$c = 18.8393(14)$ Å	$\gamma = 90^\circ$.
Volume	$3480.7(4)$ Å ³	
Z	4	
Density (calculated)	1.572 $Mg \cdot m^{-3}$	
Absorption coefficient	2.153 mm^{-1}	
F(000)	1656 e	
Crystal size	0.19 x 0.10 x 0.07 mm^3	
θ range for data collection	2.93 to 33.11°.	
Index ranges	$-18 \leq h \leq 18, -24 \leq k \leq 24, -28 \leq l \leq 28$	
Reflections collected	68603	
Independent reflections	13216 [$R_{int} = 0.0574$]	
Reflections with $I > 2\sigma(I)$	9516	

Completeness to $\theta = 27.50^\circ$	99.8 %	
Absorption correction	Gaussian	
Max. and min. transmission	0.93 and 0.80	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	13216 / 0 / 406	
Goodness-of-fit on F^2	1.060	
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0385$	$wR^2 = 0.0670$
R indices (all data)	$R_1 = 0.0731$	$wR^2 = 0.0772$
Largest diff. peak and hole	0.593 and -0.738 e · Å ⁻³	

Atomic coordinates and equivalent isotropic displacement parameters (\AA^2).

U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Ge(1)	0.4367(1)	0.7292(1)	0.4011(1)	0.011(1)
Ge(2)	0.6382(1)	0.7818(1)	0.4486(1)	0.019(1)
Cl(1)	0.4669(1)	0.5895(1)	0.3878(1)	0.019(1)
Cl(2)	0.3754(1)	0.7589(1)	0.2883(1)	0.018(1)
Cl(3)	0.6917(1)	0.8050(1)	0.3374(1)	0.033(1)
Cl(4)	0.5669(1)	0.9131(1)	0.4679(1)	0.029(1)
P(1)	0.3144(1)	0.7217(1)	0.5400(1)	0.011(1)
P(2)	0.1667(1)	0.7667(1)	0.4032(1)	0.011(1)
C(1)	0.2976(2)	0.7392(1)	0.4488(1)	0.011(1)
C(2)	0.2606(2)	0.6203(1)	0.5658(1)	0.015(1)
C(3)	0.2198(2)	0.5638(1)	0.5124(1)	0.021(1)
C(4)	0.1899(3)	0.4823(2)	0.5301(1)	0.033(1)
C(5)	0.2022(3)	0.4570(2)	0.6005(2)	0.035(1)
C(6)	0.2426(2)	0.5129(2)	0.6540(1)	0.031(1)
C(7)	0.2725(2)	0.5942(1)	0.6371(1)	0.022(1)
C(8)	0.4649(2)	0.7117(1)	0.5747(1)	0.012(1)
C(9)	0.5185(2)	0.6337(1)	0.5675(1)	0.015(1)
C(10)	0.6301(2)	0.6205(1)	0.5992(1)	0.017(1)
C(11)	0.6872(2)	0.6835(1)	0.6399(1)	0.016(1)
C(12)	0.6348(2)	0.7610(1)	0.6476(1)	0.015(1)
C(13)	0.5245(2)	0.7755(1)	0.6144(1)	0.014(1)
C(14)	0.2539(2)	0.8041(1)	0.5907(1)	0.013(1)
C(15)	0.2866(2)	0.8877(1)	0.5789(1)	0.015(1)
C(16)	0.2392(2)	0.9536(1)	0.6140(1)	0.019(1)
C(17)	0.1591(2)	0.9368(2)	0.6607(1)	0.023(1)
C(18)	0.1278(2)	0.8548(2)	0.6739(1)	0.022(1)
C(19)	0.1747(2)	0.7879(1)	0.6388(1)	0.017(1)
C(20)	0.1004(2)	0.6873(1)	0.3419(1)	0.014(1)
C(21)	-0.0152(2)	0.6964(1)	0.3145(1)	0.017(1)
C(22)	-0.0681(2)	0.6354(1)	0.2691(1)	0.021(1)
C(23)	-0.0086(2)	0.5638(1)	0.2527(1)	0.021(1)
C(24)	0.1046(2)	0.5532(1)	0.2815(1)	0.019(1)
C(25)	0.1599(2)	0.6154(1)	0.3250(1)	0.016(1)
C(26)	0.0572(2)	0.7847(1)	0.4621(1)	0.013(1)
C(27)	0.0224(2)	0.8661(1)	0.4769(1)	0.018(1)

C(28)	-0.0610(2)	0.8786(1)	0.5225(1)	0.021(1)
C(29)	-0.1091(2)	0.8105(1)	0.5536(1)	0.022(1)
C(30)	-0.0758(2)	0.7291(1)	0.5384(1)	0.021(1)
C(31)	0.0058(2)	0.7158(1)	0.4921(1)	0.017(1)
C(32)	0.1726(2)	0.8660(1)	0.3562(1)	0.014(1)
C(33)	0.2485(2)	0.9278(1)	0.3862(1)	0.016(1)
C(34)	0.2425(2)	1.0094(1)	0.3595(1)	0.019(1)
C(35)	0.1614(2)	1.0297(1)	0.3023(1)	0.020(1)
C(36)	0.0891(2)	0.9679(1)	0.2707(1)	0.019(1)
C(37)	0.0935(2)	0.8866(1)	0.2974(1)	0.017(1)

Bond lengths [Å] and angles [°].

C(1)-P(2)	1.7269(19)	C(1)-P(1)	1.7283(18)
C(1)-Ge(1)	1.9601(18)	C(2)-C(3)	1.389(3) C(2)-
C(7)	1.396(3)	C(2)-P(1)	1.8134(19)
C(3)-C(4)	1.389(3)	C(4)-C(5)	1.377(4) C(5)-
C(6)	1.384(4)	C(6)-C(7)	1.383(3) C(8)-
C(13)	1.396(3)	C(8)-C(9)	1.402(3) C(8)-
P(1)	1.8170(19)	C(9)-C(10)	1.389(3) C(10)-
C(11)	1.384(3)	C(11)-C(12)	1.388(3) C(12)-
C(13)	1.390(3)	C(14)-C(19)	1.396(3) C(14)-
C(15)	1.404(3)	C(14)-P(1)	1.8127(19)
C(15)-C(16)	1.388(3)	C(16)-C(17)	1.386(3) C(17)-
C(18)	1.381(3)	C(18)-C(19)	1.395(3) C(20)-
C(25)	1.393(3)	C(20)-C(21)	1.401(3) C(20)-
P(2)	1.8194(19)	C(21)-C(22)	1.389(3) C(22)-
C(23)	1.386(3)	C(23)-C(24)	1.386(3) C(24)-
C(25)	1.392(3)	C(26)-C(27)	1.392(3) C(26)-
C(31)	1.398(3)	C(26)-P(2)	1.8160(19)
C(27)-C(28)	1.389(3)	C(28)-C(29)	1.379(3) C(29)-
C(30)	1.388(3)	C(30)-C(31)	1.385(3) C(32)-
C(33)	1.397(3)	C(32)-C(37)	1.398(3) C(32)-
P(2)	1.811(2)	C(33)-C(34)	1.386(3) C(34)-
C(35)	1.390(3)	C(35)-C(36)	1.384(3) C(36)-
C(37)	1.383(3)	Cl(1)-Ge(1)	2.2614(5)
Cl(2)-Ge(1)	2.2124(5)	Cl(3)-Ge(2)	2.2855(7)
Cl(4)-Ge(2)	2.2865(6)	Ge(1)-Ge(2)	2.5672(4)
P(2)-C(1)-P(1)	121.79(11)	P(2)-C(1)-Ge(1)	122.20(10)
P(1)-C(1)-Ge(1)	115.98(10)	C(3)-C(2)-C(7)	119.52(19)
C(3)-C(2)-P(1)	118.54(15)	C(7)-C(2)-P(1)	121.46(16)
C(2)-C(3)-C(4)	120.0(2)	C(5)-C(4)-C(3)	120.1(2) C(4)-
C(5)-C(6)	120.2(2)	C(7)-C(6)-C(5)	120.2(2) C(6)-
C(7)-C(2)	119.9(2)	C(13)-C(8)-C(9)	119.18(17)
C(13)-C(8)-P(1)	122.40(15)	C(9)-C(8)-P(1)	118.06(14)
C(10)-C(9)-C(8)	120.20(18)	C(11)-C(10)-C(9)	120.03(19)
C(10)-C(11)-C(12)	120.29(18)	C(11)-C(12)-C(13)	120.02(18)
C(12)-C(13)-C(8)	120.23(18)	C(19)-C(14)-C(15)	119.44(18)
C(19)-C(14)-P(1)	122.80(15)	C(15)-C(14)-P(1)	117.74(14)
C(16)-C(15)-C(14)	120.14(19)	C(17)-C(16)-C(15)	119.8(2) C(18)-

C(17)-C(16)	120.7(2)	C(17)-C(18)-C(19)	120.1(2) C(18)-
C(19)-C(14)	119.9(2)	C(25)-C(20)-C(21)	119.31(18)
C(25)-C(20)-P(2)	121.48(15)	C(21)-C(20)-P(2)	119.10(15)
C(22)-C(21)-C(20)	119.9(2)	C(23)-C(22)-C(21)	120.4(2) C(22)-
C(23)-C(24)	119.81(19)	C(23)-C(24)-C(25)	120.3(2) C(24)-
C(25)-C(20)	120.14(19)	C(27)-C(26)-C(31)	119.43(18)
C(27)-C(26)-P(2)	120.91(15)	C(31)-C(26)-P(2)	119.64(15)
C(28)-C(27)-C(26)	120.07(19)	C(29)-C(28)-C(27)	120.2(2) C(28)-
C(29)-C(30)	120.04(19)	C(31)-C(30)-C(29)	120.2(2) C(30)-
C(31)-C(26)	119.95(19)	C(33)-C(32)-C(37)	119.31(18)
C(33)-C(32)-P(2)	118.09(15)	C(37)-C(32)-P(2)	121.99(16)
C(34)-C(33)-C(32)	120.29(19)	C(33)-C(34)-C(35)	119.9(2) C(36)-
C(35)-C(34)	119.95(19)	C(37)-C(36)-C(35)	120.5(2) C(36)-
C(37)-C(32)	119.9(2)	C(1)-Ge(1)-Cl(2)	103.19(5)
C(1)-Ge(1)-Cl(1)	106.24(6)	Cl(2)-Ge(1)-Cl(1)	98.00(2) C(1)-
Ge(1)-Ge(2)	126.65(5)	Cl(2)-Ge(1)-Ge(2)	116.628(17)
Cl(1)-Ge(1)-Ge(2)	101.946(16)	Cl(3)-Ge(2)-Cl(4)	98.31(2) Cl(3)-
Ge(2)-Ge(1)	94.242(19)	Cl(4)-Ge(2)-Ge(1)	90.669(18)
C(1)-P(1)-C(14)	113.68(9)	C(1)-P(1)-C(2)	114.01(9)
C(14)-P(1)-C(2)	109.10(9)	C(1)-P(1)-C(8)	111.39(9)
C(14)-P(1)-C(8)	107.25(9)	C(2)-P(1)-C(8)	100.44(9)
C(1)-P(2)-C(32)	112.30(9)	C(1)-P(2)-C(26)	112.77(9)
C(32)-P(2)-C(26)	103.45(9)	C(1)-P(2)-C(20)	115.55(9)
C(32)-P(2)-C(20)	109.22(9)	C(26)-P(2)-C(20)	102.46(9)

Anisotropic displacement parameters (\AA^2).

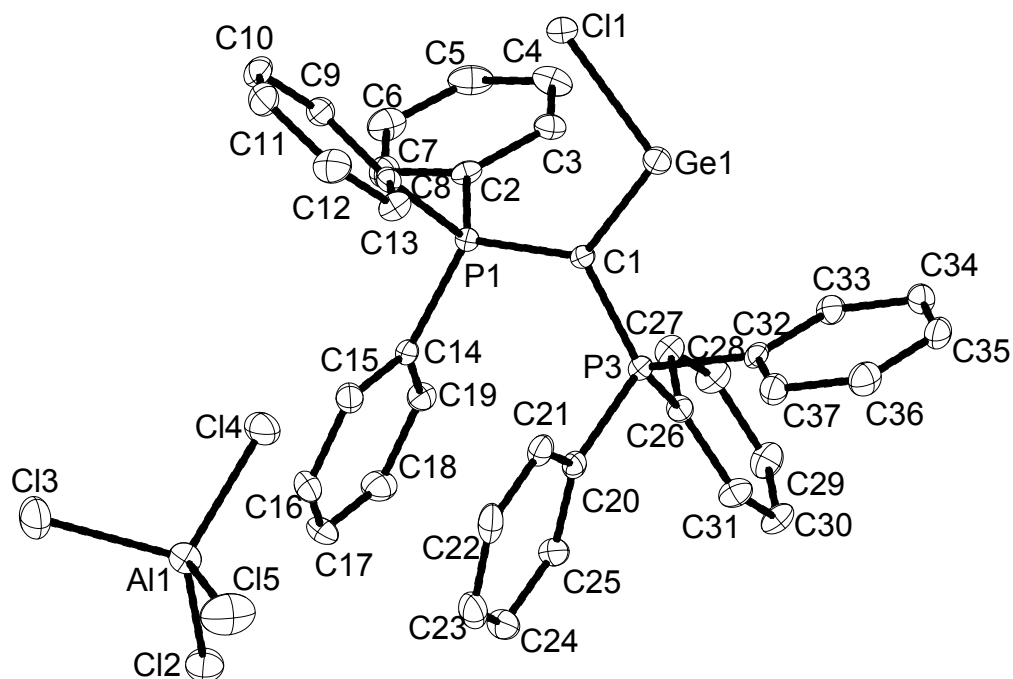
The anisotropic displacement factor exponent takes the form:

$$-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}].$$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ge(1)	0.010(1)	0.013(1)	0.010(1)	-0.001(1)	0.000(1)	-0.001(1)
Ge(2)	0.012(1)	0.023(1)	0.021(1)	-0.002(1)	-0.001(1)	-0.003(1)
Cl(1)	0.021(1)	0.015(1)	0.020(1)	-0.004(1)	-0.001(1)	0.003(1)
Cl(2)	0.017(1)	0.025(1)	0.011(1)	0.002(1)	0.001(1)	0.002(1)
Cl(3)	0.027(1)	0.044(1)	0.031(1)	-0.009(1)	0.015(1)	-0.009(1)
Cl(4)	0.033(1)	0.021(1)	0.036(1)	-0.010(1)	0.013(1)	-0.008(1)
P(1)	0.011(1)	0.011(1)	0.010(1)	0.000(1)	0.000(1)	-0.001(1)
P(2)	0.010(1)	0.014(1)	0.010(1)	0.000(1)	0.001(1)	0.000(1)
C(1)	0.010(1)	0.014(1)	0.010(1)	0.000(1)	0.001(1)	-0.001(1)
C(2)	0.014(1)	0.014(1)	0.017(1)	0.003(1)	0.002(1)	-0.002(1)
C(3)	0.029(1)	0.016(1)	0.018(1)	-0.001(1)	0.008(1)	-0.007(1)
C(4)	0.053(2)	0.018(1)	0.032(1)	-0.006(1)	0.017(1)	-0.014(1)
C(5)	0.048(2)	0.018(1)	0.041(2)	0.008(1)	0.017(1)	-0.009(1)
C(6)	0.034(1)	0.032(1)	0.025(1)	0.015(1)	0.002(1)	-0.007(1)
C(7)	0.022(1)	0.025(1)	0.018(1)	0.007(1)	-0.001(1)	-0.005(1)
C(8)	0.012(1)	0.014(1)	0.010(1)	0.002(1)	0.000(1)	0.000(1)
C(9)	0.016(1)	0.015(1)	0.014(1)	-0.001(1)	-0.001(1)	-0.001(1)
C(10)	0.016(1)	0.016(1)	0.018(1)	0.001(1)	0.001(1)	0.002(1)
C(11)	0.013(1)	0.023(1)	0.013(1)	0.003(1)	0.000(1)	0.000(1)
C(12)	0.014(1)	0.019(1)	0.012(1)	-0.003(1)	0.000(1)	-0.004(1)
C(13)	0.015(1)	0.014(1)	0.013(1)	0.000(1)	0.001(1)	0.000(1)
C(14)	0.011(1)	0.016(1)	0.012(1)	-0.002(1)	-0.001(1)	0.001(1)
C(15)	0.014(1)	0.017(1)	0.013(1)	-0.001(1)	-0.001(1)	0.001(1)
C(16)	0.018(1)	0.018(1)	0.019(1)	-0.004(1)	-0.003(1)	0.003(1)
C(17)	0.016(1)	0.031(1)	0.020(1)	-0.011(1)	-0.001(1)	0.006(1)
C(18)	0.014(1)	0.037(1)	0.015(1)	-0.007(1)	0.002(1)	0.000(1)
C(19)	0.014(1)	0.023(1)	0.014(1)	-0.001(1)	0.001(1)	-0.002(1)
C(20)	0.013(1)	0.019(1)	0.009(1)	0.000(1)	-0.001(1)	-0.004(1)
C(21)	0.014(1)	0.023(1)	0.014(1)	0.002(1)	-0.001(1)	-0.002(1)
C(22)	0.015(1)	0.032(1)	0.014(1)	0.003(1)	-0.003(1)	-0.008(1)
C(23)	0.022(1)	0.026(1)	0.013(1)	-0.002(1)	-0.001(1)	-0.011(1)
C(24)	0.021(1)	0.021(1)	0.017(1)	-0.003(1)	0.004(1)	-0.005(1)
C(25)	0.014(1)	0.021(1)	0.013(1)	-0.001(1)	0.002(1)	-0.003(1)
C(26)	0.009(1)	0.018(1)	0.011(1)	-0.001(1)	0.000(1)	-0.001(1)

