

New Sterically Hindered Tin(IV) Siloxane Precursors to Tinsilicate Materials:

Synthesis, Spectral, Structural and Photocatalytic Studies†‡

Mohan Gopalakrishnan^a and Nallasamy Palanisami^{*a}

^aMaterials Chemistry Division, School of Advanced Sciences, VIT University, Vellore 632 014,

Tamil Nadu, India.

Corresponding author: E-mail: palanisami.n@gmail.com; Tel: +91 98426 39776; Fax no:

+91416224 3092

Table S1. ^{119}Sn and ^{29}Si NMR chemical shift values for tin(IV) siloxanes **1–8**.

Compounds	$\delta(^{119}\text{Sn})$ ppm	$\delta(^{29}\text{Si})$ ppm	Reference
1	-149.60	-93.60	[1, 2]
2	-149.54	-93.37	[3, 1]
3	-148.98	-92.09	[4, 5]
4	-150.23	-91.62	[5, 6]
5	-151.31	-91.33	[7, 4]
6	-151.67	-91.32	[7, 2]
7	-151.34	-20.01	[8, 9]
8	-151.27	-20.08	[8, 9]

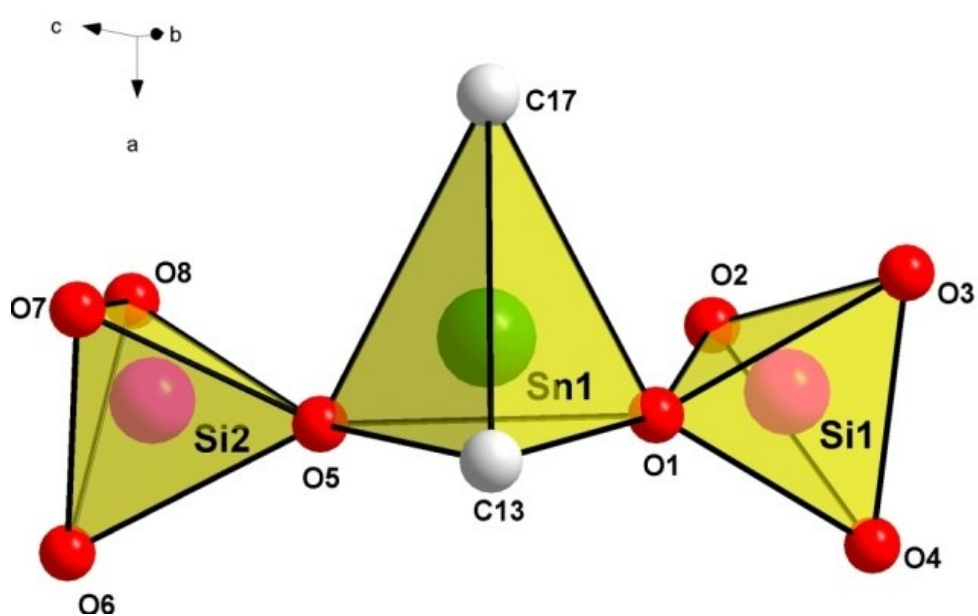


Figure S1. Geometry of tin and silicon in $(^t\text{Bu})_2\text{Sn}(\text{OSi}(\text{O}^t\text{Bu})_3)_2$ (**1**).

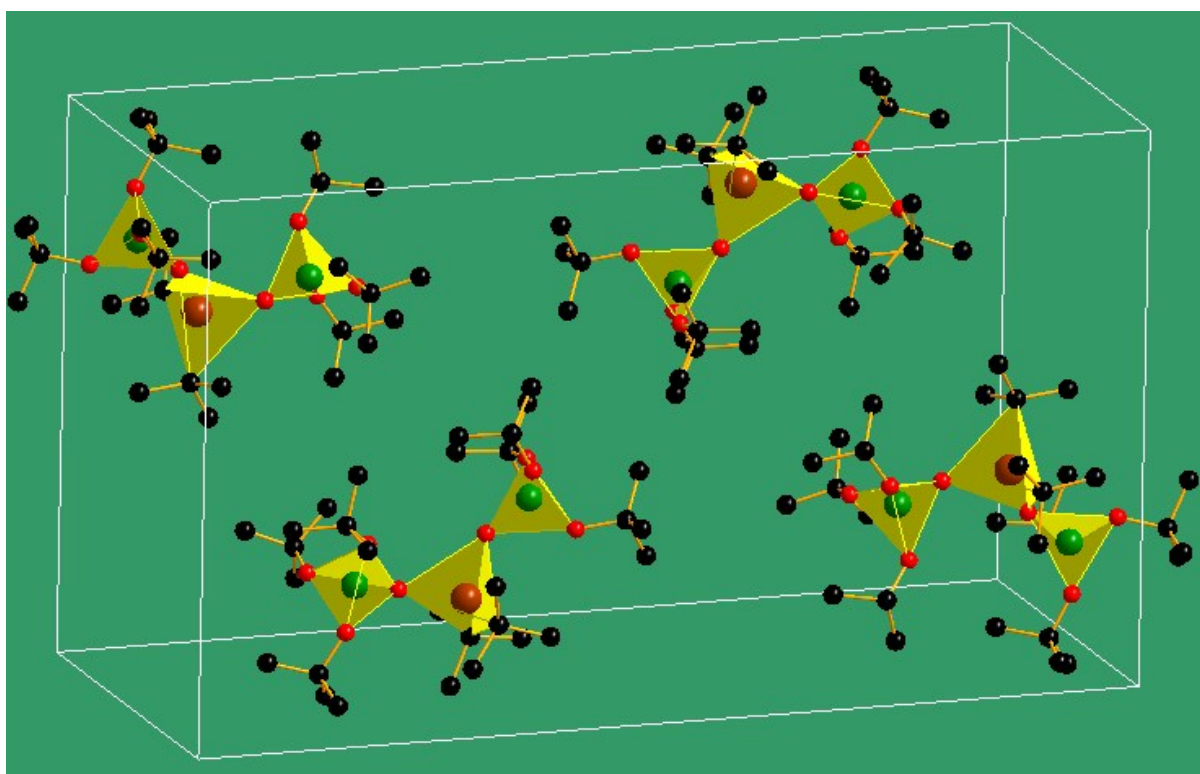


Figure S2. Unite cell packing pattern in $[(t\text{Bu})_2\text{Sn}(\text{OSi}(\text{O}^t\text{Bu})_3)_2]$ (**1**) hydrogen atoms are omitted for clarity.

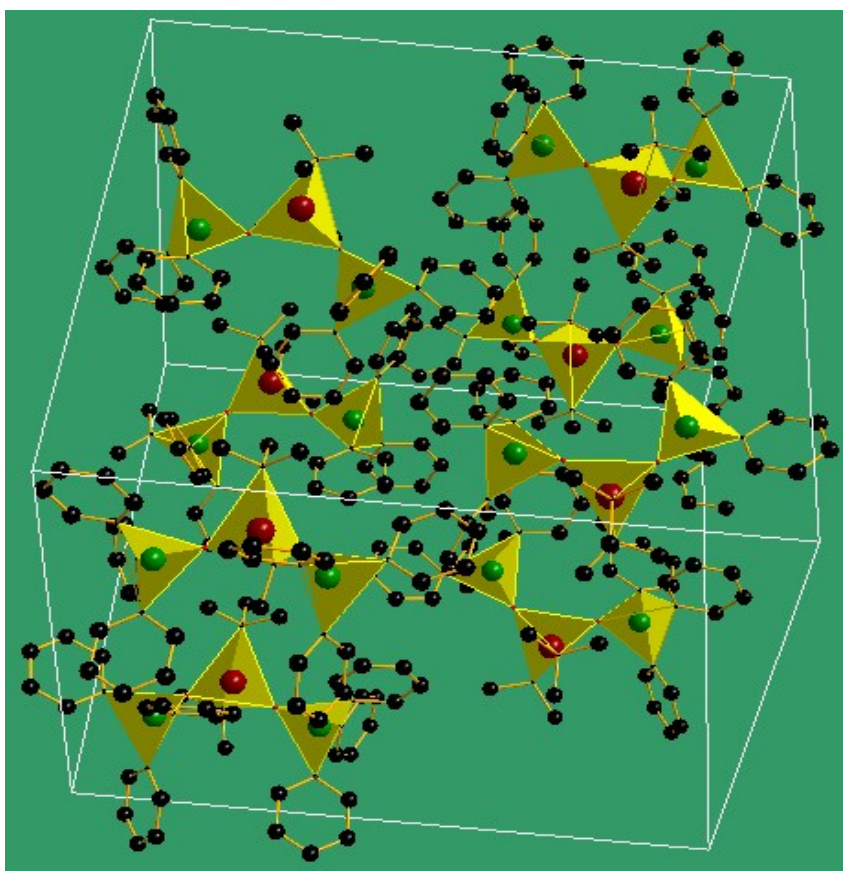


Figure S3. Unite cell packing pattern in $[(t\text{Bu})_2\text{Sn}(\text{OSiPh}_3)_2]$ (**7**) hydrogen atoms are omitted for clarity.

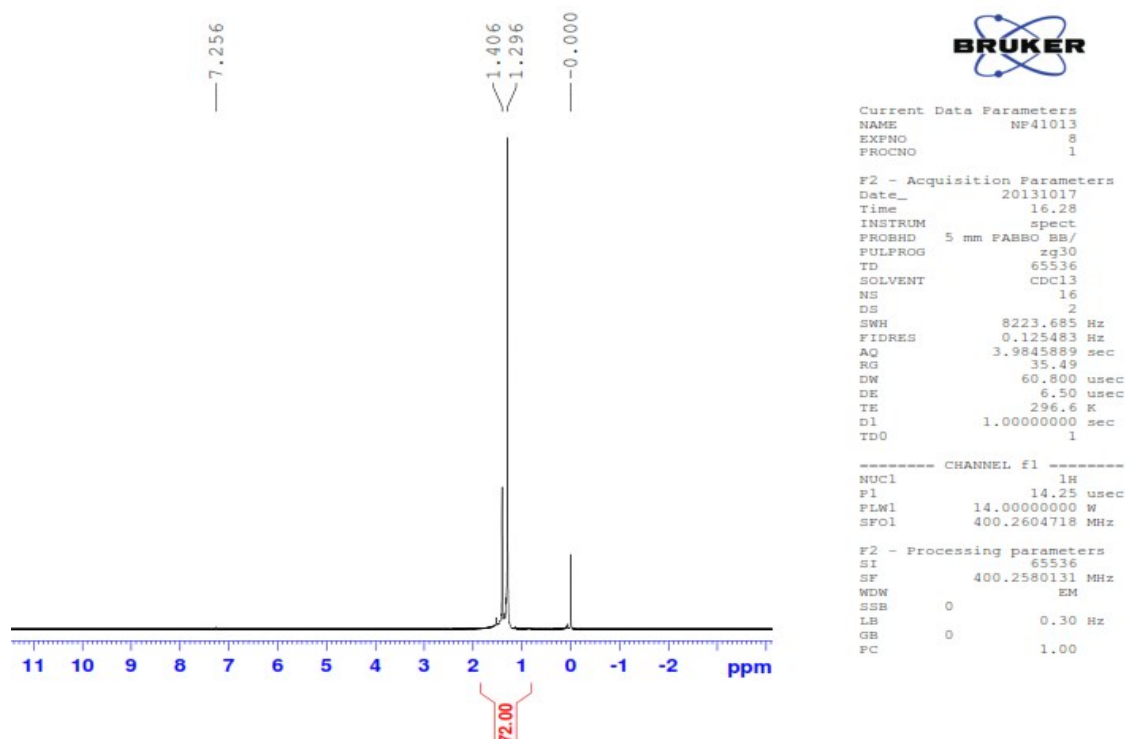


Figure S4. ^1H NMR spectrum of $[(t\text{Bu})_2\text{Sn}(\text{OSi}(\text{O}^t\text{Bu})_3)_2]$ (**1**) in CDCl_3 .

