Reactivity of Lithium *n*-Butyl Amidinates Towards Group 14 Metal(II) Chlorides Providing Series of Hetero- and Homoleptic Tetrylenes.

Tomáš Chlupatý,[a] Zdeňka Padělková,[a] Antonín Lyčka,[b] Jiří Brus,[c] Aleš Růžička,*[a]

[a] Department of General and Inorganic Chemistry, Faculty of Chemical Technology, University of Pardubice, Studentská 573, CZ-532 10, Pardubice, Czech Republic, Fax: +420-466037068, *E-mail: ales.ruzicka@upce.cz

[b] Research Institute for Organic Syntheses (VUOS), Rybitví 296, CZ-533 54 Pardubice, Czech Republic

[c] Institute of Macromolecular Chemistry, Academy of Science of the Czech Republic, Heyrovský Sqr. 2, 162 06, Praha 6, Czech Republic

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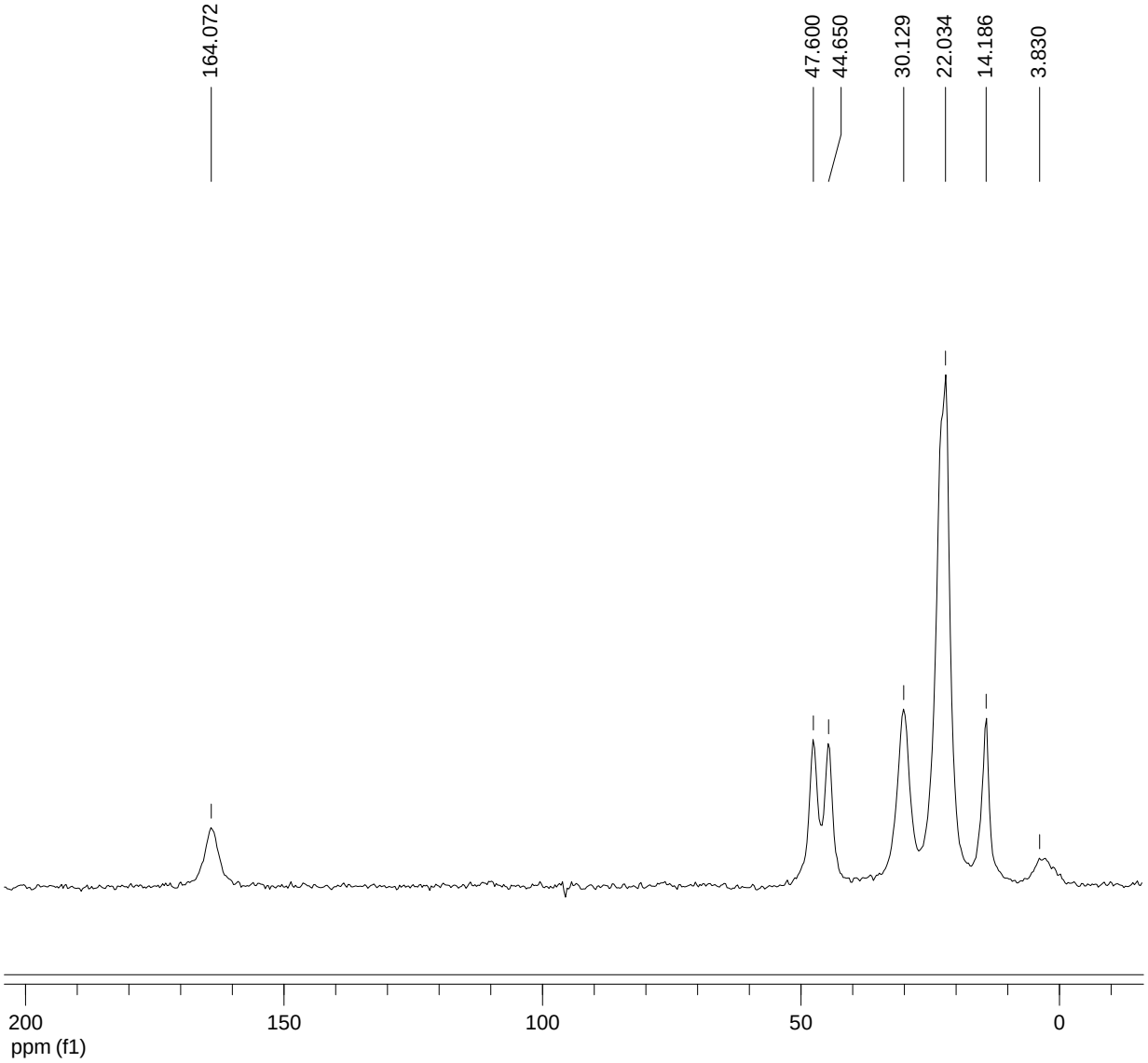
Supporting materials

^{13}C CP/MAS 11000 Hz {[(L$^{i\mathrm{Pr}}$)$_2$SnCl]OSnCl}$_2$



Date:
21 Nov 2011
Document's Title:
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Spectrum Title:
11kHz, RT, NS=7k, D1=4s.