C(27)0.016(1)	0.019(1)	0.018(1)	0.000(1)	0.004(1)	0.000(1)
C(28)0.019(1)	0.021(1)	0.025(1)	-0.004(1)	0.006(1)	0.002(1)
C(29)0.015(1)	0.030(1)	0.021(1)	-0.009(1)	0.006(1)	-0.005(1)
C(30)0.016(1)	0.026(1)	0.021(1)	-0.004(1)	0.007(1)	-0.009(1)
C(31)0.015(1)	0.019(1)	0.017(1)	-0.003(1)	0.003(1)	-0.003(1)
C(32)0.014(1)	0.016(1)	0.012(1)	0.002(1)	0.003(1)	0.003(1)
C(33)0.015(1)	0.019(1)	0.014(1)	0.002(1)	0.002(1)	0.001(1)
C(34)0.022(1)	0.017(1)	0.019(1)	0.002(1)	0.006(1)	-0.002(1)
C(35)0.024(1)	0.018(1)	0.021(1)	0.007(1)	0.009(1)	0.005(1)
C(36)0.018(1)	0.024(1)	0.017(1)	0.006(1)	0.004(1)	0.007(1)
C(37)0.015(1)	0.021(1)	0.014(1)	0.002(1)	0.002(1)	0.002(1)

Compound 4:



Empirical formula	$C_{37} H_{30} Al Cl_5 Ge P_2$	
Color	colourless	
Formula weight	813.37 $g \cdot mol^{-1}$	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	MONOCLINIC	
Space group	p 21/n, (no. 14)	
Unit cell dimensions	$a = 10.2366(15)$ Å	$\alpha = 90^\circ$.
	$b = 15.732$ (2) Å	$\beta = 90.710(3)^\circ$.
	$c = 22.963$ (3) Å	$\gamma = 90^\circ$.
Volume	$3697.7(9)$ Å ³	
Z	4	
Density (calculated)	1.461 $Mg \cdot m^{-3}$	
Absorption coefficient	1.327 mm^{-1}	
F(000)	1648 e	
Crystal size	0.12 x 0.04 x 0.03 mm ³	
θ range for data collection	1.57 to 26.57°.	
Index ranges	$-12 \leq h \leq 12, -19 \leq k \leq 19, -28 \leq l \leq 28$	
Reflections collected	77783	
Independent reflections	7681 [$R_{int} = 0.0521$]	
Reflections with $I > 2\sigma(I)$	6424	

Completeness to $\theta = 26.57^\circ$	99.6 %	
Absorption correction	Gaussian	
Max. and min. transmission	0.96231 and 0.88163	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7681 / 0 / 415	
Goodness-of-fit on F^2	1.028	
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0348$	$w R^2 = 0.0865$
R indices (all data)	$R_1 = 0.0464$	$w R^2 = 0.0927$
Largest diff. peak and hole	1.319 and -0.788 $e \cdot \text{\AA}^{-3}$	

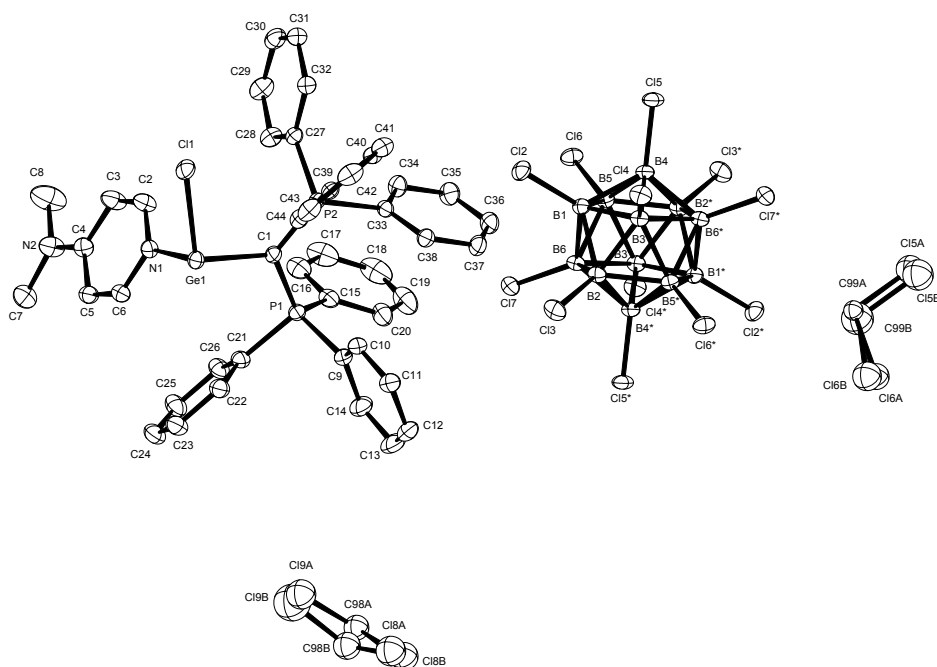
Selected bond lengths [Å] and angles [°].

Al(1)-Cl(4)	2.1311(11)	Al(1)-Cl(2)	2.1355(11)
Al(1)-Cl(5)	2.1376(12)	Al(1)-Cl(3)	2.1552(11)
C(1)-P(3)	1.741(2)	C(1)-P(1)	1.743(2) C(1)-
Ge(1)	1.954(2)	C(2)-C(3)	1.394(4) C(2)-
C(7)	1.403(4)	C(2)-P(1)	1.815(3) C(3)-
C(4)	1.387(4)	C(4)-C(5)	1.387(4) C(5)-
C(6)	1.388(4)	C(6)-C(7)	1.390(4) C(8)-
C(9)	1.394(4)	C(8)-C(13)	1.395(4) C(8)-
P(1)	1.816(3)	C(9)-C(10)	1.397(4) C(10)-
C(11)	1.385(4)	C(11)-C(12)	1.389(4) C(12)-
C(13)	1.394(4)	C(14)-C(15)	1.398(4) C(14)-
C(19)	1.400(4)	C(14)-P(1)	1.816(2) C(15)-
C(16)	1.390(4)	C(16)-C(17)	1.384(4) C(17)-
C(18)	1.385(4)	C(18)-C(19)	1.395(4) C(20)-
C(25)	1.402(4)	C(20)-C(21)	1.404(4) C(20)-
P(3)	1.807(3)	C(21)-C(22)	1.391(4) C(22)-
C(23)	1.387(4)	C(23)-C(24)	1.383(4) C(24)-
C(25)	1.396(4)	C(26)-C(27)	1.393(4) C(26)-
C(31)	1.403(4)	C(26)-P(3)	1.813(3) C(27)-
C(28)	1.391(4)	C(28)-C(29)	1.384(4) C(29)-
C(30)	1.384(4)	C(30)-C(31)	1.387(4) C(32)-
C(37)	1.394(4)	C(32)-C(33)	1.404(4) C(32)-
P(3)	1.821(3)	C(33)-C(34)	1.387(4) C(34)-
C(35)	1.387(4)	C(35)-C(36)	1.392(4) C(36)-
C(37)	1.392(4)	Cl(1)-Ge(1)	2.2527(7)
Cl(4)-Al(1)-Cl(2)	112.69(5)	Cl(4)-Al(1)-Cl(5)	109.78(5)
Cl(2)-Al(1)-Cl(5)	109.96(5)	Cl(4)-Al(1)-Cl(3)	105.82(5)
Cl(2)-Al(1)-Cl(3)	109.16(5)	Cl(5)-Al(1)-Cl(3)	109.31(5)
P(3)-C(1)-P(1)	122.12(14)	P(3)-C(1)-Ge(1)	112.51(13)
P(1)-C(1)-Ge(1)	125.19(13)	C(3)-C(2)-C(7)	119.1(2) C(3)-
C(2)-P(1)	120.10(19)	C(7)-C(2)-P(1)	120.7(2) C(4)-
C(3)-C(2)	120.6(2)	C(5)-C(4)-C(3)	120.0(3) C(4)-
C(5)-C(6)	120.1(3)	C(5)-C(6)-C(7)	120.1(3) C(6)-
C(7)-C(2)	120.1(3)	C(9)-C(8)-C(13)	119.5(2) C(9)-
C(8)-P(1)	122.0(2)	C(13)-C(8)-P(1)	118.44(19)
C(8)-C(9)-C(10)	119.7(3)	C(11)-C(10)-C(9)	120.5(3) C(10)-
C(11)-C(12)	120.0(3)	C(11)-C(12)-C(13)	119.8(3) C(12)-

C(13)-C(8)	120.4(3)	C(15)-C(14)-C(19)	119.5(2)
C(14)-P(1)	120.22(19)	C(19)-C(14)-P(1)	120.24(19)
C(16)-C(15)-C(14)	120.1(2)	C(17)-C(16)-C(15)	120.3(3)
C(17)-C(18)	120.0(2)	C(17)-C(18)-C(19)	120.5(3)
C(19)-C(14)	119.6(2)	C(25)-C(20)-C(21)	119.2(2)
C(20)-P(3)	122.8(2)	C(21)-C(20)-P(3)	118.0(2)
C(21)-C(20)	120.1(3)	C(23)-C(22)-C(21)	120.2(3)
C(23)-C(22)	120.2(3)	C(23)-C(24)-C(25)	120.3(3)
C(25)-C(20)	119.9(3)	C(27)-C(26)-C(31)	119.7(2)
C(26)-P(3)	121.01(19)	C(31)-C(26)-P(3)	118.41(19)
C(28)-C(27)-C(26)	119.7(2)	C(29)-C(28)-C(27)	120.4(2)
C(29)-C(30)	120.0(2)	C(29)-C(30)-C(31)	120.5(2)
C(31)-C(26)	119.6(2)	C(37)-C(32)-C(33)	119.5(2)
C(32)-P(3)	123.1(2)	C(33)-C(32)-P(3)	117.42(19)
C(34)-C(33)-C(32)	119.9(2)	C(35)-C(34)-C(33)	120.2(2)
C(35)-C(36)	120.4(2)	C(37)-C(36)-C(35)	119.7(3)
C(37)-C(32)	120.3(2)	C(1)-Ge(1)-Cl(1)	100.43(7)
C(1)-P(1)-C(2)	112.95(12)	C(1)-P(1)-C(8)	111.92(12)
C(2)-P(1)-C(8)	109.24(12)	C(1)-P(1)-C(14)	112.45(11)
C(2)-P(1)-C(14)	104.68(12)	C(8)-P(1)-C(14)	105.07(11)
C(1)-P(3)-C(20)	113.97(12)	C(1)-P(3)-C(26)	116.81(12)
C(20)-P(3)-C(26)	108.42(12)	C(1)-P(3)-C(32)	107.56(11)
C(20)-P(3)-C(32)	108.72(12)	C(26)-P(3)-C(32)	100.26(11)

Symmetry transformations used to generate equivalent atoms:

Compound 5:



Empirical formula

$C_{46}H_{44}B_6Cl_{11}GeN_2P_2$

Color

colourless

Formula weight

1214.17 $g \cdot mol^{-1}$

Temperature

100 K

Wavelength

0.71073 Å

Crystal system

MONOCLINIC

Space group

$P2_1/c$, (no. 14)

Unit cell dimensions

$a = 12.7024(10) \text{ Å}$ $\alpha = 90^\circ$.
 $b = 14.4943(10) \text{ Å}$ $\beta = 97.947(9)^\circ$.
 $c = 31.911(4) \text{ Å}$ $\gamma = 90^\circ$.

Volume

5818.9(9) Å³

Z

4

Density (calculated)

1.386 $Mg \cdot m^{-3}$

Absorption coefficient

1.120 mm^{-1}

F(000)

2452 e

Crystal size

0.34 x 0.34 x 0.24 mm³

θ range for data collection

2.61 to 33.13°.

Index ranges

$-19 \leq h \leq 19$, $-22 \leq k \leq 22$, $-49 \leq l \leq 49$

Reflections collected

125023

Independent reflections

22107 [$R_{int} = 0.0366$]

Reflections with $I > 2\sigma(I)$

17858

Completeness to $\theta = 33.13^\circ$

99.7 %

Absorption correction	Gaussian	
Max. and min. transmission	0.77 and 0.67	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	22107 / 0 / 609	
Goodness-of-fit on F ²	1.111	
Final R indices [I>2σ(I)]	R ₁ = 0.0660	wR ² = 0.1719
R indices (all data)	R ₁ = 0.0814	wR ² = 0.1807
Largest diff. peak and hole	1.925 and -2.599 e · Å ⁻³	

Bond lengths [Å] and angles [°].

Ge(1)-C(1)	2.053(3)	Ge(1)-N(1)	2.066(3)	Ge(1)-
Cl(1)	2.2989(8)	Cl(2)-B(1)	1.790(3)	Cl(3)-
B(2)	1.786(3)	Cl(4)-B(3)	1.791(3)	Cl(5)-
B(4)	1.784(3)	Cl(5A)-C(99A)	1.755(8)	Cl(5B)-
C(99B)	1.816(16)	Cl(6)-B(5)	1.789(3)	Cl(6A)-
C(99A)	1.781(8)	Cl(6B)-C(99B)	1.743(16)	
Cl(7)-B(6)	1.796(3)	Cl(8A)-C(98A)	1.783(9)	Cl(8B)-
C(98B)	1.753(10)	Cl(9A)-C(98A)	1.738(10)	
Cl(9B)-C(98B)	1.737(11)	P(1)-C(1)	1.715(3)	P(1)-
C(9)	1.810(3)	P(1)-C(21)	1.812(3)	P(1)-
C(15)	1.814(3)	P(2)-C(1)	1.713(3)	P(2)-
C(27)	1.815(3)	P(2)-C(33)	1.820(3)	P(2)-
C(39)	1.825(3)	N(1)-C(6)	1.342(4)	N(1)-
C(2)	1.358(4)	N(2)-C(4)	1.346(4)	N(2)-
C(7)	1.449(4)	N(2)-C(8)	1.454(5)	C(2)-
C(3)	1.359(5)	C(3)-C(4)	1.423(4)	C(4)-
C(5)	1.411(4)	C(5)-C(6)	1.369(4)	C(9)-
C(10)	1.382(4)	C(9)-C(14)	1.405(4)	C(10)-
C(11)	1.393(4)	C(11)-C(12)	1.391(5)	C(12)-
C(13)	1.372(6)	C(13)-C(14)	1.389(5)	C(15)-
C(20)	1.387(4)	C(15)-C(16)	1.400(5)	C(16)-
C(17)	1.398(5)	C(17)-C(18)	1.386(7)	C(18)-
C(19)	1.364(7)	C(19)-C(20)	1.395(5)	C(21)-
C(22)	1.391(4)	C(21)-C(26)	1.399(4)	C(22)-
C(23)	1.387(4)	C(23)-C(24)	1.385(5)	C(24)-
C(25)	1.394(5)	C(25)-C(26)	1.394(4)	C(27)-
C(28)	1.394(4)	C(27)-C(32)	1.395(4)	C(28)-
C(29)	1.390(4)	C(29)-C(30)	1.376(5)	C(30)-
C(31)	1.381(5)	C(31)-C(32)	1.392(4)	C(33)-
C(38)	1.387(4)	C(33)-C(34)	1.405(4)	C(34)-
C(35)	1.390(4)	C(35)-C(36)	1.378(5)	C(36)-
C(37)	1.390(5)	C(37)-C(38)	1.391(4)	C(39)-
C(44)	1.397(4)	C(39)-C(40)	1.403(4)	C(40)-
C(41)	1.395(4)	C(41)-C(42)	1.389(5)	C(42)-
C(43)	1.376(5)	C(43)-C(44)	1.395(4)	B(1)-
B(2)	1.780(4)	B(1)-B(6)	1.782(4)	B(1)-
B(5)	1.786(4)	B(1)-B(4)	1.789(4)	B(1)-
B(3)	1.790(4)	B(2)-B(3)	1.781(4)	B(2)-