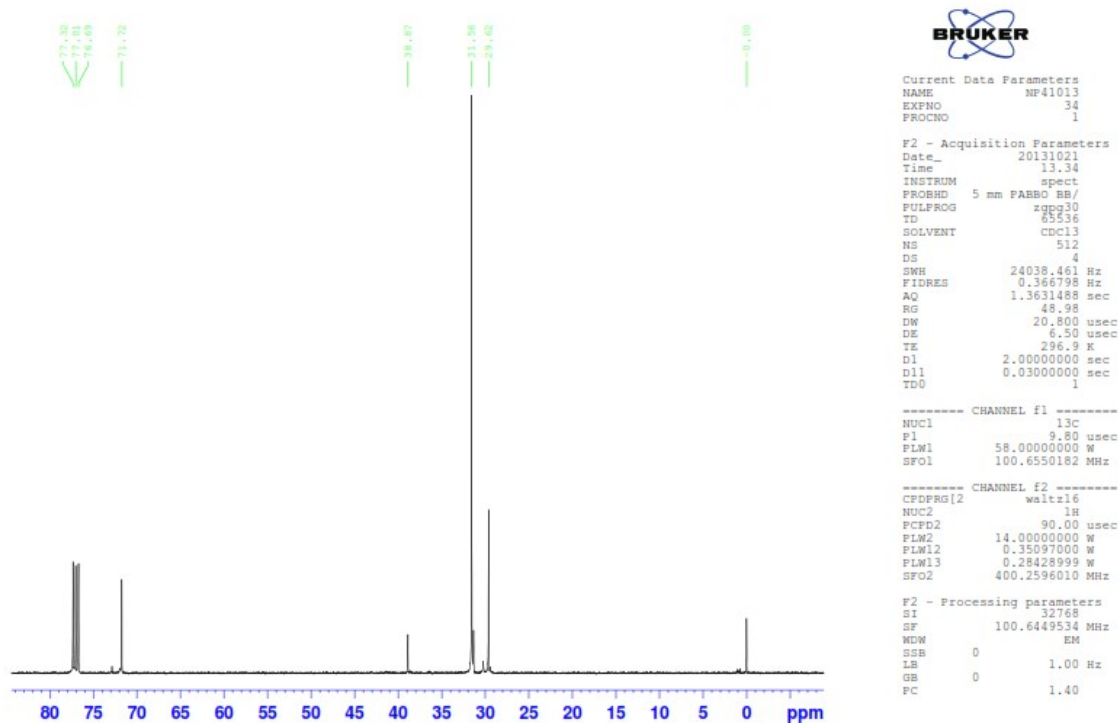


Figure S5. ^{13}C NMR spectrum of $[(t\text{Bu})_2\text{Sn}(\text{OSi}(\text{O}^t\text{Bu})_3)_2]$ (**1**) in CDCl_3 .

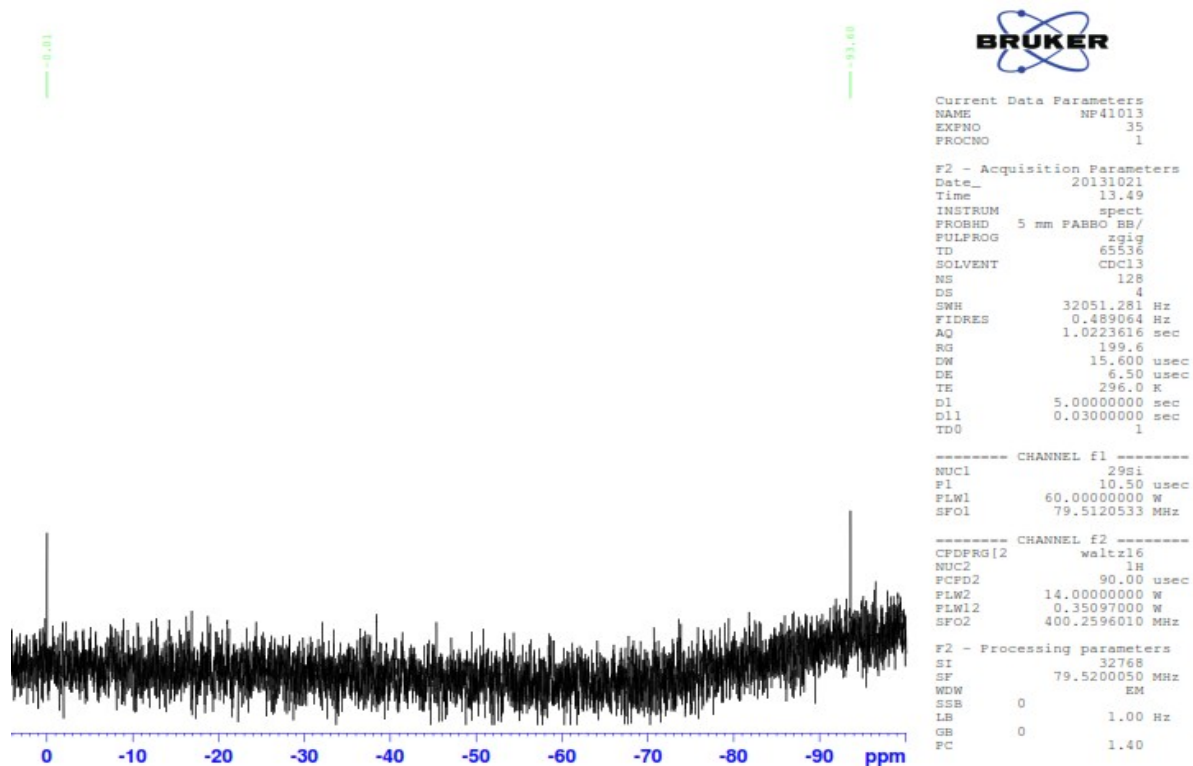


Figure S6. ^{29}Si NMR spectrum of $[(t\text{Bu})_2\text{Sn}(\text{OSi}(\text{O}^t\text{Bu})_3)_2]$ **1** in CDCl_3 .

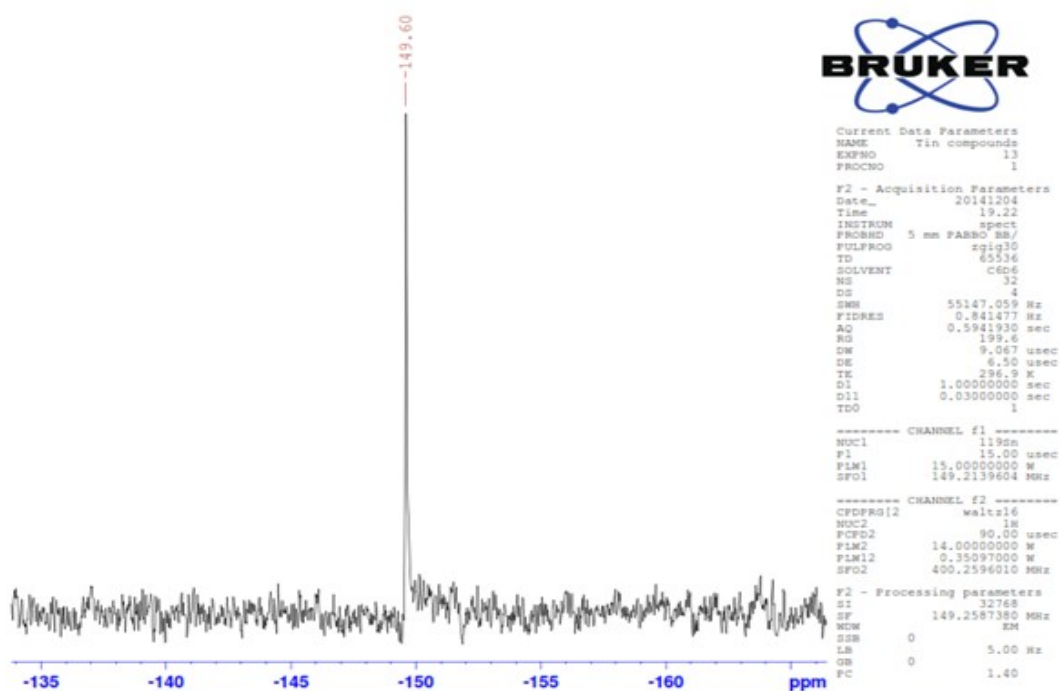


Figure S7. ^{119}Sn NMR spectrum of $[(t\text{Bu})_2\text{Sn}(\text{OSi}(\text{O}^t\text{Bu})_3)_2]$ (**1**) in C_6D_6 .

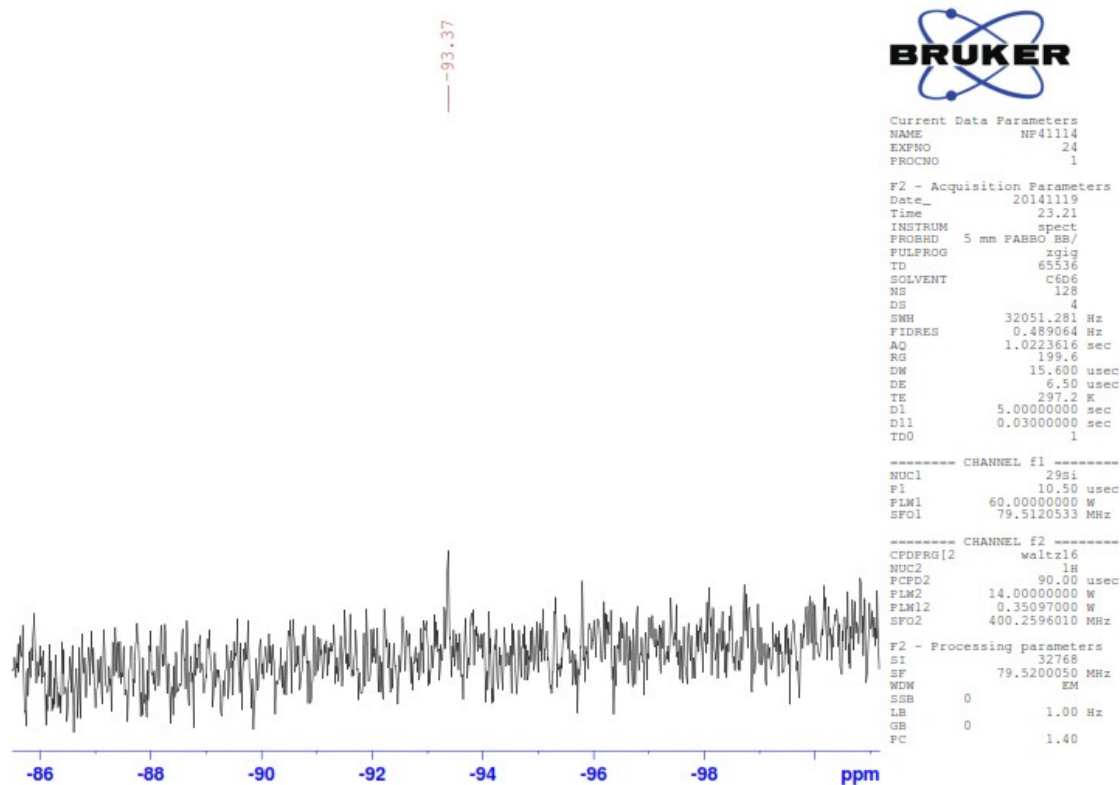


Figure S8. ^{29}Si NMR spectrum of $[(t\text{Bu})_2\text{Sn}(\text{OSi}(\text{O}^t\text{Bu})_3)\text{Cl}]$ (**2**) in C_6D_6 .

