

Table 1. Crystal data and structure refinement for AS974P.

Identification code	2(GeSn(C ₁₅ H ₂₃) ₄)	
Empirical formula	C ₁₂₀ H ₁₈₄ Ge ₂ Sn ₂	
Formula weight	2009.23	
Temperature	193(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2 ₁ /n	
Unit cell dimensions	a = 14.4059(6) Å	α = 90°.
	b = 37.5545(14) Å	β = 95.804(6)°.
	c = 21.6693(11) Å	γ = 90°.
Volume	11663.1(9) Å ³	
Z	4	
Density (calculated)	1.144 Mg/m ³	
Absorption coefficient	0.977 mm ⁻¹	
F(000)	4272	
Crystal size	0.80 x 0.38 x 0.27 mm ³	
Theta range for data collection	2.09 to 25.94°.	
Index ranges	-17 ≤ h ≤ 17, -46 ≤ k ≤ 45, -26 ≤ l ≤ 26	
Reflections collected	96389	
Independent reflections	22569 [R(int) = 0.0554]	
Observed reflections	18115 [I > 2σ(I)]	
Completeness to theta = 25.94°	97.5 %	
Absorption correction	Numerical	
Max. and min. transmission	0.7784 and 0.5088	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	22569 / 0 / 1126	
Goodness-of-fit on F ²	1.031	
Final R indices [I > 2σ(I)]	R ₁ = 0.0500, wR ₂ = 0.1395	
R indices (all data)	R ₁ = 0.0649, wR ₂ = 0.1502	
Largest diff. peak and hole	1.906 and -2.159 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for AS974P. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U(\text{eq})$
Sn(1)	525(1)	2423(1)	2493(1)	36(1)
Ge(1)	-165(1)	2633(1)	3445(1)	26(1)
C(1)	296(3)	2801(1)	1748(2)	32(1)
C(2)	-429(3)	2733(1)	1276(2)	33(1)
C(3)	-591(3)	2972(1)	783(2)	41(1)
C(4)	-52(3)	3277(1)	737(2)	44(1)
C(5)	676(3)	3339(1)	1205(2)	42(1)
C(6)	862(3)	3109(1)	1711(2)	38(1)
C(7)	-1061(3)	2404(1)	1284(2)	38(1)
C(8)	-2016(4)	2505(2)	1475(4)	79(2)
C(9)	-1129(5)	2196(1)	674(2)	62(2)
C(10)	-208(4)	3539(1)	194(2)	55(1)
C(11)	-1235(5)	3639(2)	51(3)	69(2)
C(12)	211(5)	3390(2)	-379(3)	79(2)
C(13)	1677(3)	3198(1)	2189(2)	49(1)
C(14)	2609(4)	3151(2)	1927(3)	68(2)
C(15)	1609(5)	3572(2)	2459(3)	69(2)
C(16)	1984(3)	2287(1)	2526(2)	31(1)
C(17)	2282(3)	2132(1)	1979(2)	35(1)
C(18)	3236(3)	2064(1)	1954(2)	41(1)
C(19)	3892(3)	2129(1)	2448(2)	44(1)
C(20)	3590(3)	2271(1)	2991(2)	42(1)
C(21)	2649(3)	2348(1)	3035(2)	36(1)
C(22)	1615(3)	2034(1)	1411(2)	39(1)
C(23)	1740(4)	2280(2)	850(2)	51(1)
C(24)	1712(4)	1638(1)	1231(2)	53(1)
C(25)	4933(3)	2065(2)	2415(3)	54(1)
C(26)	5137(5)	1719(2)	2123(6)	127(4)
C(27)	5351(4)	2370(2)	2097(4)	84(2)
C(28)	2399(3)	2495(2)	3660(2)	45(1)
C(29)	2674(4)	2241(2)	4196(2)	56(1)

C(30)	2825(5)	2865(2)	3800(3)	66(2)
C(31)	-1497(3)	2832(1)	3434(2)	44(1)
C(32)	-2223(3)	2643(1)	3678(2)	49(1)
C(33)	-3057(4)	2822(2)	3764(3)	65(2)
C(34)	-3189(4)	3183(2)	3610(3)	75(2)
C(35)	-2472(4)	3361(2)	3350(3)	69(2)
C(36)	-1628(4)	3194(1)	3256(2)	53(1)
C(37)	-2156(3)	2251(1)	3848(2)	49(1)
C(38)	-2207(4)	2179(2)	4550(3)	66(2)
C(39)	-2897(4)	2030(2)	3464(3)	78(2)
C(40A)	-4014(7)	3434(3)	3668(4)	42(2)
C(41A)	-4797(14)	3369(5)	3346(9)	88(6)
C(42A)	-4327(11)	3379(4)	4338(7)	77(4)
C(40B)	-4221(11)	3295(4)	3793(7)	75(4)
C(41B)	-4887(9)	3287(4)	3194(6)	52(3)
C(42B)	-4005(11)	3555(4)	4337(7)	82(4)
C(43)	-895(4)	3419(1)	2982(3)	61(1)
C(44)	-1230(5)	3558(2)	2324(3)	83(2)
C(45)	-557(6)	3729(2)	3410(3)	85(2)
C(46)	120(3)	2341(1)	4241(2)	30(1)
C(47)	176(3)	1963(1)	4277(2)	31(1)
C(48)	430(3)	1806(1)	4853(2)	36(1)
C(49)	634(3)	2005(1)	5396(2)	37(1)
C(50)	573(3)	2371(1)	5350(2)	38(1)
C(51)	324(3)	2542(1)	4790(2)	34(1)
C(52)	-41(3)	1720(1)	3711(2)	35(1)
C(53)	-722(4)	1418(1)	3832(2)	48(1)
C(54)	856(3)	1562(1)	3498(2)	43(1)
C(55)	870(3)	1827(1)	6023(2)	45(1)
C(56)	1679(4)	1564(1)	6023(3)	58(1)
C(57)	-2(5)	1656(2)	6245(3)	65(2)
C(58)	230(4)	2949(1)	4798(2)	47(1)
C(59)	1034(5)	3139(2)	5185(3)	67(2)
C(60)	-713(4)	3059(2)	5023(3)	62(1)
Sn(2)	642(1)	501(1)	2686(1)	29(1)
Ge(2)	-950(1)	271(1)	2321(1)	24(1)

Sn(2B)	-1106(6)	317(3)	2331(5)	15(2)
Sn(2C)	-960(5)	440(2)	2531(3)	9(1)
Ge(2B)	758(6)	314(3)	2577(4)	84(2)
C(61)	1715(3)	612(1)	2075(2)	32(1)
C(62)	1614(3)	542(1)	1429(2)	37(1)
C(63)	2393(3)	584(1)	1099(2)	46(1)
C(64)	3253(3)	695(1)	1376(2)	48(1)
C(65)	3325(3)	778(1)	2003(2)	44(1)
C(66)	2568(3)	740(1)	2361(2)	35(1)
C(67)	703(3)	418(2)	1076(2)	49(1)
C(68)	367(4)	667(2)	535(2)	57(1)
C(69)	775(5)	37(2)	835(2)	69(2)
C(70)	4101(4)	726(2)	1014(3)	67(2)
C(71)	4464(5)	364(2)	851(4)	99(3)
C(72)	3907(7)	954(2)	445(5)	134(4)
C(73)	2735(3)	845(1)	3046(2)	38(1)
C(74)	3440(4)	603(2)	3421(2)	54(1)
C(75)	3023(4)	1241(1)	3110(2)	49(1)
C(76)	1299(3)	117(1)	3341(2)	33(1)
C(77)	1736(3)	-196(1)	3160(2)	41(1)
C(78)	2118(4)	-432(1)	3633(3)	51(1)
C(79)	2062(3)	-366(1)	4261(2)	46(1)
C(80)	1661(3)	-54(1)	4426(2)	42(1)
C(81)	1279(3)	188(1)	3981(2)	36(1)
C(82)	1805(4)	-293(1)	2478(2)	51(1)
C(83)	1383(4)	-654(2)	2298(3)	66(2)
C(84)	2833(5)	-276(2)	2332(3)	69(2)
C(85)	2422(4)	-630(1)	4771(2)	55(1)
C(86)	1996(5)	-996(1)	4668(3)	68(2)
C(87)	3481(5)	-658(2)	4812(3)	84(2)
C(88)	826(3)	526(1)	4210(2)	39(1)
C(89)	-128(4)	443(1)	4427(3)	59(1)
C(90)	1465(5)	720(2)	4715(3)	64(2)
C(91)	-1711(3)	517(1)	1589(2)	30(1)
C(92)	-2159(3)	277(1)	1150(2)	38(1)
C(93)	-2556(4)	406(1)	583(2)	49(1)

