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Electronic Supplementary Information

Bis(pentafluorophenyl)phenothiazylborane – An Intramolecular Frustrated Lewis Pair Catalyst for Stannane Dehydrocoupling

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1 General Considerations & Procedures

All manipulations were performed using an MBraun LABstar Glove Box Workstation under N_2 atmosphere or by employing Schlenk techniques. All glassware was oven-dried at 110 °C before being transferred into the glove box. Solvents were prepared from an MBraun MB-SPS 800 solvent drying system under N_2 atmosphere. Commercially available reagents were purchased from either Sigma-Aldrich, TCI Chemicals, or Oakwood Chemicals and employed without further purification; unless otherwise stated. Chloroform-*d* and benzene-d_6 were transferred to Strauss flasks and dried over activated molecular sieves, then degassed using freeze-pump-thaw technique, followed by immediate transfer to the glovebox. Experiments monitored by NMR spectrum were conducted in NMR spectrum tubes (8" x 5 mm) sealed with standard plastic caps and wrapped with Parafilm or J-young screw cap. ^{1}H, ^{11}B, $^{13}C\{^{1}H\}$, and $^{19}F\{^{1}H\}$, and $^{31}P\{^{1}H\}$ NMR spectrum spectra were acquired at 25 ^{o}C on either a Bruker 700 MHz, Bruker DRX 600 MHz , Bruker ARX 400 MHz, or Bruker ARX 300 MHz Spectrometers. Chemical shifts are reported relative to $SiMe_4$ and referenced to the residual solvent signal (^{1}H, $^{13}C\{^{1}H\}$) of $CDCl_3$ (δ 7.26, 77.16 ppm) or C_6D_6 (δ 7.16, 128.06 ppm). ^{11}B and $^{19}F\{^{1}H\}$ NMR spectrum spectra were referenced relative to 15% BF_3-Et_2O. $^{31}P\{^{1}H\}$ NMR spectrum spectra were referenced relative to H_3PO_4. NMR spectrum spectra were analyzed using either TopSpin 4.0.1 or MestReNova 12.0.3-21384 software. Chemical shifts are reported in ppm and coupling constants as scalar values in Hz. The conventional abbreviations were used as follows: s (singlet), d (doublet), dt (doublet of triplets), t (triplet), q (quartet), dd (doublet of doublets), m (multiplet), br (broad). Absorption measurements were recorded with a Cary 5000 UV-Vis-NIR Spectrophotometer from Agilent Technologies. Recordings were obtained at 25 ^{o}C and taken with the instrument operating in single beam mode and referenced to toluene. Emission and excitation measurements were recorded with an Edinburgh Instruments FS5 fluorescence spectrometer. Emission spectra were excited at their respective absorption maxima. All absorption and fluorescence experiments were conducted in quartz cuvettes (1 cm x 1 cm) equipped with a Teflon seal.

2 Synthesis

Tris(pentafluorophenyl)borane: To a Schlenk flask of bromopentafluorobenzene (16.2704 g, 65.88 mmol) in diethylether (150 mL) at -78 °C, EtMgBr (3 M)(21.96 mL, 65.88 mmol) in diethylether was added dropwise. The solution was warmed to -50 °C and allowed to stirr for 4 hrs. The mixture was then cannula transferred to a schlenk flask of BF_3OEt_2 (3.1168 g, 2.71 mmol) in Et_2O (200 mL); the solution was stirred at room temperature for 8 hrs. The solvent was removed *in vacuo*, and the precipitate was vacuum filtered and thoroghly washed with pentanes. The solvent of the filtrate was removed *in vacuo* to yield the etherate adduct as a crude off-white powder. The powder was sublimed to yield the target product as a white crystalline powder. Yield 7.7676 g (69.1 %). **^{11}B NMR** (128 MHz, $CDCl_3$) δ 59.6 (br, s). **^{19}F NMR** (377 MHz, $CDCl_3$) δ -127.72 (dt, *J* = 6.5, 20.3 Hz, 2F), -142.45 (tt, 1F), -159.85 (tt, *J* = 6.0, 20.2 Hz, 2F).

Bis(pentafluorophenyl)borane: To a Schlenk flask of $B(C_6F_5)_3$ (7.6808 g, 15.00 mmol) in toluene (75 mL) , Et_3SiH (1.7445 g, 15.00 mmol) was added. The flask was sealed, then heated to 50 °C and stirred for 5 days. The flask was cooled to room temperture, resulting in a clear crystallined precipitate, which was vacuum filtered and washed with cold toluene and pentanes to yield the target product as a white crystalline powder. Yield 3.1069 g (59.9 %). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 4.10 (br, s, B-H). **^{11}B NMR** (128 MHz, $CDCl_3$) δ 19.43. **^{19}F NMR** (377 MHz, $CDCl_3$) δ -132.27 (d, *J* = 14.4 Hz, 2F), -147.21 (t, *J* = 20.2 Hz, 1F), -158.89 (td, *J* = 7.6, 20.9 Hz, 2F).

Bis(pentafluorophenyl)chloroborane: To a Schlenk flask of bis(pentafluorophenyl)borane (2.0132 g, 5.82 mmol) in toluene (50 mL), triphenylmethylchloride (1.622 g, 5.82 mmol) in toluene (20 mL) was added dropwise. The solution was stirred at room temperautre for 24 hrs. The solvent was removed *in vacuo*, and the crude material was washed and extracted with pentanes. The solution was concentrated and the target compound was crystallized as transparent crystalls followed by the removal of the remaining solution. The crystalls were carefully dried *in vacuo*. Yield 1.357 g (61.3%). **^{11}B NMR** (128 MHz, C_6D_6) δ: 58.33. **^{19}F NMR** (377 MHz, C_6D_6) δ: -129.24 (m, 2F), -144.35 (m, 1F), -160.92 (m, 2F).The data was in agreement with literature.[1]

N-Methyl-Phenothiazine: Sodium hydride (0.5637 g, 23.49 mmol) was added to 250 mL Schlenk flask charged with phenothiazine (2.8027 g, 14.07 mmol) and methyl iodide (3.993 g, 28.13 mmol) in THF (50 mL). The reaction was stirred at room temperature for 12 hrs. The reaction mixture was quenched with $HCl_{aq.}$, followed by the addition of DCM (100 mL). The organic material was extracted in DCM and the solvent was removed *in vacuo* to yield a crude brown solid. The crude was purified by flash silica chromatography (hexanes) to afford the product as a white powder. Yield 2.7359 g (91.2 %). The data was in agreement with literature.[2]

10-(dimesitylboraneyl)-phenothiazine: Sodium hydride (0.1700 g, 7.08 mmol) was added to a 20 mL vial of phenothiazine (0.7059 g, 3.54 mmol) in THF (10 mL). The mixture was stirred until the evolution of gas stopped. The mixture was filtered, and the solvent was removed *in vacuo* to yield a yellow precipitate. The yellow precipitate was dissolved in DCM (10 mL), to which dimesitylboron fluoride (0.9500 g, 3.54 mmol) in DCM (5 mL) was added dropwise and stirred for 16 hrs. The solvent was removed *in vacuo*, resulting in an amorphous residue that was dissolved in DCM and filtered. The solution was concentrated then triturated with MeCN to afford a white precipitate. The precipitate was vacuum filtered and rinsed with pentanes to afford the target compound as a fine white powder. Yield 1.0834 g (68.3 %). The data was in agreement with literature.[3,4]

