Supporting Information for

Do planar tetracoordinate tin complexes really exist?

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1. Tables with details of refinement of 4-sq, and the refinement replacing the Se atom for Sn (2-sq)

Table 1. Crystal data and structure refinement for **4-sq**.

Identification code	4-sq	
Empirical formula	$C_{24}H_{56}N_2P_4Se_5$	
Formula weight	891.39	
Temperature	298(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 10.3811(18) Å	α= 90°.
	b = 14.791(3) Å	β= 100.694(3)°.
	c = 12.086(2) Å	γ = 90°.
Volume	1823.6(5) $Å^3$	
Z	2	
Density (calculated)	1.623 Mg/m^3	
Absorption coefficient	5.214 mm^{-1}	
F(000)	888	
Crystal size	0.66 x 0.43 x 0.32 mm^3	
Theta range for data collection	2.20 to 28.33°.	
Index ranges	-13<=h<=13, -19<=k<=19, -16<=l<=16	
Reflections collected	30223	
Independent reflections	4493 [R(int) = 0.0643]	
Completeness to theta = 28.33°	98.9 %	
Absorption correction	Numerical	
Max. and min. transmission	0.2862 and 0.1303	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4493 / 0 / 168	
Goodness-of-fit on F^2	1.062	
Final R indices [I>2sigma(I)]	R1 = 0.0404, wR2 = 0.1061	
R indices (all data)	R1 = 0.0604, wR2 = 0.1169	
Largest diff. peak and hole	2.281 and -0.717 e.$Å^{-3}$	

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

	x	y	z	U(eq)
P(1)	-1255(1)	3855(1)	2289(1)	29(1)
P(2)	3097(1)	4928(1)	6770(1)	30(1)
Se(1)	0	5000	5000	36(1)
Se(2)	29(1)	3451(1)	3861(1)	40(1)
Se(3)	2507(1)	5274(1)	4985(1)	41(1)
N(1)	-2458(3)	4501(2)	2355(3)	36(1)
C(1)	400(5)	5253(4)	1907(4)	56(1)
C(2)	-249(4)	4392(3)	1379(4)	39(1)
C(3)	778(5)	3745(4)	1056(5)	61(1)
C(4)	-1888(4)	2810(3)	1567(4)	39(1)
C(5)	-2620(5)	2237(3)	2301(4)	55(1)
C(6)	-2769(6)	3027(4)	443(4)	68(2)
C(7)	2719(4)	3728(3)	6900(4)	43(1)
C(8)	3420(5)	3115(3)	6178(5)	58(1)
C(9)	2915(7)	3389(4)	8135(5)	72(2)
C(10)	4881(4)	5088(3)	7087(4)	44(1)
C(11)	5467(6)	4881(6)	8294(6)	94(2)
C(12)	5277(5)	6020(4)	6769(6)	65(2)

Table 3. Bond lengths [Å] and angles [°] for 4-sq.

P(1)-N(1)	1.587(3)	C(5)-H(5A)	0.9600
P(1)-C(2)	1.833(4)	C(5)-H(5B)	0.9600
P(1)-C(4)	1.835(4)	C(5)-H(5C)	0.9600
P(1)-Se(2)	2.1911(10)	C(6)-H(6A)	0.9600
P(2)-N(1)#1	1.592(3)	C(6)-H(6B)	0.9600
P(2)-C(7)	1.831(4)	C(6)-H(6C)	0.9600
P(2)-C(10)	1.835(4)	C(7)-C(8)	1.532(7)
P(2)-Se(3)	2.1905(11)	C(7)-C(9)	1.552(7)
Se(1)-Se(3)	2.6373(6)	C(7)-H(7)	0.9800
Se(1)-Se(3)#1	2.6373(6)	C(8)-H(8A)	0.9600
Se(1)-Se(2)#1	2.6766(5)	C(8)-H(8B)	0.9600
Se(1)-Se(2)	2.6766(5)	C(8)-H(8C)	0.9600
N(1)-P(2)#1	1.592(3)	C(9)-H(9A)	0.9600
C(1)-C(2)	1.524(6)	C(9)-H(9B)	0.9600
C(1)-H(1A)	0.9600	C(9)-H(9C)	0.9600
C(1)-H(1B)	0.9600	C(10)-C(11)	1.504(8)
C(1)-H(1C)	0.9600	C(10)-C(12)	1.509(7)
C(2)-C(3)	1.536(7)	C(10)-H(10)	0.9800
C(2)-H(2)	0.9800	C(11)-H(11A)	0.9600
C(3)-H(3A)	0.9600	C(11)-H(11B)	0.9600
C(3)-H(3B)	0.9600	C(11)-H(11C)	0.9600
C(3)-H(3C)	0.9600	C(12)-H(12A)	0.9600
C(4)-C(6)	1.525(6)	C(12)-H(12B)	0.9600
C(4)-C(5)	1.527(6)	C(12)-H(12C)	0.9600
C(4)-H(4)	0.9800		