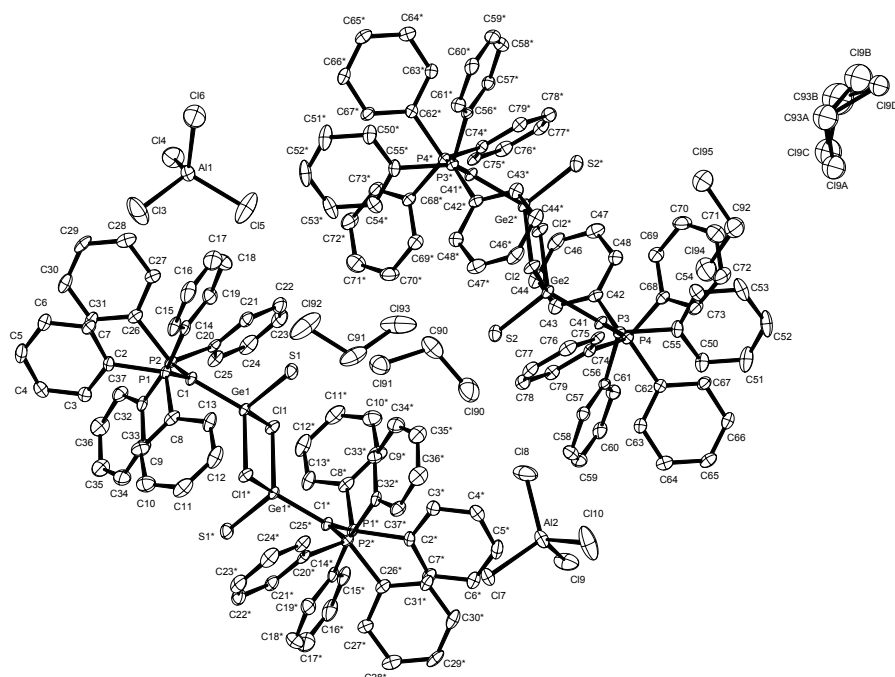
B(6)	1.783(4)	B(2)-B(5)*	1.783(4) B(2)-
B(4)*	1.784(4)	B(3)-B(5)*	1.783(4) B(3)-
B(4)	1.787(4)	B(3)-B(6)*	1.789(4) B(4)-
B(2)*	1.784(4)	B(4)-B(6)*	1.785(4) B(4)-
B(5)	1.787(4)	B(5)-B(6)	1.780(4) B(5)-
B(3)*	1.783(4)	B(5)-B(2)*	1.783(4) B(6)-
B(4)*	1.785(4)	B(6)-B(3)*	1.789(4)
C(1)-Ge(1)-N(1)	99.52(10)	C(1)-Ge(1)-Cl(1)	98.51(8) N(1)-
Ge(1)-Cl(1)	92.60(7)	C(1)-P(1)-C(9)	117.76(14)
C(1)-P(1)-C(21)	110.10(13)	C(9)-P(1)-C(21)	100.19(14)
C(1)-P(1)-C(15)	113.55(14)	C(9)-P(1)-C(15)	106.97(15)
C(21)-P(1)-C(15)	107.02(14)	C(1)-P(2)-C(27)	113.31(13)
C(1)-P(2)-C(33)	114.07(13)	C(27)-P(2)-C(33)	102.47(13)
C(1)-P(2)-C(39)	113.92(13)	C(27)-P(2)-C(39)	108.40(13)
C(33)-P(2)-C(39)	103.62(13)	C(6)-N(1)-C(2)	117.3(3) C(6)-
N(1)-Ge(1)	114.7(2)	C(2)-N(1)-Ge(1)	128.0(2) C(4)-
N(2)-C(7)	120.3(3)	C(4)-N(2)-C(8)	120.9(3) C(7)-
N(2)-C(8)	118.5(3)	P(2)-C(1)-P(1)	120.57(16)
P(2)-C(1)-Ge(1)	122.52(14)	P(1)-C(1)-Ge(1)	115.91(14)
N(1)-C(2)-C(3)	123.1(3)	C(2)-C(3)-C(4)	120.1(3) N(2)-
C(4)-C(5)	121.7(3)	N(2)-C(4)-C(3)	122.4(3) C(5)-
C(4)-C(3)	115.9(3)	C(6)-C(5)-C(4)	119.9(3) N(1)-
C(6)-C(5)	123.6(3)	C(10)-C(9)-C(14)	119.3(3) C(10)-
C(9)-P(1)	121.1(2)	C(14)-C(9)-P(1)	119.3(3) C(9)-
C(10)-C(11)	120.1(3)	C(12)-C(11)-C(10)	120.0(3) C(13)-
C(12)-C(11)	120.4(3)	C(12)-C(13)-C(14)	119.9(3) C(13)-
C(14)-C(9)	120.2(3)	C(20)-C(15)-C(16)	119.5(3) C(20)-
C(15)-P(1)	122.6(3)	C(16)-C(15)-P(1)	117.8(2) C(17)-
C(16)-C(15)	119.9(4)	C(18)-C(17)-C(16)	119.5(4) C(19)-
C(18)-C(17)	120.7(4)	C(18)-C(19)-C(20)	120.6(4) C(15)-
C(20)-C(19)	119.8(4)	C(22)-C(21)-C(26)	119.6(3) C(22)-
C(21)-P(1)	117.8(2)	C(26)-C(21)-P(1)	122.6(2) C(23)-
C(22)-C(21)	120.4(3)	C(24)-C(23)-C(22)	120.0(3) C(23)-
C(24)-C(25)	120.2(3)	C(24)-C(25)-C(26)	119.9(3) C(25)-
C(26)-C(21)	119.9(3)	C(28)-C(27)-C(32)	119.0(3) C(28)-
C(27)-P(2)	117.4(2)	C(32)-C(27)-P(2)	122.8(2) C(29)-
C(28)-C(27)	120.4(3)	C(30)-C(29)-C(28)	120.0(3) C(29)-
C(30)-C(31)	120.4(3)	C(30)-C(31)-C(32)	120.1(3) C(31)-
C(32)-C(27)	120.0(3)	C(38)-C(33)-C(34)	118.9(3) C(38)-

C(33)-P(2)	120.8(2)	C(34)-C(33)-P(2)	120.3(2)	C(35)-
C(34)-C(33)	119.8(3)	C(36)-C(35)-C(34)	120.9(3)	C(35)-
C(36)-C(37)	119.7(3)	C(36)-C(37)-C(38)	119.9(3)	C(33)-
C(38)-C(37)	120.9(3)	C(44)-C(39)-C(40)	119.5(3)	C(44)-
C(39)-P(2)	120.6(2)	C(40)-C(39)-P(2)	119.8(2)	C(41)-
C(40)-C(39)	119.8(3)	C(42)-C(41)-C(40)	120.1(3)	C(43)-
C(42)-C(41)	120.4(3)	C(42)-C(43)-C(44)	120.4(3)	C(43)-
C(44)-C(39)	119.9(3)	Cl(9A)-C(98A)-Cl(8A)	98.8(5)	Cl(9B)-
C(98B)-Cl(8B)	124.6(6)	Cl(5A)-C(99A)-Cl(6A)	110.3(4)	Cl(6B)-
C(99B)-Cl(5B)	110.1(8)	B(2)-B(1)-B(6)	60.07(17)	
B(2)-B(1)-B(5)	107.8(2)	B(6)-B(1)-B(5)	59.85(16)	
B(2)-B(1)-B(4)	107.6(2)	B(6)-B(1)-B(4)	107.8(2)	B(5)-
B(1)-B(4)	59.99(17)	B(2)-B(1)-B(3)	59.85(17)	
B(6)-B(1)-B(3)	108.0(2)	B(5)-B(1)-B(3)	107.9(2)	B(4)-
B(1)-B(3)	59.91(17)	B(2)-B(1)-Cl(2)	121.85(19)	
B(6)-B(1)-Cl(2)	121.1(2)	B(5)-B(1)-Cl(2)	121.5(2)	B(4)-
B(1)-Cl(2)	122.28(19)	B(3)-B(1)-Cl(2)	122.29(19)	
B(1)-B(2)-B(3)	60.35(17)	B(1)-B(2)-B(6)	60.00(17)	
B(3)-B(2)-B(6)	108.4(2)	B(1)-B(2)-B(5)*	108.3(2)	B(3)-
B(2)-B(5)*	60.04(17)	B(6)-B(2)-B(5)*	108.2(2)	B(1)-
B(2)-B(4)*	108.2(2)	B(3)-B(2)-B(4)*	108.3(2)	B(6)-
B(2)-B(4)*	60.07(17)	B(5)*-B(2)-B(4)*	60.14(17)	
B(1)-B(2)-Cl(3)	122.1(2)	B(3)-B(2)-Cl(3)	121.17(19)	
B(6)-B(2)-Cl(3)	122.2(2)	B(5)*-B(2)-Cl(3)	120.88(19)	
B(4)*-B(2)-Cl(3)	121.39(19)	B(2)-B(3)-B(5)*	60.04(17)	
B(2)-B(3)-B(4)	107.7(2)	B(5)*-B(3)-B(4)	107.7(2)	B(2)-
B(3)-B(6)*	107.7(2)	B(5)*-B(3)-B(6)*	59.75(16)	
B(4)-B(3)-B(6)*	59.89(16)	B(2)-B(3)-B(1)	59.81(17)	
B(5)*-B(3)-B(1)	107.9(2)	B(4)-B(3)-B(1)	60.02(17)	
B(6)*-B(3)-B(1)	107.9(2)	B(2)-B(3)-Cl(4)	121.16(19)	
B(5)*-B(3)-Cl(4)	121.71(19)	B(4)-B(3)-Cl(4)	122.41(19)	
B(6)*-B(3)-Cl(4)	122.6(2)	B(1)-B(3)-Cl(4)	121.43(19)	
B(2)*-B(4)-Cl(5)	121.11(19)	B(2)*-B(4)-B(6)*	59.94(17)	
Cl(5)-B(4)-B(6)*	121.5(2)	B(2)*-B(4)-B(5)	59.92(17)	
Cl(5)-B(4)-B(5)	121.57(19)	B(6)*-B(4)-B(5)	107.9(2)	B(2)*-
B(4)-B(3)	108.0(2)	Cl(5)-B(4)-B(3)	122.21(19)	
B(6)*-B(4)-B(3)	60.12(17)	B(5)-B(4)-B(3)	108.0(2)	B(2)*-
B(4)-B(1)	107.9(2)	Cl(5)-B(4)-B(1)	122.27(19)	
B(6)*-B(4)-B(1)	108.1(2)	B(5)-B(4)-B(1)	59.91(17)	
B(3)-B(4)-B(1)	60.07(17)	B(6)-B(5)-B(3)*	60.29(17)	

B(6)-B(5)-B(2)*	108.0(2)	B(3)*-B(5)-B(2)*	59.91(17)
B(6)-B(5)-B(1)	59.96(16)	B(3)*-B(5)-B(1)	108.3(2) B(2)*-
B(5)-B(1)	108.0(2)	B(6)-B(5)-B(4)	108.0(2) B(3)*-
B(5)-B(4)	108.1(2)	B(2)*-B(5)-B(4)	59.95(17)
B(1)-B(5)-B(4)	60.10(17)	B(6)-B(5)-Cl(6)	121.6(2) B(3)*-
B(5)-Cl(6)	121.12(19)	B(2)*-B(5)-Cl(6)	121.64(19)
B(1)-B(5)-Cl(6)	121.9(2)	B(4)-B(5)-Cl(6)	122.03(19)
B(5)-B(6)-B(1)	60.19(16)	B(5)-B(6)-B(2)	107.9(2) B(1)-
B(6)-B(2)	59.93(17)	B(5)-B(6)-B(4)*	107.9(2) B(1)-
B(6)-B(4)*	108.1(2)	B(2)-B(6)-B(4)*	59.99(17)
B(5)-B(6)-B(3)*	59.96(17)	B(1)-B(6)-B(3)*	108.2(2) B(2)-
B(6)-B(3)*	108.0(2)	B(4)*-B(6)-B(3)*	59.99(17)
B(5)-B(6)-Cl(7)	121.6(2)	B(1)-B(6)-Cl(7)	121.3(2) B(2)-
B(6)-Cl(7)	121.78(19)	B(4)*-B(6)-Cl(7)	121.99(19)
B(3)*-B(6)-Cl(7)	121.87(19)		

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

Compound 6:



Empirical formula	$C_{78}H_{68}Al_2Cl_{18}Ge_2P_4S_2$	
Color	colourless	
Formula weight	2030.56 $g \cdot mol^{-1}$	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	TRICLINIC	
Space group	$P\bar{1}$, (no. 2)	
Unit cell dimensions	$a = 15.9627(15)$ Å	$\alpha = 80.862(8)^\circ$.
	$b = 16.9274(14)$ Å	$\beta = 75.201(8)^\circ$.
	$c = 17.368(2)$ Å	$\gamma = 79.358(7)^\circ$.
Volume	4428.3(8) Å ³	
Z	2	
Density (calculated)	1.523 $Mg \cdot m^{-3}$	
Absorption coefficient	1.403 mm^{-1}	
F(000)	2048 e	
Crystal size	0.16 x 0.13 x 0.06 mm ³	
θ range for data collection	2.60 to 27.50°.	
Index ranges	-20 ≤ h ≤ 20, -21 ≤ k ≤ 21, -22 ≤ l ≤ 22	
Reflections collected	90968	
Independent reflections	20304 [$R_{int} = 0.1077$]	
Reflections with $I > 2\sigma(I)$	13526	
Completeness to $\theta = 27.50^\circ$	99.9 %	
Absorption correction	Gaussian	

Max. and min. transmission	0.93 and 0.82	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	20304 / 4 / 952	
Goodness-of-fit on F ²	1.028	
Final R indices [I>2σ(I)]	R ₁ = 0.0711	wR ² = 0.1544
R indices (all data)	R ₁ = 0.1180	wR ² = 0.1815
Largest diff. peak and hole	2.1 and -1.8 e · Å ⁻³	

Bond lengths [Å] and angles [°].

Ge(1)-C(1)	1.924(5)	Ge(1)-S(1)	2.1794(15)
Ge(1)-Cl(1)	2.2171(14)	Ge(1)-Cl(1)*	2.2323(14)
Ge(2)-C(41)	1.922(5)	Ge(2)-S(2)	2.1870(15)
Ge(2)-Cl(2)	2.2162(14)	Ge(2)-Cl(2)**	2.2273(15)
Cl(1)-Ge(1)*	2.2323(14)	Cl(2)-Ge(2)**	2.2273(15)
Cl(3)-Al(1)	2.113(3)	Cl(4)-Al(1)	2.136(3) Cl(5)-
Al(1)	2.123(3)	Cl(6)-Al(1)	2.125(3) Cl(7)-
Al(2)	2.135(2)	Cl(8)-Al(2)	2.129(3) Cl(9)-
Al(2)	2.118(2)	Cl(9A)-C(93A)	1.7004(10)
Cl(9B)-C(93A)	1.7001(10)	Cl(9C)-C(93B)	1.7000(10)
Cl(9D)-C(93B)	1.7002(10)	Cl(10)-Al(2)	2.126(3) Cl(90)-
C(90)	1.753(8)	Cl(91)-C(90)	1.772(7) Cl(92)-
C(91)	1.781(8)	Cl(93)-C(91)	1.761(9) Cl(94)-
C(92)	1.751(8)	Cl(95)-C(92)	1.765(8) P(1)-
C(1)	1.738(5)	P(1)-C(8)	1.811(6) P(1)-
C(14)	1.812(5)	P(1)-C(2)	1.812(5) P(2)-
C(1)	1.733(5)	P(2)-C(32)	1.807(5) P(2)-
C(20)	1.816(5)	P(2)-C(26)	1.822(5) P(3)-
C(41)	1.731(5)	P(3)-C(42)	1.799(5) P(3)-
C(56)	1.808(5)	P(3)-C(55)	1.816(5) P(4)-
C(41)	1.743(5)	P(4)-C(68)	1.800(6) P(4)-
C(74)	1.801(5)	P(4)-C(62)	1.819(5) C(2)-
C(3)	1.395(8)	C(2)-C(7)	1.400(7) C(3)-
C(4)	1.382(8)	C(4)-C(5)	1.397(9) C(5)-
C(6)	1.379(9)	C(6)-C(7)	1.399(8) C(8)-
C(9)	1.392(8)	C(8)-C(13)	1.409(8) C(9)-
C(10)	1.395(8)	C(10)-C(11)	1.370(9) C(11)-
C(12)	1.385(10)	C(12)-C(13)	1.392(9) C(14)-
C(19)	1.381(8)	C(14)-C(15)	1.403(8) C(15)-
C(16)	1.390(8)	C(16)-C(17)	1.372(11)
C(17)-C(18)	1.379(10)	C(18)-C(19)	1.392(8) C(20)-
C(21)	1.385(8)	C(20)-C(25)	1.391(8) C(21)-
C(22)	1.392(8)	C(22)-C(23)	1.398(9) C(23)-
C(24)	1.358(10)	C(24)-C(25)	1.392(8) C(26)-
C(31)	1.393(8)	C(26)-C(27)	1.398(8) C(27)-
C(28)	1.398(8)	C(28)-C(29)	1.385(9) C(29)-
C(30)	1.379(9)	C(30)-C(31)	1.403(8) C(32)-
C(33)	1.385(8)	C(32)-C(37)	1.408(8) C(33)-