10-(bis(perfluorophenyl)boraneyl)-phenothiazine (1): Sodium hydride (0.1 g, 4.17 mmol) was added to a 20 mL vial of phenothiazine (0.5733 g, 2.88 mmol) in THF (10 mL). The mixture was stirred until the evolution of gas stopped. The mixture was filtered, and the solvent was removed *in vacuo* to yield a yellow precipitate. The yellow precipitate was dissolved in DCM (10 mL), to which bis(pentafluorophenyl)chloroborane (1.0955 g, 2.88 mmol) in DCM (5 mL) was added dropwise and stirred for 16 hrs. The solvent was removed *in vacuo*, resulting in an amorphous residue that was dissolved in DCM and filtered. The solution was concentrated then triturated with MeCN to afford a white precipitate. The precipitate was vacuum filtered and rinsed with pentanes to afford the target compound as a fine white powder. Crystals suitable for X-ray diffraction were obtained by the slow evaporation of dichloromethane at -35 °C. Yield 1.0259 g (65.7 %). $C_{24}H_8BF_{10}NS$ (543.19 g/mol): calcd %. C 53.07; H 1.48; N 2.58, S 5.90%; found C 53.31, H 1.42, N 2.93, S 5.78%. **^{1}H NMR** (300 MHz, C_6D_6) δ 6.97 – 7.06 (m, 4H), 6.51 – 6.63 (m, 4H). **^{11}B NMR** (128 MHz, C_6D6_6) δ 38.5. **^{13}C NMR** (101 MHz, C_6D_6) δ 146.31 (d, *J* = 243.8 Hz), 142.16, 142.15 (d, *J* = 254.6 Hz), 137.60 (d, *J* = 252.6 Hz), 132.88, 128.21, 127.22, 127.13, 124.04, 111.25. **^{19}F NMR** (282 MHz, C_6D6_6) δ -130.41 (br, m), -151.57 (t, *J* = 20.6 Hz), -161.12 (br, m).