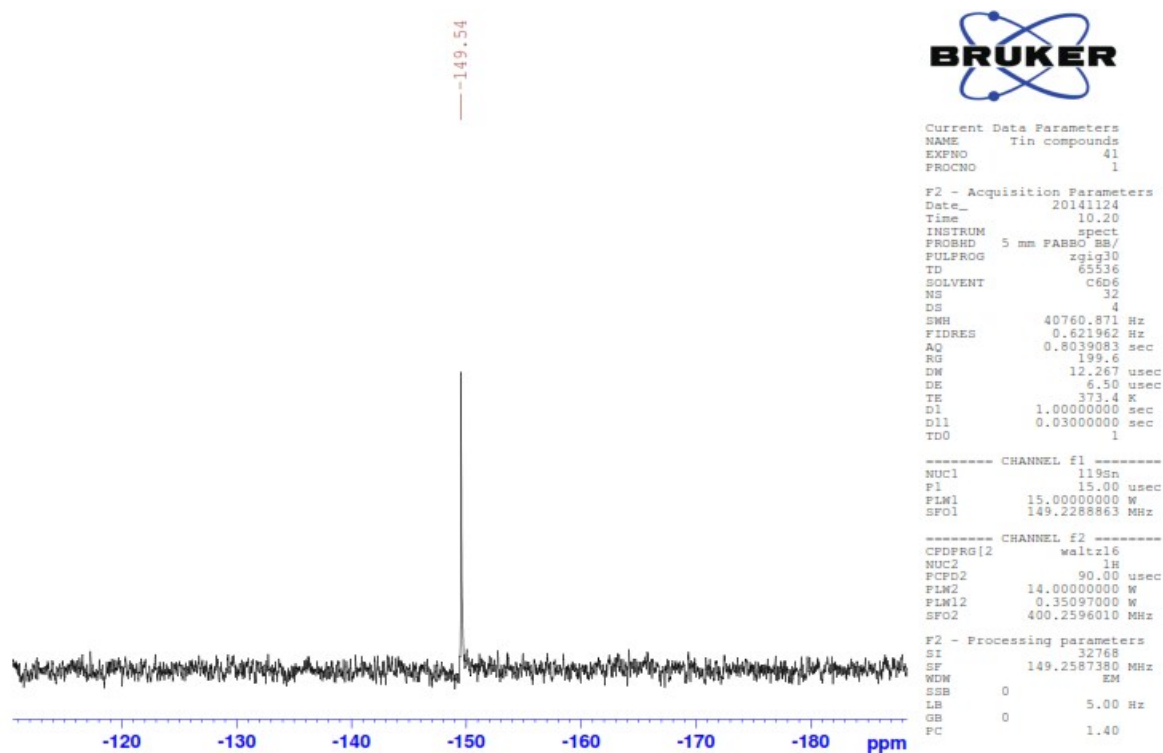


Figure S9. ^{119}Sn NMR spectrum of $[(t\text{Bu})_2\text{Sn}(\text{OSi}(\text{O}^t\text{Bu})_3)\text{Cl}]$ (**2**) in C_6D_6 .

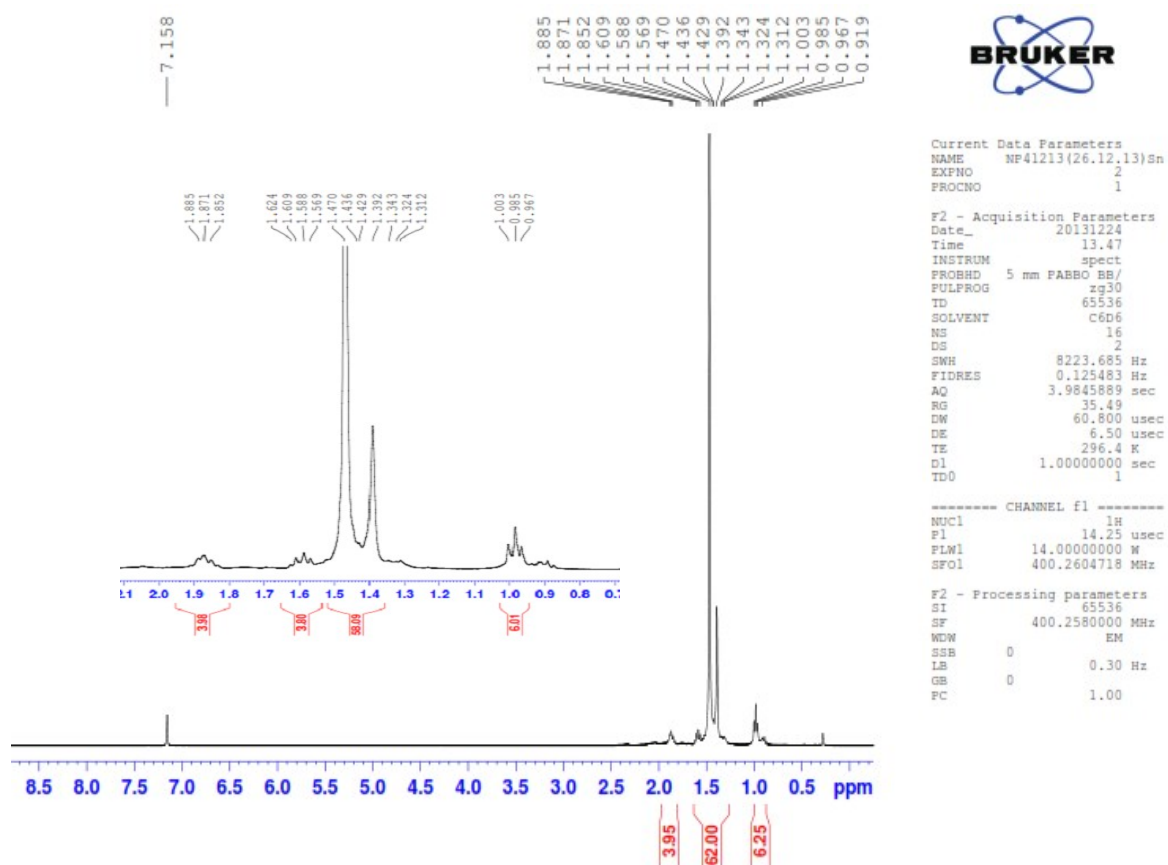


Figure S10. ^1H NMR spectrum of $[(n\text{-Bu})_2\text{Sn}(\text{OSi}(\text{O}^t\text{Bu})_3)_2]$ (**3**) in C_6D_6 .

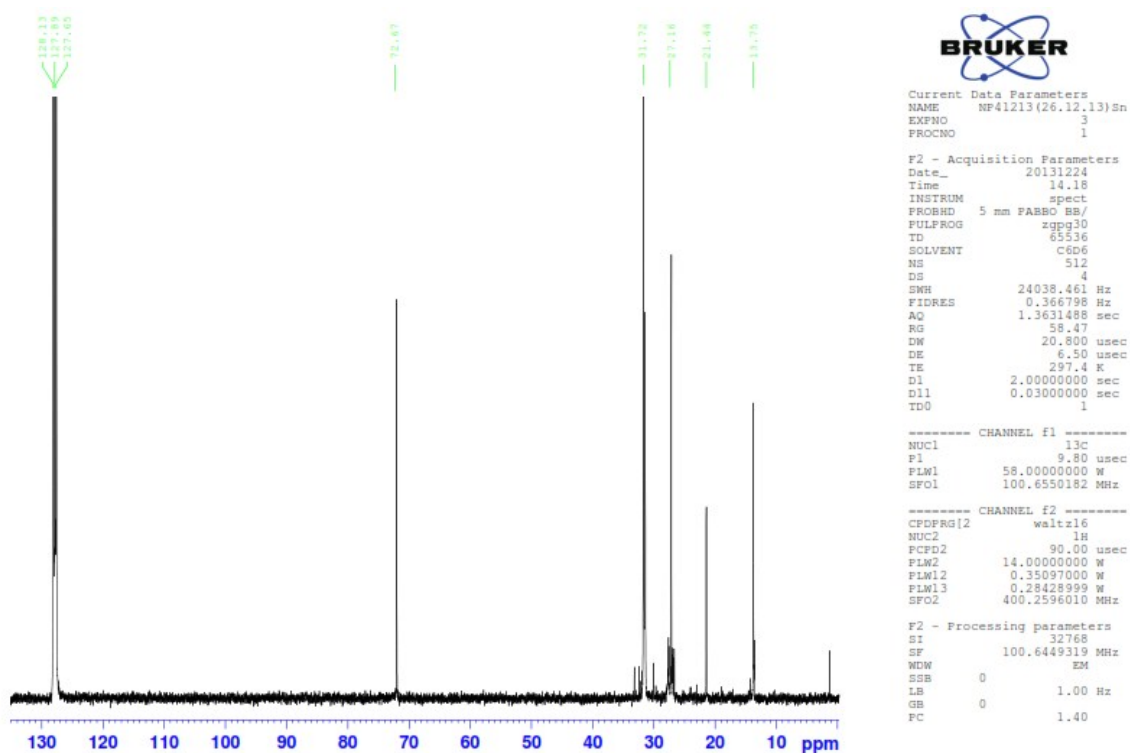


Figure S11. ^{13}C NMR spectrum of $[(n\text{-Bu})_2\text{Sn}(\text{OSi}(\text{O}^t\text{Bu})_3)_2]$ (**3**) in C_6D_6 .

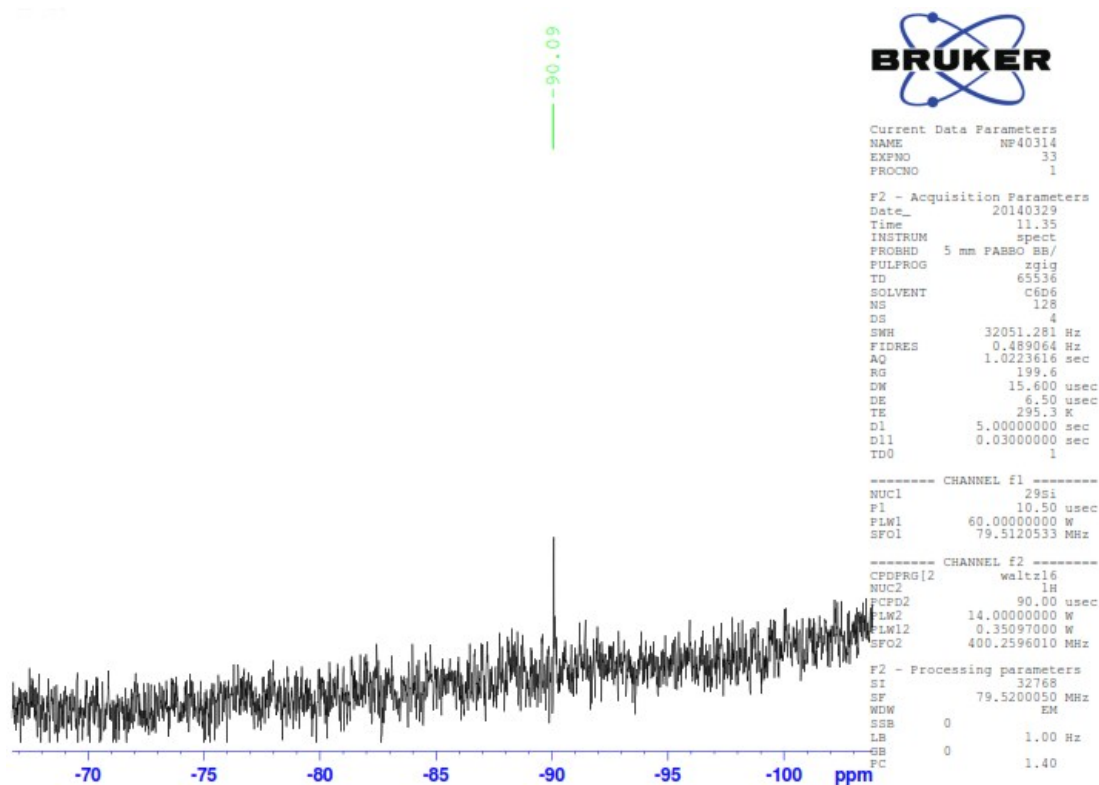


Figure S12. ^{29}Si NMR spectrum of $[(n\text{-Bu})_2\text{Sn}(\text{OSi}(\text{O}^t\text{Bu})_3)_2]$ (**3**) in C_6D_6 .