N(1)-P(1)-C(2)	108.1(2)	C(7)-P(2)-C(10)	109.3(2)
N(1)-P(1)-C(4)	108.4(2)	N(1)#1-P(2)-Se(3)	117.11(13)
C(2)-P(1)-C(4)	105.8(2)	C(7)-P(2)-Se(3)	106.61(16)
N(1)-P(1)-Se(2)	118.63(13)	C(10)-P(2)-Se(3)	105.21(17)
C(2)-P(1)-Se(2)	108.40(15)	Se(3)-Se(1)-Se(3)#1	180.0
C(4)-P(1)-Se(2)	106.83(14)	Se(3)-Se(1)-Se(2)#1	88.709(15)
N(1)#1-P(2)-C(7)	109.6(2)	Se(3)#1-Se(1)-Se(2)#1	91.291(15)
N(1)#1-P(2)-C(10)	108.7(2)	Se(3)-Se(1)-Se(2)	91.291(15)

Se(3)#1-Se(1)-Se(2)	88.709(15)	C(4)-C(6)-H(6B)	109.5
Se(2)#1-Se(1)-Se(2)	180.0	H(6A)-C(6)-H(6B)	109.5
P(1)-Se(2)-Se(1)	98.59(3)	C(4)-C(6)-H(6C)	109.5
P(2)-Se(3)-Se(1)	93.07(3)	H(6A)-C(6)-H(6C)	109.5
P(1)-N(1)-P(2)#1	141.4(2)	H(6B)-C(6)-H(6C)	109.5
C(2)-C(1)-H(1A)	109.5	C(8)-C(7)-C(9)	111.5(4)
C(2)-C(1)-H(1B)	109.5	C(8)-C(7)-P(2)	113.1(3)
H(1A)-C(1)-H(1B)	109.5	C(9)-C(7)-P(2)	113.8(4)
C(2)-C(1)-H(1C)	109.5	C(8)-C(7)-H(7)	105.9
H(1A)-C(1)-H(1C)	109.5	C(9)-C(7)-H(7)	105.9
H(1B)-C(1)-H(1C)	109.5	P(2)-C(7)-H(7)	105.9
C(1)-C(2)-C(3)	110.7(4)	C(7)-C(8)-H(8A)	109.5
C(1)-C(2)-P(1)	111.6(3)	C(7)-C(8)-H(8B)	109.5
C(3)-C(2)-P(1)	112.5(3)	H(8A)-C(8)-H(8B)	109.5
C(1)-C(2)-H(2)	107.3	C(7)-C(8)-H(8C)	109.5
C(3)-C(2)-H(2)	107.3	H(8A)-C(8)-H(8C)	109.5
P(1)-C(2)-H(2)	107.3	H(8B)-C(8)-H(8C)	109.5
C(2)-C(3)-H(3A)	109.5	C(7)-C(9)-H(9A)	109.5
C(2)-C(3)-H(3B)	109.5	C(7)-C(9)-H(9B)	109.5
H(3A)-C(3)-H(3B)	109.5	H(9A)-C(9)-H(9B)	109.5
C(2)-C(3)-H(3C)	109.5	C(7)-C(9)-H(9C)	109.5
H(3A)-C(3)-H(3C)	109.5	H(9A)-C(9)-H(9C)	109.5
H(3B)-C(3)-H(3C)	109.5	H(9B)-C(9)-H(9C)	109.5
C(6)-C(4)-C(5)	110.7(4)	C(11)-C(10)-C(12)	110.6(5)
C(6)-C(4)-P(1)	110.5(3)	C(11)-C(10)-P(2)	112.8(4)
C(5)-C(4)-P(1)	111.3(3)	C(12)-C(10)-P(2)	112.1(3)
C(6)-C(4)-H(4)	108.1	C(11)-C(10)-H(10)	107.0
C(5)-C(4)-H(4)	108.1	C(12)-C(10)-H(10)	107.0
P(1)-C(4)-H(4)	108.1	P(2)-C(10)-H(10)	107.0
C(4)-C(5)-H(5A)	109.5	C(10)-C(11)-H(11A)	109.5
C(4)-C(5)-H(5B)	109.5	C(10)-C(11)-H(11B)	109.5
H(5A)-C(5)-H(5B)	109.5	H(11A)-C(11)-H(11B)	109.5
C(4)-C(5)-H(5C)	109.5	C(10)-C(11)-H(11C)	109.5
H(5A)-C(5)-H(5C)	109.5	H(11A)-C(11)-H(11C)	109.5
H(5B)-C(5)-H(5C)	109.5	H(11B)-C(11)-H(11C)	109.5
C(4)-C(6)-H(6A)	109.5	C(10)-C(12)-H(12A)	109.5