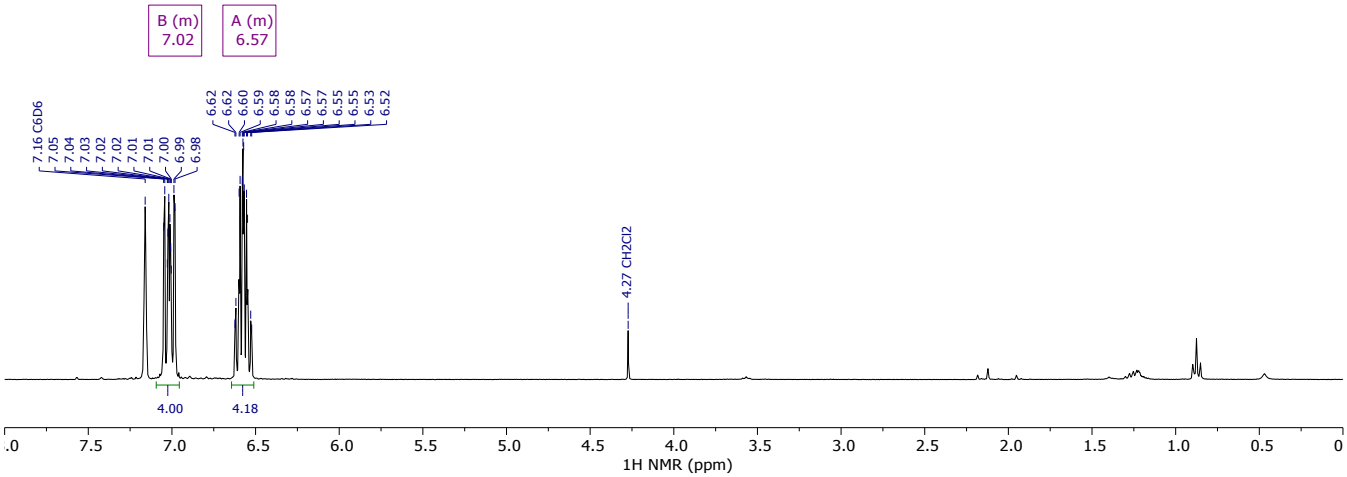

*Figure S1. ^{1}H NMR spectrum of **1** in C_6D_6.*

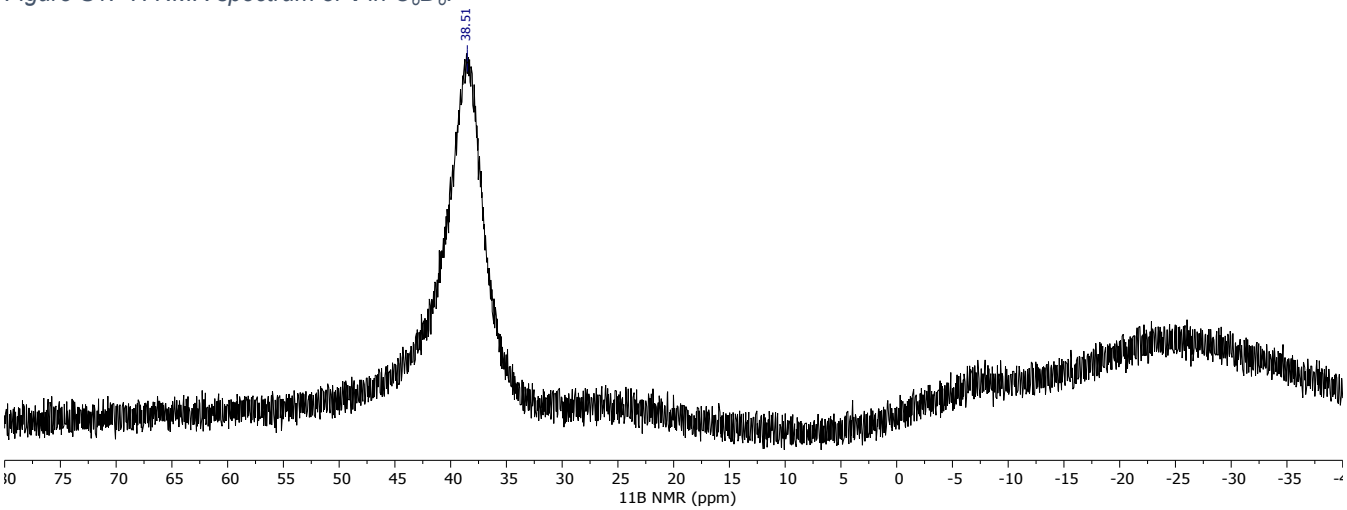

*Figure S2. ^{11}B NMR spectrum of **1** in C_6D_6.*

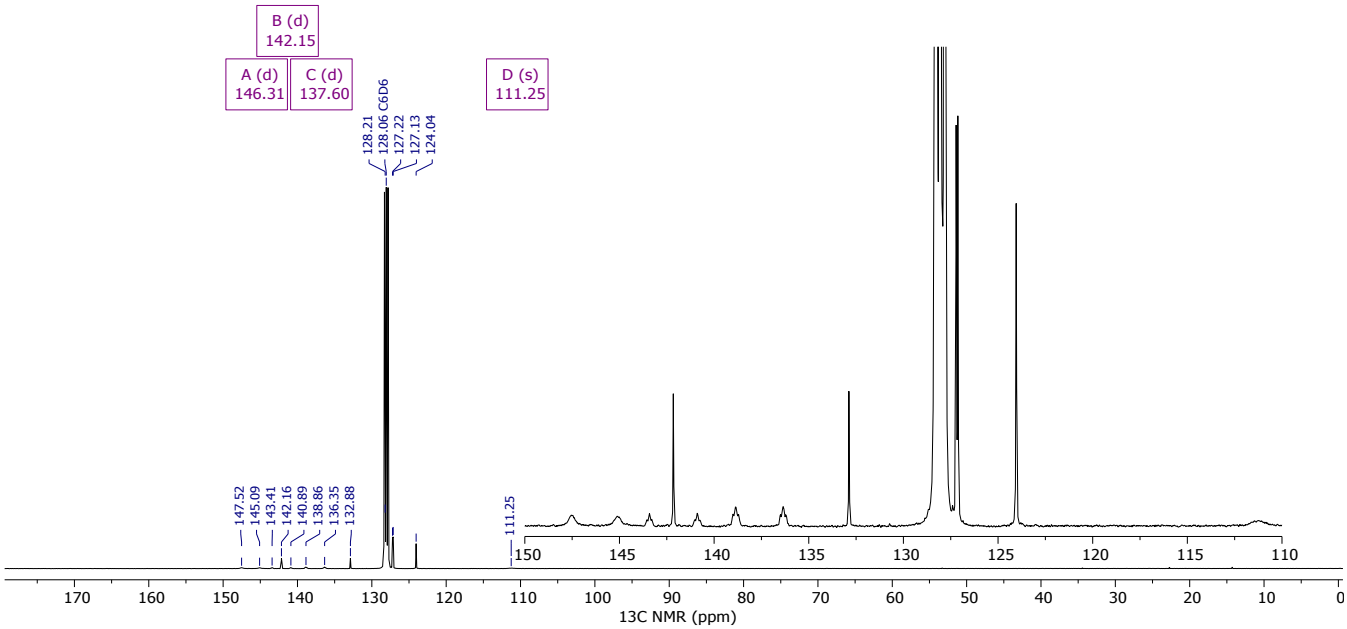

*Figure S3. ^{13}C NMR spectrum of **1** in C_6D_6.*

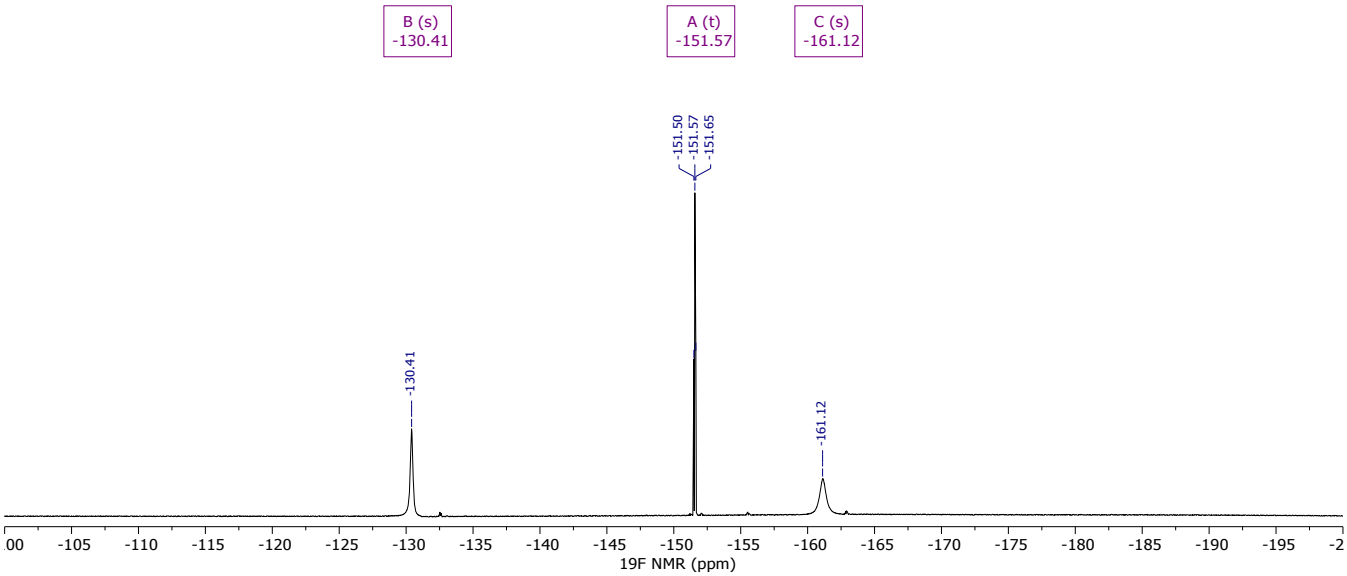

*Figure S4. ^{19}F NMR spectrum of **1** in C_6D_6.*

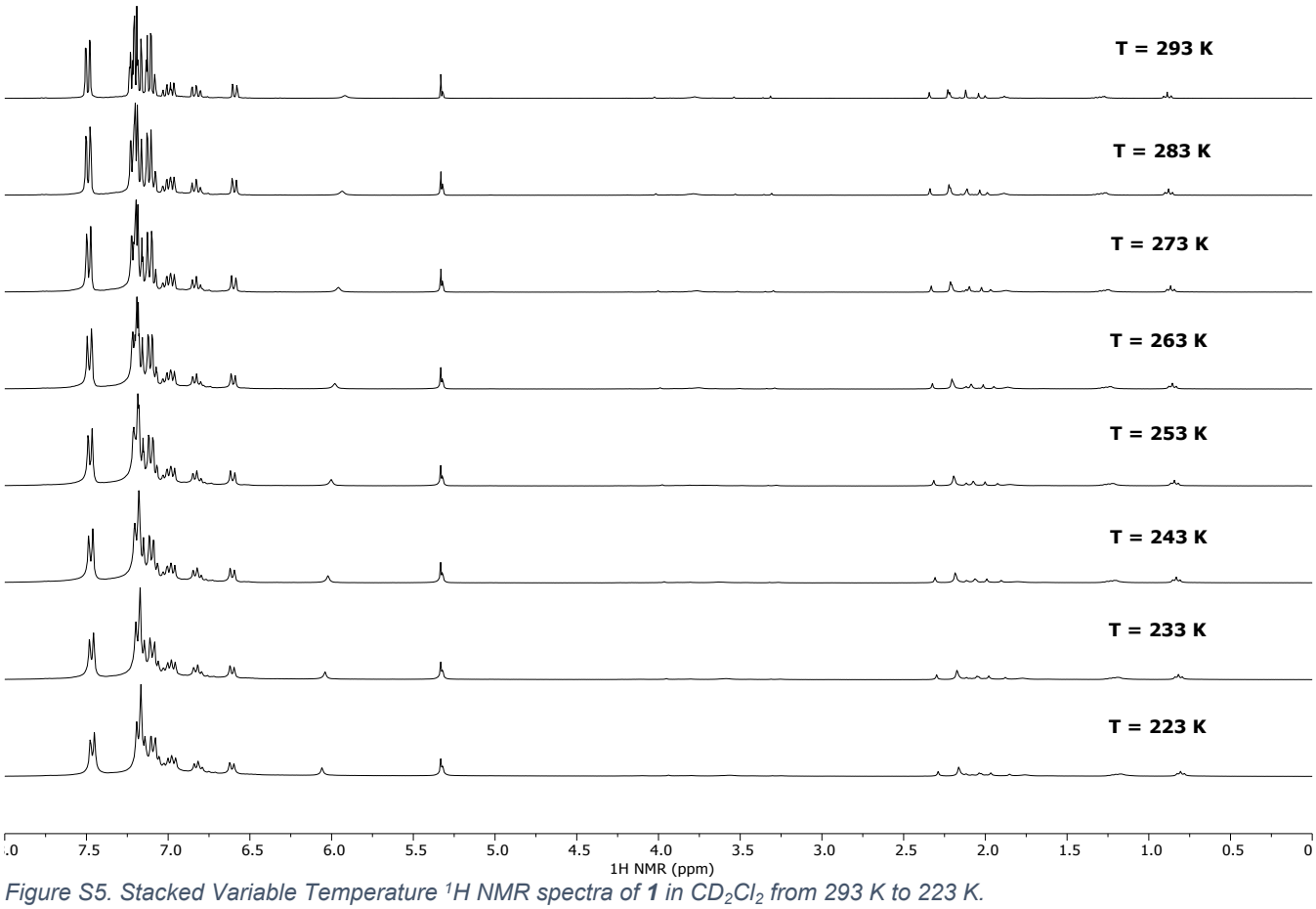

*Figure S5. Stacked Variable Temperature ^1H NMR spectra of **1** in CD_2Cl_2 from 293 K to 223 K.*