C(94)	-2529(4)	765(2)	425(2)	53(1)
C(95)	-2122(4)	997(1)	869(2)	47(1)
C(96)	-1708(3)	885(1)	1449(2)	35(1)
C(97)	-2255(3)	-121(1)	1299(2)	43(1)
C(98)	-1889(5)	-363(2)	812(3)	70(2)
C(99)	-3228(5)	-221(2)	1414(4)	84(2)
C(100)	-2905(6)	912(2)	-211(3)	90(3)
C(101)	-3572(6)	663(3)	-581(3)	110(3)
C(102)	-2097(8)	1027(3)	-579(3)	119(3)
C(103)	-1288(3)	1167(1)	1907(2)	38(1)
C(104)	-1993(4)	1464(1)	2025(3)	53(1)
C(105)	-390(3)	1332(1)	1705(2)	46(1)
C(106)	-1867(3)	91(1)	2925(2)	36(1)
C(107)	-1734(3)	-265(1)	3135(2)	41(1)
C(108)	-2424(4)	-430(1)	3449(2)	55(1)
C(109)	-3240(4)	-254(2)	3560(3)	62(2)
C(110)	-3340(4)	99(2)	3377(3)	58(1)
C(111)	-2672(3)	278(1)	3054(2)	43(1)
C(112)	-891(4)	-490(1)	3030(2)	45(1)
C(113)	-362(4)	-616(1)	3639(2)	58(1)
C(114)	-1163(4)	-810(1)	2599(2)	57(1)
C(115)	-4011(5)	-451(2)	3870(3)	84(2)
C(116)	-4070(6)	-338(3)	4507(3)	102(3)
C(117)	-4840(6)	-512(3)	3437(4)	110(3)
C(118)	-2868(3)	663(1)	2868(2)	47(1)
C(119)	-3719(4)	697(2)	2393(3)	63(1)
C(120)	-2968(5)	898(2)	3436(3)	72(2)

Table 3. Bond lengths [Å] and angles [°] for AS974P.

Sn(1)-C(1)	2.150(4)	C(28)-C(30)	1.536(8)
Sn(1)-C(16)	2.158(4)	C(31)-C(32)	1.412(7)
Sn(1)-Ge(1)	2.5065(5)	C(31)-C(36)	1.421(7)
Ge(1)-C(46)	2.051(4)	C(32)-C(33)	1.406(7)
Ge(1)-C(31)	2.056(4)	C(32)-C(37)	1.518(8)
C(1)-C(2)	1.408(6)	C(33)-C(34)	1.404(10)
C(1)-C(6)	1.421(6)	C(34)-C(35)	1.396(10)
C(2)-C(3)	1.398(6)	C(34)-C(40A)	1.531(11)
C(2)-C(7)	1.536(6)	C(34)-C(40B)	1.632(16)
C(3)-C(4)	1.391(6)	C(35)-C(36)	1.400(7)
C(4)-C(5)	1.403(6)	C(36)-C(43)	1.520(9)
C(4)-C(10)	1.533(6)	C(37)-C(39)	1.530(7)
C(5)-C(6)	1.400(6)	C(37)-C(38)	1.554(8)
C(6)-C(13)	1.523(6)	C(40A)-C(41A)	1.29(2)
C(7)-C(8)	1.524(7)	C(40A)-C(42A)	1.577(17)
C(7)-C(9)	1.531(7)	C(40B)-C(41B)	1.53(2)
C(10)-C(11)	1.527(8)	C(40B)-C(42B)	1.54(2)
C(10)-C(12)	1.539(9)	C(43)-C(45)	1.535(8)
C(13)-C(14)	1.521(8)	C(43)-C(44)	1.549(8)
C(13)-C(15)	1.528(8)	C(46)-C(51)	1.415(5)
C(16)-C(21)	1.404(6)	C(46)-C(47)	1.424(5)
C(16)-C(17)	1.425(6)	C(47)-C(48)	1.396(6)
C(17)-C(18)	1.405(6)	C(47)-C(52)	1.534(5)
C(17)-C(22)	1.527(6)	C(48)-C(49)	1.398(6)
C(18)-C(19)	1.377(7)	C(49)-C(50)	1.382(6)
C(19)-C(20)	1.399(7)	C(49)-C(55)	1.523(6)
C(19)-C(25)	1.529(6)	C(50)-C(51)	1.390(6)
C(20)-C(21)	1.400(6)	C(51)-C(58)	1.532(6)
C(21)-C(28)	1.539(6)	C(52)-C(54)	1.535(6)
C(22)-C(24)	1.546(7)	C(52)-C(53)	1.540(6)
C(22)-C(23)	1.551(6)	C(55)-C(56)	1.528(7)
C(25)-C(26)	1.486(10)	C(55)-C(57)	1.530(7)
C(25)-C(27)	1.496(8)	C(58)-C(59)	1.537(8)
C(28)-C(29)	1.525(7)	C(58)-C(60)	1.545(7)

Sn(2)-C(76)	2.170(4)	C(80)-C(81)	1.398(6)
Sn(2)-C(61)	2.175(4)	C(81)-C(88)	1.532(6)
Sn(2)-Ge(2)	2.5025(13)	C(82)-C(83)	1.521(7)
Ge(2)-C(91)	2.054(4)	C(82)-C(84)	1.546(8)
Ge(2)-C(106)	2.065(4)	C(85)-C(86)	1.512(8)
Sn(2B)-Sn(2C)	0.653(12)	C(85)-C(87)	1.523(9)
Sn(2B)-C(91)	1.903(11)	C(88)-C(89)	1.529(7)
Sn(2B)-C(106)	1.966(10)	C(88)-C(90)	1.541(7)
Sn(2B)-Ge(2B)	2.685(13)	C(91)-C(96)	1.415(6)
Sn(2C)-C(106)	2.092(8)	C(91)-C(92)	1.417(6)
Sn(2C)-C(91)	2.230(8)	C(92)-C(93)	1.389(6)
Sn(2C)-Ge(2B)	2.513(12)	C(92)-C(97)	1.538(6)
Ge(2B)-C(76)	1.905(10)	C(93)-C(94)	1.394(7)
Ge(2B)-C(61)	2.154(10)	C(94)-C(95)	1.384(7)
C(61)-C(66)	1.404(6)	C(94)-C(100)	1.532(7)
C(61)-C(62)	1.417(5)	C(95)-C(96)	1.400(6)
C(62)-C(63)	1.399(6)	C(96)-C(103)	1.534(6)
C(62)-C(67)	1.523(6)	C(97)-C(99)	1.496(8)
C(63)-C(64)	1.385(7)	C(97)-C(98)	1.525(7)
C(64)-C(65)	1.388(7)	C(100)-C(101)	1.511(12)
C(64)-C(70)	1.521(6)	C(100)-C(102)	1.538(12)
C(65)-C(66)	1.408(6)	C(103)-C(105)	1.537(6)
C(66)-C(73)	1.533(6)	C(103)-C(104)	1.547(6)
C(67)-C(69)	1.532(8)	C(106)-C(111)	1.407(6)
C(67)-C(68)	1.538(8)	C(106)-C(107)	1.418(6)
C(70)-C(72)	1.506(11)	C(107)-C(108)	1.406(6)
C(70)-C(71)	1.510(9)	C(107)-C(112)	1.515(7)
C(73)-C(74)	1.533(7)	C(108)-C(109)	1.391(8)
C(73)-C(75)	1.546(6)	C(109)-C(110)	1.388(8)
C(76)-C(77)	1.409(6)	C(109)-C(115)	1.544(7)
C(76)-C(81)	1.414(6)	C(110)-C(111)	1.414(6)
C(77)-C(78)	1.424(7)	C(111)-C(118)	1.522(7)
C(77)-C(82)	1.536(7)	C(112)-C(113)	1.530(7)
C(78)-C(79)	1.392(7)	C(112)-C(114)	1.548(6)
C(79)-C(80)	1.370(7)	C(115)-C(116)	1.454(10)
C(79)-C(85)	1.535(7)	C(115)-C(117)	1.461(11)