C(10)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(10)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5

Symmetry transformations used to generate equivalent atoms:

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

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

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
P(1)	31(1)	30(1)	26(1)	-1(1)	3(1)	2(1)
P(2)	26(1)	29(1)	33(1)	0(1)	2(1)	3(1)
Se(1)	35(1)	42(1)	26(1)	1(1)	-3(1)	7(1)
Se(2)	46(1)	38(1)	32(1)	0(1)	-3(1)	13(1)
Se(3)	41(1)	53(1)	31(1)	4(1)	9(1)	5(1)
N(1)	36(2)	40(2)	31(2)	0(1)	4(1)	9(2)
C(1)	62(3)	58(3)	49(3)	-1(2)	15(2)	-20(2)
C(2)	38(2)	47(2)	34(2)	-1(2)	12(2)	-2(2)
C(3)	56(3)	68(3)	66(3)	-3(3)	30(3)	5(3)
C(4)	46(2)	34(2)	38(2)	-7(2)	7(2)	0(2)
C(5)	64(3)	42(3)	60(3)	-8(2)	17(2)	-14(2)
C(6)	98(5)	54(3)	41(3)	-7(2)	-12(3)	-15(3)
C(7)	41(2)	33(2)	53(3)	4(2)	8(2)	0(2)
C(8)	63(3)	31(2)	83(4)	-8(2)	22(3)	4(2)
C(9)	93(5)	58(3)	67(4)	27(3)	16(3)	0(3)
C(10)	28(2)	46(2)	58(3)	-6(2)	8(2)	1(2)
C(11)	46(3)	143(7)	79(5)	19(4)	-22(3)	-7(4)
C(12)	42(3)	57(3)	97(4)	-10(3)	15(3)	-17(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 4-sq.

	x	y	z	U(eq)
H(1A)	985	5106	2596	83
H(1B)	-261	5663	2062	83
H(1C)	885	5532	1395	83
H(2)	-838	4566	681	47
H(3A)	1350	4074	661	91
H(3B)	345	3275	580	91
H(3C)	1282	3482	1725	91
H(4)	-1140	2458	1415	47
H(5A)	-3352	2573	2467	83
H(5B)	-2039	2086	2990	83
H(5C)	-2928	1693	1906	83
H(6A)	-3090	2475	74	101
H(6B)	-2277	3354	-24	101
H(6C)	-3496	3389	570	101
H(7)	1781	3665	6596	51
H(8A)	4345	3118	6474	87
H(8B)	3265	3334	5417	87
H(8C)	3090	2510	6191	87
H(9A)	2421	2844	8166	109
H(9B)	2616	3843	8596	109
H(9C)	3828	3271	8408	109
H(10)	5259	4656	6621	53
H(11A)	6375	5052	8441	140
H(11B)	5393	4246	8430	140
H(11C)	5008	5215	8782	140
H(12A)	4933	6463	7217	97
H(12B)	4933	6127	5986	97
H(12C)	6215	6062	6901	97

Table 6. Torsion angles [°] for 4-sq.