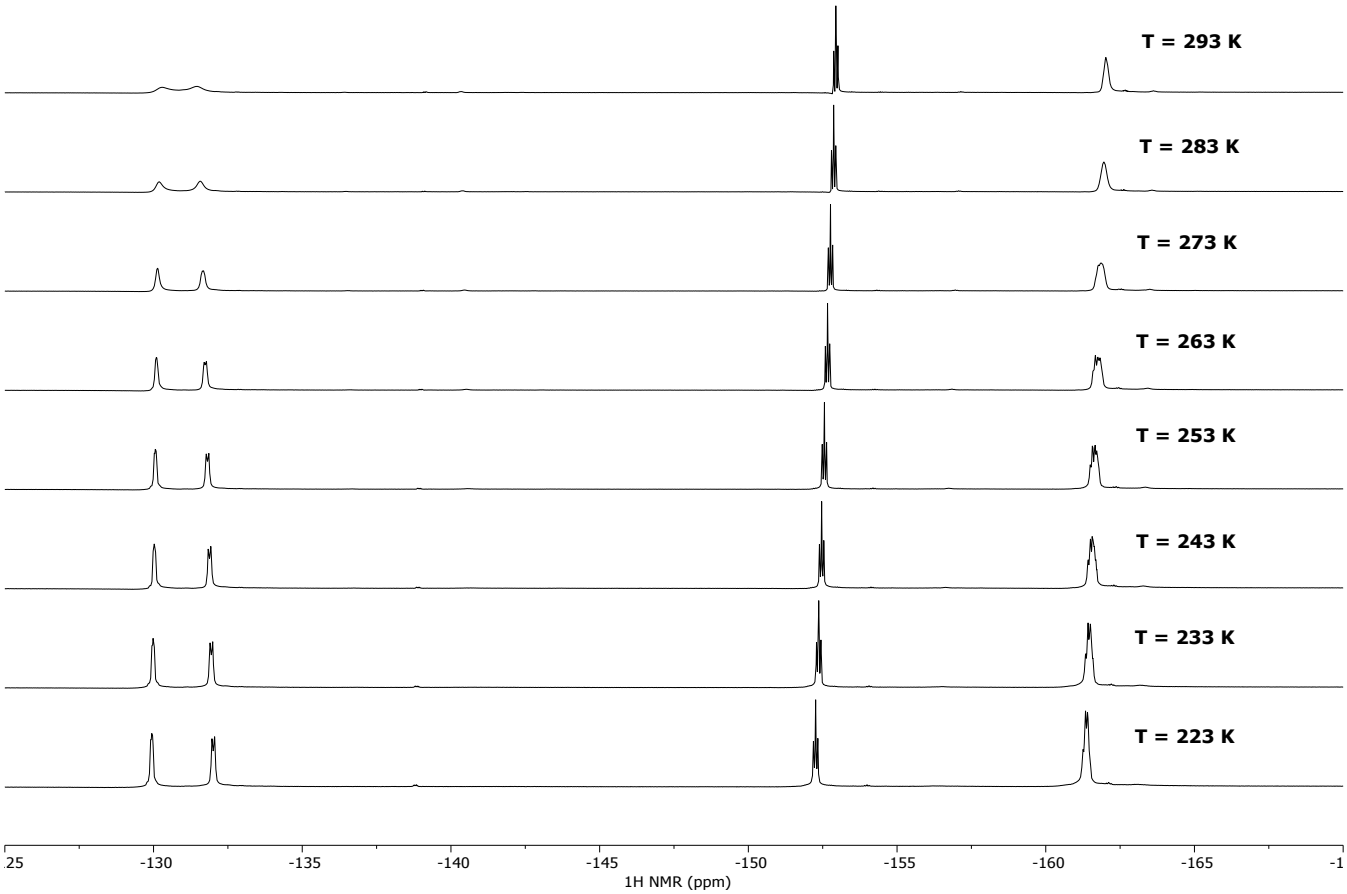

*Figure S6. Stacked Variable Temperature ^{19}F NMR spectra of **1** in CD_2Cl_2 from 293 K to 223 K.*

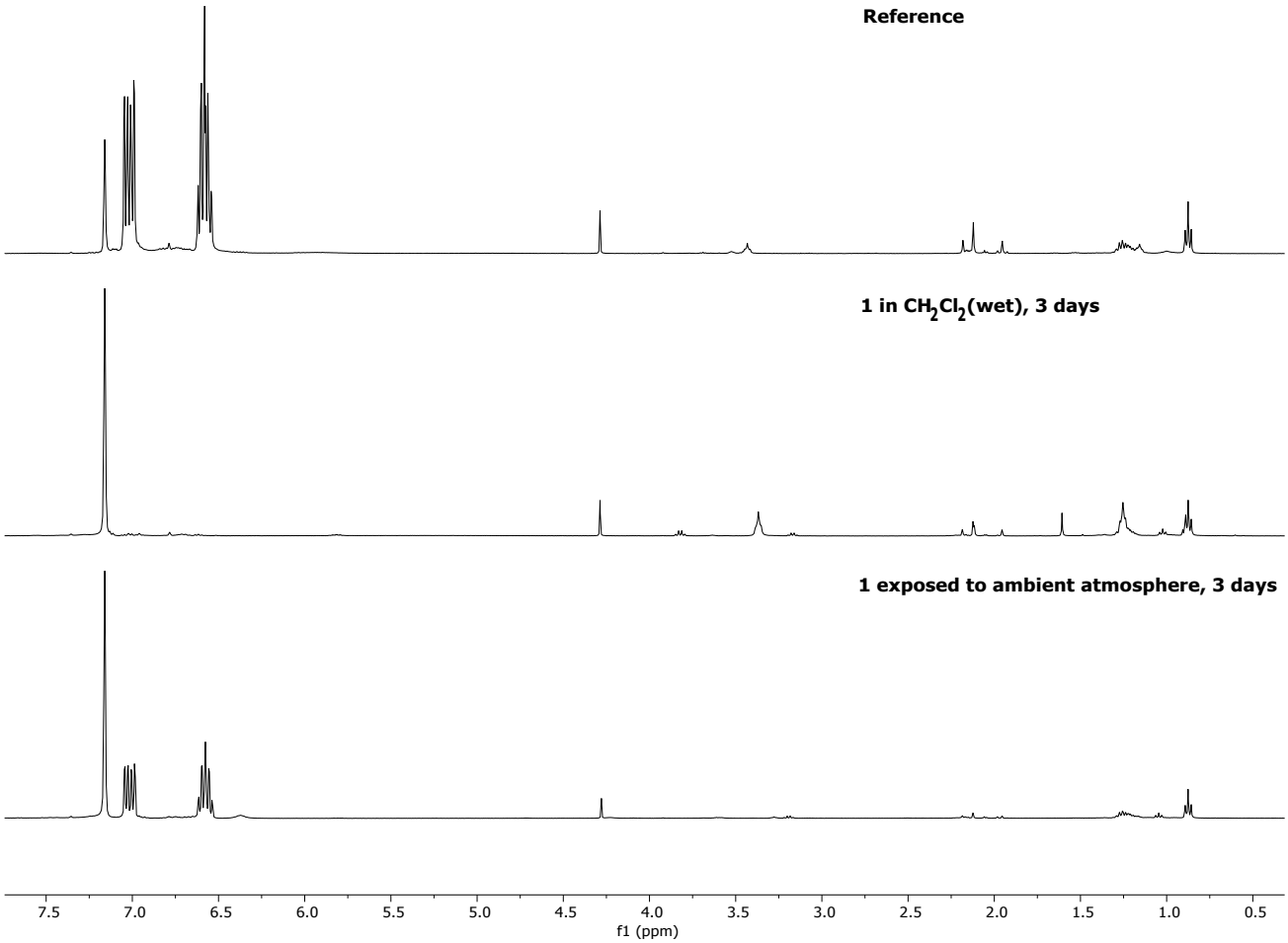

*Figure S7. Stacked ^{1}H NMR spectra of **1** exposed to wet solvent (middle) and ambient atmosphere (bottom) in C_6D_6.*