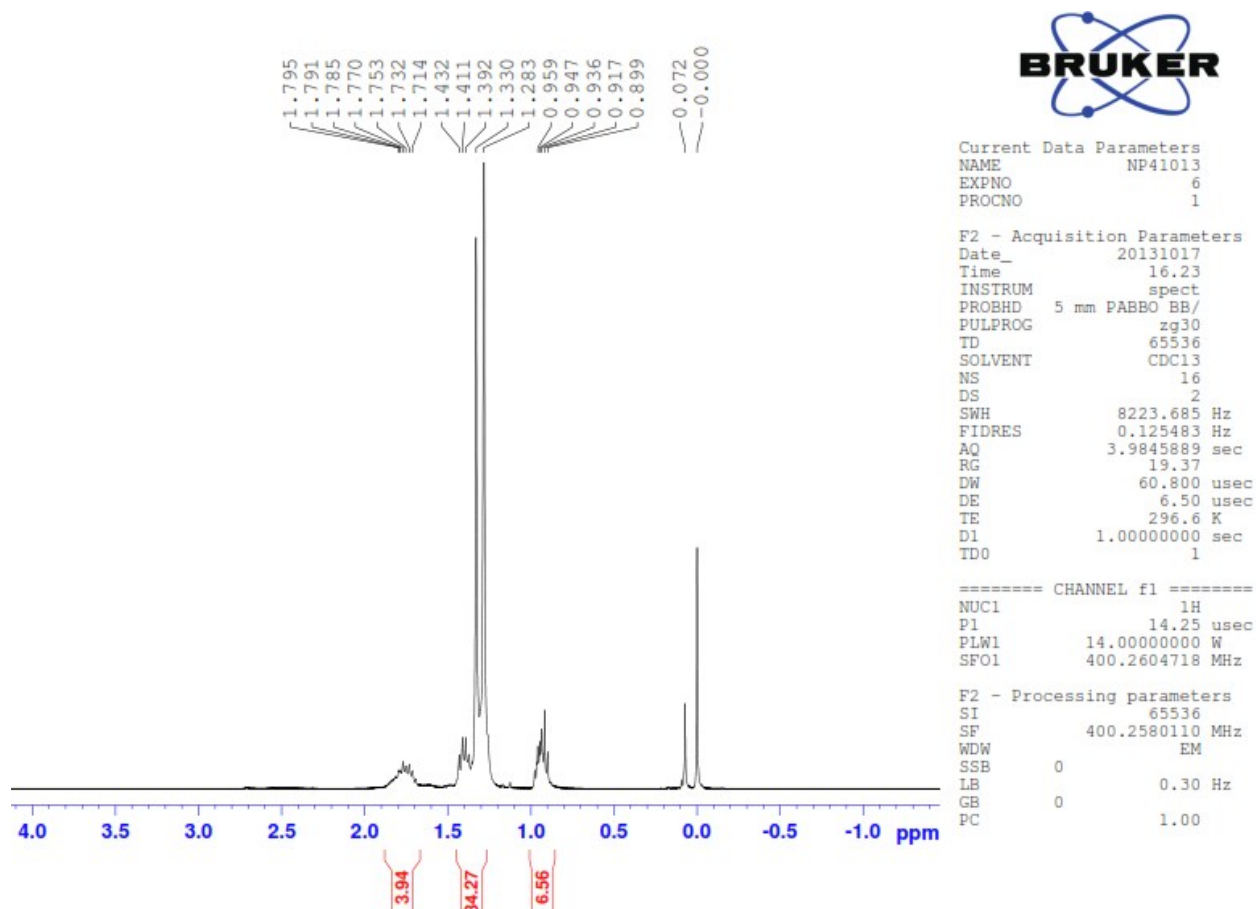


Figure S13. ^1H NMR spectrum of $[(n\text{-Bu})_2\text{Sn}(\text{OSi}(\text{O}^t\text{Bu})_3)\text{Cl}]$ (**4**) in CDCl_3 .

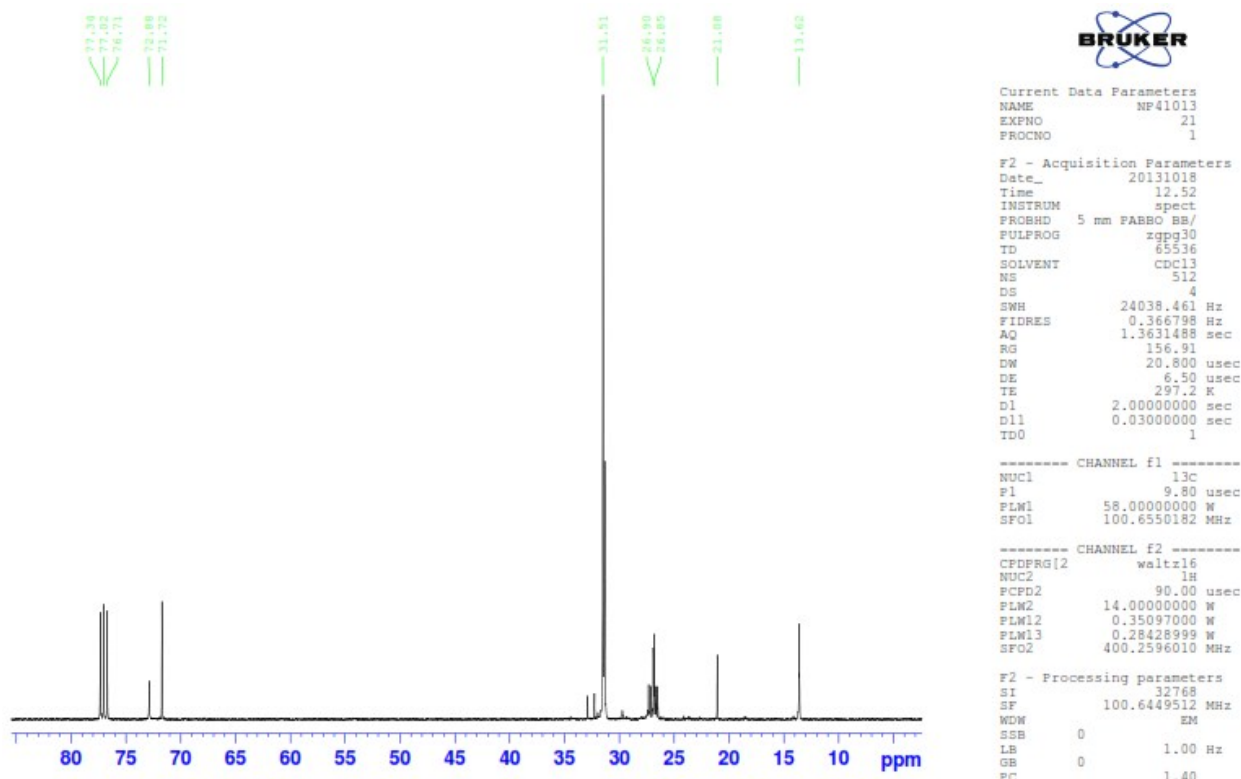


Figure S14. ^{13}C NMR spectrum of $[(n\text{-Bu})_2\text{Sn}(\text{OSi}(\text{O}^t\text{Bu})_3)\text{Cl}]$ (**4**) in CDCl_3 .

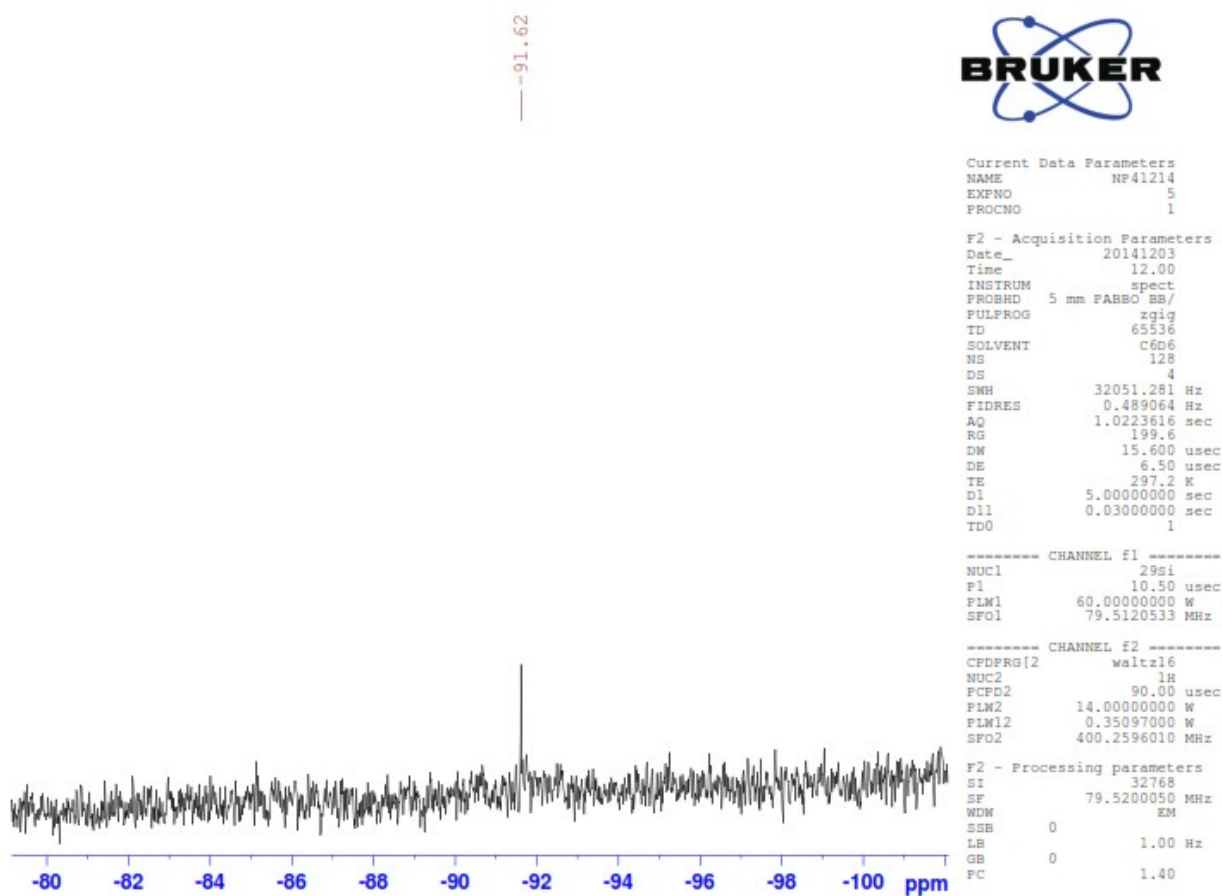


Figure S15. ^{29}Si NMR spectrum of $[(n\text{-Bu})_2\text{Sn}(\text{OSi}(\text{O}^t\text{Bu})_3)\text{Cl}]$ (**4**) in C_6D_6 .

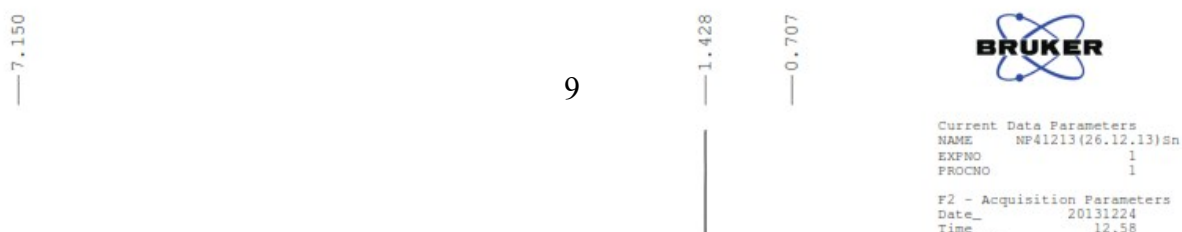
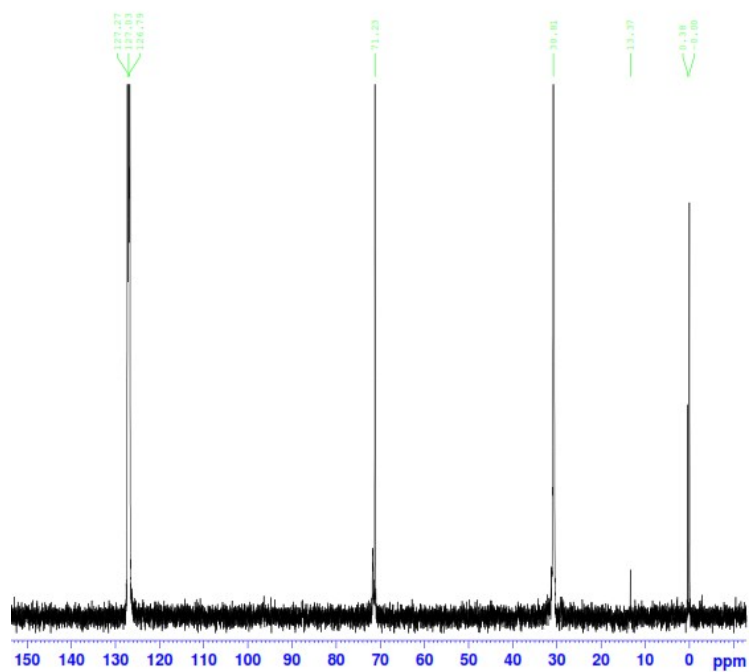


