

Reactivity of N-Heterocyclic Stannylenes: Oxidative Addition of Chalcogen Elements to a Chiral NH-Sn System

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Supplementary Information

Table S1: Experimental Single-crystal X-ray crystallographic parameters for complexes **2-6**

Compound reference	2	3	4	5	6
Chemical formula	C ₂₀ H ₄₄ N ₄ Sn ₂	C ₃₆ H ₇₈ N ₆ O ₃ Sn ₃ · ½(C ₆ H ₁₄)	C ₂₄ H ₅₂ N ₄ S ₂ Sn ₂	C ₂₄ H ₅₂ N ₄ Se ₂ Sn ₂	C ₂₄ H ₅₂ N ₄ Sn ₂ Te ₂
Formula Mass	577.97	1042.19	698.19	791.99	889.27
Crystal system	Monoclinic	Triclinic	Monoclinic	Monoclinic	Monoclinic
<i>a</i> /Å	9.91798(14)	10.8990(4)	9.32547(18)	9.38243(8)	9.45210(6)
<i>b</i> /Å	13.5756(2)	16.4550(4)	17.0121(3)	17.04431(14)	17.30526(10)
<i>c</i> /Å	19.0840(3)	16.5995(4)	9.87122(18)	9.86411(8)	9.95026(6)
<i>α</i> /°	90	119.163(3)	90	90	90
<i>β</i> /°	95.5413(14)	103.209(3)	95.9146(17)	95.8668(7)	96.0099(6)
<i>γ</i> /°	90	95.724(2)	90	90	90
Unit cell volume/Å ³	2557.51(7)	2451.59(14)	1557.69(5)	1569.18(2)	1618.629(17)
Temperature/K	150(2)	150(2)	150(2)	150(2)	150(2)
Space group	<i>P</i> 21/ <i>c</i>	<i>P</i> $\bar{1}$	<i>P</i> 21/ <i>n</i>	<i>P</i> 21/ <i>n</i>	<i>P</i> 21/ <i>n</i>
No. of formula units per unit cell, <i>Z</i>	4	2	2	2	2
Radiation type	Mo Kα	Cu Kα	Mo Kα	Cu Kα	Cu Kα
Absorption coefficient, μ/mm ⁻¹	1.964	12.344	1.755	15.433	26.329
No. of reflections measured	115034	43453	37439	16083	32107
No. of independent reflections	5854	8999	3581	3140	3247
<i>R</i> _{int}	0.0554	0.0537	0.0567	0.0305	0.0621
Final <i>R</i> ₁ (<i>I</i> > 2σ(<i>I</i>))	0.0352	0.0443	0.0219	0.0200	0.0254
Final <i>wR</i> (<i>F</i> ²) (<i>I</i> > 2σ(<i>I</i>))	0.0772	0.1222	0.0476	0.0488	0.0675
Final <i>R</i> ₁ (all data)	0.0397	0.0499	0.0234	0.0204	0.0258
Final <i>wR</i> (<i>F</i> ²) (all data)	0.0792	0.1274	0.0482	0.0490	0.0679
Goodness of fit on <i>F</i> ²	1.126	1.057	1.133	1.115	1.159
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