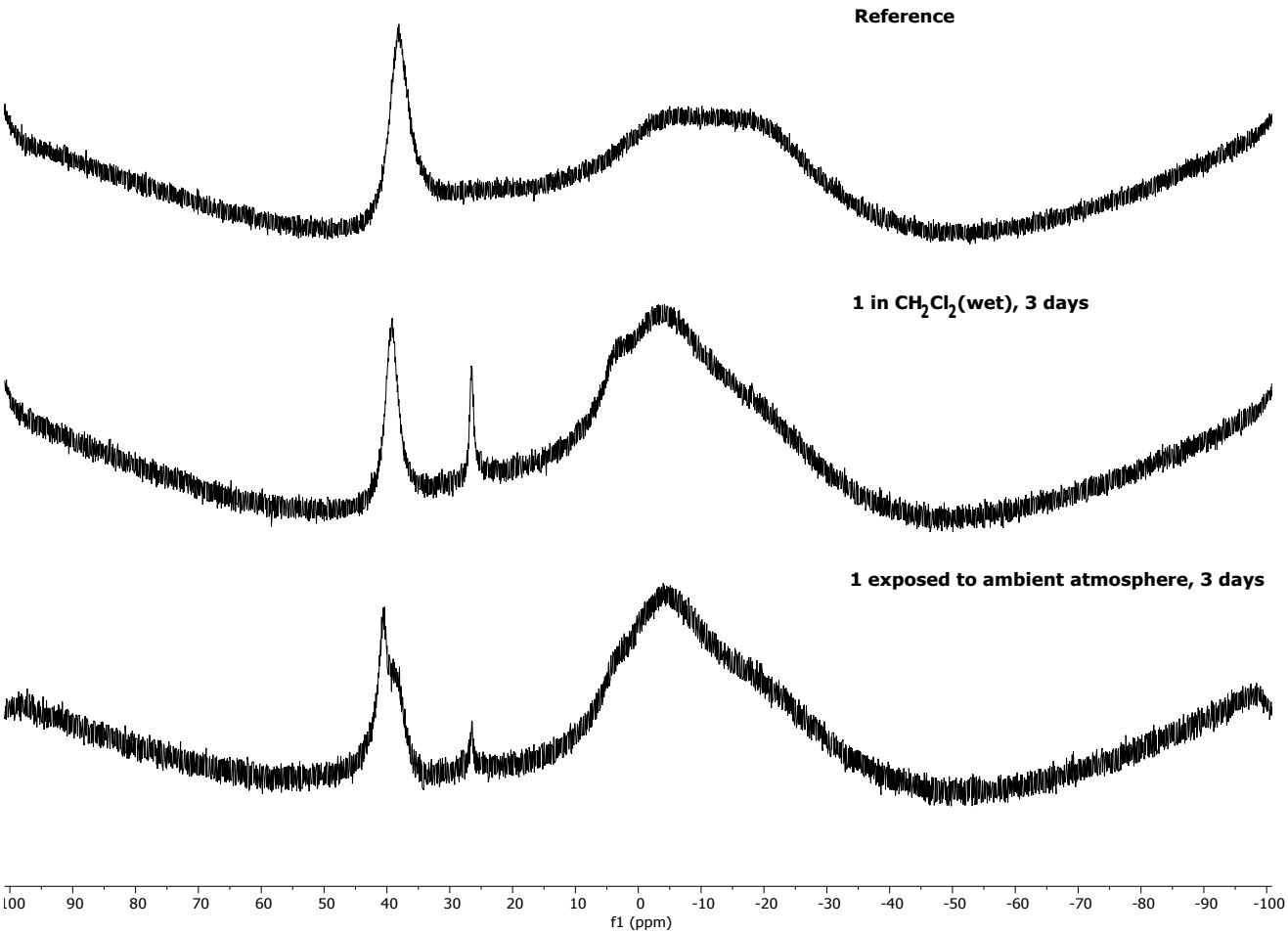

*Figure S8. Stacked ^{11}B NMR spectra of **1** exposed to wet solvent (middle) and ambient atmosphere (bottom) in C_6D_6.*