C(118)-C(119)	1.525(8)	C(118)-C(120)	1.533(7)
C(1)-Sn(1)-C(16)	104.92(14)	C(18)-C(17)-C(22)	117.7(4)
C(1)-Sn(1)-Ge(1)	111.50(11)	C(16)-C(17)-C(22)	123.4(3)
C(16)-Sn(1)-Ge(1)	120.90(11)	C(19)-C(18)-C(17)	122.4(4)
C(46)-Ge(1)-C(31)	108.13(17)	C(18)-C(19)-C(20)	118.4(4)
C(46)-Ge(1)-Sn(1)	117.45(10)	C(18)-C(19)-C(25)	122.3(4)
C(31)-Ge(1)-Sn(1)	123.49(12)	C(20)-C(19)-C(25)	119.3(4)
C(2)-C(1)-C(6)	119.7(3)	C(19)-C(20)-C(21)	121.4(4)
C(2)-C(1)-Sn(1)	118.1(3)	C(20)-C(21)-C(16)	120.1(4)
C(6)-C(1)-Sn(1)	122.2(3)	C(20)-C(21)-C(28)	116.6(4)
C(3)-C(2)-C(1)	119.5(4)	C(16)-C(21)-C(28)	123.3(4)
C(3)-C(2)-C(7)	118.1(4)	C(17)-C(22)-C(24)	111.6(4)
C(1)-C(2)-C(7)	122.4(3)	C(17)-C(22)-C(23)	112.0(4)
C(4)-C(3)-C(2)	122.1(4)	C(24)-C(22)-C(23)	110.7(4)
C(3)-C(4)-C(5)	117.8(4)	C(26)-C(25)-C(27)	111.5(6)
C(3)-C(4)-C(10)	122.9(4)	C(26)-C(25)-C(19)	113.3(5)
C(5)-C(4)-C(10)	119.3(4)	C(27)-C(25)-C(19)	110.0(4)
C(6)-C(5)-C(4)	122.2(4)	C(29)-C(28)-C(30)	110.3(4)
C(5)-C(6)-C(1)	118.7(4)	C(29)-C(28)-C(21)	112.3(4)
C(5)-C(6)-C(13)	118.0(4)	C(30)-C(28)-C(21)	112.0(4)
C(1)-C(6)-C(13)	123.3(4)	C(32)-C(31)-C(36)	119.9(4)
C(8)-C(7)-C(9)	112.5(5)	C(32)-C(31)-Ge(1)	122.7(4)
C(8)-C(7)-C(2)	110.8(4)	C(36)-C(31)-Ge(1)	116.7(4)
C(9)-C(7)-C(2)	112.8(4)	C(33)-C(32)-C(31)	119.0(5)
C(11)-C(10)-C(4)	112.2(4)	C(33)-C(32)-C(37)	117.9(5)
C(11)-C(10)-C(12)	112.1(5)	C(31)-C(32)-C(37)	123.2(4)
C(4)-C(10)-C(12)	110.4(5)	C(34)-C(33)-C(32)	121.9(6)
C(14)-C(13)-C(6)	111.6(4)	C(35)-C(34)-C(33)	118.0(5)
C(14)-C(13)-C(15)	110.0(5)	C(35)-C(34)-C(40A)	110.6(7)
C(6)-C(13)-C(15)	112.9(4)	C(33)-C(34)-C(40A)	131.4(8)
C(21)-C(16)-C(17)	118.8(3)	C(35)-C(34)-C(40B)	134.9(8)
C(21)-C(16)-Sn(1)	124.8(3)	C(33)-C(34)-C(40B)	107.1(8)
C(17)-C(16)-Sn(1)	116.3(3)	C(40A)-C(34)-C(40B)	24.3(6)
C(18)-C(17)-C(16)	118.9(4)	C(34)-C(35)-C(36)	122.2(6)

C(35)-C(36)-C(31)	118.9(6)	C(51)-C(58)-C(60)	110.7(4)
C(35)-C(36)-C(43)	117.0(5)	C(59)-C(58)-C(60)	109.9(4)
C(31)-C(36)-C(43)	124.0(4)	C(76)-Sn(2)-C(61)	103.63(15)
C(32)-C(37)-C(39)	111.7(5)	C(76)-Sn(2)-Ge(2)	107.66(11)
C(32)-C(37)-C(38)	113.5(4)	C(61)-Sn(2)-Ge(2)	123.93(11)
C(39)-C(37)-C(38)	109.8(5)	C(91)-Ge(2)-C(106)	108.09(17)
C(41A)-C(40A)-C(34)	118.9(12)	C(91)-Ge(2)-Sn(2)	119.37(12)
C(41A)-C(40A)-C(42A)	99.1(12)	C(106)-Ge(2)-Sn(2)	122.48(13)
C(34)-C(40A)-C(42A)	107.0(9)	Sn(2C)-Sn(2B)-C(91)	111.8(12)
C(41B)-C(40B)-C(42B)	136.0(13)	Sn(2C)-Sn(2B)-C(106)	91.9(11)
C(41B)-C(40B)-C(34)	107.3(10)	C(91)-Sn(2B)-C(106)	119.0(5)
C(42B)-C(40B)-C(34)	103.4(11)	Sn(2C)-Sn(2B)-Ge(2B)	67.9(9)
C(36)-C(43)-C(45)	112.1(5)	C(91)-Sn(2B)-Ge(2B)	122.2(5)
C(36)-C(43)-C(44)	112.5(5)	C(106)-Sn(2B)-Ge(2B)	118.7(5)
C(45)-C(43)-C(44)	110.6(5)	Sn(2B)-Sn(2C)-C(106)	69.9(10)
C(51)-C(46)-C(47)	118.7(4)	Sn(2B)-Sn(2C)-C(91)	52.5(10)
C(51)-C(46)-Ge(1)	115.3(3)	C(106)-Sn(2C)-C(91)	100.9(4)
C(47)-C(46)-Ge(1)	125.9(3)	Sn(2B)-Sn(2C)-Ge(2B)	98.2(11)
C(48)-C(47)-C(46)	118.6(4)	C(106)-Sn(2C)-Ge(2B)	121.3(4)
C(48)-C(47)-C(52)	118.6(3)	C(91)-Sn(2C)-Ge(2B)	116.5(4)
C(46)-C(47)-C(52)	122.8(3)	C(76)-Ge(2B)-C(61)	114.5(5)
C(47)-C(48)-C(49)	122.8(4)	C(76)-Ge(2B)-Sn(2C)	115.0(5)
C(50)-C(49)-C(48)	117.7(4)	C(61)-Ge(2B)-Sn(2C)	124.1(5)
C(50)-C(49)-C(55)	120.5(4)	C(76)-Ge(2B)-Sn(2B)	119.2(5)
C(48)-C(49)-C(55)	121.7(4)	C(61)-Ge(2B)-Sn(2B)	125.1(5)
C(49)-C(50)-C(51)	122.1(4)	Sn(2C)-Ge(2B)-Sn(2B)	13.9(3)
C(50)-C(51)-C(46)	120.1(4)	C(66)-C(61)-C(62)	119.8(3)
C(50)-C(51)-C(58)	117.8(4)	C(66)-C(61)-Ge(2B)	122.1(4)
C(46)-C(51)-C(58)	122.1(4)	C(62)-C(61)-Ge(2B)	113.3(4)
C(47)-C(52)-C(54)	111.2(4)	C(66)-C(61)-Sn(2)	116.2(3)
C(47)-C(52)-C(53)	112.6(3)	C(62)-C(61)-Sn(2)	123.9(3)
C(54)-C(52)-C(53)	109.6(3)	Ge(2B)-C(61)-Sn(2)	20.3(3)
C(49)-C(55)-C(56)	112.7(4)	C(63)-C(62)-C(61)	118.4(4)
C(49)-C(55)-C(57)	110.3(4)	C(63)-C(62)-C(67)	118.3(4)
C(56)-C(55)-C(57)	112.3(4)	C(61)-C(62)-C(67)	123.3(3)
C(51)-C(58)-C(59)	114.1(4)	C(64)-C(63)-C(62)	122.8(4)