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Original Points Count:
(f1) 512
Actual Points Count:
(f1) 1024
Acquisition Time (sec):
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Spectral Width (ppm):
(f1) 298.880
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Fig. S1: ^{13}C CP/MAS NMR spectrum of **5a**

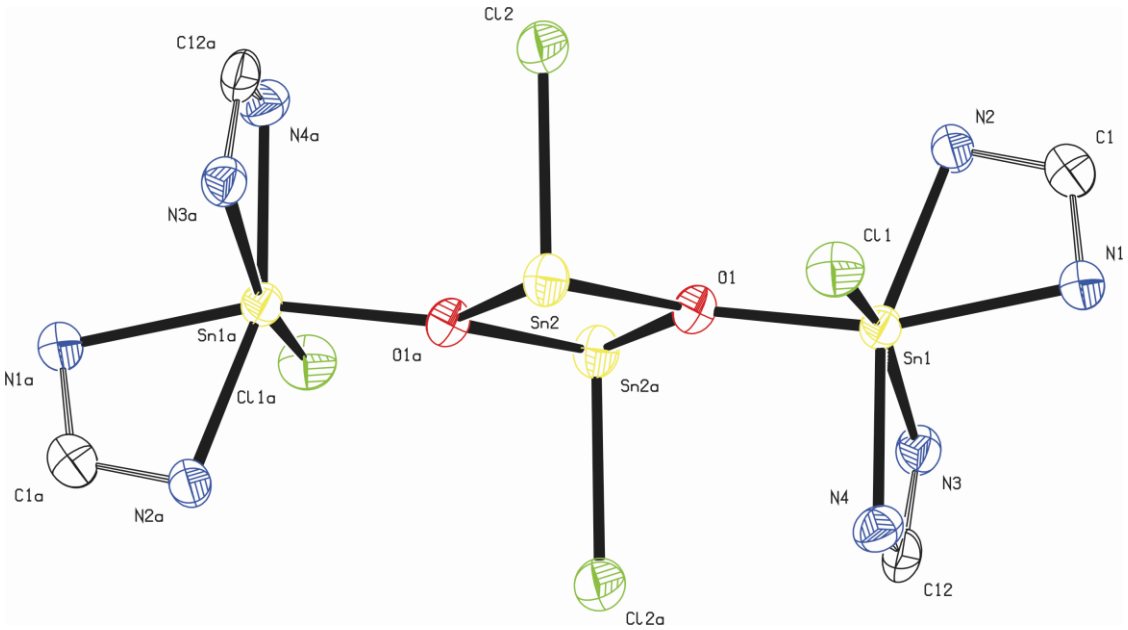

Fig. S2: Detail of the coordination sphere of tin atoms in molecular structure of **5a**

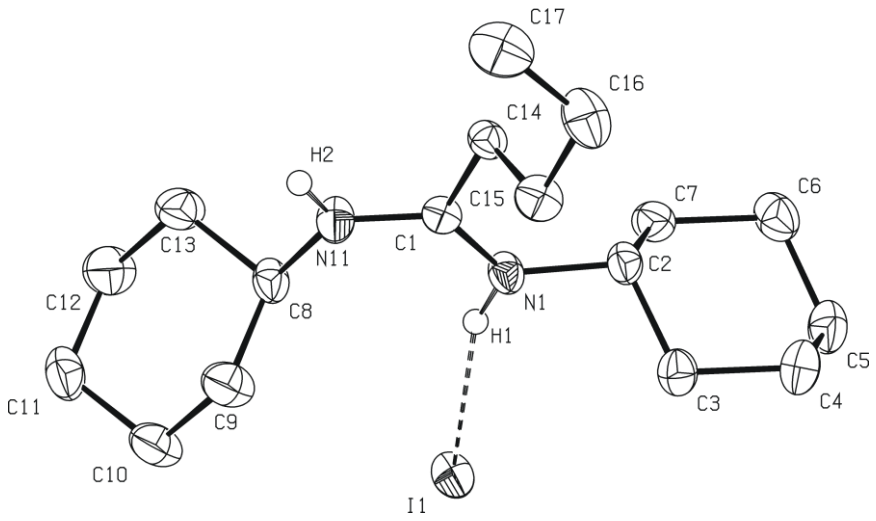

Fig. S3: Molecular structure of $\mathbf{L^{Cy}HI{\cdot}C_6H_6}$ (ORTEP view, 50% probability level). Hydrogen atoms are omitted for clarity. Selected interatomic distances [Å] and angles [°]: N1-C1 1.317(3); N1-C2 1.474(3); N11-C1 1.316(3); N11-C8 1.473(3); C1-C14 1.509(4); N1-I1 3.723(2); N1-C1-N11 121.9(2); C2-C1-C8 121.90(13).

In the $\mathbf{L^{Cy}HI{\cdot}C_6H_6}$, there is no acyclic protonated amidine structure reported up to now except of N-[(3-methoxyphenyl)(methylamino)methylene]methanaminium[1] chloride monohydrate which is difficult to compare with $\mathbf{L^{Cy}HI}$ because of extensive hydrogen bonding with the water molecule(s). On the other hand, in $\mathbf{L^{Cy}HI}$ there are only NH...I contacts forming nonlinear infinite

chain in the solid state. The central NC(*n*-Bu)N moiety is nearly planar due to high degree of delocalization of π-electrons within this fragment (Fig. S3). The differences in the bond lengths and angles between $\mathbf{L^{Cy}HI}$ and previously reported protonated amidine are negligible but the N11-C1-N1 angle is about 10 degrees wider in comparison with the same type of angles in coordinated amidinates.

Reference

1 W.-Z. Chen, G.-L. Xu, C.G. Jablonski and T. Ren, *J. Mol. Struct.*, 2008, **890**, 90-94.