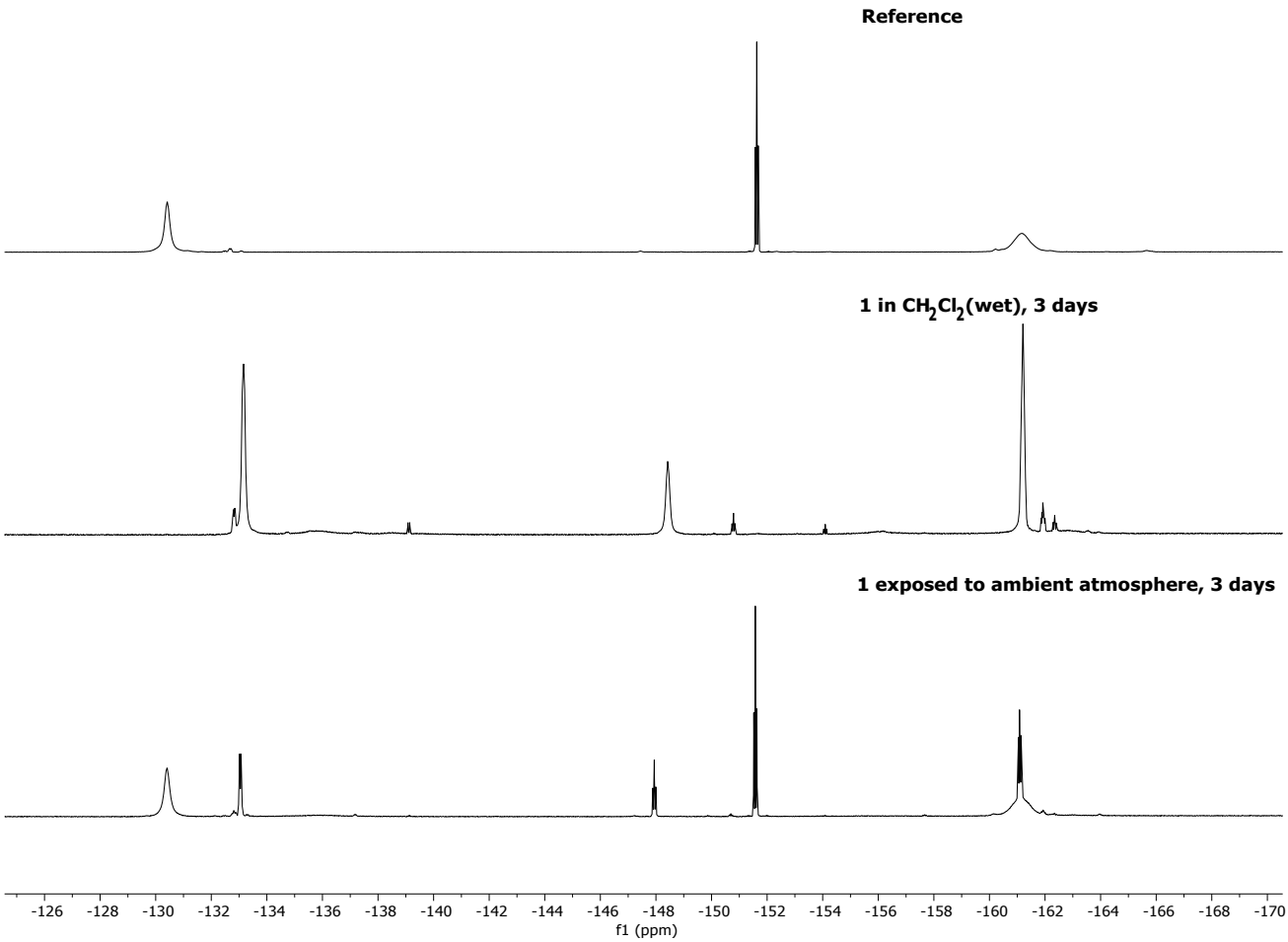

*Figure S9. Stacked ^{19}F NMR spectra of **1** exposed to wet solvent (middle) and ambient atmosphere (bottom) in C_6D_6.*

3 Catalytic Hydrosilylation Experiments

In the glovebox, acetophenone (0.33 mmol) and triethylsilane (1.1 eq) were massed out into a 5 mL scintillation vial and dissolved in C_6D_6 (0.5 mL). Compound **1** (10 mol%) was massed out into a separate vial and dissolved in C_6D_6 (0.2 mL). The solution of substrates was transferred to a J-young tap NMR spectrum tube, followed by the careful addition of the solution of respective catalyst. The NMR tube was promptly sealed. The reaction was monitored by the ^1H nuclei at specific time intervals at room temperature. The reaction was deemed complete upon either no observable progression or complete conversion. The resulting silyl ether was in agreement with literature.[5]</sup>

The reaction does indeed proceed to complete conversion. For the purpose of observing the reaction overtime it was necessary to prepare dilute samples; the reaction was othewise completed too quickly before any possible NMR spectra acquisition.

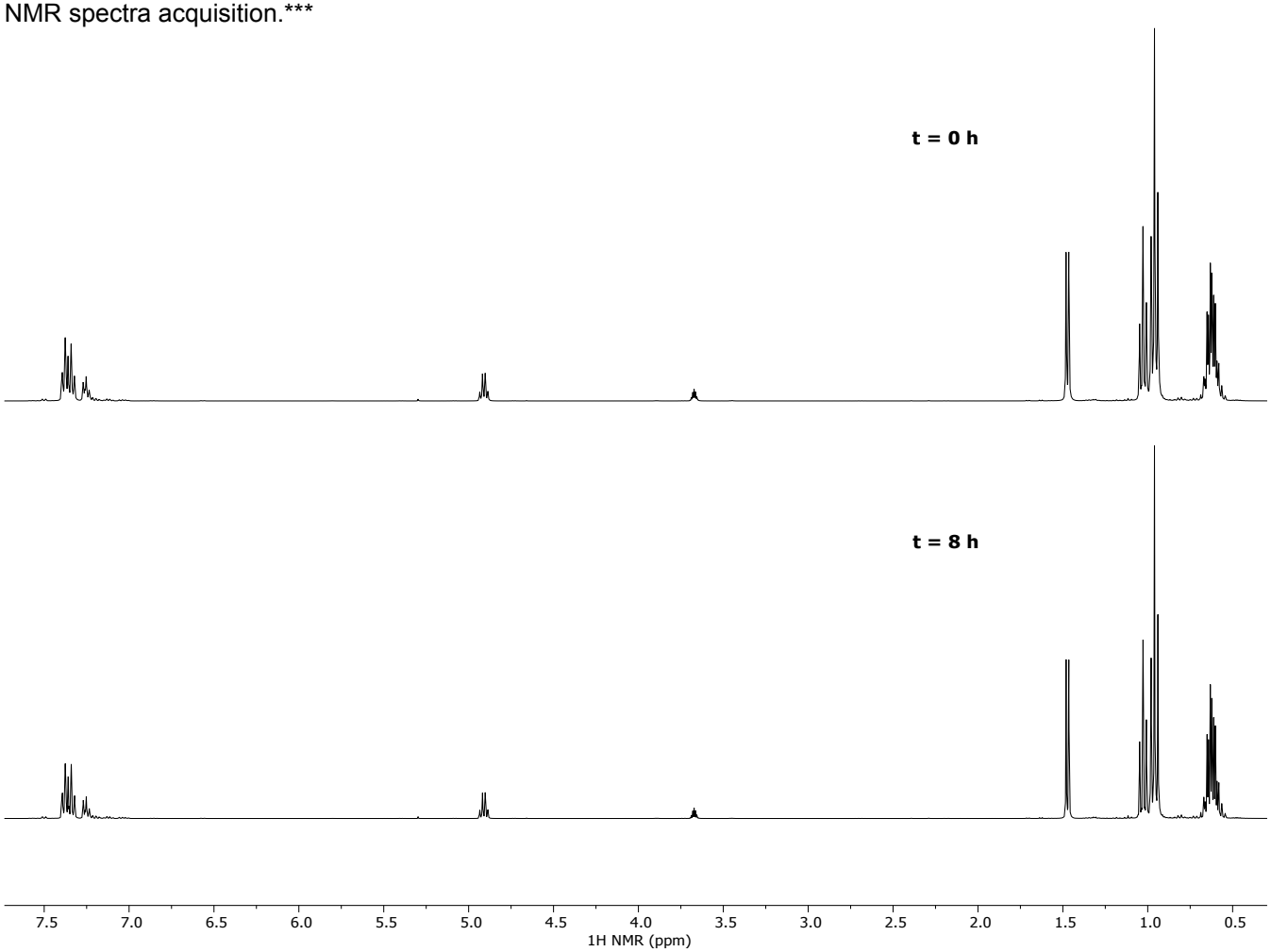

*Figure S10. Stacked ^1H NMR spectra of Et_3SiH (1.1 eq.) and acetophenone (1 eq.) with **1** (10 mol%) in C_6D_6 (concentrated).*