N(1)-P(1)-Se(2)-Se(1)	-36.56(16)
C(2)-P(1)-Se(2)-Se(1)	87.11(15)
C(4)-P(1)-Se(2)-Se(1)	-159.23(15)
Se(3)-Se(1)-Se(2)-P(1)	-113.33(3)
Se(3)#1-Se(1)-Se(2)-P(1)	66.67(3)
Se(2)#1-Se(1)-Se(2)-P(1)	90(65)
N(1)#1-P(2)-Se(3)-Se(1)	-57.26(16)
C(7)-P(2)-Se(3)-Se(1)	65.81(15)
C(10)-P(2)-Se(3)-Se(1)	-178.16(15)
Se(3)#1-Se(1)-Se(3)-P(2)	-17(49)
Se(2)#1-Se(1)-Se(3)-P(2)	73.85(3)
Se(2)-Se(1)-Se(3)-P(2)	-106.15(3)
C(2)-P(1)-N(1)-P(2)#1	-118.2(4)
C(4)-P(1)-N(1)-P(2)#1	127.5(4)
Se(2)-P(1)-N(1)-P(2)#1	5.6(5)
N(1)-P(1)-C(2)-C(1)	66.9(4)
C(4)-P(1)-C(2)-C(1)	-177.2(3)
Se(2)-P(1)-C(2)-C(1)	-62.9(4)
N(1)-P(1)-C(2)-C(3)	-168.1(3)
C(4)-P(1)-C(2)-C(3)	-52.2(4)
Se(2)-P(1)-C(2)-C(3)	62.1(4)
N(1)-P(1)-C(4)-C(6)	52.6(4)
C(2)-P(1)-C(4)-C(6)	-63.1(4)
Se(2)-P(1)-C(4)-C(6)	-178.5(3)
N(1)-P(1)-C(4)-C(5)	-70.8(4)
C(2)-P(1)-C(4)-C(5)	173.4(3)
Se(2)-P(1)-C(4)-C(5)	58.0(3)
N(1)#1-P(2)-C(7)-C(8)	-173.7(3)
C(10)-P(2)-C(7)-C(8)	-54.7(4)
Se(3)-P(2)-C(7)-C(8)	58.6(4)
N(1)#1-P(2)-C(7)-C(9)	-45.2(4)
C(10)-P(2)-C(7)-C(9)	73.9(4)
Se(3)-P(2)-C(7)-C(9)	-172.9(4)
N(1)#1-P(2)-C(10)-C(11)	53.6(5)

C(7)-P(2)-C(10)-C(11)	-66.0(5)
Se(3)-P(2)-C(10)-C(11)	179.8(4)
N(1)#1-P(2)-C(10)-C(12)	-72.1(4)
C(7)-P(2)-C(10)-C(12)	168.3(4)
Se(3)-P(2)-C(10)-C(12)	54.2(4)

Symmetry transformations used to generate equivalent atoms:

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

Table 1. Crystal data and structure refinement for **2-sq**.

Identification code	2-sq	
Empirical formula	$C_{24}H_{56}N_2P_4Se_4Sn$	
Formula weight	931.12	
Temperature	298(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 10.3811(18) Å	α= 90°.
	b = 14.791(3) Å	β= 100.694(3)°.
	c = 12.086(2) Å	γ = 90°.
Volume	1823.6(5) $Å^3$	
Z	2	
Density (calculated)	1.696 Mg/m^3	
Absorption coefficient	4.885 mm^{-1}	
F(000)	920	
Crystal size	0.66 x 0.43 x 0.32 mm^3	
Theta range for data collection	2.20 to 28.33°.	
Index ranges	-13<=h<=13, -19<=k<=19, -16<=l<=16	
Reflections collected	30223	
Independent reflections	4493 [R(int) = 0.0643]	
Completeness to theta = 28.33°	98.9 %	
Absorption correction	None	
Max. and min. transmission	0.3040 and 0.1408	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4493 / 0 / 168	
Goodness-of-fit on F^2	2.234	
Final R indices [I>2sigma(I)]	R1 = 0.0777, wR2 = 0.2290	
R indices (all data)	R1 = 0.1000, wR2 = 0.2362	
Largest diff. peak and hole	2.501 and -4.623 $e.Å^{-3}$	

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

	x	y	z	U(eq)
P(1)	-1256(2)	3855(1)	2290(2)	24(1)
P(2)	3098(2)	4928(1)	6773(2)	24(1)
Sn(1)	0	5000	5000	55(1)
Se(2)	29(1)	3451(1)	3861(1)	35(1)
Se(3)	2507(1)	5272(1)	4986(1)	36(1)
N(1)	-2460(7)	4498(5)	2368(6)	31(2)
C(1)	428(11)	5247(7)	1926(9)	50(3)
C(2)	-255(9)	4386(6)	1373(7)	33(2)
C(3)	777(11)	3737(8)	1056(11)	56(3)
C(4)	-1896(9)	2807(6)	1561(7)	32(2)
C(5)	-2613(11)	2220(7)	2301(10)	51(3)
C(6)	-2790(13)	3028(8)	458(9)	62(3)
C(7)	2731(9)	3735(6)	6890(8)	38(2)
C(8)	3401(11)	3118(7)	6180(10)	52(3)
C(9)	2899(14)	3398(8)	8155(11)	63(3)
C(10)	4882(8)	5091(7)	7068(9)	40(2)
C(11)	5428(13)	4868(13)	8322(13)	95(6)
C(12)	5287(11)	5992(8)	6785(12)	60(3)

Table 3. Bond lengths [Å] and angles [°] for 2-sq.