C(63)-C(64)-C(65)	117.8(4)	C(86)-C(85)-C(87)	109.7(5)
C(63)-C(64)-C(70)	122.0(5)	C(86)-C(85)-C(79)	112.3(5)
C(65)-C(64)-C(70)	120.2(5)	C(87)-C(85)-C(79)	110.5(5)
C(64)-C(65)-C(66)	122.0(4)	C(89)-C(88)-C(81)	110.9(4)
C(61)-C(66)-C(65)	119.0(4)	C(89)-C(88)-C(90)	111.6(4)
C(61)-C(66)-C(73)	124.1(3)	C(81)-C(88)-C(90)	112.3(4)
C(65)-C(66)-C(73)	117.0(4)	C(96)-C(91)-C(92)	119.3(4)
C(62)-C(67)-C(69)	111.7(5)	C(96)-C(91)-Sn(2B)	123.7(5)
C(62)-C(67)-C(68)	112.7(4)	C(92)-C(91)-Sn(2B)	117.0(4)
C(69)-C(67)-C(68)	109.6(4)	C(96)-C(91)-Ge(2)	126.2(3)
C(72)-C(70)-C(71)	111.1(6)	C(92)-C(91)-Ge(2)	113.9(3)
C(72)-C(70)-C(64)	111.9(6)	Sn(2B)-C(91)-Ge(2)	7.0(3)
C(71)-C(70)-C(64)	111.6(5)	C(96)-C(91)-Sn(2C)	108.1(3)
C(74)-C(73)-C(66)	113.0(4)	C(92)-C(91)-Sn(2C)	132.7(4)
C(74)-C(73)-C(75)	111.4(4)	Sn(2B)-C(91)-Sn(2C)	15.8(4)
C(66)-C(73)-C(75)	110.4(4)	Ge(2)-C(91)-Sn(2C)	20.5(2)
C(77)-C(76)-C(81)	118.9(4)	C(93)-C(92)-C(91)	119.4(4)
C(77)-C(76)-Ge(2B)	103.6(4)	C(93)-C(92)-C(97)	119.1(4)
C(81)-C(76)-Ge(2B)	137.1(4)	C(91)-C(92)-C(97)	121.5(4)
C(77)-C(76)-Sn(2)	123.3(3)	C(92)-C(93)-C(94)	122.4(5)
C(81)-C(76)-Sn(2)	117.8(3)	C(95)-C(94)-C(93)	117.3(4)
Ge(2B)-C(76)-Sn(2)	20.3(3)	C(95)-C(94)-C(100)	119.1(5)
C(76)-C(77)-C(78)	118.1(4)	C(93)-C(94)-C(100)	123.6(5)
C(76)-C(77)-C(82)	122.8(4)	C(94)-C(95)-C(96)	123.3(4)
C(78)-C(77)-C(82)	119.1(4)	C(95)-C(96)-C(91)	118.3(4)
C(79)-C(78)-C(77)	122.4(4)	C(95)-C(96)-C(103)	118.6(4)
C(80)-C(79)-C(78)	118.3(4)	C(91)-C(96)-C(103)	123.1(4)
C(80)-C(79)-C(85)	119.0(4)	C(99)-C(97)-C(98)	111.1(5)
C(78)-C(79)-C(85)	122.7(4)	C(99)-C(97)-C(92)	112.5(4)
C(79)-C(80)-C(81)	121.5(4)	C(98)-C(97)-C(92)	113.0(4)
C(80)-C(81)-C(76)	120.6(4)	C(101)-C(100)-C(94)	113.7(6)
C(80)-C(81)-C(88)	117.8(4)	C(101)-C(100)-C(102)	112.0(6)
C(76)-C(81)-C(88)	121.6(4)	C(94)-C(100)-C(102)	110.4(6)
C(83)-C(82)-C(77)	113.3(4)	C(96)-C(103)-C(105)	112.5(3)
C(83)-C(82)-C(84)	110.6(4)	C(96)-C(103)-C(104)	112.5(4)
C(77)-C(82)-C(84)	110.1(4)	C(105)-C(103)-C(104)	110.0(4)

C(111)-C(106)-C(107)	119.5(4)	C(110)-C(109)-C(115)	121.7(6)
C(111)-C(106)-Sn(2B)	116.2(4)	C(108)-C(109)-C(115)	120.3(5)
C(107)-C(106)-Sn(2B)	123.4(4)	C(109)-C(110)-C(111)	122.6(5)
C(111)-C(106)-Ge(2)	123.8(3)	C(106)-C(111)-C(110)	118.6(4)
C(107)-C(106)-Ge(2)	115.9(3)	C(106)-C(111)-C(118)	123.7(4)
Sn(2B)-C(106)-Ge(2)	7.6(3)	C(110)-C(111)-C(118)	117.7(4)
C(111)-C(106)-Sn(2C)	109.3(4)	C(107)-C(112)-C(113)	112.4(4)
C(107)-C(106)-Sn(2C)	130.6(4)	C(107)-C(112)-C(114)	111.4(4)
Sn(2B)-C(106)-Sn(2C)	18.2(3)	C(113)-C(112)-C(114)	110.7(4)
Ge(2)-C(106)-Sn(2C)	21.6(2)	C(116)-C(115)-C(117)	122.3(6)
C(108)-C(107)-C(106)	119.5(5)	C(116)-C(115)-C(109)	112.7(6)
C(108)-C(107)-C(112)	116.2(4)	C(117)-C(115)-C(109)	111.9(6)
C(106)-C(107)-C(112)	124.2(4)	C(111)-C(118)-C(119)	112.0(4)
C(109)-C(108)-C(107)	121.7(5)	C(111)-C(118)-C(120)	111.3(4)
C(110)-C(109)-C(108)	118.0(4)	C(119)-C(118)-C(120)	111.1(5)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for AS974P. 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}
Sn(1)	36(1)	39(1)	31(1)	5(1)	-1(1)	5(1)
Ge(1)	27(1)	26(1)	25(1)	0(1)	-4(1)	10(1)
C(1)	33(2)	34(2)	29(2)	10(2)	2(2)	1(2)
C(2)	34(2)	32(2)	33(2)	5(2)	2(2)	3(2)
C(3)	41(2)	43(2)	36(2)	10(2)	-8(2)	-1(2)
C(4)	51(3)	41(2)	38(2)	12(2)	-2(2)	-3(2)
C(5)	44(2)	38(2)	42(2)	11(2)	-1(2)	-8(2)
C(6)	38(2)	38(2)	37(2)	5(2)	-1(2)	-4(2)
C(7)	37(2)	35(2)	41(2)	10(2)	-7(2)	1(2)
C(8)	41(3)	50(3)	151(7)	8(4)	27(4)	-7(2)
C(9)	85(4)	49(3)	48(3)	4(2)	-17(3)	-16(3)
C(10)	69(3)	49(3)	44(3)	21(2)	-11(2)	-14(2)
C(11)	88(4)	54(3)	60(3)	22(3)	-14(3)	8(3)
C(12)	82(4)	100(5)	58(3)	32(3)	16(3)	2(4)
C(13)	51(3)	47(3)	46(3)	13(2)	-9(2)	-17(2)
C(14)	42(3)	74(4)	83(4)	17(3)	-14(3)	-13(3)
C(15)	75(4)	57(3)	70(4)	-2(3)	-18(3)	-15(3)
C(16)	25(2)	37(2)	31(2)	11(2)	3(2)	1(2)
C(17)	29(2)	42(2)	34(2)	6(2)	7(2)	-1(2)
C(18)	34(2)	49(2)	42(2)	6(2)	10(2)	2(2)
C(19)	27(2)	55(3)	49(2)	16(2)	5(2)	2(2)
C(20)	25(2)	58(3)	41(2)	13(2)	-3(2)	-1(2)
C(21)	29(2)	46(2)	34(2)	10(2)	3(2)	0(2)
C(22)	31(2)	53(3)	35(2)	-2(2)	7(2)	-1(2)
C(23)	48(3)	68(3)	34(2)	6(2)	0(2)	-2(2)
C(24)	45(3)	61(3)	52(3)	-11(2)	7(2)	-7(2)
C(25)	27(2)	76(3)	59(3)	16(3)	9(2)	8(2)
C(26)	42(3)	79(5)	265(13)	5(6)	34(5)	25(3)
C(27)	48(3)	99(5)	112(6)	31(4)	36(4)	-1(3)
C(28)	30(2)	75(3)	30(2)	-3(2)	-5(2)	6(2)
C(29)	54(3)	77(4)	36(2)	6(2)	-7(2)	-13(3)