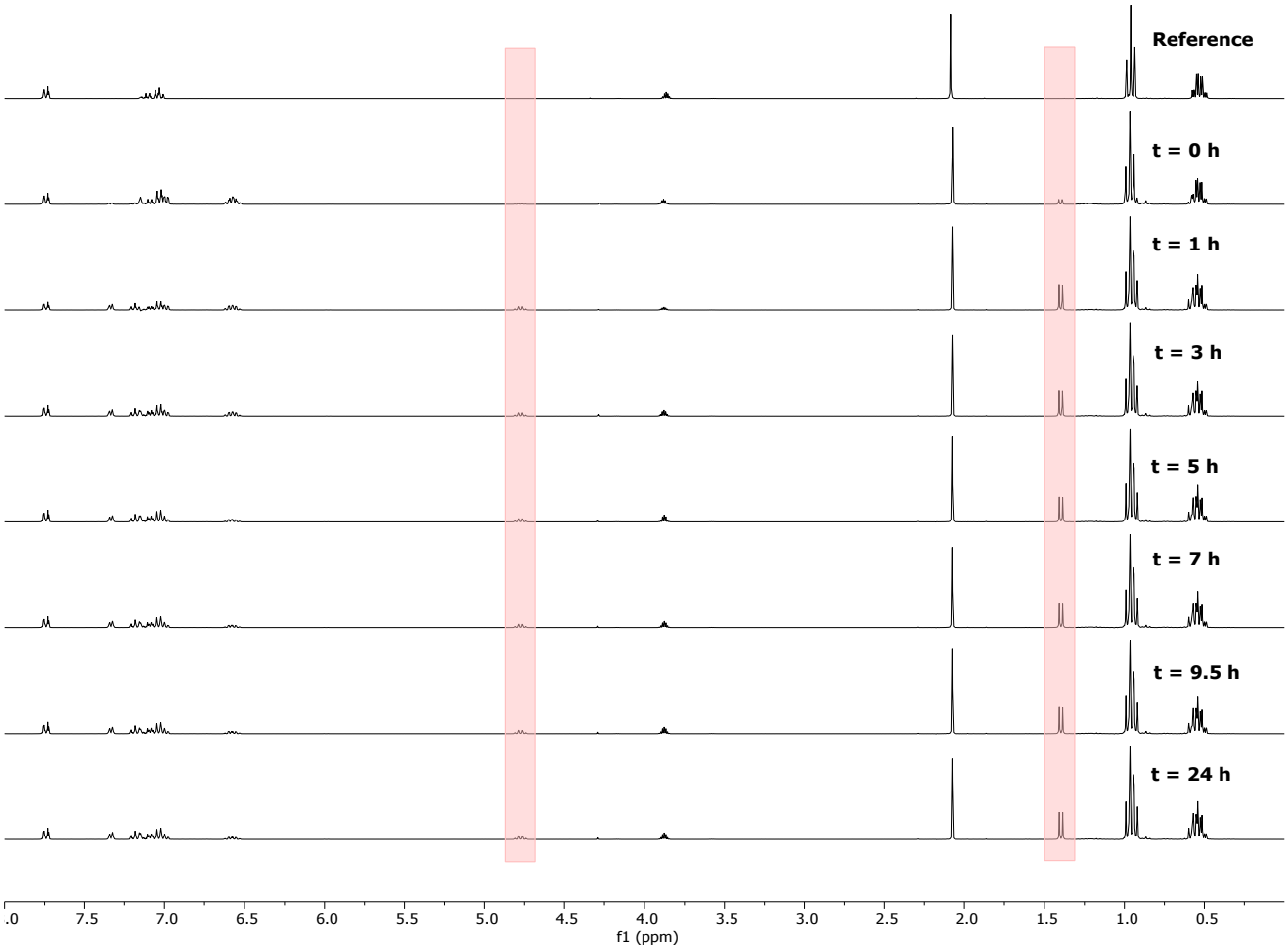

*Figure S11. Stacked ^{1}H NMR spectra of Et_3SiH (1.1 eq.) and acetophenone (1 eq.) with **1** (10 mol%) in C_6D_6 (dilute).*

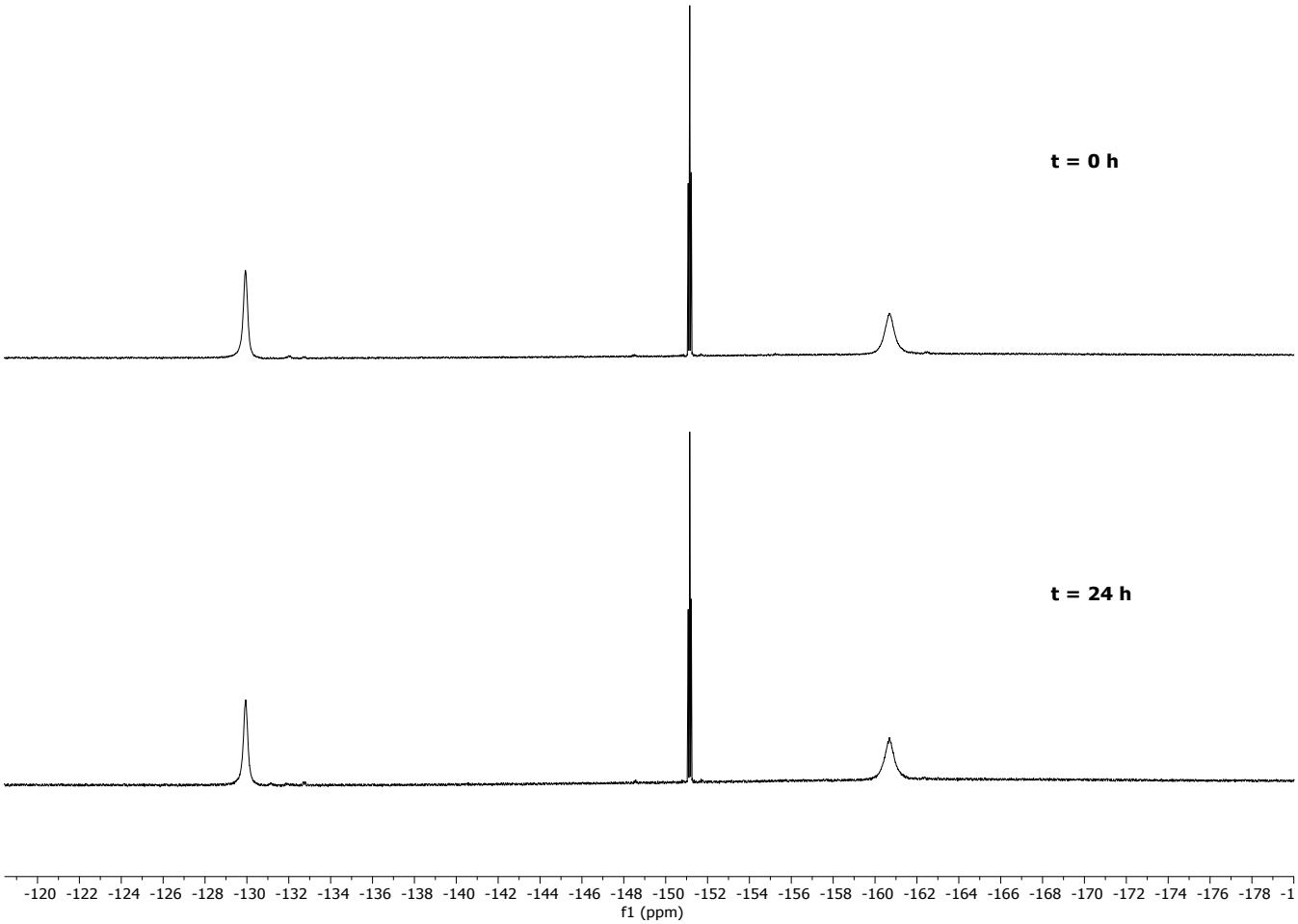

*Figure S12. Stacked ^{19}F NMR spectra of Et_3SiH (1.1 eq.) and acetophenone (1 eq.) with **1** (10 mol%) in C_6D_6 (dilute).*

4 Stoichiometric Experiments

In the glovebox, Ph_3SnH (51.3 mg, 0.148 mmol) and Mes_3P (28.4 mg, 0.074 mmol) were massed out into separate 5 mL scintillation vial, and each were dissolved in C_6D_6 (0.3 mL). The two solutions were ccombined. Compound **1** (39.7 mg, 0.074 mmol) was massed out into a separate vial and dissolved in C_6D_6 (0.2 mL). The solution of **1** was added to the other mixture, then transferred to a J-young tap NMR spectrum tube, followed by the careful addition of the solution of **1**. The NMR spectrum tube was promptly sealed. The reaction was monitored by ^{1}H and ^{119}Sn NMR spectrum overtime; and heated as necessary. The reaction was deemed complete upon either no observable progression or complete conversion.