P(1)-N(1)	1.587(7)	C(5)-H(5A)	0.9600
P(1)-C(2)	1.831(9)	C(5)-H(5B)	0.9600
P(1)-C(4)	1.845(8)	C(5)-H(5C)	0.9600
P(1)-Se(2)	2.190(2)	C(6)-H(6A)	0.9600
P(2)-N(1)#1	1.578(7)	C(6)-H(6B)	0.9600
P(2)-C(7)	1.817(9)	C(6)-H(6C)	0.9600
P(2)-C(10)	1.836(9)	C(7)-C(8)	1.509(14)
P(2)-Se(3)	2.193(2)	C(7)-C(9)	1.586(15)
Sn(1)-Se(3)	2.6362(10)	C(7)-H(7)	0.9800
Sn(1)-Se(3)#1	2.6362(10)	C(8)-H(8A)	0.9600
Sn(1)-Se(2)	2.6768(9)	C(8)-H(8B)	0.9600
Sn(1)-Se(2)#1	2.6768(9)	C(8)-H(8C)	0.9600
N(1)-P(2)#1	1.578(7)	C(9)-H(9A)	0.9600
C(1)-C(2)	1.548(13)	C(9)-H(9B)	0.9600
C(1)-H(1A)	0.9600	C(9)-H(9C)	0.9600
C(1)-H(1B)	0.9600	C(10)-C(12)	1.458(15)
C(1)-H(1C)	0.9600	C(10)-C(11)	1.552(17)
C(2)-C(3)	1.539(13)	C(10)-H(10)	0.9800
C(2)-H(2)	0.9800	C(11)-H(11A)	0.9600
C(3)-H(3A)	0.9600	C(11)-H(11B)	0.9600
C(3)-H(3B)	0.9600	C(11)-H(11C)	0.9600
C(3)-H(3C)	0.9600	C(12)-H(12A)	0.9600
C(4)-C(6)	1.512(13)	C(12)-H(12B)	0.9600
C(4)-C(5)	1.535(13)	C(12)-H(12C)	0.9600
C(4)-H(4)	0.9800		

N(1)-P(1)-C(2)	108.6(4)	C(7)-P(2)-C(10)	109.3(4)
N(1)-P(1)-C(4)	108.3(4)	N(1)#1-P(2)-Se(3)	116.6(3)
C(2)-P(1)-C(4)	105.4(4)	C(7)-P(2)-Se(3)	106.1(3)
N(1)-P(1)-Se(2)	118.2(3)	C(10)-P(2)-Se(3)	104.4(3)
C(2)-P(1)-Se(2)	108.6(3)	Se(3)-Sn(1)-Se(3)#1	180.0
C(4)-P(1)-Se(2)	107.0(3)	Se(3)-Sn(1)-Se(2)	91.26(3)
N(1)#1-P(2)-C(7)	110.6(4)	Se(3)#1-Sn(1)-Se(2)	88.74(3)
N(1)#1-P(2)-C(10)	109.4(4)	Se(3)-Sn(1)-Se(2)#1	88.74(3)

