

Inorganic Chemistry

including bioinorganic chemistry

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Table S1. Crystal data and structure refinement details (V)

Empirical formula	C ₂₁ H ₂₄ Sn ₂
Formula weight	513.78
Temperature, K	293(2)
Wavelength, Å	0.71073
Crystal system	Trigonal
Space group	$P\bar{3}$ (No. 147)
Unit cell dimensions	
<i>a</i> ,	11.739(3) Å
<i>c</i> ,	8.871(4) Å
<i>V</i> ,	1058.7(6) Å ³
<i>Z</i>	2
<i>D_x</i> , g/cm ³	1.612
μ	23.57 cm ⁻¹
<i>F</i> (000)	500
θ range for data collection,	2.00 ≤ θ ≤ 22.54
Index ranges	-12 ≤ <i>h</i> ≤ 3; 0 ≤ <i>k</i> ≤ 12; -9 ≤ <i>l</i> ≤ 9
Reflections collected	1661
Independent reflections	930 [<i>R</i> (int) = 0.055]
Absorption correction	Semiempirical (Psi-scan)
Max. and min. transmission	0.481 and 0.335
Refinement method	Full-matrix least-squares on <i>F</i> ²
Data / parameters	930 / 72
Goodness-of-fit on <i>F</i> ²	1.038
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> 1 = 0.0243, <i>wR</i> 2 = 0.0619
<i>R</i> indices (all data)	<i>R</i> 1 = 0.0301, <i>wR</i> 2 = 0.0651
Largest difference peak and hole, e.Å ⁻³	0.454; -0.391

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Table S2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$).^a

	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> (eq)
Sn1	1/3	2/3	4549(1)	55(1)
Sn2	1/3	2/3	7685(1)	64(1)
C1	5240(4)	7953(4)	3593(4)	54(1)
C2	5685(4)	7548(5)	2391(5)	68(1)
C3	6910(6)	8351(6)	1769(7)	92(2)
C4	7724(5)	9556(6)	2373(7)	90(2)
C5	7312(5)	9979(5)	3602(7)	90(2)
C6	6086(5)	9182(4)	4191(6)	74(1)
C7	3865(7)	5294(6)	8541(6)	102(2)
H2	5115	6768	1829	108(8)
H3	7286	7951	1153	108(8)
H4	8540	10122	1870	108(8)
H5	7846	10843	4017	108(8)
H6	5775	9510	4988	108(8)
H7a	3849	5330	9621	156(16)
H7b	4737	5541	8210	156(16)
H7c	3262	4415	8210	156(16)

^a *U*(eq) is defined as one third of the trace of the orthogonalized *U*_{ij} tensor.

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Table S.3. Bond lengths [Å] and angles [°]

Sn(1)-C(1)#1	2.152(4)	C(1)-C(2)	1.373(6)
Sn(1)-C(1)	2.152(4)	C(1)-C(6)	1.384(6)
Sn(1)-C(1)#2	2.152(4)	C(2)-C(3)	1.380(7)
Sn(1)-Sn(2)	2.7820(14)	C(3)-C(4)	1.360(8)
Sn(2)-C(7)#2	2.138(5)	C(4)-C(5)	1.382(8)
Sn(2)-C(7)#1	2.138(5)	C(5)-C(6)	1.368(7)
Sn(2)-C(7)	2.138(5)		
C(1)#1-Sn(1)-C(1)	105.48(11)	C(7)#1-Sn(2)-Sn(1)	110.8(2)
C(1)#1-Sn(1)-C(1)#2	105.48(12)	C(7)-Sn(2)-Sn(1)	110.8(2)
C(1)-Sn(1)-C(1)#2	105.48(12)	C(2)-C(1)-C(6)	117.4(4)
C(1)#1-Sn(1)-Sn(2)	113.21(10)	C(2)-C(1)-Sn(1)	120.4(3)
C(1)-Sn(1)-Sn(2)	113.21(10)	C(6)-C(1)-Sn(1)	122.2(3)
C(1)#2-Sn(1)-Sn(2)	113.21(10)	C(3)-C(2)-C(1)	121.4(4)
C(7)#2-Sn(2)-C(7)#1	108.1(2)	C(4)-C(3)-C(2)	120.2(5)
C(7)#2-Sn(2)-C(7)	108.1(2)	C(3)-C(4)-C(5)	119.6(5)
C(7)#1-Sn(2)-C(7)	108.1(2)	C(6)-C(5)-C(4)	119.5(5)
C(7)#2-Sn(2)-Sn(1)	110.8(2)	C(5)-C(6)-C(1)	121.9(5)

Symmetry transformations used to generate equivalent atoms:

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

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

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Table S4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$). 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}
Sn1	55(1)	55(1)	54(1)	0	0	28(1)
Sn2	69(1)	69(1)	55(1)	0	0	34(1)
C1	53(2)	52(2)	59(2)	1(2)	-3(2)	28(2)
C2	62(3)	71(3)	64(3)	-7(2)	5(2)	28(2)
C3	83(4)	97(4)	98(4)	4(3)	26(3)	47(3)
C4	60(3)	74(3)	122(5)	27(3)	15(3)	23(3)
C5	75(3)	60(3)	118(4)	-4(3)	-2(3)	21(3)
C6	74(3)	58(3)	91(3)	-5(2)	1(3)	34(2)
C7	133(5)	112(4)	84(4)	11(3)	-3(3)	78(4)

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Table S5 Hydrogen atomic coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$)

	x	y	z	U(eq)
H2	5115(4)	6768(5)	1829(5)	108(8)
H3	7286(6)	7951(6)	1153(7)	108(8)
H4	8540(5)	10122(6)	1870(7)	108(8)
H5	7846(5)	10843(5)	4017(7)	108(8)
H6	5775(5)	9510(4)	4988(6)	108(8)
H7A	3849(7)	5330(6)	9621(6)	156(16)
H7B	4737(7)	5541(6)	8210(6)	156(16)
H7A	3262(7)	4415(6)	8210(6)	156(16)