Figure S16. ¹H NMR spectrum of [(Me)₂Sn(OSi(O^tBu)₃)₂] (5) in C₆D₆.



```

Current Data Parameters
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EXPNO    5
PROCNO   1

F2 - Acquisition Parameters
Date_    20131224
Time     13.29
INSTRUM  spect
PROBHD   5 mm PABBO BB/
PULPROG  zgpg30
TD       65536
SOLVENT  CDCl3
NS       512
DS       4
SWH      24038.461 Hz
FIDRES   0.366798 Hz
AQ       1.3631488 sec
RG       143.73
DM       20.800 usec
DE       6.50 usec
TE       297.4 K
D1       2.00000000 sec
D11      0.03000000 sec
TD0      1

----- CHANNEL f1 -----
NUC1     13C
P1       9.80 usec
PLM1     58.00000000 W
SFO1     100.6250182 MHz

----- CHANNEL f2 -----
CPDPRG2  waltz16
NUC2     1H
PCPD2    90.00 usec
PLM2     14.00000000 W
PLM12    0.35097000 W
PLM13    0.28428999 W
SFO2     400.2536810 MHz

F2 - Processing parameters
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SF       100.6250184 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
    
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Figure S17. ¹³C NMR spectrum of [(Me)₂Sn(OSi(O^tBu)₃)₂] (5) in C₆D₆.



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Current Data Parameters
NAME      NP41213(26.12.13)Sn
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PROCNO   1

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INSTRUM
    
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Figure S18. ^{29}Si NMR spectrum of $[(\text{Me})_2\text{Sn}(\text{OSi}(\text{O}^t\text{Bu})_3)_2]$ (**5**) in C_6D_6 .

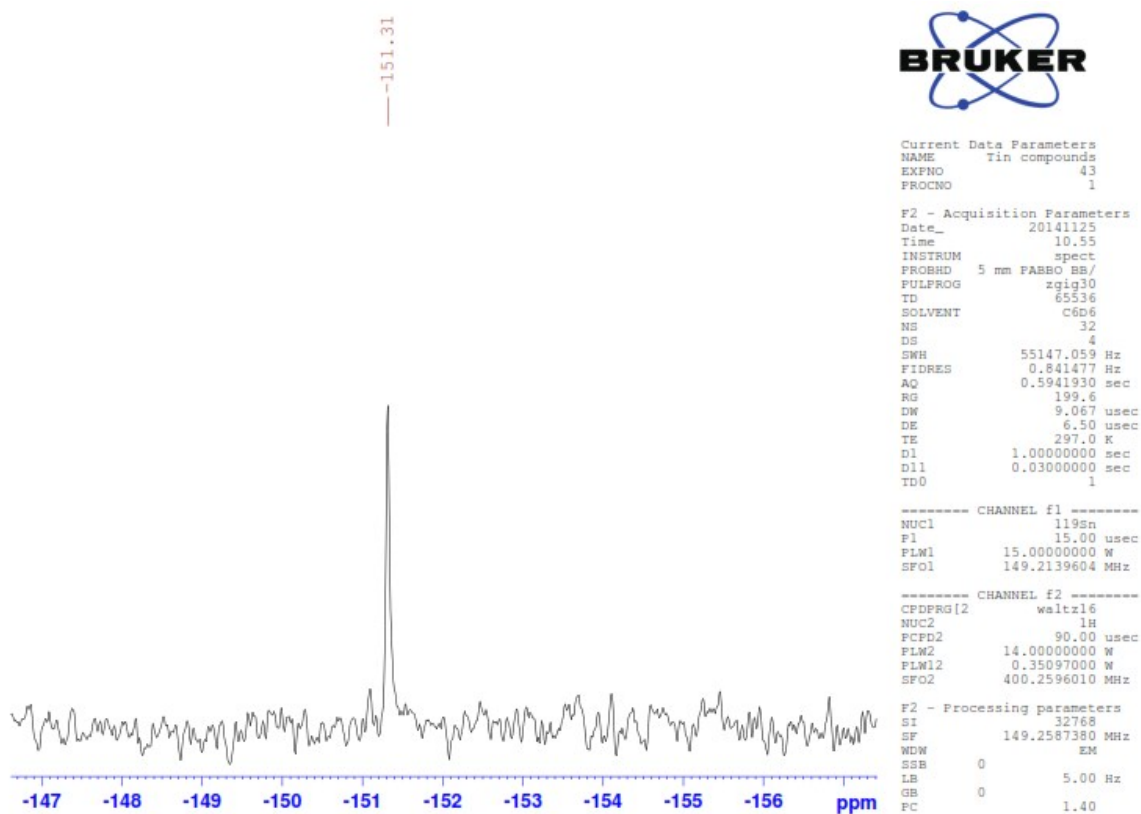


Figure S19. ^{119}Sn NMR spectrum of $[(\text{Me})_2\text{Sn}(\text{OSi}(\text{O}^t\text{Bu})_3)_2]$ (**5**) in C_6D_6 .

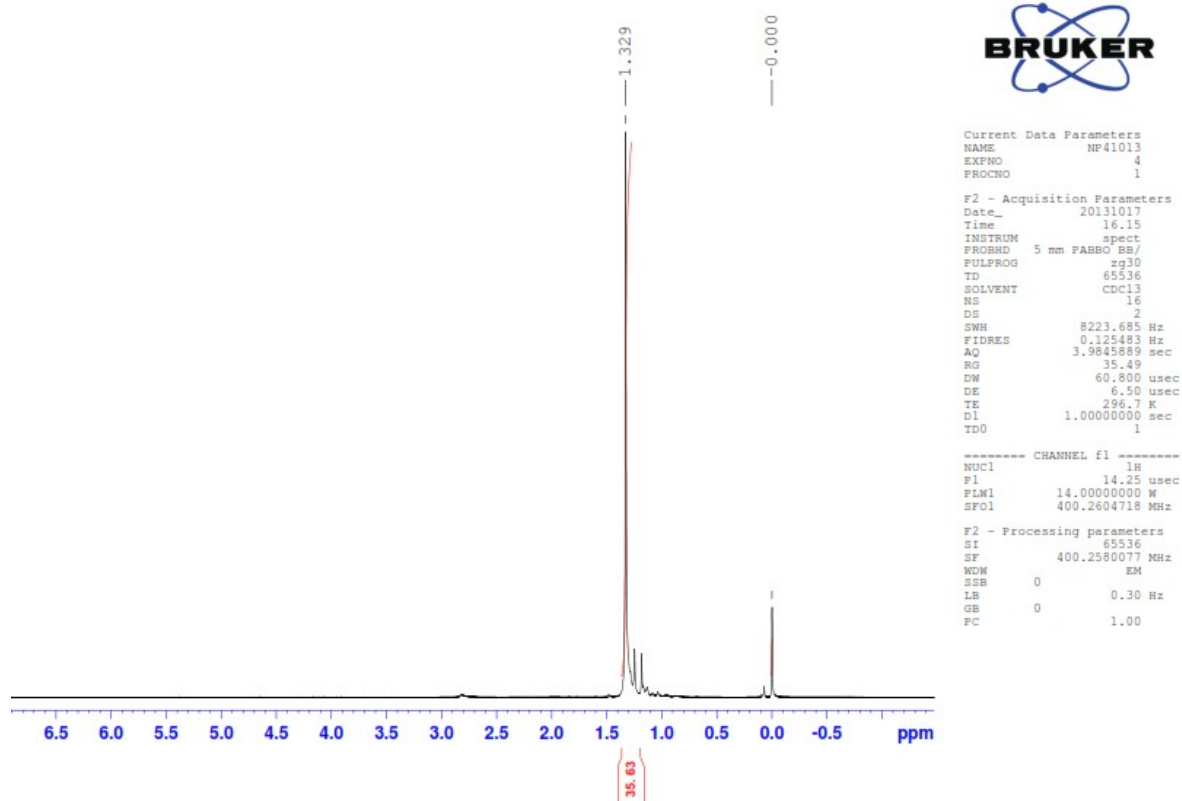


Figure S20. ^1H NMR spectrum of $[(\text{Me})_2\text{Sn}(\text{OSi}(\text{O}^t\text{Bu})_3)\text{Cl}]$ (**6**) in CDCl_3 .

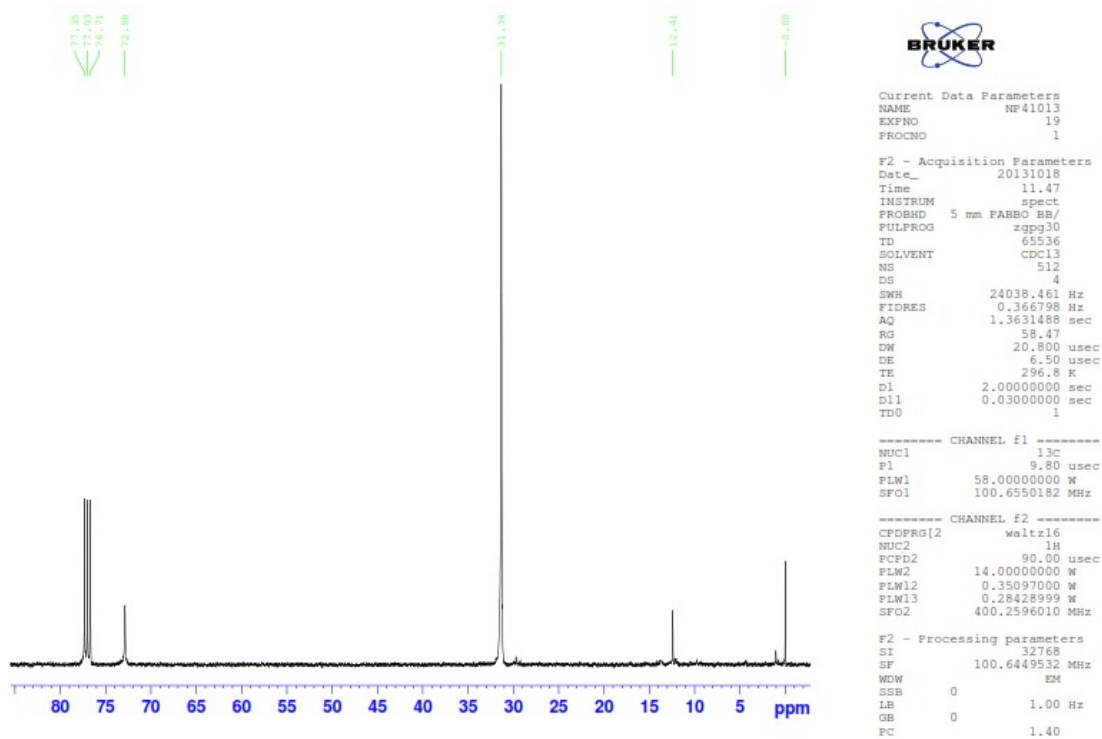