Se(3)#1-Sn(1)-Se(2)#1	91.26(3)	C(4)-C(6)-H(6B)	109.5
Se(2)-Sn(1)-Se(2)#1	180.0	H(6A)-C(6)-H(6B)	109.5
P(1)-Se(2)-Sn(1)	98.56(6)	C(4)-C(6)-H(6C)	109.5
P(2)-Se(3)-Sn(1)	93.11(6)	H(6A)-C(6)-H(6C)	109.5
P(2)#1-N(1)-P(1)	142.4(5)	H(6B)-C(6)-H(6C)	109.5
C(2)-C(1)-H(1A)	109.5	C(8)-C(7)-C(9)	112.2(9)
C(2)-C(1)-H(1B)	109.5	C(8)-C(7)-P(2)	114.7(7)
H(1A)-C(1)-H(1B)	109.5	C(9)-C(7)-P(2)	113.2(7)
C(2)-C(1)-H(1C)	109.5	C(8)-C(7)-H(7)	105.2
H(1A)-C(1)-H(1C)	109.5	C(9)-C(7)-H(7)	105.2
H(1B)-C(1)-H(1C)	109.5	P(2)-C(7)-H(7)	105.2
C(3)-C(2)-C(1)	109.7(8)	C(7)-C(8)-H(8A)	109.5
C(3)-C(2)-P(1)	112.5(7)	C(7)-C(8)-H(8B)	109.5
C(1)-C(2)-P(1)	111.0(6)	H(8A)-C(8)-H(8B)	109.5
C(3)-C(2)-H(2)	107.9	C(7)-C(8)-H(8C)	109.5
C(1)-C(2)-H(2)	107.9	H(8A)-C(8)-H(8C)	109.5
P(1)-C(2)-H(2)	107.9	H(8B)-C(8)-H(8C)	109.5
C(2)-C(3)-H(3A)	109.5	C(7)-C(9)-H(9A)	109.5
C(2)-C(3)-H(3B)	109.5	C(7)-C(9)-H(9B)	109.5
H(3A)-C(3)-H(3B)	109.5	H(9A)-C(9)-H(9B)	109.5
C(2)-C(3)-H(3C)	109.5	C(7)-C(9)-H(9C)	109.5
H(3A)-C(3)-H(3C)	109.5	H(9A)-C(9)-H(9C)	109.5
H(3B)-C(3)-H(3C)	109.5	H(9B)-C(9)-H(9C)	109.5
C(6)-C(4)-C(5)	110.6(8)	C(12)-C(10)-C(11)	110.8(10)
C(6)-C(4)-P(1)	110.3(6)	C(12)-C(10)-P(2)	113.4(7)
C(5)-C(4)-P(1)	111.5(6)	C(11)-C(10)-P(2)	109.6(8)
C(6)-C(4)-H(4)	108.1	C(12)-C(10)-H(10)	107.6
C(5)-C(4)-H(4)	108.1	C(11)-C(10)-H(10)	107.6
P(1)-C(4)-H(4)	108.1	P(2)-C(10)-H(10)	107.6
C(4)-C(5)-H(5A)	109.5	C(10)-C(11)-H(11A)	109.5
C(4)-C(5)-H(5B)	109.5	C(10)-C(11)-H(11B)	109.5
H(5A)-C(5)-H(5B)	109.5	H(11A)-C(11)-H(11B)	109.5
C(4)-C(5)-H(5C)	109.5	C(10)-C(11)-H(11C)	109.5
H(5A)-C(5)-H(5C)	109.5	H(11A)-C(11)-H(11C)	109.5
H(5B)-C(5)-H(5C)	109.5	H(11B)-C(11)-H(11C)	109.5
C(4)-C(6)-H(6A)	109.5	C(10)-C(12)-H(12A)	109.5

C(10)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(10)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5

Symmetry transformations used to generate equivalent atoms:

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

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

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
P(1)	25(1)	25(1)	21(1)	-1(1)	2(1)	3(1)
P(2)	20(1)	25(1)	28(1)	0(1)	1(1)	3(1)
Sn(1)	55(1)	62(1)	44(1)	0(1)	-2(1)	9(1)
Se(2)	40(1)	33(1)	27(1)	0(1)	-4(1)	13(1)
Se(3)	35(1)	47(1)	25(1)	4(1)	7(1)	5(1)
N(1)	30(4)	33(4)	29(4)	-2(3)	2(3)	9(3)
C(1)	59(7)	50(6)	46(6)	-5(5)	17(5)	-24(5)
C(2)	37(4)	37(5)	29(4)	1(4)	13(4)	-3(4)
C(3)	50(6)	59(7)	67(7)	0(6)	33(6)	3(5)
C(4)	37(4)	28(4)	32(4)	-4(3)	8(4)	-1(3)
C(5)	57(6)	39(5)	59(6)	-3(5)	14(5)	-10(5)
C(6)	93(9)	53(7)	33(5)	-11(5)	-7(6)	-20(6)
C(7)	35(5)	30(4)	49(5)	5(4)	8(4)	-1(4)
C(8)	59(7)	28(5)	71(7)	-8(5)	18(6)	4(4)
C(9)	82(9)	41(6)	66(8)	22(5)	12(7)	-2(6)
C(10)	22(4)	41(5)	54(6)	-6(4)	3(4)	2(4)
C(11)	40(7)	160(17)	71(10)	22(10)	-29(7)	-9(8)
C(12)	35(5)	60(7)	85(9)	-1(6)	11(5)	-17(5)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 2-sq.