C(30)	86(4)	66(3)	45(3)	-2(2)	-4(3)	14(3)
C(31)	38(2)	53(3)	40(2)	-13(2)	-2(2)	12(2)
C(32)	32(2)	66(3)	47(3)	-21(2)	-2(2)	10(2)
C(33)	39(3)	97(5)	59(3)	-25(3)	2(2)	12(3)
C(34)	60(4)	92(5)	68(4)	-29(3)	-13(3)	42(3)
C(35)	64(4)	73(4)	66(4)	-16(3)	-8(3)	36(3)
C(36)	55(3)	52(3)	48(3)	-11(2)	-10(2)	21(2)
C(37)	29(2)	61(3)	56(3)	-16(2)	8(2)	-1(2)
C(38)	57(3)	81(4)	63(3)	-12(3)	17(3)	-8(3)
C(39)	50(3)	87(5)	94(5)	-34(4)	-10(3)	-4(3)
C(43)	68(3)	45(3)	66(3)	-2(2)	-8(3)	23(3)
C(44)	90(5)	88(5)	68(4)	12(3)	-4(3)	35(4)
C(45)	114(6)	53(3)	86(5)	-10(3)	-3(4)	0(4)
C(46)	28(2)	31(2)	30(2)	-2(2)	5(2)	2(2)
C(47)	32(2)	31(2)	30(2)	3(2)	6(2)	1(2)
C(48)	44(2)	31(2)	34(2)	2(2)	7(2)	2(2)
C(49)	37(2)	45(2)	31(2)	5(2)	5(2)	1(2)
C(50)	44(2)	42(2)	28(2)	-5(2)	4(2)	0(2)
C(51)	35(2)	37(2)	31(2)	-3(2)	8(2)	0(2)
C(52)	44(2)	31(2)	30(2)	1(2)	5(2)	0(2)
C(53)	55(3)	39(2)	49(3)	-2(2)	6(2)	-8(2)
C(54)	53(3)	37(2)	39(2)	-4(2)	12(2)	2(2)
C(55)	55(3)	48(2)	30(2)	5(2)	0(2)	-1(2)
C(56)	69(3)	47(3)	52(3)	8(2)	-13(3)	2(2)
C(57)	85(4)	69(4)	43(3)	14(2)	9(3)	-16(3)
C(58)	66(3)	37(2)	38(2)	-5(2)	6(2)	2(2)
C(59)	78(4)	46(3)	78(4)	-12(3)	14(3)	-21(3)
C(60)	70(4)	52(3)	63(3)	-22(3)	-2(3)	19(3)
Sn(2)	34(1)	28(1)	25(1)	1(1)	4(1)	-2(1)
Ge(2)	29(1)	22(1)	22(1)	2(1)	7(1)	-1(1)
C(61)	29(2)	37(2)	30(2)	-2(2)	8(2)	-2(2)
C(62)	37(2)	46(2)	29(2)	-7(2)	10(2)	-5(2)
C(63)	49(3)	54(3)	37(2)	-13(2)	19(2)	-12(2)
C(64)	41(2)	53(3)	55(3)	-9(2)	22(2)	-9(2)
C(65)	33(2)	48(2)	53(3)	-10(2)	8(2)	-9(2)
C(66)	33(2)	36(2)	37(2)	-5(2)	5(2)	-1(2)

C(67)	39(2)	81(3)	29(2)	-11(2)	13(2)	-19(2)
C(68)	54(3)	80(4)	36(2)	-13(2)	5(2)	9(3)
C(69)	97(5)	66(3)	40(3)	5(2)	-10(3)	-41(3)
C(70)	53(3)	81(4)	74(4)	-21(3)	37(3)	-22(3)
C(71)	74(4)	94(5)	140(7)	17(5)	69(5)	27(4)
C(72)	124(7)	106(6)	193(10)	67(7)	119(8)	20(5)
C(73)	31(2)	48(2)	36(2)	-7(2)	1(2)	-4(2)
C(74)	49(3)	61(3)	50(3)	-1(2)	-7(2)	-1(2)
C(75)	49(3)	53(3)	45(3)	-13(2)	4(2)	-7(2)
C(76)	34(2)	29(2)	34(2)	5(2)	-3(2)	-2(2)
C(77)	44(2)	35(2)	44(2)	1(2)	0(2)	2(2)
C(78)	51(3)	29(2)	71(3)	2(2)	0(2)	11(2)
C(79)	49(3)	42(2)	44(2)	6(2)	-6(2)	-5(2)
C(80)	52(3)	34(2)	36(2)	4(2)	-6(2)	-7(2)
C(81)	40(2)	32(2)	35(2)	4(2)	-1(2)	-9(2)
C(82)	63(3)	39(2)	49(3)	-7(2)	6(2)	11(2)
C(83)	74(4)	55(3)	69(4)	-24(3)	11(3)	7(3)
C(84)	75(4)	65(4)	70(4)	-12(3)	24(3)	5(3)
C(85)	68(3)	51(3)	44(3)	6(2)	6(2)	10(2)
C(86)	99(5)	42(3)	62(3)	15(2)	8(3)	6(3)
C(87)	69(4)	97(5)	86(5)	36(4)	13(3)	24(4)
C(88)	54(3)	33(2)	29(2)	3(2)	4(2)	-5(2)
C(89)	61(3)	48(3)	72(4)	13(2)	28(3)	6(2)
C(90)	89(4)	49(3)	50(3)	-15(2)	-9(3)	-2(3)
C(91)	30(2)	33(2)	29(2)	1(2)	8(2)	2(2)
C(92)	39(2)	40(2)	35(2)	-1(2)	6(2)	1(2)
C(93)	53(3)	57(3)	34(2)	-5(2)	-3(2)	6(2)
C(94)	63(3)	61(3)	33(2)	4(2)	-3(2)	21(2)
C(95)	57(3)	42(2)	43(2)	8(2)	6(2)	14(2)
C(96)	36(2)	37(2)	33(2)	1(2)	9(2)	6(2)
C(97)	51(3)	38(2)	39(2)	-5(2)	4(2)	-4(2)
C(98)	103(5)	53(3)	57(3)	-12(3)	23(3)	6(3)
C(99)	77(4)	58(4)	122(6)	-7(4)	41(4)	-21(3)
C(100)	138(7)	86(5)	40(3)	1(3)	-17(4)	56(5)
C(101)	107(6)	168(9)	46(4)	18(4)	-32(4)	19(6)
C(102)	188(10)	122(7)	44(4)	32(4)	4(5)	-16(7)