C(34)	1.393(8)	C(34)-C(35)	1.381(9) C(35)-
C(36)	1.375(9)	C(36)-C(37)	1.391(8) C(42)-
C(48)	1.400(8)	C(42)-C(43)	1.405(8) C(43)-
C(44)	1.385(8)	C(44)-C(46)	1.373(9) C(46)-
C(47)	1.372(9)	C(47)-C(48)	1.396(8) C(50)-
C(51)	1.385(8)	C(50)-C(55)	1.395(8) C(51)-
C(52)	1.376(10)	C(52)-C(53)	1.412(10)
C(53)-C(54)	1.381(8)	C(54)-C(55)	1.394(8) C(56)-
C(57)	1.374(7)	C(56)-C(61)	1.413(7) C(57)-
C(58)	1.399(8)	C(58)-C(59)	1.386(8) C(59)-
C(60)	1.367(9)	C(60)-C(61)	1.386(8) C(62)-
C(63)	1.394(7)	C(62)-C(67)	1.397(7) C(63)-
C(64)	1.400(7)	C(64)-C(65)	1.390(8) C(65)-
C(66)	1.378(8)	C(66)-C(67)	1.398(8) C(68)-
C(69)	1.393(8)	C(68)-C(73)	1.405(7) C(69)-
C(70)	1.383(8)	C(70)-C(71)	1.391(9) C(71)-
C(72)	1.379(9)	C(72)-C(73)	1.387(8) C(74)-
C(79)	1.403(7)	C(74)-C(75)	1.405(7) C(75)-
C(76)	1.382(8)	C(76)-C(77)	1.385(9) C(77)-
C(78)	1.390(8)	C(78)-C(79)	1.389(7)
C(1)-Ge(1)-S(1)	107.55(16)	C(1)-Ge(1)-Cl(1)	118.34(16)
S(1)-Ge(1)-Cl(1)	108.20(6)	C(1)-Ge(1)-Cl(1)*	118.30(17)
S(1)-Ge(1)-Cl(1)*	107.14(6)	Cl(1)-Ge(1)-Cl(1)*	96.39(5) C(41)-
Ge(2)-S(2)	108.82(16)	C(41)-Ge(2)-Cl(2)	117.22(15)
S(2)-Ge(2)-Cl(2)	107.80(6)	C(41)-Ge(2)-Cl(2)**	118.71(16)
S(2)-Ge(2)-Cl(2)**	106.78(6)	Cl(2)-Ge(2)-Cl(2)**	96.39(5) Ge(1)-
Cl(1)-Ge(1)*	83.61(5)	Ge(2)-Cl(2)-Ge(2)**	83.61(5) C(1)-
P(1)-C(8)	112.6(2)	C(1)-P(1)-C(14)	115.0(3) C(8)-
P(1)-C(14)	103.6(3)	C(1)-P(1)-C(2)	110.8(2) C(8)-
P(1)-C(2)	107.4(2)	C(14)-P(1)-C(2)	106.9(2) C(1)-
P(2)-C(32)	113.5(3)	C(1)-P(2)-C(20)	109.6(2) C(32)-
P(2)-C(20)	106.4(3)	C(1)-P(2)-C(26)	113.4(2) C(32)-
P(2)-C(26)	107.3(2)	C(20)-P(2)-C(26)	106.1(2) C(41)-
P(3)-C(42)	110.7(2)	C(41)-P(3)-C(56)	115.0(2) C(42)-
P(3)-C(56)	102.2(2)	C(41)-P(3)-C(55)	111.2(2) C(42)-
P(3)-C(55)	110.4(3)	C(56)-P(3)-C(55)	107.1(2) C(41)-
P(4)-C(68)	113.9(3)	C(41)-P(4)-C(74)	109.8(2) C(68)-
P(4)-C(74)	106.4(2)	C(41)-P(4)-C(62)	113.1(2) C(68)-
P(4)-C(62)	106.6(2)	C(74)-P(4)-C(62)	106.6(2) Cl(3)-

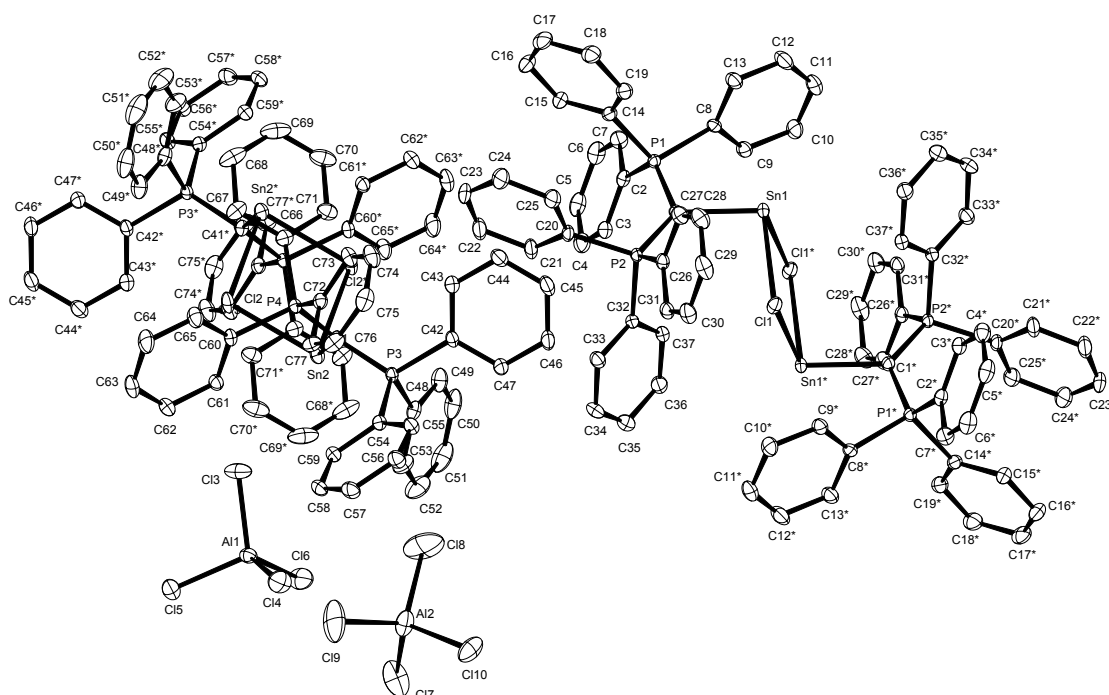
Al(1)-Cl(5)	109.86(13)	Cl(3)-Al(1)-Cl(6)	109.55(13)
Cl(5)-Al(1)-Cl(6)	109.22(12)	Cl(3)-Al(1)-Cl(4)	108.96(11)
Cl(5)-Al(1)-Cl(4)	109.12(11)	Cl(6)-Al(1)-Cl(4)	110.12(12)
Cl(9)-Al(2)-Cl(10)	111.29(12)	Cl(9)-Al(2)-Cl(8)	108.70(11)
Cl(10)-Al(2)-Cl(8)	107.15(13)	Cl(9)-Al(2)-Cl(7)	109.57(10)
Cl(10)-Al(2)-Cl(7)	108.49(11)	Cl(8)-Al(2)-Cl(7)	111.64(10)
P(2)-C(1)-P(1)	124.7(3)	P(2)-C(1)-Ge(1)	117.3(3) P(1)-
C(1)-Ge(1)	117.8(3)	C(3)-C(2)-C(7)	120.1(5) C(3)-
C(2)-P(1)	119.3(4)	C(7)-C(2)-P(1)	120.6(4) C(4)-
C(3)-C(2)	120.4(5)	C(3)-C(4)-C(5)	119.4(5) C(6)-
C(5)-C(4)	120.8(5)	C(5)-C(6)-C(7)	120.0(5) C(6)-
C(7)-C(2)	119.2(5)	C(9)-C(8)-C(13)	119.1(5) C(9)-
C(8)-P(1)	121.8(4)	C(13)-C(8)-P(1)	119.0(5) C(8)-
C(9)-C(10)	120.5(6)	C(11)-C(10)-C(9)	119.8(6) C(10)-
C(11)-C(12)	120.9(6)	C(11)-C(12)-C(13)	120.1(6) C(12)-
C(13)-C(8)	119.6(6)	C(19)-C(14)-C(15)	120.1(5) C(19)-
C(14)-P(1)	121.0(4)	C(15)-C(14)-P(1)	119.0(4) C(16)-
C(15)-C(14)	119.6(6)	C(17)-C(16)-C(15)	119.9(6) C(16)-
C(17)-C(18)	120.6(6)	C(17)-C(18)-C(19)	120.4(7) C(14)-
C(19)-C(18)	119.4(6)	C(21)-C(20)-C(25)	119.4(5) C(21)-
C(20)-P(2)	120.0(4)	C(25)-C(20)-P(2)	120.7(4) C(20)-
C(21)-C(22)	121.0(6)	C(21)-C(22)-C(23)	118.3(6) C(24)-
C(23)-C(22)	121.3(6)	C(23)-C(24)-C(25)	120.2(6) C(20)-
C(25)-C(24)	119.8(6)	C(31)-C(26)-C(27)	119.5(5) C(31)-
C(26)-P(2)	121.7(4)	C(27)-C(26)-P(2)	118.7(4) C(28)-
C(27)-C(26)	120.0(5)	C(29)-C(28)-C(27)	119.9(6) C(30)-
C(29)-C(28)	120.7(5)	C(29)-C(30)-C(31)	119.8(5) C(26)-
C(31)-C(30)	120.1(6)	C(33)-C(32)-C(37)	119.9(5) C(33)-
C(32)-P(2)	120.0(4)	C(37)-C(32)-P(2)	120.0(4) C(32)-
C(33)-C(34)	119.7(5)	C(35)-C(34)-C(33)	120.2(6) C(36)-
C(35)-C(34)	120.4(6)	C(35)-C(36)-C(37)	120.4(6) C(36)-
C(37)-C(32)	119.3(6)	P(3)-C(41)-P(4)	123.6(3) P(3)-
C(41)-Ge(2)	118.0(3)	P(4)-C(41)-Ge(2)	118.4(3) C(48)-
C(42)-C(43)	118.8(5)	C(48)-C(42)-P(3)	122.7(4) C(43)-
C(42)-P(3)	118.5(4)	C(44)-C(43)-C(42)	120.4(6) C(46)-
C(44)-C(43)	120.0(6)	C(47)-C(46)-C(44)	120.7(6) C(46)-
C(47)-C(48)	120.5(6)	C(47)-C(48)-C(42)	119.5(5) C(51)-
C(50)-C(55)	119.6(6)	C(52)-C(51)-C(50)	121.3(6) C(51)-
C(52)-C(53)	119.1(6)	C(54)-C(53)-C(52)	119.9(6) C(53)-
C(54)-C(55)	120.3(6)	C(54)-C(55)-C(50)	119.7(5) C(54)-

C(55)-P(3)	118.7(4)	C(50)-C(55)-P(3)	121.5(4)	C(57)-
C(56)-C(61)	119.7(5)	C(57)-C(56)-P(3)	121.5(4)	C(61)-
C(56)-P(3)	118.7(4)	C(56)-C(57)-C(58)	120.4(5)	C(59)-
C(58)-C(57)	119.0(5)	C(60)-C(59)-C(58)	121.2(5)	C(59)-
C(60)-C(61)	120.2(5)	C(60)-C(61)-C(56)	119.4(5)	C(63)-
C(62)-C(67)	119.8(5)	C(63)-C(62)-P(4)	118.7(4)	C(67)-
C(62)-P(4)	121.5(4)	C(62)-C(63)-C(64)	120.0(5)	C(65)-
C(64)-C(63)	120.0(5)	C(66)-C(65)-C(64)	119.9(5)	C(65)-
C(66)-C(67)	120.9(5)	C(62)-C(67)-C(66)	119.4(5)	C(69)-
C(68)-C(73)	118.6(5)	C(69)-C(68)-P(4)	119.8(4)	C(73)-
C(68)-P(4)	121.5(4)	C(70)-C(69)-C(68)	120.8(5)	C(69)-
C(70)-C(71)	119.8(6)	C(72)-C(71)-C(70)	120.3(6)	C(71)-
C(72)-C(73)	120.1(6)	C(72)-C(73)-C(68)	120.3(5)	C(79)-
C(74)-C(75)	119.3(5)	C(79)-C(74)-P(4)	119.6(4)	C(75)-
C(74)-P(4)	121.1(4)	C(76)-C(75)-C(74)	119.9(5)	C(75)-
C(76)-C(77)	120.6(5)	C(76)-C(77)-C(78)	120.1(5)	C(79)-
C(78)-C(77)	120.1(6)	C(78)-C(79)-C(74)	120.0(5)	Cl(90)-
C(90)-Cl(91)	111.7(4)	Cl(93)-C(91)-Cl(92)	113.3(4)	Cl(94)-
C(92)-Cl(95)	112.1(4)	Cl(9B)-C(93A)-Cl(9A)	116.3(3)	Cl(9C)-
C(93B)-Cl(9D)	117.7(7)			

Symmetry transformations used to generate equivalent atoms:

* $-x+2, -y+1, -z$ ** $-x+2, -y, -z+1$

Compound 9:



Empirical formula

$C_{74}H_{60}Al_2Cl_{10}P_4Sn_2$

Color

colourless

Formula weight

1718.94 $g \cdot mol^{-1}$

Temperature

100 K

Wavelength

0.71073 Å

Crystal system

TRICLINIC

Space group

$P\bar{1}$, (no. 2)

Unit cell dimensions

$a = 14.8877(15) \text{ \AA}$ $\alpha = 93.175(5)^\circ$
 $b = 15.2192(17) \text{ \AA}$ $\beta = 94.331(5)^\circ$
 $c = 17.0271(5) \text{ \AA}$ $\gamma = 97.118(8)^\circ$

Volume

3809.1(6) Å³

Z

2

Density (calculated)

1.499 $Mg \cdot m^{-3}$

Absorption coefficient

1.154 mm^{-1}

F(000)

1720 e

Crystal size

0.41 x 0.20 x 0.10 mm³

θ range for data collection

2.67 to 33.07°.

Index ranges

$-22 \leq h \leq 22$, $-23 \leq k \leq 23$, $-26 \leq l \leq 26$

Reflections collected

105812

Independent reflections

28837 [$R_{int} = 0.0501$]

Reflections with $I > 2\sigma(I)$

23324

Completeness to $\theta = 33.07^\circ$

99.9 %

Absorption correction	Gaussian	
Max. and min. transmission	0.89 and 0.72	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	28837 / 0 / 829	
Goodness-of-fit on F ²	1.056	
Final R indices [I>2σ(I)]	R ₁ = 0.0410	wR ² = 0.1028
R indices (all data)	R ₁ = 0.0544	wR ² = 0.1088
Largest diff. peak and hole	1.803 and -2.021 e · Å ⁻³	

Bond lengths [Å] and angles [°].