Figure S21. ^{13}C NMR spectrum of $[(\text{Me})_2\text{Sn}(\text{OSi}(\text{O}^t\text{Bu})_3)\text{Cl}]$ (**6**) in CDCl_3 .

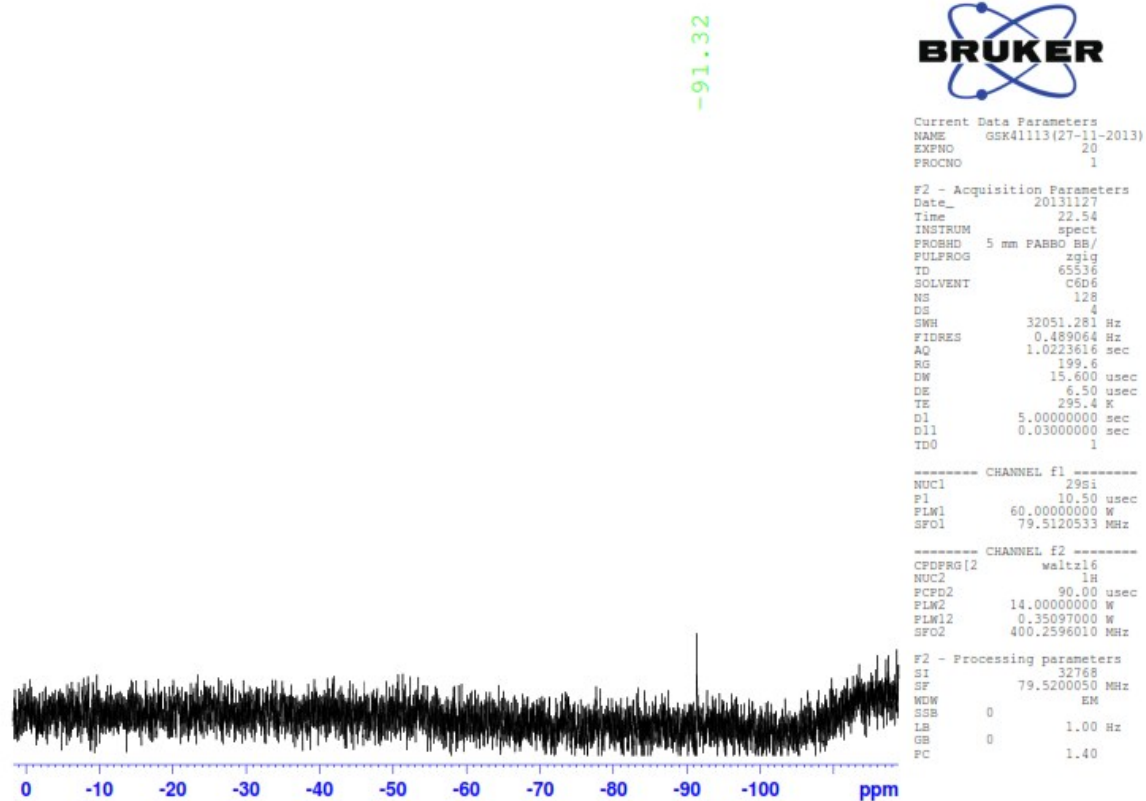


Figure S22. ^{29}Si NMR spectrum of $[(\text{Me})_2\text{Sn}(\text{OSi}(\text{O}^t\text{Bu})_3)\text{Cl}]$ (**6**) in C_6D_6 .

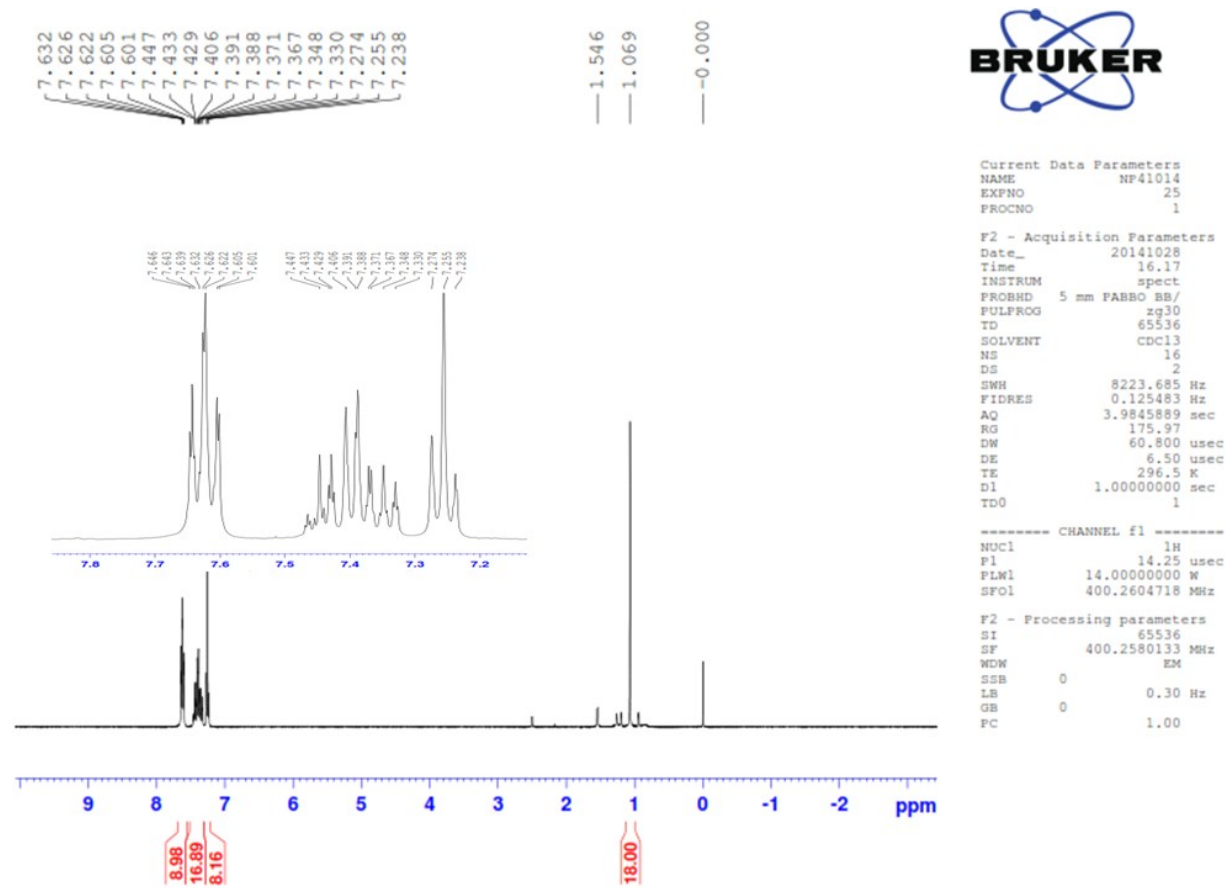


Figure S23. ^1H NMR spectrum of $[(^t\text{Bu})_2\text{Sn}(\text{OSiPh}_3)_2]$ (**7**) in CDCl_3 .

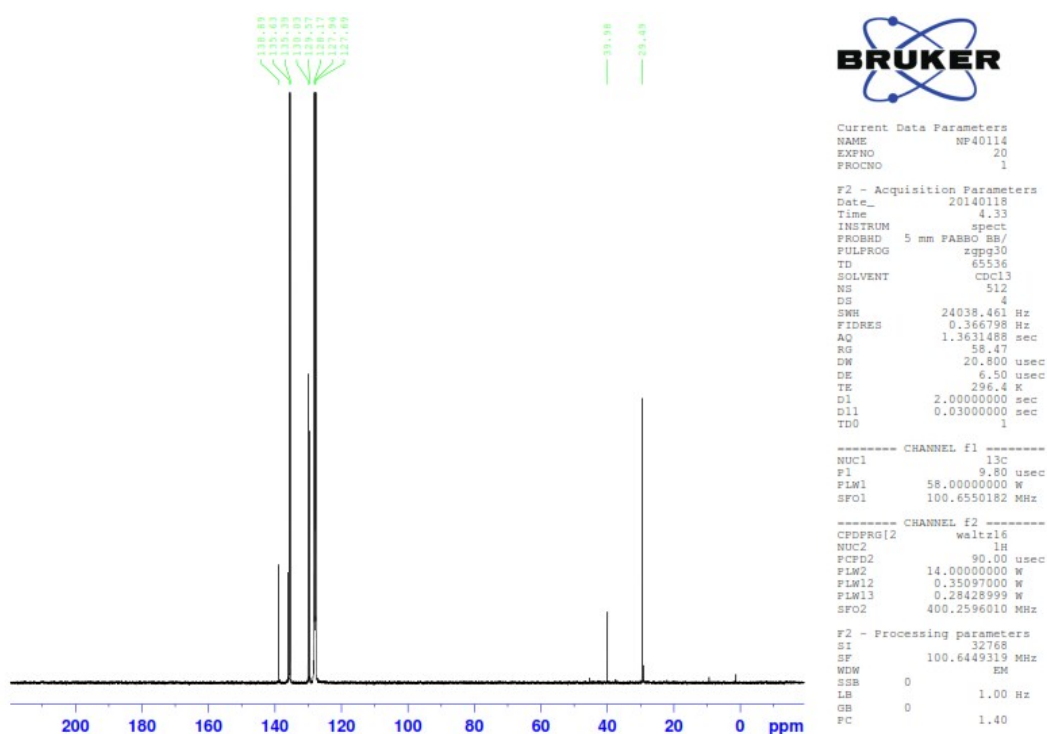


Figure S24. ^{13}C NMR spectrum of $[(t\text{Bu})_2\text{Sn}(\text{OSiPh}_3)_2]$ (**7**) in CDCl_3 .

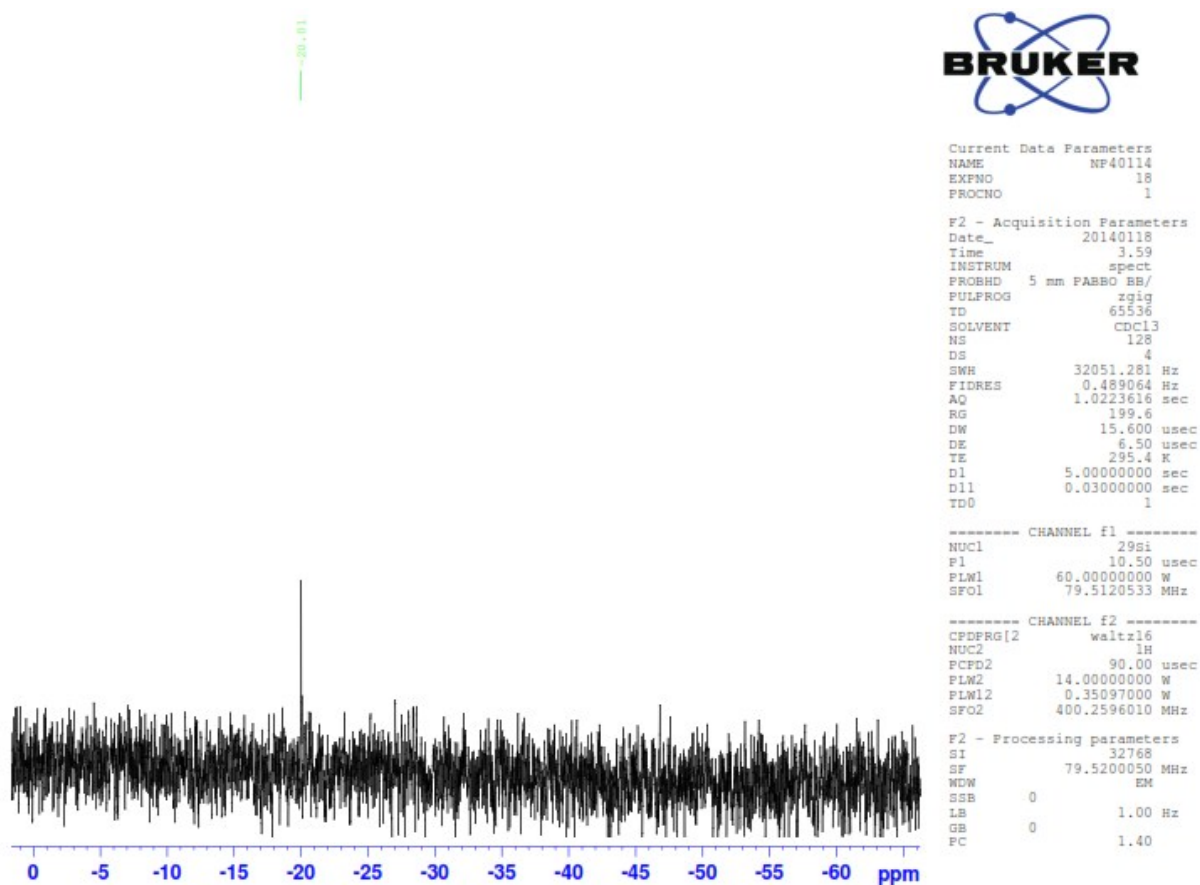


Figure S25. ^{29}Si NMR spectrum of $[(t\text{Bu})_2\text{Sn}(\text{OSiPh}_3)_2]$ (**7**) in CDCl_3 .

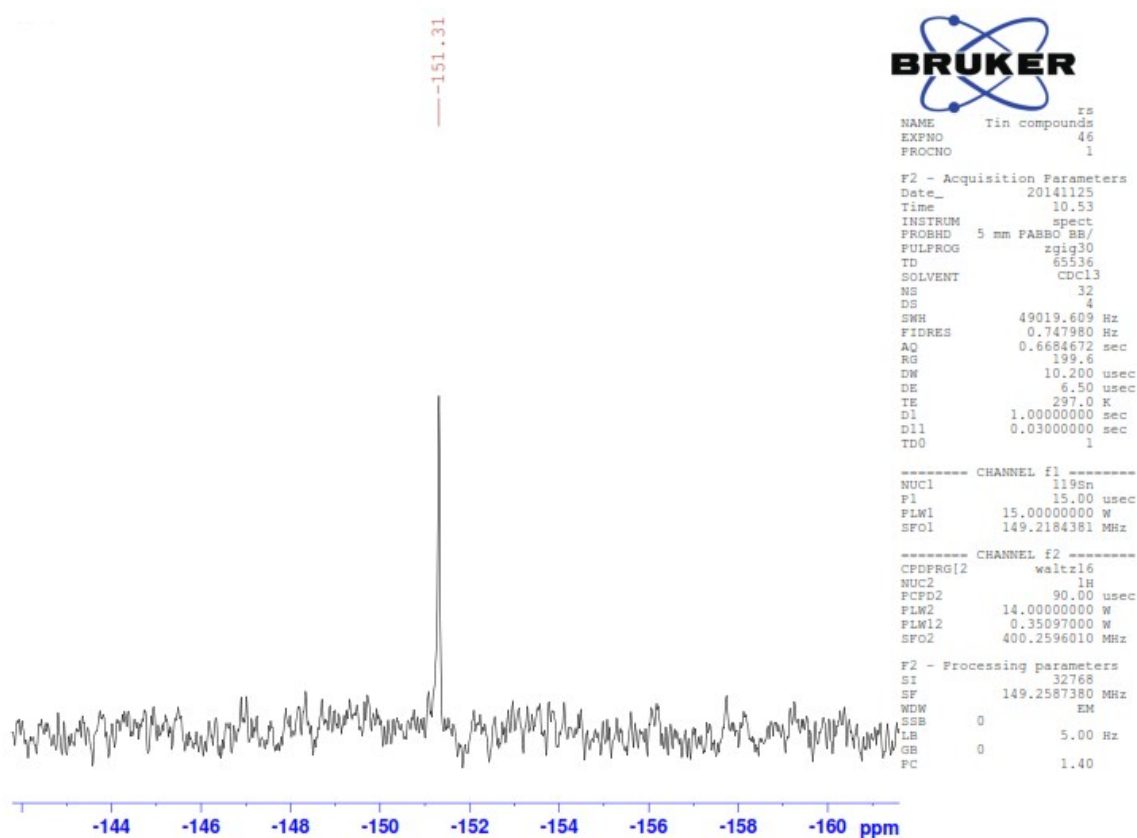


Figure S26. ^{119}Sn NMR spectrum of $[(t\text{Bu})_2\text{Sn}(\text{OSiPh}_3)_2]$ (**7**) in CDCl_3 .

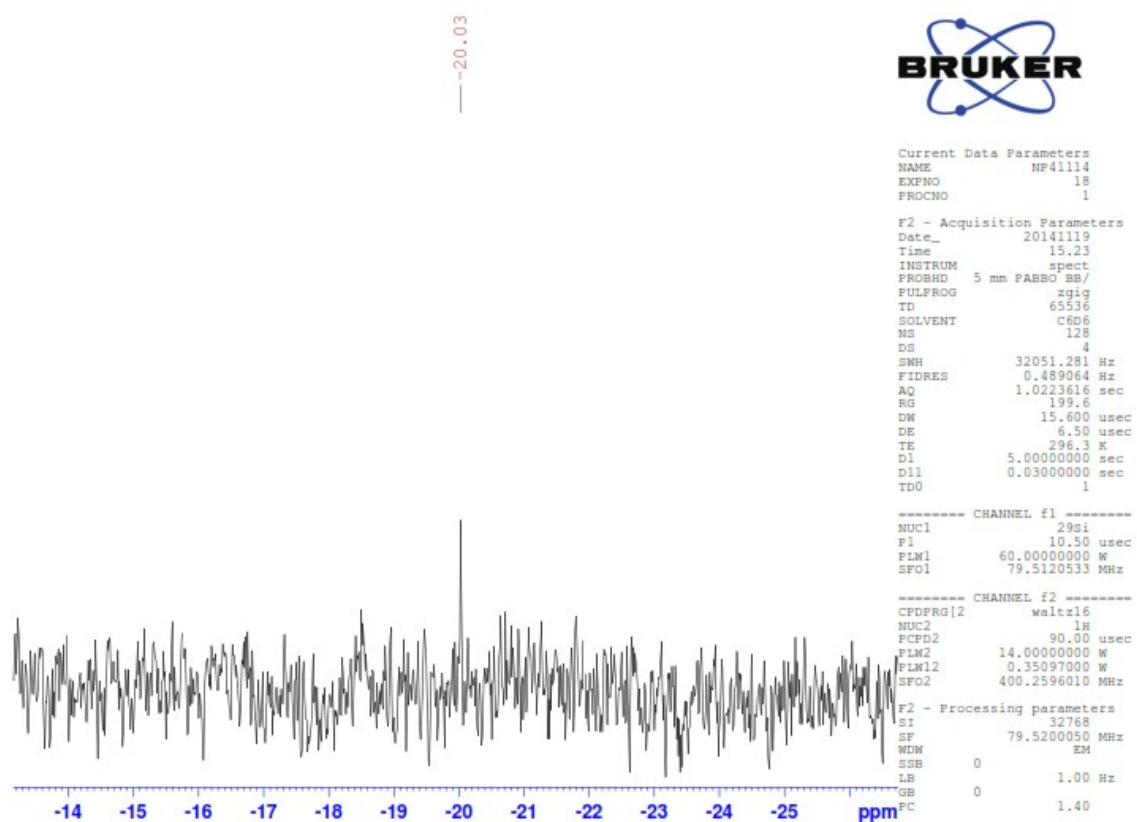


Figure S27. ^{29}Si NMR spectrum of $[(t\text{Bu})_2\text{Sn}(\text{OSiPh}_3)\text{Cl}]$ (**8**) in C_6D_6 .