C(103)	45(2)	29(2)	41(2)	3(2)	11(2)	3(2)
C(104)	62(3)	38(2)	61(3)	-2(2)	16(3)	10(2)
C(105)	50(3)	35(2)	52(3)	0(2)	11(2)	-2(2)
C(106)	41(2)	39(2)	28(2)	-4(2)	6(2)	-13(2)
C(107)	49(3)	41(2)	33(2)	1(2)	4(2)	-17(2)
C(108)	63(3)	53(3)	49(3)	7(2)	10(2)	-25(2)
C(109)	63(3)	67(3)	60(3)	8(3)	23(3)	-28(3)
C(110)	48(3)	71(3)	60(3)	-6(3)	27(2)	-16(3)
C(111)	42(2)	48(2)	42(2)	-2(2)	11(2)	-15(2)
C(112)	56(3)	33(2)	46(2)	9(2)	3(2)	-13(2)
C(113)	72(3)	46(3)	52(3)	12(2)	-7(3)	-16(2)
C(114)	82(4)	38(2)	49(3)	-1(2)	-3(3)	-13(2)
C(115)	76(4)	94(5)	88(5)	16(4)	42(4)	-31(4)
C(116)	90(5)	146(8)	76(5)	5(5)	40(4)	-48(5)
C(117)	89(5)	130(7)	119(7)	-32(5)	60(5)	-66(5)
C(118)	44(2)	47(3)	54(3)	-6(2)	21(2)	-5(2)
C(119)	47(3)	57(3)	84(4)	-4(3)	10(3)	3(2)
C(120)	91(5)	60(3)	70(4)	-19(3)	35(3)	-16(3)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for AS974P.

	x	y	z	U(eq)
H(3)	-1086	2925	469	49
H(5)	1055	3544	1178	50
H(7)	-766	2241	1613	46
H(8A)	-2407	2292	1479	119
H(8B)	-2314	2678	1179	119
H(8C)	-1942	2611	1891	119
H(9A)	-500	2137	570	93
H(9B)	-1448	2341	342	93
H(9C)	-1482	1976	718	93
H(10)	140	3762	320	66
H(11A)	-1302	3807	-297	103
H(11B)	-1460	3750	417	103
H(11C)	-1601	3424	-59	103
H(12A)	869	3331	-268	119
H(12B)	161	3570	-709	119
H(12C)	-130	3176	-525	119
H(13)	1661	3026	2539	59
H(14A)	3116	3209	2247	101
H(14B)	2638	3311	1571	101
H(14C)	2673	2904	1793	101
H(15A)	2146	3615	2766	103
H(15B)	1032	3593	2660	103
H(15C)	1607	3748	2125	103
H(18)	3437	1969	1583	50
H(20)	4034	2315	3338	50
H(22)	965	2069	1524	47
H(23A)	1300	2209	497	76
H(23B)	2380	2258	737	76
H(23C)	1621	2527	962	76
H(24A)	1275	1584	867	79

Table 1. Crystal data and structure refinement for MA436.

Identification code	MA436	
Empirical formula	C60 H92 Ge O2 Sn	
Formula weight	1036.62	
Temperature	193(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2 ₁ /n	
Unit cell dimensions	a = 12.465(3) Å	α = 90°.
	b = 28.216(7) Å	β = 104.43(2)°.
	c = 17.473(3) Å	γ = 90°.
Volume	5951(2) Å ³	
Z	4	
Density (calculated)	1.157 Mg/m ³	
Absorption coefficient	0.961 mm ⁻¹	
F(000)	2200	
Crystal size	0.55 x 0.26 x 0.16 mm ³	
Theta range for data collection	2.22 to 25.99°.	
Index ranges	-15 ≤ h ≤ 15, -34 ≤ k ≤ 34, -21 ≤ l ≤ 21	
Reflections collected	70531	
Independent reflections	10904 [R(int) = 0.0703]	
Observed reflections	8484 [I > 2σ(I)]	
Completeness to theta = 25.99°	91.3 %	
Absorption correction	Numerical	
Max. and min. transmission	0.8614 and 0.6199	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	10904 / 0 / 568	
Goodness-of-fit on F ²	1.018	
Final R indices [I > 2σ(I)]	R1 = 0.0350, wR2 = 0.0857	
R indices (all data)	R1 = 0.0500, wR2 = 0.0912	
Largest diff. peak and hole	0.758 and -0.588 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for MA436. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{\dagger} tensor.

	x	y	z	$U(\text{eq})$
Sn(1)	4823(1)	1485(1)	7563(1)	30(1)
Sn(2)	5018(1)	2413(1)	7694(1)	26(1)
Ge(1)	4823(1)	1485(1)	7563(1)	30(1)
Ge(2)	5018(1)	2413(1)	7694(1)	26(1)
O(1)	4205(2)	1766(1)	6517(1)	41(1)
O(2)	3911(2)	2267(1)	6718(1)	38(1)
C(1)	5920(3)	988(1)	7318(2)	44(1)
C(2)	7053(3)	985(1)	7697(2)	50(1)
C(3)	7700(3)	611(2)	7530(3)	76(1)
C(4)	7271(4)	246(2)	7016(4)	89(2)
C(5)	6174(4)	262(2)	6640(3)	81(1)
C(6)	5482(3)	629(1)	6775(2)	59(1)
C(7)	7621(2)	1373(1)	8264(2)	54(1)
C(8)	8209(3)	1173(2)	9082(3)	68(1)
C(9)	8430(3)	1667(2)	7918(3)	72(1)
C(10A)	7936(8)	-129(3)	6686(7)	73(2)
C(11A)	9193(7)	-17(3)	6893(5)	60(2)
C(12A)	7598(9)	-589(4)	6979(7)	86(3)
C(13A)	4388(6)	640(2)	6238(4)	42(2)
C(14A)	4313(9)	756(4)	5370(6)	80(3)
C(15A)	3776(9)	179(4)	6330(7)	79(3)
C(10B)	8008(11)	-250(5)	7069(9)	101(4)
C(11B)	8644(12)	-174(4)	6556(8)	104(4)
C(12B)	7870(11)	-621(4)	7517(8)	103(3)
C(13B)	4102(7)	584(3)	6416(5)	56(2)
C(14B)	3901(10)	566(4)	5520(7)	95(3)
C(15B)	3576(9)	177(4)	6743(7)	84(3)
C(16)	3659(2)	1163(1)	8071(2)	36(1)
C(17)	4066(2)	904(1)	8774(2)	39(1)
C(18)	3331(3)	708(1)	9168(2)	50(1)
C(19)	2193(3)	762(1)	8888(2)	55(1)

C(20)	1815(3)	1009(1)	8190(2)	55(1)
C(21)	2511(2)	1209(1)	7765(2)	45(1)
C(22)	5295(2)	830(1)	9134(2)	42(1)
C(23)	5626(3)	320(1)	8967(3)	58(1)
C(24)	5659(3)	944(2)	10016(2)	63(1)
C(25)	1389(3)	551(2)	9320(3)	78(2)
C(26)	1288(5)	23(2)	9215(4)	114(2)
C(27)	1703(5)	674(2)	10200(4)	101(2)
C(28)	1979(3)	1488(2)	7017(2)	59(1)
C(29)	1122(4)	1194(2)	6430(3)	91(2)
C(30)	1467(4)	1957(2)	7213(3)	80(2)
C(31)	6477(2)	2711(1)	7558(2)	30(1)
C(32)	6743(2)	2744(1)	6823(2)	36(1)
C(33)	7785(3)	2918(1)	6812(2)	49(1)
C(34)	8551(3)	3066(1)	7476(2)	55(1)
C(35)	8264(3)	3046(1)	8197(2)	47(1)
C(36)	7242(2)	2868(1)	8251(2)	35(1)
C(37)	5970(2)	2585(1)	6048(2)	42(1)
C(38)	6384(3)	2128(1)	5730(2)	57(1)
C(39)	5766(3)	2982(1)	5426(2)	54(1)
C(40A)	9767(6)	3153(3)	7434(4)	37(2)
C(41A)	10644(8)	2979(4)	8089(6)	69(2)
C(42A)	9824(10)	3756(4)	7473(8)	99(3)
C(40B)	9622(7)	3332(4)	7419(5)	57(2)
C(41B)	10551(9)	3197(4)	8088(7)	85(3)
C(42B)	9595(8)	3710(3)	6952(6)	70(2)
C(43)	7015(2)	2851(1)	9068(2)	40(1)
C(44)	7926(3)	2597(2)	9684(2)	63(1)
C(45)	6793(3)	3350(2)	9340(2)	61(1)
C(46)	4212(2)	2898(1)	8237(2)	30(1)
C(47)	3878(2)	3334(1)	7830(2)	35(1)
C(48)	3483(2)	3705(1)	8222(2)	42(1)
C(49)	3405(2)	3661(1)	8999(2)	43(1)
C(50)	3692(2)	3223(1)	9375(2)	41(1)
C(51)	4089(2)	2838(1)	9005(2)	33(1)
C(52)	3871(3)	3401(1)	6970(2)	46(1)

C(53)	2706(4)	3325(2)	6454(3)	92(2)
C(54)	4352(7)	3870(2)	6796(3)	145(3)
C(55)	3027(3)	4094(1)	9396(2)	58(1)
C(56)	3942(4)	4456(1)	9630(3)	69(1)
C(57)	2501(5)	3977(2)	10040(4)	118(2)
C(58)	4341(2)	2363(1)	9453(2)	39(1)
C(59)	5055(3)	2423(1)	10294(2)	57(1)
C(60)	3272(3)	2103(1)	9459(2)	51(1)

Table 3. Bond lengths [Å] and angles [°] for MA436.