Sn(1)-C(1)	2.2011(18)	Sn(1)-Cl(1)	2.6220(5)
Sn(1)-Cl(1)*	2.7279(5)	Sn(2)-C(41)	2.2398(19)
Sn(2)-Cl(2)	2.6052(6)	Sn(2)-Cl(2)**	2.7129(5)
Cl(1)-Sn(1)*	2.7279(5)	Cl(2)-Sn(2)**	2.7129(5)
Cl(3)-Al(1)	2.1353(9)	Cl(4)-Al(1)	2.1370(9)
Cl(5)-Al(1)	2.1397(9)	Cl(6)-Al(1)	2.1302(9)
Cl(7)-Al(2)	2.1376(12)	Cl(8)-Al(2)	2.1273(13)
Cl(9)-Al(2)	2.1243(11)	Cl(10)-Al(2)	2.1280(10)
P(1)-C(1)	1.7101(19)	P(1)-C(2)	1.807(2) P(1)-
C(14)	1.8190(19)	P(1)-C(8)	1.8227(19)
P(2)-C(1)	1.7200(19)	P(2)-C(32)	1.8099(19)
P(2)-C(20)	1.8118(19)	P(2)-C(26)	1.812(2) P(3)-
C(41)	1.7163(19)	P(3)-C(54)	1.810(2) P(3)-
C(48)	1.817(2)	P(3)-C(42)	1.820(2) P(4)-
C(41)	1.7250(19)	P(4)-C(60)	1.8154(19)
P(4)-C(66)	1.818(2)	P(4)-C(72)	1.821(2) C(2)-
C(3)	1.391(3)	C(2)-C(7)	1.406(3) C(3)-
C(4)	1.397(3)	C(4)-C(5)	1.380(3) C(5)-
C(6)	1.389(4)	C(6)-C(7)	1.384(3) C(8)-
C(13)	1.400(3)	C(8)-C(9)	1.406(3) C(9)-
C(10)	1.397(3)	C(10)-C(11)	1.385(3) C(11)-
C(12)	1.393(3)	C(12)-C(13)	1.392(3) C(14)-
C(19)	1.398(3)	C(14)-C(15)	1.402(3) C(15)-
C(16)	1.397(3)	C(16)-C(17)	1.384(4) C(17)-
C(18)	1.392(3)	C(18)-C(19)	1.391(3) C(20)-
C(25)	1.391(3)	C(20)-C(21)	1.400(3) C(21)-
C(22)	1.387(3)	C(22)-C(23)	1.378(4) C(23)-
C(24)	1.379(5)	C(24)-C(25)	1.393(3) C(26)-
C(31)	1.397(3)	C(26)-C(27)	1.404(3) C(27)-
C(28)	1.391(3)	C(28)-C(29)	1.390(3) C(29)-
C(30)	1.385(3)	C(30)-C(31)	1.393(3) C(32)-
C(37)	1.397(3)	C(32)-C(33)	1.407(3) C(33)-
C(34)	1.387(3)	C(34)-C(35)	1.388(3) C(35)-
C(36)	1.390(3)	C(36)-C(37)	1.391(3) C(42)-
C(43)	1.389(3)	C(42)-C(47)	1.405(3) C(43)-
C(44)	1.395(3)	C(44)-C(45)	1.390(3) C(45)-
C(46)	1.392(3)	C(46)-C(47)	1.385(3) C(48)-
C(53)	1.387(3)	C(48)-C(49)	1.410(3) C(49)-

C(50)	1.390(3)	C(50)-C(51)	1.379(5)	C(51)-
C(52)	1.385(4)	C(52)-C(53)	1.402(3)	C(54)-
C(55)	1.396(3)	C(54)-C(59)	1.403(3)	C(55)-
C(56)	1.391(3)	C(56)-C(57)	1.391(3)	C(57)-
C(58)	1.389(3)	C(58)-C(59)	1.390(3)	C(60)-
C(61)	1.390(3)	C(60)-C(65)	1.403(3)	C(61)-
C(62)	1.393(3)	C(62)-C(63)	1.388(3)	C(63)-
C(64)	1.390(3)	C(64)-C(65)	1.388(3)	C(66)-
C(71)	1.398(3)	C(66)-C(67)	1.400(3)	C(67)-
C(68)	1.392(3)	C(68)-C(69)	1.380(4)	C(69)-
C(70)	1.385(4)	C(70)-C(71)	1.389(3)	C(72)-
C(73)	1.398(3)	C(72)-C(77)	1.402(3)	C(73)-
C(74)	1.392(3)	C(74)-C(75)	1.390(4)	C(75)-
C(76)	1.385(3)	C(76)-C(77)	1.392(3)	
C(1)-Sn(1)-Cl(1)	97.70(5)	C(1)-Sn(1)-Cl(1)*	98.56(5)	Cl(1)-
Sn(1)-Cl(1)*	78.353(17)	C(41)-Sn(2)-Cl(2)	95.77(5)	C(41)-
Sn(2)-Cl(2)**	101.85(5)	Cl(2)-Sn(2)-Cl(2)**	80.870(17)	
Sn(1)-Cl(1)-Sn(1)*	101.646(17)	Sn(2)-Cl(2)-Sn(2)**	99.130(17)	
C(1)-P(1)-C(2)	117.59(9)	C(1)-P(1)-C(14)	115.43(9)	
C(2)-P(1)-C(14)	106.12(9)	C(1)-P(1)-C(8)	105.33(9)	
C(2)-P(1)-C(8)	103.07(9)	C(14)-P(1)-C(8)	108.31(9)	
C(1)-P(2)-C(32)	113.91(9)	C(1)-P(2)-C(20)	113.53(9)	
C(32)-P(2)-C(20)	104.67(9)	C(1)-P(2)-C(26)	109.47(9)	
C(32)-P(2)-C(26)	107.68(9)	C(20)-P(2)-C(26)	107.18(9)	
C(41)-P(3)-C(54)	114.28(9)	C(41)-P(3)-C(48)	106.27(9)	
C(54)-P(3)-C(48)	108.28(9)	C(41)-P(3)-C(42)	118.78(9)	
C(54)-P(3)-C(42)	106.68(9)	C(48)-P(3)-C(42)	101.39(9)	
C(41)-P(4)-C(60)	114.73(9)	C(41)-P(4)-C(66)	110.02(9)	
C(60)-P(4)-C(66)	108.29(10)	C(41)-P(4)-C(72)	114.81(9)	
C(60)-P(4)-C(72)	102.56(9)	C(66)-P(4)-C(72)	105.77(9)	
Cl(6)-Al(1)-Cl(3)	111.65(4)	Cl(6)-Al(1)-Cl(4)	109.62(4)	
Cl(3)-Al(1)-Cl(4)	108.84(4)	Cl(6)-Al(1)-Cl(5)	109.78(4)	
Cl(3)-Al(1)-Cl(5)	106.88(4)	Cl(4)-Al(1)-Cl(5)	110.03(4)	
Cl(9)-Al(2)-Cl(8)	110.94(6)	Cl(9)-Al(2)-Cl(10)	110.12(5)	
Cl(8)-Al(2)-Cl(10)	107.25(6)	Cl(9)-Al(2)-Cl(7)	110.52(5)	
Cl(8)-Al(2)-Cl(7)	110.82(5)	Cl(10)-Al(2)-Cl(7)	107.07(5)	
P(1)-C(1)-P(2)	126.11(11)	P(1)-C(1)-Sn(1)	111.48(9)	
P(2)-C(1)-Sn(1)	121.94(10)	C(3)-C(2)-C(7)	119.56(19)	
C(3)-C(2)-P(1)	120.81(15)	C(7)-C(2)-P(1)	119.61(16)	

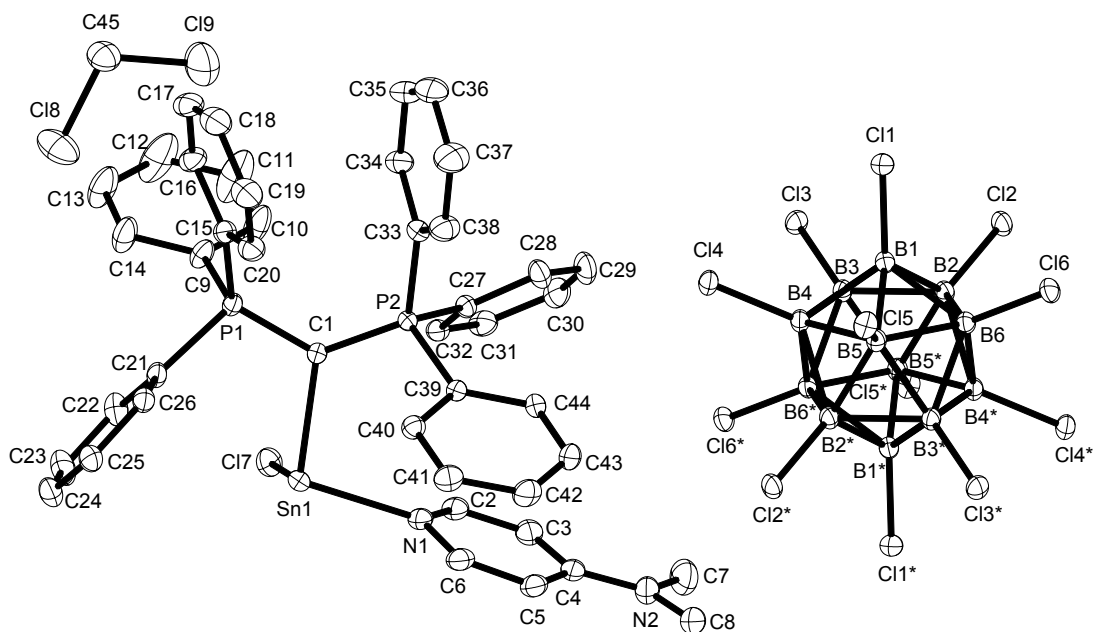
C(2)-C(3)-C(4)	120.08(19)	C(5)-C(4)-C(3)	119.7(2) C(4)-
C(5)-C(6)	120.8(2)	C(7)-C(6)-C(5)	119.9(2) C(6)-
C(7)-C(2)	120.0(2)	C(13)-C(8)-C(9)	119.43(17)
C(13)-C(8)-P(1)	123.85(14)	C(9)-C(8)-P(1)	116.34(14)
C(10)-C(9)-C(8)	120.07(19)	C(11)-C(10)-C(9)	120.0(2) C(10)-
C(11)-C(12)	120.2(2)	C(13)-C(12)-C(11)	120.4(2) C(12)-
C(13)-C(8)	119.90(19)	C(19)-C(14)-C(15)	119.37(18)
C(19)-C(14)-P(1)	119.12(15)	C(15)-C(14)-P(1)	121.50(16)
C(16)-C(15)-C(14)	119.9(2)	C(17)-C(16)-C(15)	120.2(2) C(16)-
C(17)-C(18)	120.4(2)	C(19)-C(18)-C(17)	119.8(2) C(18)-
C(19)-C(14)	120.4(2)	C(25)-C(20)-C(21)	119.73(19)
C(25)-C(20)-P(2)	120.92(17)	C(21)-C(20)-P(2)	119.23(16)
C(22)-C(21)-C(20)	120.0(2)	C(23)-C(22)-C(21)	120.0(2) C(22)-
C(23)-C(24)	120.3(2)	C(23)-C(24)-C(25)	120.6(3) C(20)-
C(25)-C(24)	119.3(2)	C(31)-C(26)-C(27)	118.87(18)
C(31)-C(26)-P(2)	122.62(15)	C(27)-C(26)-P(2)	118.50(15)
C(28)-C(27)-C(26)	120.4(2)	C(29)-C(28)-C(27)	120.2(2) C(30)-
C(29)-C(28)	119.8(2)	C(29)-C(30)-C(31)	120.4(2) C(30)-
C(31)-C(26)	120.29(19)	C(37)-C(32)-C(33)	119.59(18)
C(37)-C(32)-P(2)	119.59(14)	C(33)-C(32)-P(2)	120.80(15)
C(34)-C(33)-C(32)	119.71(19)	C(33)-C(34)-C(35)	120.2(2) C(34)-
C(35)-C(36)	120.5(2)	C(35)-C(36)-C(37)	119.8(2) C(36)-
C(37)-C(32)	120.18(19)	P(3)-C(41)-P(4)	124.10(11)
P(3)-C(41)-Sn(2)	110.21(9)	P(4)-C(41)-Sn(2)	124.43(10)
C(43)-C(42)-C(47)	119.11(18)	C(43)-C(42)-P(3)	121.94(15)
C(47)-C(42)-P(3)	118.87(15)	C(42)-C(43)-C(44)	120.65(19)
C(45)-C(44)-C(43)	119.9(2)	C(44)-C(45)-C(46)	119.9(2) C(47)-
C(46)-C(45)	120.3(2)	C(46)-C(47)-C(42)	120.2(2) C(53)-
C(48)-C(49)	120.4(2)	C(53)-C(48)-P(3)	123.01(17)
C(49)-C(48)-P(3)	116.42(17)	C(50)-C(49)-C(48)	119.4(2) C(51)-
C(50)-C(49)	120.3(2)	C(50)-C(51)-C(52)	120.4(2) C(51)-
C(52)-C(53)	120.5(3)	C(48)-C(53)-C(52)	119.0(2) C(55)-
C(54)-C(59)	119.47(18)	C(55)-C(54)-P(3)	122.30(15)
C(59)-C(54)-P(3)	118.01(15)	C(56)-C(55)-C(54)	120.16(19)
C(57)-C(56)-C(55)	120.1(2)	C(58)-C(57)-C(56)	119.99(19)
C(57)-C(58)-C(59)	120.27(19)	C(58)-C(59)-C(54)	119.95(19)
C(61)-C(60)-C(65)	118.92(18)	C(61)-C(60)-P(4)	121.18(14)
C(65)-C(60)-P(4)	119.85(15)	C(60)-C(61)-C(62)	120.75(18)
C(63)-C(62)-C(61)	119.8(2)	C(62)-C(63)-C(64)	120.0(2) C(65)-
C(64)-C(63)	120.2(2)	C(64)-C(65)-C(60)	120.3(2) C(71)-

C(66)-C(67)	119.4(2)	C(71)-C(66)-P(4)	117.53(16)
C(67)-C(66)-P(4)	122.99(17)	C(68)-C(67)-C(66)	119.4(2) C(69)-
C(68)-C(67)	120.9(2)	C(68)-C(69)-C(70)	119.9(2) C(69)-
C(70)-C(71)	120.3(2)	C(70)-C(71)-C(66)	120.1(2) C(73)-
C(72)-C(77)	119.17(18)	C(73)-C(72)-P(4)	121.77(15)
C(77)-C(72)-P(4)	119.02(15)	C(74)-C(73)-C(72)	120.2(2) C(75)-
C(74)-C(73)	120.1(2)	C(76)-C(75)-C(74)	120.0(2) C(75)-
C(76)-C(77)	120.3(2)	C(76)-C(77)-C(72)	120.0(2)

Symmetry transformations used to generate equivalent atoms:

* $-x+2, -y+1, -z+2$ ** $-x+1, -y, -z+1$

Compound 10:



Empirical formula	$C_{45} H_{42} B_6 Cl_9 N_2 P_2 Sn$	
Colour	colourless	
Formula weight	1175.35 $g \cdot mol^{-1}$	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	TRICLINIC	
Space group	p -1, (no. 2)	
Unit cell dimensions	$a = 13.4966(15) \text{ \AA}$	$\alpha = 75.335(2)^\circ$.
	$b = 13.8369(15) \text{ \AA}$	$\beta = 78.243(2)^\circ$.
	$c = 15.8174(17) \text{ \AA}$	$\gamma = 89.307(2)^\circ$.
Volume	$2795.3(5) \text{ \AA}^3$	
Z	2	
Density (calculated)	1.396 $Mg \cdot m^{-3}$	
Absorption coefficient	0.977 mm^{-1}	
F(000)	1178 e	
Crystal size	0.16 x 0.15 x 0.13 mm^3	
θ range for data collection	1.76 to 31.38°.	
Index ranges	$-19 \leq h \leq 19, -20 \leq k \leq 20, -23 \leq l \leq 23$	
Reflections collected	83085	
Independent reflections	18121 [$R_{int} = 0.0204$]	
Reflections with $I > 2\sigma(I)$	16507	
Completeness to $\theta = 27.50^\circ$	99.7 %	

Absorption correction	Gaussian	
Max. and min. transmission	0.92312 and 0.86886	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	18121 / 0 / 588	
Goodness-of-fit on F ²	1.061	
Final R indices [I > 2σ(I)]	R ₁ = 0.0246	wR ² = 0.0644
R indices (all data)	R ₁ = 0.0273	wR ² = 0.0656
Largest diff. peak and hole	1.327 and -0.891 e · Å ⁻³	

Selected bond lengths [Å] and angles [°].