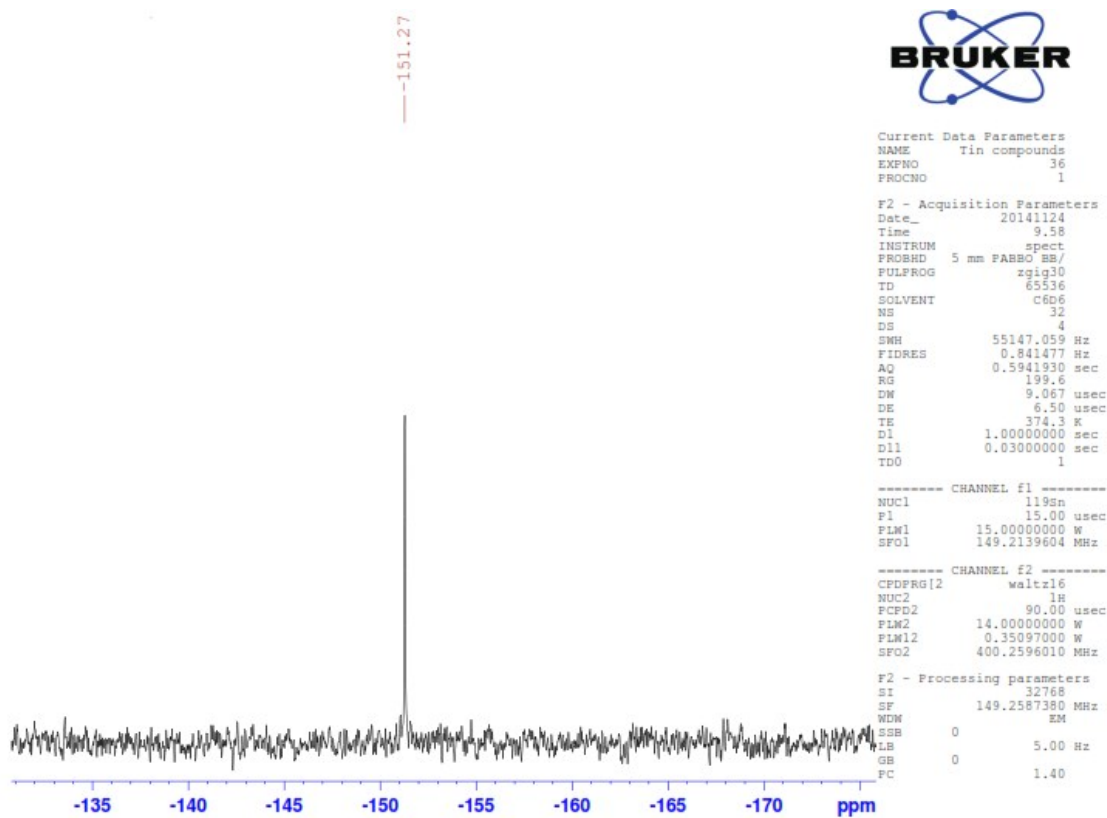


Figure S28. ^{119}Sn NMR spectrum of $[(t\text{Bu})_2\text{Sn}(\text{OSiPh}_3)\text{Cl}]$ (**8**) in C_6D_6 .

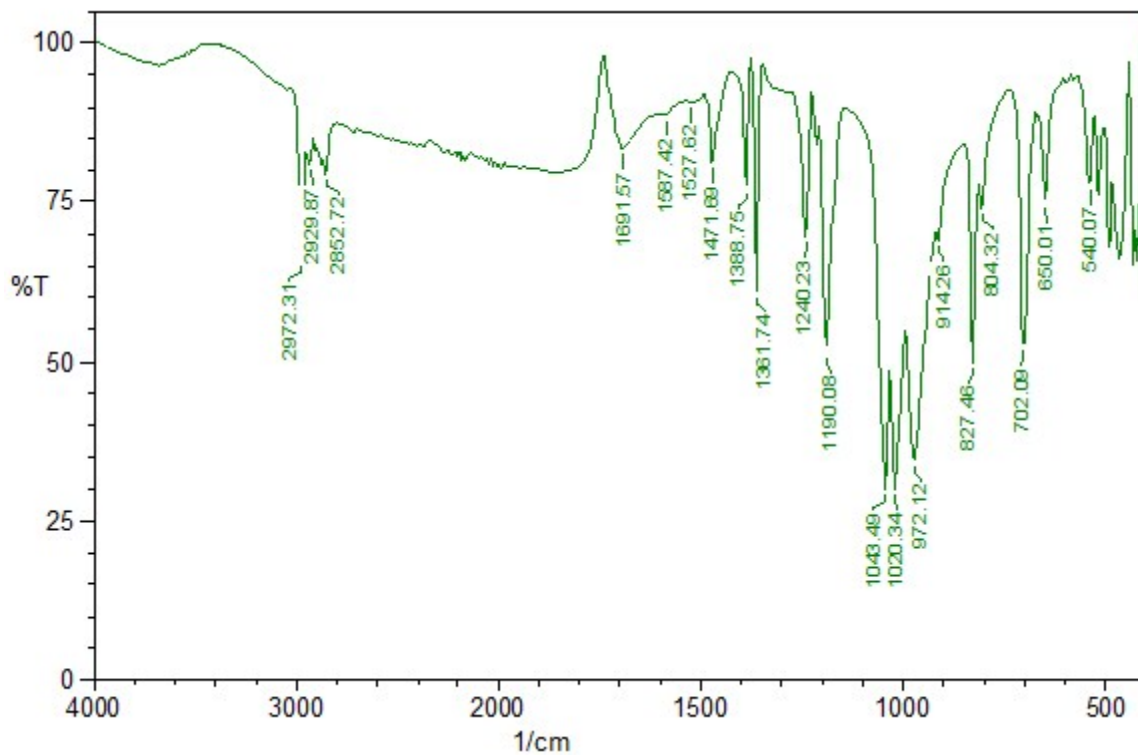


Figure S29. FT-IR spectrum of $[(t\text{Bu})_2\text{Sn}(\text{OSi}(t\text{Bu})_3)_2]$ (**1**).

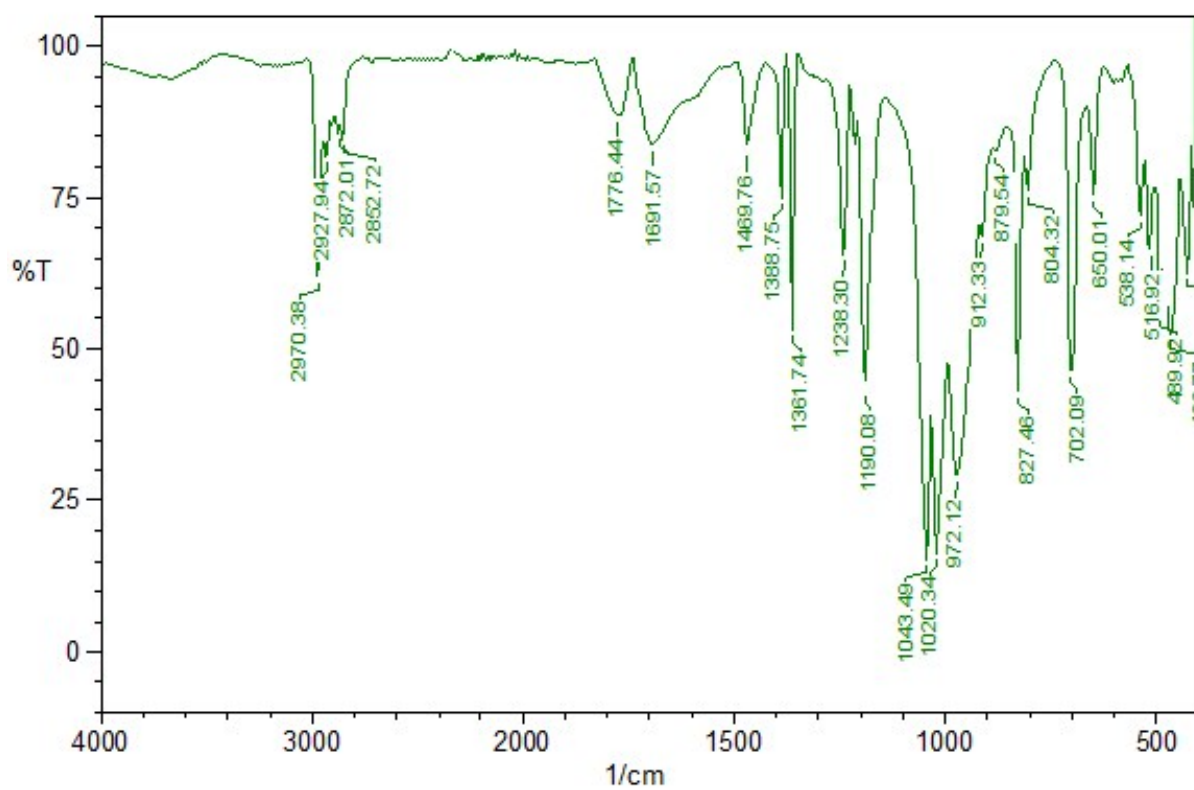


Figure S30. FT-IR spectrum of $[(n\text{-Bu})_2\text{Sn}(\text{OSi}(\text{O}^t\text{Bu})_3)_2]$ (**3**)

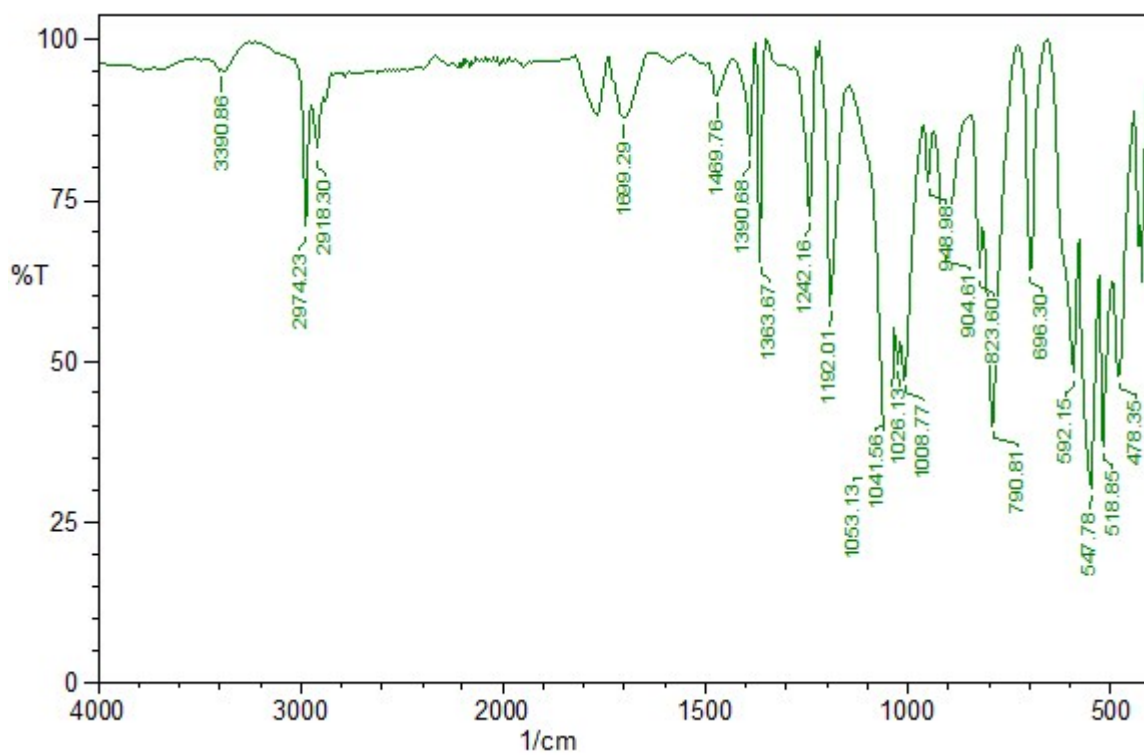


Figure S31. FT-IR spectrum of $[(\text{Me})_2\text{Sn}(\text{OSi}(\text{O}^t\text{Bu})_3)_2]$ (**5**).

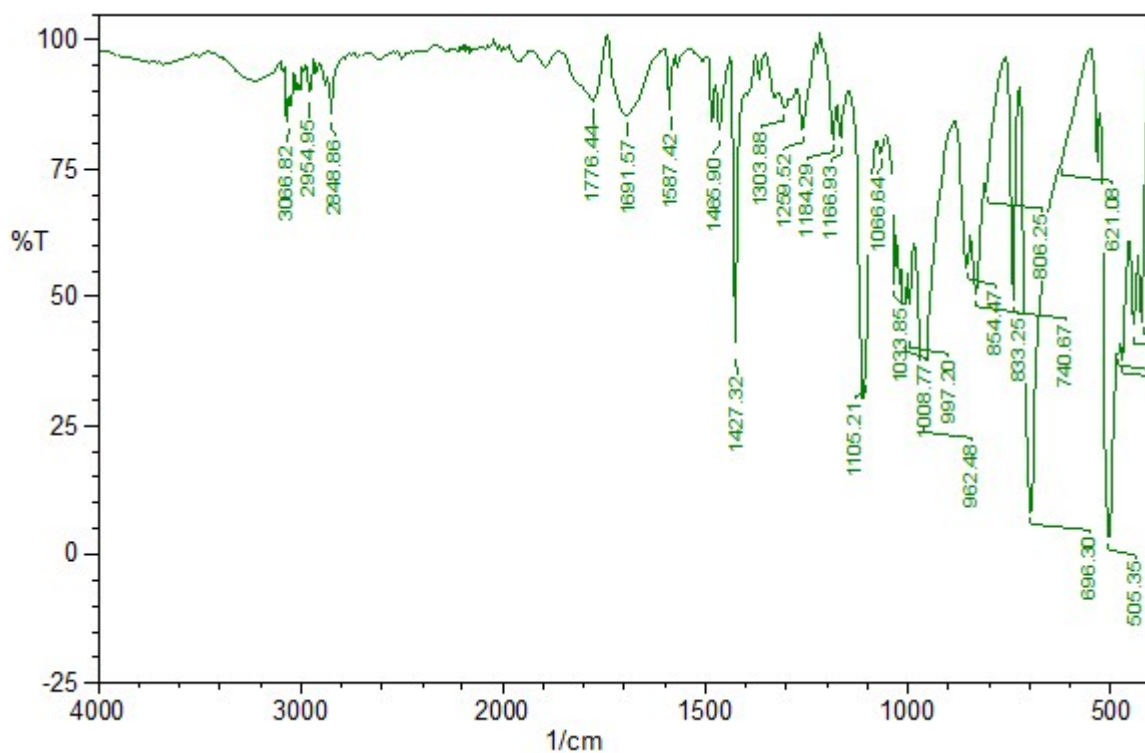


Figure S32. FT-IR spectrum of $[(t\text{Bu})_2\text{Sn}(\text{OSiPh}_3)_2]$ (**7**)

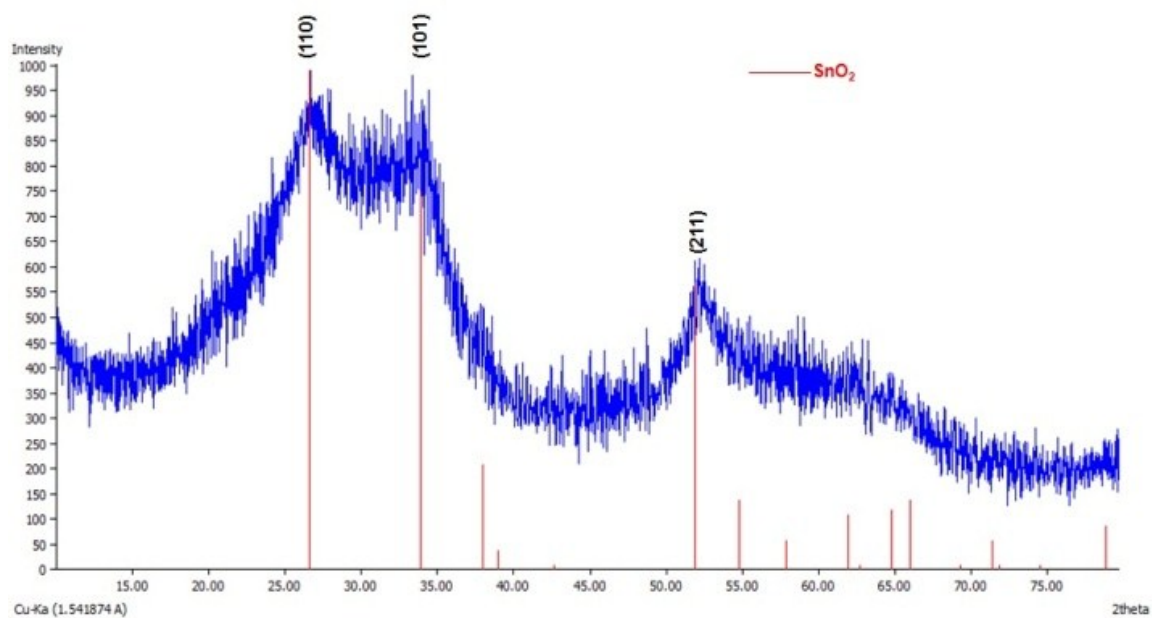


Figure S33. Powder XRD patterns of the tinsilicate material obtained from degradation of **1**.

References

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