Sn(1)-O(1)	1.965(2)	C(19)-C(20)	1.383(5)
Sn(1)-C(1)	2.077(3)	C(19)-C(25)	1.519(5)
Sn(1)-C(16)	2.088(3)	C(20)-C(21)	1.393(4)
Sn(1)-Ge(2)	2.6347(7)	C(21)-C(28)	1.529(5)
Ge(2)-O(2)	1.952(2)	C(22)-C(24)	1.528(5)
Ge(2)-C(46)	2.064(3)	C(22)-C(23)	1.543(5)
Ge(2)-C(31)	2.071(2)	C(25)-C(26)	1.500(7)
O(1)-O(2)	1.521(3)	C(25)-C(27)	1.530(7)
C(1)-C(2)	1.402(5)	C(28)-C(29)	1.529(6)
C(1)-C(6)	1.402(5)	C(28)-C(30)	1.543(6)
C(2)-C(3)	1.401(5)	C(31)-C(32)	1.408(4)
C(2)-C(7)	1.528(5)	C(31)-C(36)	1.412(4)
C(3)-C(4)	1.385(6)	C(32)-C(33)	1.394(4)
C(4)-C(5)	1.361(7)	C(32)-C(37)	1.520(4)
C(4)-C(10A)	1.542(11)	C(33)-C(34)	1.371(5)
C(4)-C(10B)	1.664(14)	C(34)-C(35)	1.395(5)
C(5)-C(6)	1.405(5)	C(34)-C(40A)	1.555(7)
C(6)-C(13A)	1.451(8)	C(34)-C(40B)	1.556(9)
C(6)-C(13B)	1.683(9)	C(35)-C(36)	1.394(4)
C(7)-C(9)	1.540(5)	C(36)-C(43)	1.524(4)
C(7)-C(8)	1.542(6)	C(37)-C(39)	1.536(5)
C(10A)-C(12A)	1.494(15)	C(37)-C(38)	1.543(5)
C(10A)-C(11A)	1.550(13)	C(40A)-C(41A)	1.457(12)
C(13A)-C(14A)	1.531(12)	C(40A)-C(42A)	1.703(14)
C(13A)-C(15A)	1.535(12)	C(40B)-C(42B)	1.337(13)
C(10B)-C(12B)	1.343(17)	C(40B)-C(41B)	1.476(14)
C(10B)-C(11B)	1.353(17)	C(43)-C(45)	1.533(5)
C(13B)-C(15B)	1.504(13)	C(43)-C(44)	1.535(5)
C(13B)-C(14B)	1.524(14)	C(46)-C(51)	1.399(4)
C(16)-C(21)	1.403(4)	C(46)-C(47)	1.430(4)
C(16)-C(17)	1.410(4)	C(47)-C(48)	1.404(4)
C(17)-C(18)	1.389(4)	C(47)-C(52)	1.513(4)
C(17)-C(22)	1.519(4)	C(48)-C(49)	1.390(5)
C(18)-C(19)	1.389(4)	C(49)-C(50)	1.403(5)

C(49)-C(55)	1.536(4)	C(55)-C(57)	1.475(6)
C(50)-C(51)	1.415(4)	C(55)-C(56)	1.508(5)
C(51)-C(58)	1.545(4)	C(58)-C(60)	1.523(4)
C(52)-C(54)	1.515(5)	C(58)-C(59)	1.527(5)
C(52)-C(53)	1.522(6)		
O(1)-Sn(1)-C(1)	101.94(11)	C(5)-C(6)-C(13A)	115.1(4)
O(1)-Sn(1)-C(16)	114.74(10)	C(1)-C(6)-C(13B)	119.8(4)
C(1)-Sn(1)-C(16)	110.92(12)	C(5)-C(6)-C(13B)	119.7(4)
O(1)-Sn(1)-Ge(2)	71.67(6)	C(13A)-C(6)-C(13B)	18.4(4)
C(1)-Sn(1)-Ge(2)	129.62(9)	C(2)-C(7)-C(9)	112.0(3)
C(16)-Sn(1)-Ge(2)	117.01(8)	C(2)-C(7)-C(8)	112.1(3)
O(2)-Ge(2)-C(46)	102.88(10)	C(9)-C(7)-C(8)	110.8(3)
O(2)-Ge(2)-C(31)	115.79(10)	C(12A)-C(10A)-C(4)	104.2(8)
C(46)-Ge(2)-C(31)	108.96(11)	C(12A)-C(10A)-C(11A)	116.9(9)
O(2)-Ge(2)-Sn(1)	71.58(6)	C(4)-C(10A)-C(11A)	112.3(7)
C(46)-Ge(2)-Sn(1)	130.90(7)	C(6)-C(13A)-C(14A)	117.4(7)
C(31)-Ge(2)-Sn(1)	117.31(8)	C(6)-C(13A)-C(15A)	109.1(6)
O(2)-O(1)-Sn(1)	102.80(13)	C(14A)-C(13A)-C(15A)	112.1(7)
O(1)-O(2)-Ge(2)	103.87(13)	C(12B)-C(10B)-C(11B)	133.6(13)
C(2)-C(1)-C(6)	119.4(3)	C(12B)-C(10B)-C(4)	122.6(11)
C(2)-C(1)-Sn(1)	123.0(2)	C(11B)-C(10B)-C(4)	103.7(11)
C(6)-C(1)-Sn(1)	117.5(3)	C(15B)-C(13B)-C(14B)	112.9(9)
C(3)-C(2)-C(1)	118.1(3)	C(15B)-C(13B)-C(6)	114.7(7)
C(3)-C(2)-C(7)	118.4(3)	C(14B)-C(13B)-C(6)	106.0(7)
C(1)-C(2)-C(7)	123.4(3)	C(21)-C(16)-C(17)	119.4(3)
C(4)-C(3)-C(2)	123.0(4)	C(21)-C(16)-Sn(1)	123.2(2)
C(5)-C(4)-C(3)	117.9(4)	C(17)-C(16)-Sn(1)	117.29(19)
C(5)-C(4)-C(10A)	114.3(6)	C(18)-C(17)-C(16)	119.9(3)
C(3)-C(4)-C(10A)	126.6(5)	C(18)-C(17)-C(22)	117.5(3)
C(5)-C(4)-C(10B)	121.9(6)	C(16)-C(17)-C(22)	122.6(3)
C(3)-C(4)-C(10B)	118.1(7)	C(19)-C(18)-C(17)	121.6(3)
C(10A)-C(4)-C(10B)	26.2(5)	C(20)-C(19)-C(18)	117.4(3)
C(4)-C(5)-C(6)	121.9(4)	C(20)-C(19)-C(25)	121.0(3)
C(1)-C(6)-C(5)	119.6(4)	C(18)-C(19)-C(25)	121.7(3)
C(1)-C(6)-C(13A)	124.6(4)	C(19)-C(20)-C(21)	123.6(3)

