

Supplementary material for:

Straightforward Synthesis of Novel Cyclic Metallasiloxanes Supported by a *N,C,N* - Chelating Ligand.

Adéla Fridrichová,^a Barbora Mairychová,^a Zdeňka Padělková,^a Antonín Lyčka,^b Klaus Jurkschat,^c Roman Jambor^{a*} and Libor Dostál^{a*}

^a Department of General and Inorganic Chemistry, Faculty of Chemical Technology, University of Pardubice, Studentská 573, CZ - 532 10, Pardubice, Czech Republic Fax: +420466037068; Tel: +420466037163; E-mail: libor.dostal@upce.cz, roman.jambor@upce.cz

^b Research Institute for Organic Syntheses, Rybitví 296, CZ-533 54 Pardubice, Czech Republic

^c Technische Universität Dortmund, Lehrstuhl für Anorganische Chemie II, Otto-Hahn-Str. 6, D-44227 Dortmund, Germany

Table S1. Crystallographic Data for 4, 5, 6 and 7

	4	5	6	7
empirical formula	C ₄₂ H ₄₄ O ₃ Si ₂ Sn	C ₆₀ H ₆₈ N ₄ O ₄ Si ₂ Sn ₂ ·0.5(CH ₂ Cl ₂)	C ₃₆ H ₃₉ N ₂ O ₃ SbSi ₂	C ₃₆ H ₃₉ BiN ₂ O ₃ Si ₂
cryst syst	triclinic	monoclinic	orthorhombic	orthorhombic
space group	P-1	P21/c	Pna21	Pna21
<i>a</i> [Å]	10.7320(2)	17.5356(3)	14.2341(16)	14.1440(10)
<i>b</i> [Å]	13.1811(8)	16.2802(3)	20.3199(11)	20.3112(12)
<i>c</i> [Å]	13.5121(8)	21.3586(4)	11.8500(14)	11.9648(11)
α [deg]	89.060(5)	90	90	90
β [deg]	84.317(4)	100.403(2)	90	90
γ [deg]	87.989(3)	90	90	90
<i>Z</i>	2	4	4	4
μ [mm ⁻¹]	0.776	0.965	0.912	5.236
<i>D_x</i> [Mg m ⁻³]	1.397	1.379	1.406	1.571
cryst size [mm]	0.36x0.31x0.29	0.40x0.32x0.22	0.36x0.25x0.22	0.44x0.30x0.22
θ range, [deg]	1 – 27.5	1 – 27.5	1 – 27.5	1 – 27.5
<i>T_{min}</i> <i>T_{max}</i>	0.801, 0.848	0.883, 1.000	0.798, 0.888	0.169, 0.384
no. of reflections measured	36 963	29 851	16 428	25 644
no. of unique reflns, <i>R_{int}</i> ^a	8664, 0.033	11137, 0.040	6646, 0.048	7029, 0.037
no. of observed reflns [<i>I</i> >2 σ (<i>I</i>)]	7598	8759	5804	6378
no. of parameters	451	657	397	397
<i>S</i> ^b all data	1.078	0.928	1.100	1.106
final <i>R</i> ^b indices [<i>I</i> >2 σ (<i>I</i>)]	0.027	0.023	0.036	0.029
w <i>R</i> ^{2b} indices (all data)	0.059	0.056	0.065	0.066
$\Delta\rho$, max., min. [e Å ⁻³]	0.480, -0.609	0.560, -0.255	0.482, -0.546	0.951, -1.453

$$^a R_{\text{int}} = \frac{\sum |F_o^2 - F_{o,\text{mean}}^2|}{\sum F_o^2}, \quad ^b S = \left[\frac{\sum (w(F_o^2 - F_c^2)^2)}{(N_{\text{diffrs}} - N_{\text{params}})} \right]^{1/2}, \quad ^b R(F) = \frac{\sum |F_o| - |F_c|}{\sum |F_o|},$$

$$wR(F^2) = \left[\frac{\sum (w(F_o^2 - F_c^2)^2)}{\sum w(F_o^2)^2} \right]^{1/2}$$

Table S1 (continue). Crystallographic Data for 8 and 11

	8	11
empirical formula	C ₄₈ H ₅₈ N ₄ O ₄ Sb ₂ Si ₂	C ₁₆ H ₃₁ BiN ₂ O ₃ Si ₂
cryst syst	monoclinic	monoclinic
space group	P21/c	P21/c
a[Å]	11.7080(5)	13.1780(12)
b[Å]	15.9991(10)	11.1920(10)
c[Å]	13.7490(6)	15.8121(19)
α[deg]	90	90
β[deg]	113.078(4)	105.551(6)
γ[deg]	90	90
Z	2	4
μ[mm ⁻¹]	1.237	7.969
D _x [Mg m ⁻³]	1.478	1.669
cryst size [mm]	0.39x0.34x0.15	0.59x0.29x0.26
θ range, [deg]	1 – 27.5	1 – 27.5
T _{min} , T _{max}	0.699, 0.902	0.087, 0.309
no. of reflections measured	20 039	22 262
no. of unique reflns, R _{int} ^a	5376, 0.037	5118, 0.096
no. of observed reflns [I>2σ(I)]	4424	3437
no. of parameters	271	217
S ^b all data	1.093	1.090
final R ^b indices [I>2σ(I)]	0.029	0.061
wR ^b indices (all data)	0.059	0.130
Δρ, max., min. [e Å ⁻³]	0.975, -0.744	2.360, -2.973

$$^a R_{\text{int}} = \frac{\sum |F_o^2 - F_{o,\text{mean}}^2|}{\sum F_o^2}, \quad ^b S = \left[\frac{\sum (w(F_o^2 - F_c^2)^2)}{(N_{\text{diffs}} - N_{\text{params}})} \right]^{1/2}, \quad ^b R(F) = \frac{\sum ||F_o| - |F_c||}{\sum |F_o|}, \quad wR(F^2) = \left[\frac{\sum (w(F_o^2 - F_c^2)^2)}{(\sum w(F_o^2)^2)} \right]^{1/2}$$