B(1)-B(5)	1.7830(18)	B(1)-B(6)	1.7864(19)
B(1)-B(2)	1.7895(18)	B(1)-B(3)	1.7906(19)
B(1)-Cl(1)	1.7927(13)	B(1)-B(4)	1.7947(18)
B(2)-B(3)	1.7862(18)	B(2)-B(6)	1.7937(19)
B(2)-Cl(2)	1.7958(13)	B(3)-B(4)	1.7879(18)
B(3)-Cl(3)	1.7952(13)	B(4)-B(5)	1.7911(19)
B(4)-Cl(4)	1.7964(13)	B(5)-B(6)	1.7928(18)
B(5)-Cl(5)	1.7988(13)	B(6)-Cl(6)	1.7943(13)
C(1)-P(1)	1.7007(12)	C(1)-P(2)	1.7012(12)
C(1)-Sn(1)	2.2721(12)	C(2)-N(1)	1.3522(17)
C(2)-C(3)	1.3764(19)	C(3)-C(4)	1.414(2) C(4)-
N(2)	1.3530(18)	C(4)-C(5)	1.416(2) C(5)-
C(6)	1.3726(19)	C(6)-N(1)	1.3558(17)
C(7)-N(2)	1.451(3)	C(8)-N(2)	1.458(2) C(9)-
C(10)	1.3917(19)	C(9)-C(14)	1.4002(19)
C(9)-P(1)	1.8139(13)	C(10)-C(11)	1.392(2) C(11)-
C(12)	1.388(3)	C(12)-C(13)	1.383(3) C(13)-
C(14)	1.388(2)	C(15)-C(20)	1.4005(19)
C(15)-C(16)	1.4008(18)	C(15)-P(1)	1.8218(13)
C(16)-C(17)	1.393(2)	C(17)-C(18)	1.383(3) C(18)-
C(19)	1.392(2)	C(19)-C(20)	1.3936(19)
C(21)-C(22)	1.3999(18)	C(21)-C(26)	1.4015(17)
C(21)-P(1)	1.8253(13)	C(22)-C(23)	1.397(2) C(23)-
C(24)	1.388(2)	C(24)-C(25)	1.388(2) C(25)-
C(26)	1.3930(18)	C(27)-C(32)	1.3956(18)
C(27)-C(28)	1.4037(17)	C(27)-P(2)	1.8197(12)
C(28)-C(29)	1.3908(19)	C(29)-C(30)	1.387(2) C(30)-
C(31)	1.392(2)	C(31)-C(32)	1.3978(17)
C(33)-C(38)	1.3970(19)	C(33)-C(34)	1.3995(18)
C(33)-P(2)	1.8110(12)	C(34)-C(35)	1.3883(19)
C(35)-C(36)	1.390(2)	C(36)-C(37)	1.388(2) C(37)-
C(38)	1.396(2)	C(39)-C(44)	1.4011(16)
C(39)-C(40)	1.4038(17)	C(39)-P(2)	1.8095(12)
C(40)-C(41)	1.3870(18)	C(41)-C(42)	1.391(2) C(42)-
C(43)	1.389(2)	C(43)-C(44)	1.3899(19)
C(45)-Cl(9)	1.7422(18)	C(45)-Cl(8)	1.7642(17)
Cl(7)-Sn(1)	2.5035(4)	N(1)-Sn(1)	2.2975(11)

B(5)-B(1)-B(6)	60.30(7)	B(5)-B(1)-B(2)	108.35(9)
B(6)-B(1)-B(2)	60.21(7)	B(5)-B(1)-B(3)	108.01(9)
B(6)-B(1)-B(3)	108.11(9)	B(2)-B(1)-B(3)	59.86(7) B(5)-
B(1)-Cl(1)	121.17(9)	B(6)-B(1)-Cl(1)	121.57(8)
B(2)-B(1)-Cl(1)	122.09(8)	B(3)-B(1)-Cl(1)	121.98(9)
B(5)-B(1)-B(4)	60.08(7)	B(6)-B(1)-B(4)	108.29(9)
B(2)-B(1)-B(4)	107.89(9)	B(3)-B(1)-B(4)	59.82(7) Cl(1)-
B(1)-B(4)	121.40(8)	B(3)-B(2)-B(1)	60.10(7) B(3)-
B(2)-B(6)	107.99(9)	B(1)-B(2)-B(6)	59.81(7) B(3)-
B(2)-Cl(2)	119.24(8)	B(1)-B(2)-Cl(2)	120.89(8)
B(6)-B(2)-Cl(2)	123.62(8)	B(2)-B(3)-B(4)	108.34(9)
B(2)-B(3)-B(1)	60.04(7)	B(4)-B(3)-B(1)	60.20(7) B(2)-
B(3)-Cl(3)	121.03(8)	B(4)-B(3)-Cl(3)	121.91(8)
B(1)-B(3)-Cl(3)	121.42(8)	B(3)-B(4)-B(5)	107.77(9)
B(3)-B(4)-B(1)	59.97(7)	B(5)-B(4)-B(1)	59.64(7) B(3)-
B(4)-Cl(4)	119.78(8)	B(5)-B(4)-Cl(4)	123.35(8)
B(1)-B(4)-Cl(4)	121.21(8)	B(1)-B(5)-B(4)	60.28(7) B(1)-
B(5)-B(6)	59.94(7)	B(4)-B(5)-B(6)	108.17(9)
B(1)-B(5)-Cl(5)	121.74(8)	B(4)-B(5)-Cl(5)	121.91(8)
B(6)-B(5)-Cl(5)	121.47(9)	B(1)-B(6)-B(5)	59.76(7) B(1)-
B(6)-B(2)	59.98(7)	B(5)-B(6)-B(2)	107.73(9)
B(1)-B(6)-Cl(6)	122.81(8)	B(5)-B(6)-Cl(6)	122.08(9)
B(2)-B(6)-Cl(6)	122.21(8)	P(1)-C(1)-P(2)	129.02(7)
P(1)-C(1)-Sn(1)	111.95(6)	P(2)-C(1)-Sn(1)	118.84(6)
N(1)-C(2)-C(3)	123.39(13)	C(2)-C(3)-C(4)	120.29(13)
N(2)-C(4)-C(3)	122.11(15)	N(2)-C(4)-C(5)	122.01(14)
C(3)-C(4)-C(5)	115.87(12)	C(6)-C(5)-C(4)	119.63(13)
N(1)-C(6)-C(5)	124.11(13)	C(10)-C(9)-C(14)	119.00(13)
C(10)-C(9)-P(1)	119.80(11)	C(14)-C(9)-P(1)	120.64(10)
C(11)-C(10)-C(9)	120.15(15)	C(12)-C(11)-C(10)	120.25(17)
C(13)-C(12)-C(11)	120.11(16)	C(12)-C(13)-C(14)	119.82(16)
C(13)-C(14)-C(9)	120.66(15)	C(20)-C(15)-C(16)	119.11(12)
C(20)-C(15)-P(1)	119.68(10)	C(16)-C(15)-P(1)	121.21(11)
C(17)-C(16)-C(15)	119.91(15)	C(18)-C(17)-C(16)	120.56(14)
C(17)-C(18)-C(19)	120.18(14)	C(18)-C(19)-C(20)	119.65(15)
C(19)-C(20)-C(15)	120.58(13)	C(22)-C(21)-C(26)	119.15(12)
C(22)-C(21)-P(1)	121.35(10)	C(26)-C(21)-P(1)	119.25(10)
C(23)-C(22)-C(21)	120.04(13)	C(24)-C(23)-C(22)	120.16(14)
C(25)-C(24)-C(23)	120.30(13)	C(24)-C(25)-C(26)	119.85(13)
C(25)-C(26)-C(21)	120.51(12)	C(32)-C(27)-C(28)	119.51(11)

C(32)-C(27)-P(2)	119.26(9)	C(28)-C(27)-P(2)	121.20(10)
C(29)-C(28)-C(27)	120.01(13)	C(30)-C(29)-C(28)	120.12(13)
C(29)-C(30)-C(31)	120.43(13)	C(30)-C(31)-C(32)	119.68(13)
C(27)-C(32)-C(31)	120.21(12)	C(38)-C(33)-C(34)	119.43(12)
C(38)-C(33)-P(2)	121.53(10)	C(34)-C(33)-P(2)	119.03(10)
C(35)-C(34)-C(33)	120.09(14)	C(34)-C(35)-C(36)	120.27(14)
C(37)-C(36)-C(35)	120.09(14)	C(36)-C(37)-C(38)	119.96(15)
C(37)-C(38)-C(33)	120.14(14)	C(44)-C(39)-C(40)	119.34(11)
C(44)-C(39)-P(2)	123.08(9)	C(40)-C(39)-P(2)	117.47(9)
C(41)-C(40)-C(39)	120.31(12)	C(40)-C(41)-C(42)	120.00(13)
C(43)-C(42)-C(41)	120.04(13)	C(42)-C(43)-C(44)	120.49(12)
C(43)-C(44)-C(39)	119.81(12)	Cl(9)-C(45)-Cl(8)	111.73(9)
C(2)-N(1)-C(6)	116.41(12)	C(2)-N(1)-Sn(1)	127.78(9)
C(6)-N(1)-Sn(1)	115.75(9)	C(4)-N(2)-C(7)	120.51(15)
C(4)-N(2)-C(8)	120.47(15)	C(7)-N(2)-C(8)	118.89(14)
C(1)-P(1)-C(9)	117.79(6)	C(1)-P(1)-C(15)	115.53(6)
C(9)-P(1)-C(15)	103.60(6)	C(1)-P(1)-C(21)	107.13(6)
C(9)-P(1)-C(21)	105.05(6)	C(15)-P(1)-C(21)	106.84(6)
C(1)-P(2)-C(39)	108.39(6)	C(1)-P(2)-C(33)	118.02(6)
C(39)-P(2)-C(33)	104.56(6)	C(1)-P(2)-C(27)	114.60(6)
C(39)-P(2)-C(27)	107.26(6)	C(33)-P(2)-C(27)	103.12(6)
C(1)-Sn(1)-N(1)	101.61(4)	C(1)-Sn(1)-Cl(7)	93.82(3) N(1)-
Sn(1)-Cl(7)	88.00(3)		

Symmetry transformations used to generate equivalent atoms:

Computational Methods

Geometry optimizations were carried out using the BP86^{1, 2} functional in combination with def2-TZVP basis sets.³ The resolution-of-identity (RI) approximation⁴⁻⁶ was applied in conjunction with the appropriate auxiliary basis sets to speed up the calculations. Relevant stationary points were characterized as minima, by evaluating harmonic vibrational frequencies at the same level (RI-BP86/def2-TZVP). All geometry optimizations were performed using the TURBOMOLE (version 6.4) suite of programs.^{7, 8} In order to gain insight into the electronic structure of the complexes, a Natural Bond Orbital (NBO) analysis was carried out at the BP86/6-31G* level using NBO version 3.1⁹⁻¹⁵ as implemented in the Gaussian 09 program package.¹⁶ Additionally, the σ -donation and π -(back)donation effects were rationalized by performing a fragment analysis on the molecules considered in the present study. In this analysis, the molecule is built from user-defined fragments, and the symmetrized fragment orbitals (SFOs) are used as new basis functions. These computations employed the *Amsterdam Density Functional* (ADF) program package,¹⁷⁻¹⁹ where the molecular orbitals (MOs) are expanded in terms of Slater-type orbitals (STOs), employing a triple- ζ basis set (TZP) with one polarization function.

Computational Results

Tables S1-S7 present the computed NBO charges and Wiberg bond indices for species **2**, **3**, **4**, **5**, **7**, **8**, and **10** (see main paper). The atom labels in these tables are identical to those used in the figures of the main paper and in the crystal structures (see above). Tables S8 and S9 contain selected results from a fragment analysis (see below) for complexes **4** and **8**, respectively, while Table S10 provides an energy decomposition analysis for complex **4**. Figures S1-S4 show the optimized geometries for species **2-5**, respectively, and compare the experimental and theoretical values of some key bond lengths. Figures S5 and S6 present an MO interaction diagram and a LUMO isosurface plot for complex **4**, respectively. Finally, Cartesian coordinates are listed for all optimized geometries.

Fragment Analysis

In the case of complex **4**, the optimized molecule is divided into two fragments: GeCl^+ and $\text{C}(\text{PPh}_3)_2$. Molecular orbitals are generated for each of these fragments, and the electronic structure is then recomputed based on the fragment orbitals. Please refer Figure S5 for the MO interaction diagram and the local axis frame. The mixing of the HOMO-1 of $\text{C}(\text{PPh}_3)_2$ and the GeCl^+ orbital of matching symmetry (π^*_y) gives the HOMO of **4** (20.9% from HOMO-1 of $\text{C}(\text{PPh}_3)_2$ and 32% from π^*_y of GeCl^+). Similarly, the LUMO of **4** results from the mixing of the HOMO of $\text{C}(\text{PPh}_3)_2$ and the π^*_x orbital of GeCl^+ (65.8% from HOMO of $\text{C}(\text{PPh}_3)_2$ and 8% from π^*_x of GeCl^+). The gross population of the symmetrized fragment orbitals provide an estimate of σ -donation and π -(back)donation (see Table S8). An analogous analysis has been applied for complex **8**, the results of which are summarized in Table S9.

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TABLES

Table S1. The calculated NBO charges and Wiberg bond indices for **2**.

<i>Atoms</i>	<i>NBO charges^a</i>	<i>Wiberg bond indices^b in a.u. (Wi)</i>	
		<i>bond</i>	<i>Wi</i>
<i>P1</i>	<i>1.60</i>	<i>Cl-P1</i>	<i>1.17</i>
<i>P2</i>	<i>1.60</i>	<i>Cl-P2</i>	<i>1.13</i>
<i>Cl</i>	<i>-1.53</i>	<i>Cl-Ge</i>	<i>0.54</i>
<i>Ge1</i>	<i>0.81</i>	<i>Ge1-Cl1</i>	<i>0.65</i>
<i>Cl1</i>	<i>-0.55</i>	<i>Ge1-Cl2</i>	<i>0.72</i>
<i>Cl2</i>	<i>-0.51</i>		

^a at BP86/def2-TZVP level

^b at BP86/6-31G* level

Table S2. The calculated NBO charges and Wiberg bond indices for **3**.

<i>Atoms</i>	<i>NBO charges^a</i>	<i>Wiberg bond indices^b in a.u. (Wi)</i>	
		<i>bond</i>	<i>Wi</i>
<i>P1</i>	<i>1.61</i>	<i>Cl-P1</i>	<i>1.11</i>
<i>P2</i>	<i>1.61</i>	<i>Cl-P2</i>	<i>1.08</i>
<i>Cl</i>	<i>-1.55</i>	<i>Cl-Ge1</i>	<i>0.61</i>
<i>Ge1</i>	<i>0.93</i>	<i>Ge1-Cl1</i>	<i>0.69</i>
<i>Cl1</i>	<i>-0.48</i>	<i>Ge1-Cl2</i>	<i>0.78</i>
<i>Cl2</i>	<i>-0.42</i>	<i>Ge1-Ge2</i>	<i>0.68</i>
<i>Ge2</i>	<i>0.60</i>	<i>Ge2-Cl3</i>	<i>0.80</i>
<i>Cl3</i>	<i>-0.47</i>	<i>Ge2-Cl4</i>	<i>0.65</i>
<i>Cl4</i>	<i>-0.55</i>		

^a at BP86/def2-TZVP level

^b at BP86/6-31G* level

Table S3. The calculated NBO charges and Wiberg bond indices for **4**.

<i>Atoms</i>	<i>NBO charges^a</i>	<i>Wiberg bond indices^b in a.u. (Wi)</i>	
		<i>bond</i>	<i>Wi</i>
<i>P1</i>	<i>1.61</i>	<i>Cl-P1</i>	<i>1.06</i>
<i>P2</i>	<i>1.60</i>	<i>Cl-P2</i>	<i>1.02</i>
<i>Cl</i>	<i>-1.57</i>	<i>Cl-Ge1</i>	<i>0.84</i>
<i>Ge1</i>	<i>0.94</i>	<i>Ge1-Cl1</i>	<i>0.84</i>
<i>Cl1</i>	<i>-0.46</i>		

^a at BP86/def2-TZVP level^b at BP86/6-31G* level**Table S4.** The calculated NBO charges and Wiberg bond indices for **5**.

<i>Atoms</i>	<i>NBO charges^a</i>	<i>Wiberg bond indices^b in a.u. (Wi)</i>	
		<i>bond</i>	<i>Wi</i>
<i>P1</i>	<i>1.60</i>	<i>Cl-P1</i>	<i>1.08</i>
<i>P2</i>	<i>1.60</i>	<i>Cl-P2</i>	<i>1.13</i>
<i>Cl</i>	<i>-1.55</i>	<i>Cl-Ge</i>	<i>0.64</i>
<i>Ge1</i>	<i>0.92</i>	<i>Ge1-Cl1</i>	<i>0.74</i>
<i>Cl1</i>	<i>-0.50</i>	<i>Ge1-N1</i>	<i>0.36</i>
<i>N1</i>	<i>-0.52</i>		

^a at BP86/def2-TZVP level^b at BP86/6-31G* level

Table S5. The calculated NBO charges and Wiberg bond indices for **7**.

<i>Atoms</i>	<i>NBO charges^a</i>	<i>Wiberg bond indices^b in a.u. (Wi)</i>	
		<i>bond</i>	<i>Wi</i>
<i>P1</i>	<i>1.58</i>	<i>C1-P1</i>	<i>1.20</i>
<i>P2</i>	<i>1.59</i>	<i>C1-P2</i>	<i>1.16</i>
<i>C1</i>	<i>-1.53</i>	<i>C1-Sn</i>	<i>0.41</i>
<i>Sn1</i>	<i>0.97</i>	<i>Sn1-C11</i>	<i>0.56</i>
<i>C11</i>	<i>-0.61</i>	<i>Sn1-C12</i>	<i>0.61</i>
<i>C12</i>	<i>-0.58</i>		

^a at BP86/def2-TZVP level^b at BP86/6-31G* level. The LANL2DZ basis set was used for Sn.**Table S6.** The calculated NBO charges and Wiberg bond indices for **8**.