C(20)-C(21)-C(16)	118.1(3)	C(41A)-C(40A)-C(34)	117.3(6)
C(20)-C(21)-C(28)	117.9(3)	C(41A)-C(40A)-C(42A)	106.9(7)
C(16)-C(21)-C(28)	123.9(3)	C(34)-C(40A)-C(42A)	100.8(6)
C(17)-C(22)-C(24)	113.8(3)	C(42B)-C(40B)-C(41B)	125.8(9)
C(17)-C(22)-C(23)	109.9(3)	C(42B)-C(40B)-C(34)	122.1(8)
C(24)-C(22)-C(23)	111.1(3)	C(41B)-C(40B)-C(34)	109.9(7)
C(26)-C(25)-C(19)	112.0(4)	C(36)-C(43)-C(45)	110.6(3)
C(26)-C(25)-C(27)	110.0(4)	C(36)-C(43)-C(44)	113.2(3)
C(19)-C(25)-C(27)	111.9(4)	C(45)-C(43)-C(44)	111.8(3)
C(21)-C(28)-C(29)	112.0(3)	C(51)-C(46)-C(47)	119.6(3)
C(21)-C(28)-C(30)	111.6(3)	C(51)-C(46)-Ge(2)	122.8(2)
C(29)-C(28)-C(30)	110.9(3)	C(47)-C(46)-Ge(2)	117.2(2)
C(32)-C(31)-C(36)	120.0(2)	C(48)-C(47)-C(46)	119.4(3)
C(32)-C(31)-Ge(2)	123.0(2)	C(48)-C(47)-C(52)	118.5(3)
C(36)-C(31)-Ge(2)	117.00(19)	C(46)-C(47)-C(52)	122.0(3)
C(33)-C(32)-C(31)	117.9(3)	C(49)-C(48)-C(47)	122.0(3)
C(33)-C(32)-C(37)	118.5(3)	C(48)-C(49)-C(50)	117.6(3)
C(31)-C(32)-C(37)	123.5(2)	C(48)-C(49)-C(55)	118.4(3)
C(34)-C(33)-C(32)	123.5(3)	C(50)-C(49)-C(55)	124.1(3)
C(33)-C(34)-C(35)	118.0(3)	C(49)-C(50)-C(51)	122.7(3)
C(33)-C(34)-C(40A)	119.3(4)	C(46)-C(51)-C(50)	118.6(3)
C(35)-C(34)-C(40A)	121.5(4)	C(46)-C(51)-C(58)	122.3(3)
C(33)-C(34)-C(40B)	121.4(4)	C(50)-C(51)-C(58)	119.0(3)
C(35)-C(34)-C(40B)	119.7(4)	C(47)-C(52)-C(54)	113.8(3)
C(40A)-C(34)-C(40B)	19.8(4)	C(47)-C(52)-C(53)	109.8(3)
C(36)-C(35)-C(34)	121.4(3)	C(54)-C(52)-C(53)	111.8(5)
C(35)-C(36)-C(31)	119.2(3)	C(57)-C(55)-C(56)	113.2(4)
C(35)-C(36)-C(43)	117.4(3)	C(57)-C(55)-C(49)	114.4(3)
C(31)-C(36)-C(43)	123.3(2)	C(56)-C(55)-C(49)	111.4(3)
C(32)-C(37)-C(39)	111.8(3)	C(60)-C(58)-C(59)	110.3(3)
C(32)-C(37)-C(38)	111.9(3)	C(60)-C(58)-C(51)	110.7(3)
C(39)-C(37)-C(38)	111.4(3)	C(59)-C(58)-C(51)	112.7(3)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for MA436. 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}
Sn(1)	22(1)	35(1)	34(1)	2(1)	8(1)	0(1)
Sn(2)	18(1)	38(1)	24(1)	-2(1)	7(1)	-2(1)
Ge(1)	22(1)	35(1)	34(1)	2(1)	8(1)	0(1)
Ge(2)	18(1)	38(1)	24(1)	-2(1)	7(1)	-2(1)
O(1)	41(1)	52(1)	32(1)	-7(1)	11(1)	-5(1)
O(2)	27(1)	49(1)	37(1)	4(1)	6(1)	4(1)
C(1)	47(2)	42(2)	43(2)	-4(1)	14(2)	2(1)
C(2)	42(2)	47(2)	66(3)	-7(2)	23(2)	5(1)
C(3)	55(2)	70(3)	110(4)	-19(3)	33(3)	13(2)
C(4)	83(3)	71(3)	116(4)	-26(3)	32(3)	23(2)
C(5)	93(3)	66(3)	87(4)	-35(2)	26(3)	6(2)
C(6)	71(2)	44(2)	60(2)	-12(2)	13(2)	5(2)
C(7)	27(1)	55(2)	82(3)	-6(2)	14(2)	4(1)
C(8)	35(2)	77(3)	88(3)	-1(2)	7(2)	3(2)
C(9)	41(2)	70(3)	107(4)	5(2)	27(2)	-1(2)
C(16)	27(1)	35(2)	44(2)	5(1)	4(1)	-5(1)
C(17)	30(1)	35(2)	50(2)	6(1)	5(1)	-1(1)
C(18)	37(2)	50(2)	60(2)	24(2)	9(2)	0(1)
C(19)	33(2)	58(2)	75(3)	26(2)	15(2)	1(1)
C(20)	26(1)	62(2)	75(3)	25(2)	6(2)	-3(1)
C(21)	27(1)	54(2)	50(2)	14(2)	4(2)	-5(1)
C(22)	30(1)	42(2)	49(2)	12(1)	2(1)	1(1)
C(23)	44(2)	50(2)	77(3)	16(2)	5(2)	14(2)
C(24)	42(2)	82(3)	58(3)	4(2)	0(2)	-2(2)
C(25)	40(2)	91(3)	108(4)	57(3)	24(2)	3(2)
C(26)	122(4)	106(4)	127(5)	-3(4)	55(4)	-70(4)
C(27)	107(4)	84(3)	144(5)	3(3)	90(4)	-9(3)
C(28)	26(1)	87(3)	57(2)	27(2)	-1(2)	-9(2)
C(29)	58(2)	132(5)	67(3)	23(3)	-12(2)	-29(3)
C(30)	57(2)	95(3)	81(4)	45(3)	5(2)	17(2)
C(31)	21(1)	39(2)	31(2)	2(1)	10(1)	-1(1)

C(32)	27(1)	51(2)	33(2)	-1(1)	15(1)	0(1)
C(33)	35(2)	80(2)	36(2)	0(2)	17(2)	-11(2)
C(34)	35(2)	82(3)	50(2)	-1(2)	15(2)	-14(2)
C(35)	30(2)	70(2)	39(2)	-4(2)	4(2)	-13(1)
C(36)	28(1)	43(2)	34(2)	-1(1)	9(1)	-1(1)
C(37)	31(1)	69(2)	30(2)	-4(1)	15(1)	-8(1)
C(38)	59(2)	73(3)	42(2)	-9(2)	21(2)	-11(2)
C(39)	38(2)	85(3)	40(2)	8(2)	13(2)	2(2)
C(43)	28(1)	62(2)	27(2)	-2(1)	2(1)	-5(1)
C(44)	41(2)	107(3)	38(2)	12(2)	2(2)	4(2)
C(45)	60(2)	73(3)	54(2)	-22(2)	24(2)	-11(2)
C(46)	23(1)	35(2)	30(2)	-2(1)	4(1)	-4(1)
C(47)	27(1)	35(2)	40(2)	1(1)	4(1)	-2(1)
C(48)	40(2)	36(2)	49(2)	1(1)	8(2)	1(1)
C(49)	35(2)	40(2)	56(2)	-8(2)	16(2)	2(1)
C(50)	36(2)	53(2)	39(2)	-4(1)	20(2)	0(1)
C(51)	25(1)	41(2)	36(2)	0(1)	10(1)	-1(1)
C(52)	61(2)	38(2)	38(2)	6(1)	11(2)	5(1)
C(53)	70(3)	151(5)	43(3)	-7(3)	-9(2)	43(3)
C(54)	307(10)	71(3)	84(4)	-10(3)	100(6)	-79(5)
C(55)	59(2)	51(2)	70(3)	-10(2)	27(2)	8(2)
C(56)	77(3)	50(2)	83(3)	-21(2)	27(2)	-3(2)
C(57)	156(5)	62(3)	186(6)	-19(3)	136(5)	5(3)
C(58)	39(2)	46(2)	36(2)	4(1)	19(1)	5(1)
C(59)	58(2)	74(3)	38(2)	12(2)	11(2)	7(2)
C(60)	55(2)	50(2)	56(2)	1(2)	29(2)	-4(2)