	x	y	z	U(eq)
H(1A)	1210	5080	2443	76
H(1B)	-155	5561	2326	76
H(1C)	652	5635	1354	76
H(2)	-841	4568	677	40
H(3A)	1350	4065	662	83
H(3B)	345	3266	581	83
H(3C)	1278	3477	1728	83
H(4)	-1151	2460	1393	39
H(5A)	-3252	2580	2581	77
H(5B)	-1991	1985	2923	77
H(5C)	-3043	1728	1863	77
H(6A)	-3184	2483	123	93
H(6B)	-2290	3307	-43	93
H(6C)	-3464	3436	593	93
H(7)	1792	3678	6583	46
H(8A)	4285	3007	6558	78
H(8B)	3411	3398	5465	78
H(8C)	2935	2555	6065	78
H(9A)	2261	2938	8208	95
H(9B)	2774	3897	8631	95
H(9C)	3764	3155	8390	95
H(10)	5263	4656	6608	48
H(11A)	6208	5216	8578	143
H(11B)	5633	4235	8397	143
H(11C)	4782	5015	8768	143
H(12A)	4971	6430	7257	90
H(12B)	4928	6120	6010	90
H(12C)	6226	6020	6901	90

Table 6. Torsion angles [°] for 2-sq.

N(1)-P(1)-Se(2)-Sn(1)	-36.8(3)
C(2)-P(1)-Se(2)-Sn(1)	87.4(3)
C(4)-P(1)-Se(2)-Sn(1)	-159.2(3)
Se(3)-Sn(1)-Se(2)-P(1)	-113.39(6)
Se(3)#1-Sn(1)-Se(2)-P(1)	66.61(6)
Se(2)#1-Sn(1)-Se(2)-P(1)	104(85)
N(1)#1-P(2)-Se(3)-Sn(1)	-57.3(3)
C(7)-P(2)-Se(3)-Sn(1)	66.3(3)
C(10)-P(2)-Se(3)-Sn(1)	-178.2(3)
Se(3)#1-Sn(1)-Se(3)-P(2)	0(100)
Se(2)-Sn(1)-Se(3)-P(2)	-106.25(6)
Se(2)#1-Sn(1)-Se(3)-P(2)	73.75(6)
C(2)-P(1)-N(1)-P(2)#1	-117.6(8)
C(4)-P(1)-N(1)-P(2)#1	128.3(8)
Se(2)-P(1)-N(1)-P(2)#1	6.6(10)
N(1)-P(1)-C(2)-C(3)	-168.7(7)
C(4)-P(1)-C(2)-C(3)	-52.8(8)
Se(2)-P(1)-C(2)-C(3)	61.6(8)
N(1)-P(1)-C(2)-C(1)	68.1(8)
C(4)-P(1)-C(2)-C(1)	-176.0(7)
Se(2)-P(1)-C(2)-C(1)	-61.6(7)
N(1)-P(1)-C(4)-C(6)	52.0(8)
C(2)-P(1)-C(4)-C(6)	-64.1(8)
Se(2)-P(1)-C(4)-C(6)	-179.6(7)
N(1)-P(1)-C(4)-C(5)	-71.3(7)
C(2)-P(1)-C(4)-C(5)	172.5(7)
Se(2)-P(1)-C(4)-C(5)	57.0(7)
N(1)#1-P(2)-C(7)-C(8)	-174.6(7)
C(10)-P(2)-C(7)-C(8)	-54.0(9)
Se(3)-P(2)-C(7)-C(8)	58.0(8)
N(1)#1-P(2)-C(7)-C(9)	-44.1(9)
C(10)-P(2)-C(7)-C(9)	76.5(8)
Se(3)-P(2)-C(7)-C(9)	-171.5(7)
N(1)#1-P(2)-C(10)-C(12)	-70.0(9)
C(7)-P(2)-C(10)-C(12)	168.8(8)
Se(3)-P(2)-C(10)-C(12)	55.6(9)

N(1)#1-P(2)-C(10)-C(11)	54.3(10)
C(7)-P(2)-C(10)-C(11)	-66.9(10)
Se(3)-P(2)-C(10)-C(11)	179.9(9)

Symmetry transformations used to generate equivalent atoms:

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

2. Cartesian coordinates of the theoretical models

0,1

7	-4.042104000	0.643268000	0.502433000
15	-3.949241000	-0.319876000	-0.793860000
34	-2.396260000	-1.845534000	-0.832023000
50	0.000001000	-0.000004000	-1.070157000
34	0.968935000	-1.909960000	0.673925000
15	2.864537000	-1.088079000	1.495712000
7	4.042103000	-0.643263000	0.502444000
15	3.949242000	0.319877000	-0.793851000
34	2.396259000	1.845534000	-0.832021000
15	-2.864539000	1.088084000	1.495702000
34	-0.968933000	1.909959000	0.673918000
6	-2.431173000	-0.229099000	2.679959000
6	-3.554862000	2.439503000	2.498166000
6	-3.844357000	0.721069000	-2.292202000
6	-5.570464000	-1.139953000	-0.914071000
6	3.554860000	-2.439493000	2.498182000
6	2.431164000	0.229106000	2.679965000
6	5.570466000	1.139954000	-0.914061000
6	3.844362000	-0.721072000	-2.292191000
1	4.678230000	-1.431348000	-2.298226000
1	2.904086000	-1.279273000	-2.263887000
1	3.869040000	-0.098532000	-3.190542000
1	6.360991000	0.382198000	-0.899686000
1	5.625818000	1.724234000	-1.836465000
1	5.689861000	1.806466000	-0.056609000
1	4.470670000	-2.087451000	2.984410000
1	2.829860000	-2.760445000	3.250810000
1	3.794296000	-3.278522000	1.840767000
1	3.346640000	0.589004000	3.162029000
1	1.959918000	1.049565000	2.131724000
1	1.734850000	-0.158155000	3.428997000
1	-4.470675000	2.087465000	2.984392000
1	-2.829864000	2.760454000	3.250795000
1	-3.794294000	3.278530000	1.840748000
1	-3.346652000	-0.588994000	3.162022000
1	-1.959928000	-1.049561000	2.131721000
1	-1.734860000	0.158160000	3.428993000
1	-6.360990000	-0.382197000	-0.899700000
1	-5.625815000	-1.724236000	-1.836473000
1	-5.689862000	-1.806463000	-0.056617000
1	-4.678224000	1.431346000	-2.298241000
1	-2.904081000	1.279269000	-2.263898000
1	-3.869034000	0.098526000	-3.190551000

0,1

7	0.087709000	3.789807000	0.000000000
15	0.000000000	3.205221000	-1.488471000
34	-1.271784000	1.462430000	-1.881951000
34	0.000000000	0.000000000	0.000000000
34	1.271784000	-1.462430000	1.881951000
15	0.000000000	-3.205221000	1.488471000
7	-0.087709000	-3.789807000	0.000000000
15	0.000000000	-3.205221000	-1.488471000
34	1.271784000	-1.462430000	-1.881951000

15	0.000000000	3.205221000	1.488471000
34	-1.271784000	1.462430000	1.881951000
6	-0.628949000	4.557179000	2.534064000
6	1.678109000	2.860654000	2.119308000
6	1.678109000	2.860654000	-2.119308000
6	-0.628949000	4.557179000	-2.534064000
6	-1.678109000	-2.860654000	2.119308000
6	0.628949000	-4.557179000	2.534064000
6	0.628949000	-4.557179000	-2.534064000
6	-1.678109000	-2.860654000	-2.119308000
1	-2.314798000	-3.737090000	-1.956813000
1	-2.085519000	-2.006221000	-1.572354000
1	-1.636078000	-2.615061000	-3.183897000
1	-0.005987000	-5.439286000	-2.399666000
1	0.630287000	-4.254283000	-3.584615000
1	1.648669000	-4.795019000	-2.222009000
1	-2.314798000	-3.737090000	1.956813000
1	-1.636078000	-2.615061000	3.183897000
1	-2.085519000	-2.006221000	1.572354000
1	-0.005987000	-5.439286000	2.399666000
1	1.648669000	-4.795019000	2.222009000
1	0.630287000	-4.254283000	3.584615000
1	0.005987000	5.439286000	-2.399666000
1	-0.630287000	4.254283000	-3.584615000
1	-1.648669000	4.795019000	-2.222009000
1	2.314798000	3.737090000	-1.956813000
1	2.085519000	2.006221000	-1.572354000
1	1.636078000	2.615061000	-3.183897000
1	0.005987000	5.439286000	2.399666000
1	-1.648669000	4.795019000	2.222009000
1	-0.630287000	4.254283000	3.584615000
1	2.314798000	3.737090000	1.956813000
1	1.636078000	2.615061000	3.183897000
1	2.085519000	2.006221000	1.572354000