<i>Atoms</i>	<i>NBO charges^a</i>	<i>Wiberg bond indices^b in a.u. (Wi)</i>	
		<i>Bond</i>	<i>Wi</i>
<i>P1</i>	<i>1.60</i>	<i>C1-P1</i>	<i>1.11</i>
<i>P2</i>	<i>1.60</i>	<i>C1-P2</i>	<i>1.14</i>
<i>C1</i>	<i>-1.60</i>	<i>C1-Sn1</i>	<i>0.49</i>
<i>Sn1</i>	<i>1.14</i>	<i>Sn1-C11</i>	<i>0.69</i>
<i>C11</i>	<i>-0.56</i>		

^a at BP86/def2-TZVP level^b at BP86/6-31G* level. The LANL2DZ basis set was used for Sn.

Table S7. The calculated NBO charges and Wiberg bond indices for **10**.

<i>Atoms</i>	<i>NBO charges^a</i>	<i>Wiberg bond indices^b in a.u. (Wi)</i>	
		<i>Bond</i>	<i>Wi</i>
<i>P1</i>	<i>1.58</i>	<i>C1-P1</i>	<i>1.15</i>
<i>P2</i>	<i>1.59</i>	<i>C1-P2</i>	<i>1.15</i>
<i>C1</i>	<i>-1.58</i>	<i>C1-Sn1</i>	<i>0.47</i>
<i>Sn1</i>	<i>1.12</i>	<i>Sn1-Cl1</i>	<i>0.59</i>
<i>Cl1</i>	<i>-0.60</i>	<i>Sn1-N1</i>	<i>0.29</i>
<i>N1</i>	<i>-0.54</i>		

^a at BP86/def2-TZVP level^b at BP86/6-31G* level. The LANL2DZ basis set was used for Sn.**Table S8.** Fragment analysis of **4**. The gross populations (summation over all occupied MOs) of relevant symmetrised fragment orbitals (SFOs) are given at BP86/TZP level.

<i>Orbitals of GeCl⁺ fragment</i>	<i>SFO gross populations</i>	<i>Orbitals of C(PPh₃)₂ fragment</i>	<i>SFO gross populations</i>
σ	<i>1.96</i>	<i>HOMO-1</i>	
π_x	<i>1.97</i>	<i>(\sigma)</i>	<i>1.72</i>
π_y	<i>1.96</i>		
π_y^*	<i>0.38</i>	<i>HOMO</i>	
π_x^*	<i>0.47</i>	<i>(\pi)</i>	<i>1.47</i>
σ^*	<i>0.05</i>		

Table S9. Fragment analysis of **8**. The gross populations (summation over all occupied MOs) of relevant symmetrised fragment orbitals (SFOs) are given at BP86/TZP level.

<i>Orbitals of SnCl⁺ fragment</i>	<i>SFO gross populations</i>	<i>Orbitals of C(PPh₃)₂ fragment</i>	<i>SFO gross populations</i>
σ	1.96	<i>HOMO</i> (π)	1.90
π_x	1.97		
π_y	1.97		
π_y^*	0.40	<i>HOMO-1</i> (σ)	1.60
π_x^*	0.26		
σ^*	0.06		

Table S10. Summary of the results from energy decomposition analysis (in kcal/mol) for complex **4** performed at BP86/TZP level (with GeCl⁺ as fragment-1 and C(PPh₃)₂ as fragment-2).

Total bonding energy of complex 4	-128.16
Total steric interaction between fragment 1 and fragment 2	46.20
Total orbital interactions between fragment 1 and fragment 2	-174.36
σ -orbital interaction energy in HOMO	-97.20
π -orbital interaction energy in HOMO-1	-111.43

FIGURES

Figure S1. Optimized geometry of **2** at the BP86/def2-TZVP level. The hydrogen atoms are omitted for clarity (colour code: gray balls are carbon; orange balls are phosphorous; green balls are chlorine). Some important bond lengths are also given (calculated values in black and experimental values in blue).

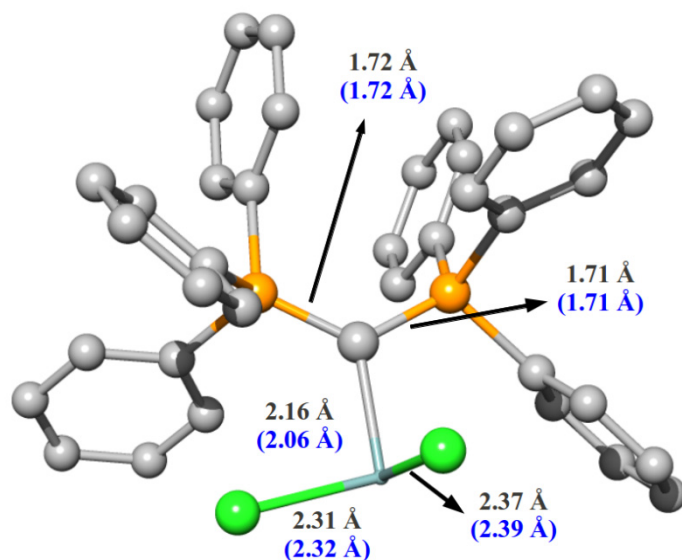


Figure S2. Optimized geometry of **3** at the BP86/def2-TZVP level. The hydrogen atoms are omitted for clarity (please refer to Figure S1 for colour code). Some important bond lengths are also given (calculated values in black and experimental values in blue).

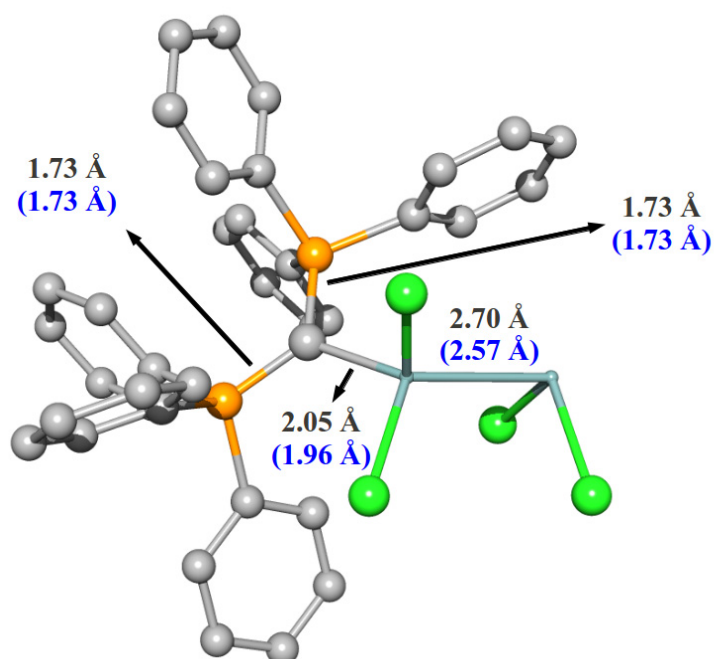


Figure S3. Optimized geometry of **4** at the BP86/def2-TZVP level. The hydrogen atoms are omitted for clarity (please refer to Figure S1 for colour code). Some important bond lengths are also given (calculated values in black and experimental values in blue).

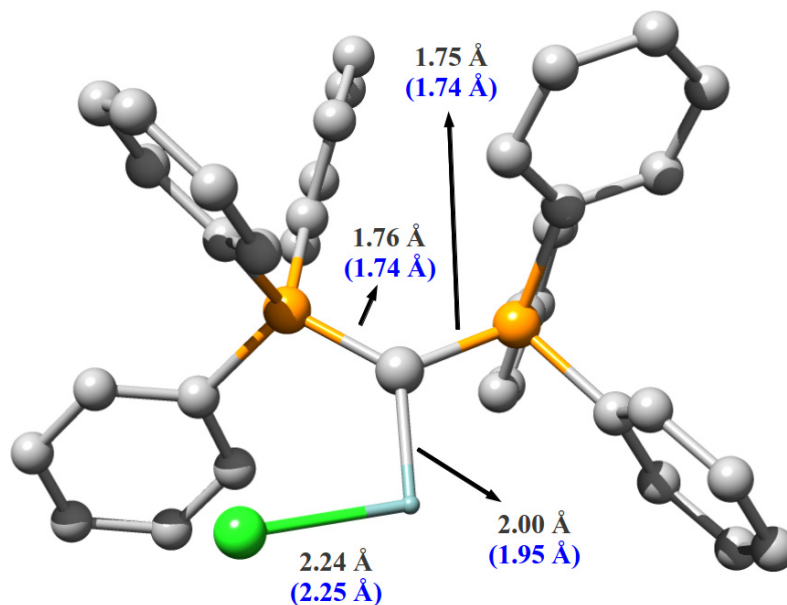


Figure S4. Optimized geometry of **5** at the BP86/def2-TZVP level. The hydrogen atoms are omitted for clarity (please refer to Figure S1 for colour code). Some important bond lengths are also given (calculated values in black and experimental values in blue).

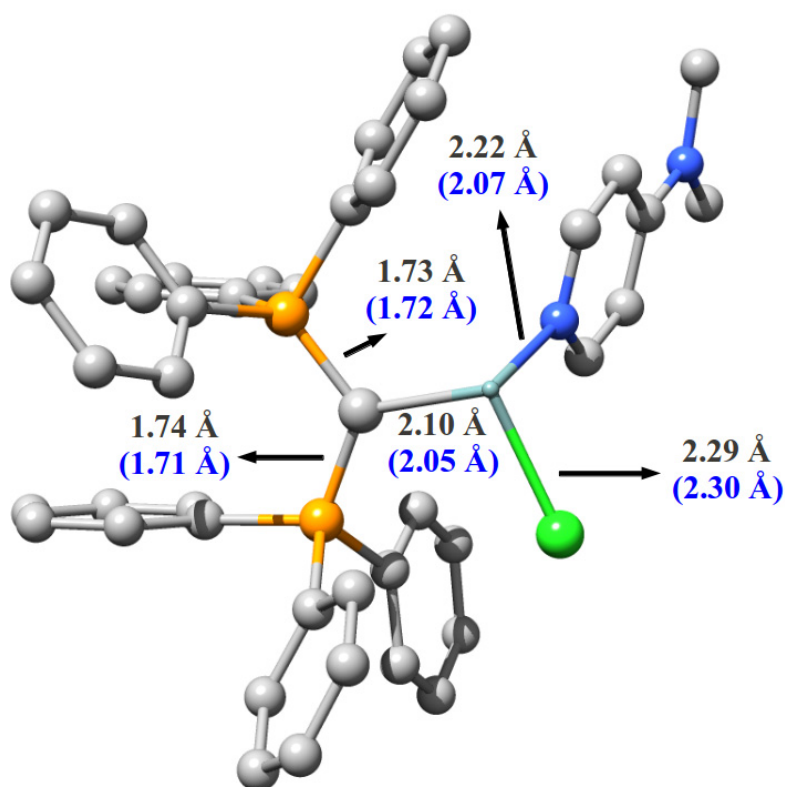


Figure S5. MO interaction diagram for complex **4** showing the composition and relative energies of the fragment orbitals of GeCl^+ and $\text{C}(\text{PPh}_3)_2$. The local axis frame is also specified in the figure.

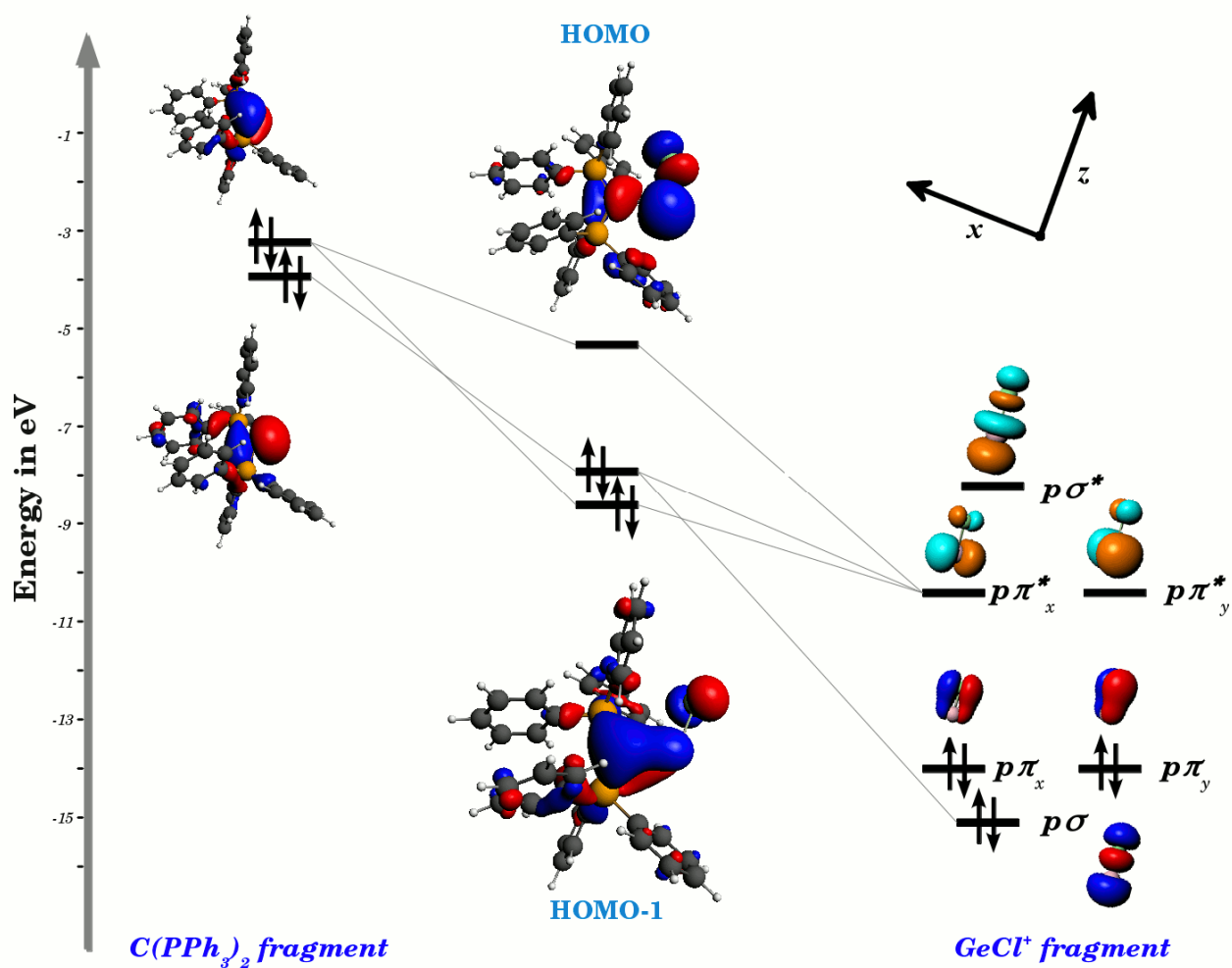
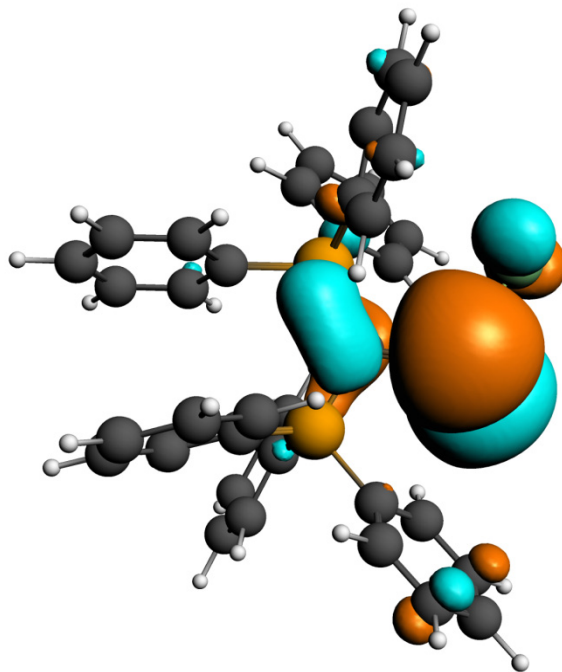


Figure S6. The calculated isosurface of the lowest unoccupied molecular orbital (LUMO) for complex **4**.



CARTESIAN COORDINATES OF OPTIMIZED GEOMETRIES (BP86/def2-TZVP, Å)

2

c	2.4408017568	11.7288341624	8.4064002271
c	2.1594082338	10.8322808560	9.4472217012
c	1.5004578876	9.6313768874	9.1520676940
c	1.1424913237	9.3221827870	7.8390797502
c	1.4339608415	10.2151012866	6.8058028285
c	2.0784270199	11.4206343044	7.0940490515
p	2.6836197850	11.1478600631	11.1828871448
c	4.4717696823	10.7032690681	11.1874187768
c	5.0184223903	9.8563866784	10.2119712153
c	6.3782892182	9.5362622524	10.2353171180
c	7.2077359188	10.0599434754	11.2287706970
c	6.6712011912	10.9041589463	12.2053671604
c	5.3135901952	11.2233819741	12.1860672737
c	1.6987773951	10.2885926275	12.2967594102
p	2.3053881891	9.2374352814	13.4983371044
c	3.5645371634	8.0233947194	12.9170570243
c	3.2665721911	7.2706726877	11.7672135267
c	4.1455572652	6.2895282829	11.3091287357
c	5.3486865444	6.0585400045	11.9813927343
c	5.6691645903	6.8229682247	13.1040273886
c	4.7829453662	7.7967422071	13.5725553823
ge	-0.4600634083	10.4316365097	12.3135055522
cl	-0.7159302161	11.9713020946	14.1004150558
cl	-0.7342209154	11.9696052812	10.6119436597
c	2.9953104297	10.0256461993	15.0121600287
c	3.0657384882	11.4220090599	15.0789003213
c	3.5387745087	12.0517414934	16.2338828274
c	3.9402113387	11.2891220446	17.3316920060
c	3.8515872971	9.8934940375	17.2814942693
c	3.3736445286	9.2637728791	16.1322011029
c	0.9562615212	8.2028673596	14.2120749527
c	0.1126628344	8.7761561556	15.1800508070
c	-0.9296159502	8.0324332256	15.7352095259
c	-1.1352499245	6.7076141196	15.3452851165
c	-0.2923807142	6.1268033943	14.3953906551
c	0.7474717504	6.8683871057	13.8310021895
c	2.7543549875	12.9738712231	11.3892874655
c	3.7836226020	13.7193306608	10.7832454303
c	3.8277060754	15.1072168893	10.9230944468
c	2.8508823002	15.7661200818	11.6753265387
c	1.8370518850	15.0300598477	12.2907235807
c	1.7840376867	13.6406225539	12.1499902432
h	2.7091106220	12.0137203502	14.2346195483
h	3.5760232713	13.1408737774	16.2776209478

h	4.3053824762	11.7797428519	18.2352479639
h	4.1427881936	9.2946661595	18.1457965773
h	3.2753484837	8.1770168585	16.1162382394
h	0.2479176503	9.8149612845	15.4814258459
h	-1.5865029327	8.4998564565	16.4694443466
h	-1.9497940665	6.1278052529	15.7820185185
h	-0.4404202383	5.0898224433	14.0904393169
h	1.4018267825	6.3924138818	13.1023288368
h	2.3434355389	7.4660647308	11.2208362023
h	3.8922483909	5.7092178433	10.4205962636
h	6.0391520397	5.2935875464	11.6231831751
h	6.6158934483	6.6647771262	13.6226184376
h	5.0522174286	8.3883916231	14.4463904500
h	4.5685110316	13.2168162412	10.2168516173
h	4.6315618542	15.6722979566	10.4487055130
h	2.8862898999	16.8511805352	11.7858586372
h	1.0715510567	15.5320580112	12.8837623773
h	0.9856575383	13.0848202904	12.6432493214
h	4.3823602204	9.4549138971	9.4232631070
h	6.7896407027	8.8791899153	9.4677688212
h	8.2707802980	9.8149135352	11.2405523708
h	7.3125110809	11.3224773467	12.9825710327
h	4.9108816231	11.8952232414	12.9445556720
h	1.2383002017	8.9578413920	9.9684190430
h	0.6179860041	8.3894530944	7.6269089367
h	1.1449469741	9.9803263773	5.7803379391
h	2.2903460316	12.1332314125	6.2955651336
h	2.9191471434	12.6847806706	8.6171706333

3

c	2.4713895595	11.7327960700	8.4384599309
c	1.7987182908	9.7767254796	10.6396129884
c	1.3084092694	8.8994801306	9.6651649325
h	1.3326434598	9.1982195041	8.6165644898
c	0.8314699785	7.6356384336	10.0260627436
h	0.4616459505	6.9584779302	9.2552256286
c	0.8448167230	7.2391328234	11.3639862259
h	0.4757149369	6.2521885475	11.6466198549
c	1.3537576930	8.1015125649	12.3414717003
h	1.3864542396	7.7875081577	13.3856729684
c	1.8377957000	9.3592296035	11.9826993547
h	2.2671861441	10.0077620067	12.7476496275
c	4.2200752987	11.2420045579	10.7809358541
c	4.8966795431	10.0215721047	10.5971315492
h	4.4403355883	9.2216909562	10.0161866673
c	6.1655964354	9.8315530547	11.1434026524
h	6.6831964047	8.8862211399	10.9773003398
c	6.7669205281	10.8437552074	11.8947396651

h	7.7578880966	10.6912817307	12.3244228224
c	6.1000349498	12.0543478340	12.0861862916
h	6.5640674382	12.8544340845	12.6635318496
c	4.8346516666	12.2574286478	11.5317206419
h	4.3339616261	13.2092745845	11.6928305247
c	1.7026492953	12.6890593346	11.1589611096
c	2.1328012983	14.0169584441	10.9801383470
h	2.8980152439	14.2527945264	10.2366645684
c	1.5967722069	15.0408187950	11.7622896095
h	1.9510256003	16.0628363508	11.6215664822
c	0.6154136169	14.7577327216	12.7162346069
h	0.1961404531	15.5598039273	13.3254321360
c	0.1664167392	13.4458275918	12.8794446307
h	-0.6124655367	13.2191844040	13.6087638240
c	0.7078856939	12.4140134392	12.1084678333
h	0.3381129320	11.3981017781	12.2399142229
c	0.3912130145	10.8736365179	6.4251403975
c	-0.9373165670	10.9241111686	5.9623529963
h	-1.6167964065	11.6980676055	6.3217155618
c	-1.4073712660	9.9717234499	5.0569459596
h	-2.4391880061	10.0234650700	4.7064850361
c	-0.5606260975	8.9543731440	4.6082550582
h	-0.9280234762	8.2100215818	3.9001403724
c	0.7536257479	8.8904622852	5.0746724131
h	1.4223463275	8.0993021881	4.7334640297
c	1.2307519655	9.8434981277	5.9780172522
h	2.2597051866	9.7732949318	6.3318388272
c	-0.4399904802	12.4549089590	8.6681114820
c	-0.8355905082	13.7644766117	8.9815391185
h	-0.2656172178	14.6110366814	8.5993266922
c	-1.9675072999	13.9895386685	9.7679708423
h	-2.2660860506	15.0126295850	9.9993842175
c	-2.7182826074	12.9132775445	10.2457642078
h	-3.6081531614	13.0922566908	10.8509778373
c	-2.3297642433	11.6061929852	9.9400853033
h	-2.9134197082	10.7596035382	10.3042833017
c	-1.1982752814	11.3768543616	9.1564388434
h	-0.9175613723	10.3529898869	8.9100416742
c	1.1988582179	13.7062259211	6.6343489458
c	2.1071770915	14.6730692202	7.0863711962
h	2.7576429046	14.4660346981	7.9366987586
c	2.2295684557	15.8914042733	6.4159839024
h	2.9618342672	16.6191533797	6.7668456301
c	1.4451675379	16.1547455285	5.2917043537
h	1.5494007944	17.1017596564	4.7602233674
c	0.5424064316	15.1909437196	4.8333157127
h	-0.0584703215	15.3812125785	3.9429269732
c	0.4179402229	13.9708160581	5.4986748951
h	-0.2675566965	13.2186764374	5.1102641014
cl	4.6843544742	9.4117430069	7.2518024353
cl	3.7399237172	12.0970465040	5.3472943603
cl	7.1485757973	13.5935479448	6.3319242880

cl	5.2430585519	14.8303171880	8.9944475142
ge	4.2750092013	11.6617796251	7.4754564368
ge	6.4780123093	12.9354789695	8.3849083467
p	2.5060283292	11.3973881565	10.1317691742
p	1.0186863497	12.1513844255	7.5884297144

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c	7.7834158874	1.2836765923	14.0143816955
c	6.5089893058	1.6967437184	13.5999238758
c	5.6863282186	2.4050835382	14.4984876715
c	6.1259647504	2.6686471733	15.7951101168
c	7.3910328953	2.2385349635	16.2067567717
c	8.2185079851	1.5541855836	15.3149355109
p	5.8442388028	1.3651573126	11.9248669410
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c	3.8908493707	3.2448656623	11.1531692229
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c	5.6955152497	5.3781987442	11.0858003379
c	6.1470916900	4.0970078837	11.4000685918
c	4.6308500727	0.1147620242	12.0635438347
p	3.7849607692	-0.5718375359	10.6825984747
c	4.5327587816	-0.1751024388	9.0566464367
c	5.3812887474	-1.0939292752	8.4176880714
c	5.9408246714	-0.7887050600	7.1757224834
c	5.6568924565	0.4301757789	6.5565310535
c	4.8102960149	1.3479504402	7.1840680185
c	4.2502302643	1.0500034235	8.4264970565
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cl	2.6401909151	-1.8342164307	13.8559438298
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c	3.7874072901	-2.3953651996	10.7866495184
c	2.6687544716	-3.1442260763	10.3943588882
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c	4.9824014471	-4.4560137745	11.2597551978
c	4.9448998819	-3.0616664268	11.2211738122
c	7.2524961493	0.9014940851	10.8572685939
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c	9.0040197946	-0.7098624412	10.3601649699
c	9.4586622767	0.1028658228	9.3177623218
c	8.8024225123	1.3016966616	9.0347912635
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h	1.8736117312	-0.5967018986	8.4482802401
h	1.7531339068	-2.6455625656	10.0789928702
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h	3.8896798456	-6.2864079346	10.9089726954
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h	5.8168426633	-2.4882499728	11.5373377475
h	5.5919367386	-2.0588002737	8.8780180218
h	6.5906001845	-1.5146918354	6.6861712659
h	6.0851799607	0.6609329284	5.5804178713
h	4.5735660692	2.2962782702	6.7001659872
h	3.5756850208	1.7677223862	8.8919322527
h	7.5453993739	-0.9656700324	11.9229754547
h	9.5074515977	-1.6515781391	10.5817950220
h	10.3200382614	-0.2029385124	8.7229378834
h	9.1437790182	1.9321165230	8.2131052483
h	7.1992355632	2.6380825142	9.5611261445
h	3.1767156327	2.4230359675	11.2119790042
h	2.3826606005	4.7013392407	10.6469938767
h	3.9919911747	6.6016107803	10.5645555233
h	6.3996879201	6.2106220014	11.0733910034
h	7.1979866153	3.9463684865	11.6519902990
h	4.7067559777	2.7643327618	14.1790028564
h	5.4806841257	3.2153189913	16.4832304670
h	7.7344806445	2.4468192929	17.2204204115
h	9.2118523585	1.2309373794	15.6271502687
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c	4.7566821961	16.3413290132	8.9378367104
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c	6.4319110333	15.3192893872	10.3552788294
c	5.2309570483	15.2357845998	9.6474546684
p	4.8690678088	19.0057376342	8.0010837494
c	6.4132722711	19.6665337467	7.2423497112
c	6.6917838616	21.0428227895	7.2296350694
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c	8.5243922997	19.2620293515	6.1018989597
c	7.3463702387	18.7805717894	6.6744330842
c	3.5657548647	18.6878732559	6.8955178725
p	3.8155256701	18.6494299204	5.1852049098
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c	5.3324552198	16.2764467631	5.3185901363
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c	4.7419014261	20.1443793225	10.5990970066
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c	-2.7806248256	23.8606772109	6.9367857821
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c	16.3061296781	10.1788383508	-2.8655874006
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p	16.2091660838	5.7043358962	0.1170991584
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h	11.9655699019	10.9438071114	-1.9905835189
h	10.1990960696	9.1887058261	-1.9399818648
h	10.8383420253	6.7818536304	-2.0174774089

h	13.2340873807	6.1362733144	-2.1367139696
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h	18.5811491912	6.3847382390	-6.1280869975
h	16.7180835360	6.2844152337	-7.7829631369
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h	18.8338532049	6.0492227746	-0.4440352488
h	15.0278659484	8.4032268479	0.8834606861
h	13.0472602248	9.1962877828	2.1177923230
h	11.4149878368	7.5648946469	3.0589203853
h	11.7896344759	5.1210394547	2.7523122250
h	13.7686630110	4.3105973565	1.5140880219
h	14.2645627669	3.7722678670	-1.1397733728
h	14.3018435445	1.2963139079	-1.2630663865
h	16.0023277382	0.0079064778	0.0243583305
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h	17.6762380552	3.6848524787	1.5152648573

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n	13.4526052612	5.9817817075	1.1370296940
c	14.5924184546	6.7105776441	1.1350483795
c	14.7246852102	7.9182128740	1.7921778694
c	13.6334891429	8.4544380318	2.5287451169
c	12.4453340777	7.6721185206	2.5303384671
c	12.4088714138	6.4771795712	1.8410231462
n	13.7224869260	9.6344627389	3.1980873420
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sn	13.3116830616	3.6730650378	0.5090657838
cl	15.7901150888	3.6908925434	0.2474053867
c	14.9777723969	10.3812050528	3.2090591633
c	12.7504242823	3.7045663332	-1.7539895049
p	12.2977152805	5.1406592096	-2.5716970473
c	11.1219869976	6.1031051530	-1.5338489998
c	10.1678175362	5.4001635427	-0.7796778038
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c	9.1371636733	7.4796243940	-0.0945599809
c	10.0975116558	8.1873533320	-0.8222851560
c	11.0834073112	7.5058359747	-1.5396920768
p	12.8242623874	2.1314094717	-2.4375435371
c	12.9554905440	0.8980344107	-1.0779894700
c	14.2205352967	0.6203584494	-0.5258685724
c	14.3436527653	-0.2829986943	0.5328410933
c	13.2140385305	-0.9248965783	1.0436998267
c	11.9563430032	-0.6614701213	0.4943162818

c	11.8249901164	0.2443483670	-0.5595661620
c	14.2796232461	1.7256733162	-3.4795158988
c	15.1312485443	2.7436716711	-3.9248295529
c	16.2441216081	2.4414955079	-4.7146620201
c	16.5172031678	1.1171127402	-5.0604342466
c	15.6816068049	0.0914009494	-4.6058954739
c	14.5712338543	0.3905805510	-3.8163602938
c	11.3441690862	1.6312517152	-3.4066732384
c	11.4359763556	0.9377107387	-4.6232216373
c	10.2803763433	0.5107248109	-5.2818152262
c	9.0217176656	0.7648232123	-4.7343017691
c	8.9190097105	1.4680648353	-3.5312504851
c	10.0709881778	1.9048249476	-2.8771837592
c	13.6731833690	6.2887394317	-2.9805305810
c	13.4862972254	7.3395676696	-3.8979895343
c	14.5393789073	8.2029872908	-4.2034011739
c	15.7910964701	8.0219455953	-3.6070381560
c	15.9862747346	6.9721759769	-2.7071999880
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c	11.5662653603	4.4793491580	-6.5637338164
c	10.1939125804	4.7142376824	-6.6883267462
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c	10.0635958718	5.1919802619	-4.3180271256
h	15.4352342832	6.2712484651	0.6005357810
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h	11.5588867590	7.9865419156	3.0753981495
h	11.5016653457	5.8700820978	1.8510064625
h	15.7894021122	9.8056004542	3.6822186348
h	14.8377918251	11.3049735069	3.7781334874
h	15.2895023013	10.6531970238	2.1889527358
h	11.6960490962	10.2495403915	3.3602510487
h	12.8501124808	11.0977509195	4.4089155596
h	12.3493895121	9.4398727842	4.8148663861
h	14.9413952121	3.7742404930	-3.6241676726
h	16.9043599725	3.2428900908	-5.0479515443
h	17.3886483331	0.8795554345	-5.6716395144
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h	13.9401885948	-0.4204901649	-3.4494992150
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h	8.1219562342	0.4235551917	-5.2475920191
h	7.9390454253	1.6815460478	-3.1026960895
h	9.9840945759	2.4697094008	-1.9488307090
h	15.1112880366	1.1117149214	-0.9161407387
h	15.3290519555	-0.4824042963	0.9545365777
h	13.3136572734	-1.6355813739	1.8649128463
h	11.0720274373	-1.1692534361	0.8810077989
h	10.8400656223	0.4233874511	-0.9892092219
h	12.5238540144	7.4729697807	-4.3936636167
h	14.3846171632	9.0109572238	-4.9195923483

h	16.6156964927	8.6912016144	-3.8561170674
h	16.9650105904	6.8122546635	-2.2525596045
h	15.1046167025	5.2754967096	-1.7065298255
h	13.2625943194	4.4347190201	-5.2436908066
h	12.1576741407	4.2060685103	-7.4382829085
h	9.7104739619	4.6257678650	-7.6620278633
h	8.3758463925	5.2610377153	-5.6569962985
h	9.4694170692	5.4810982834	-3.4514568552
h	10.2065864079	4.3105023651	-0.7561786732
h	8.4361201638	5.5225422349	0.5018936793
h	8.3603564795	8.0149424891	0.4529524069
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