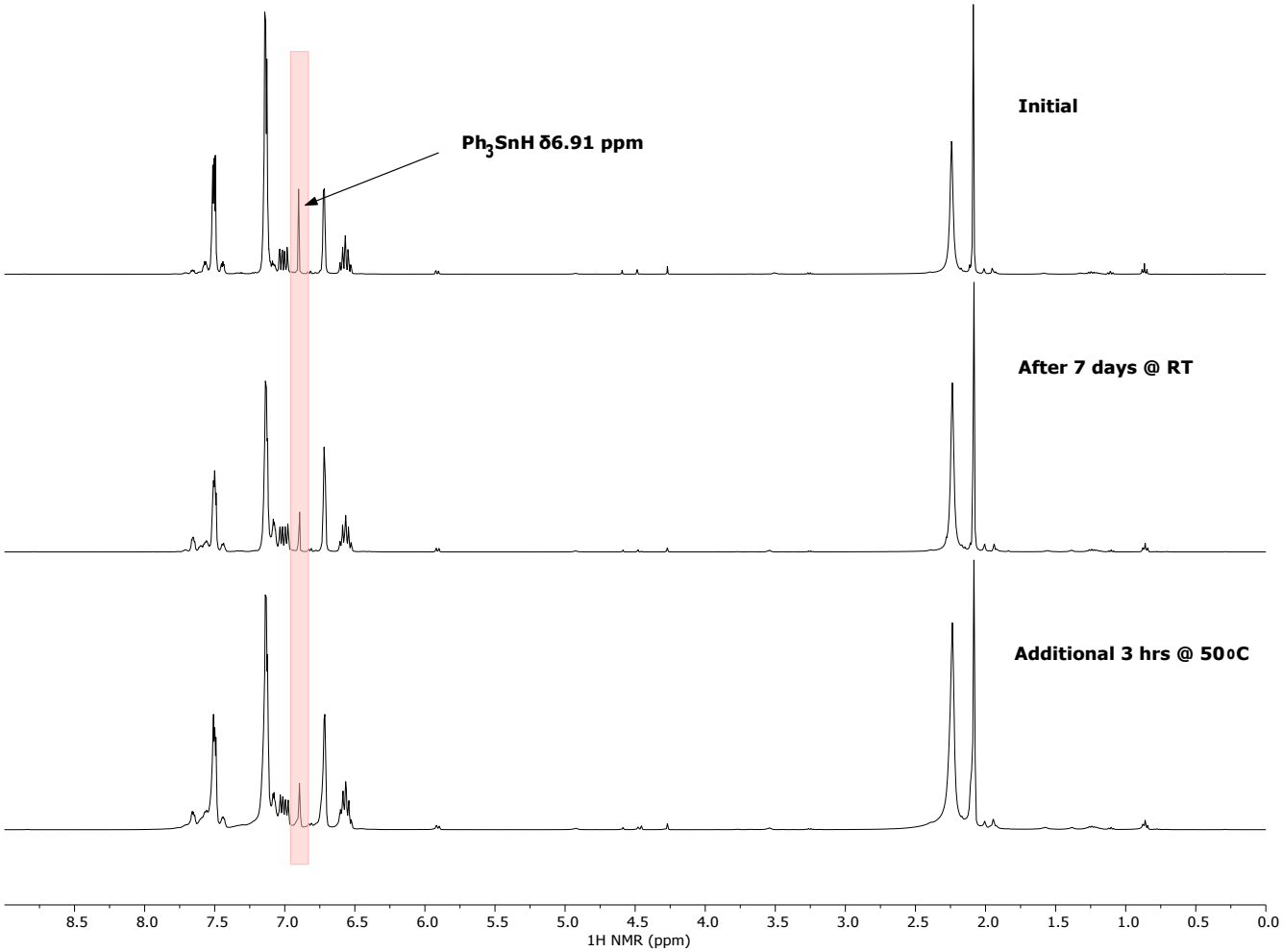

*Figure S13. Stacked ^{1}H NMR spectra of Ph_3SnH with **1** (1 eq.) and Mes_3P (1 eq.) in C_6D_6 at ambient temperature over time.*

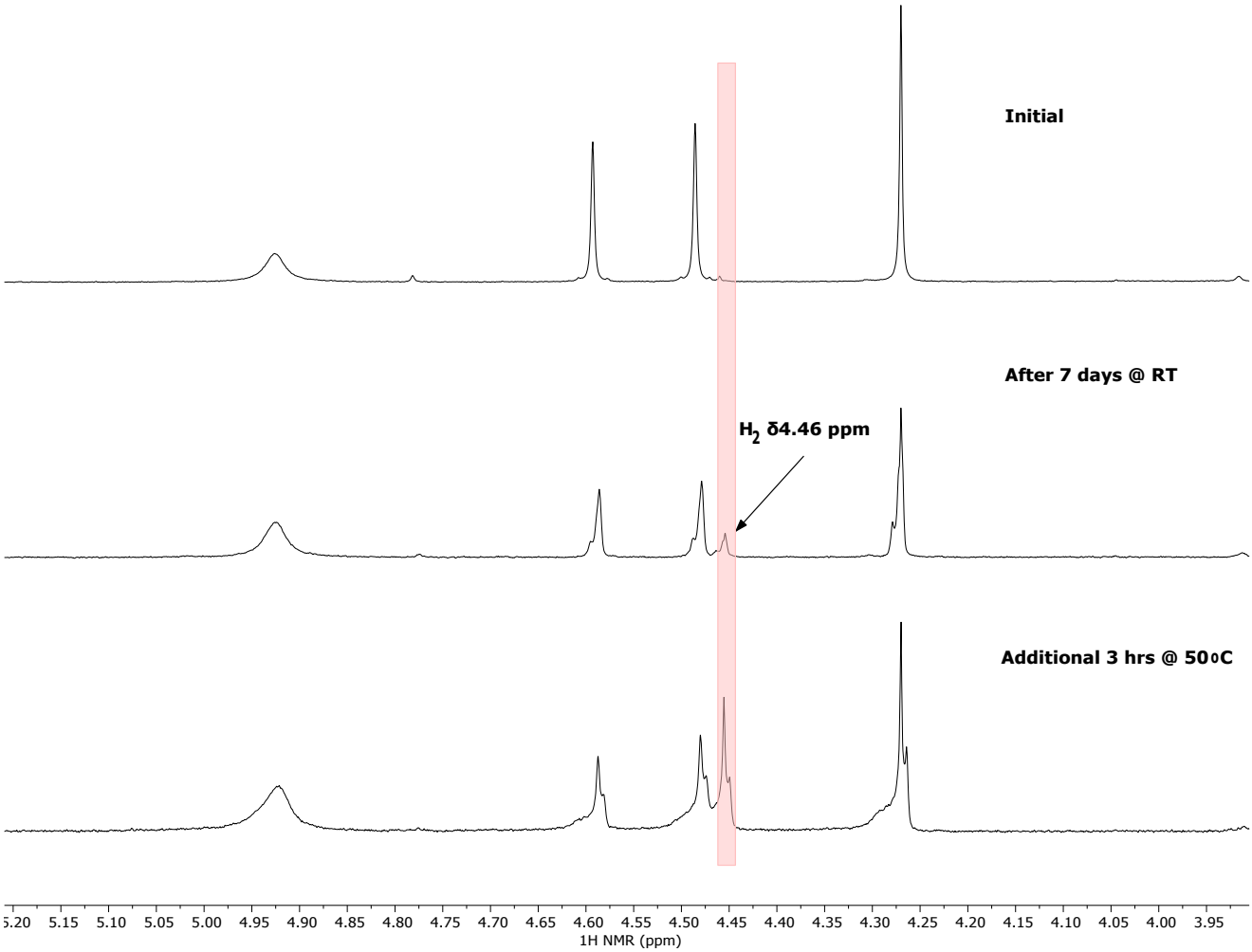

*Figure S14. Stacked ^{1}H NMR spectra of Ph_3SnH with **1** (1 eq.) and Mes_3P (1 eq.) in C_6D_6 at ambient temperature over time; expanded region.*

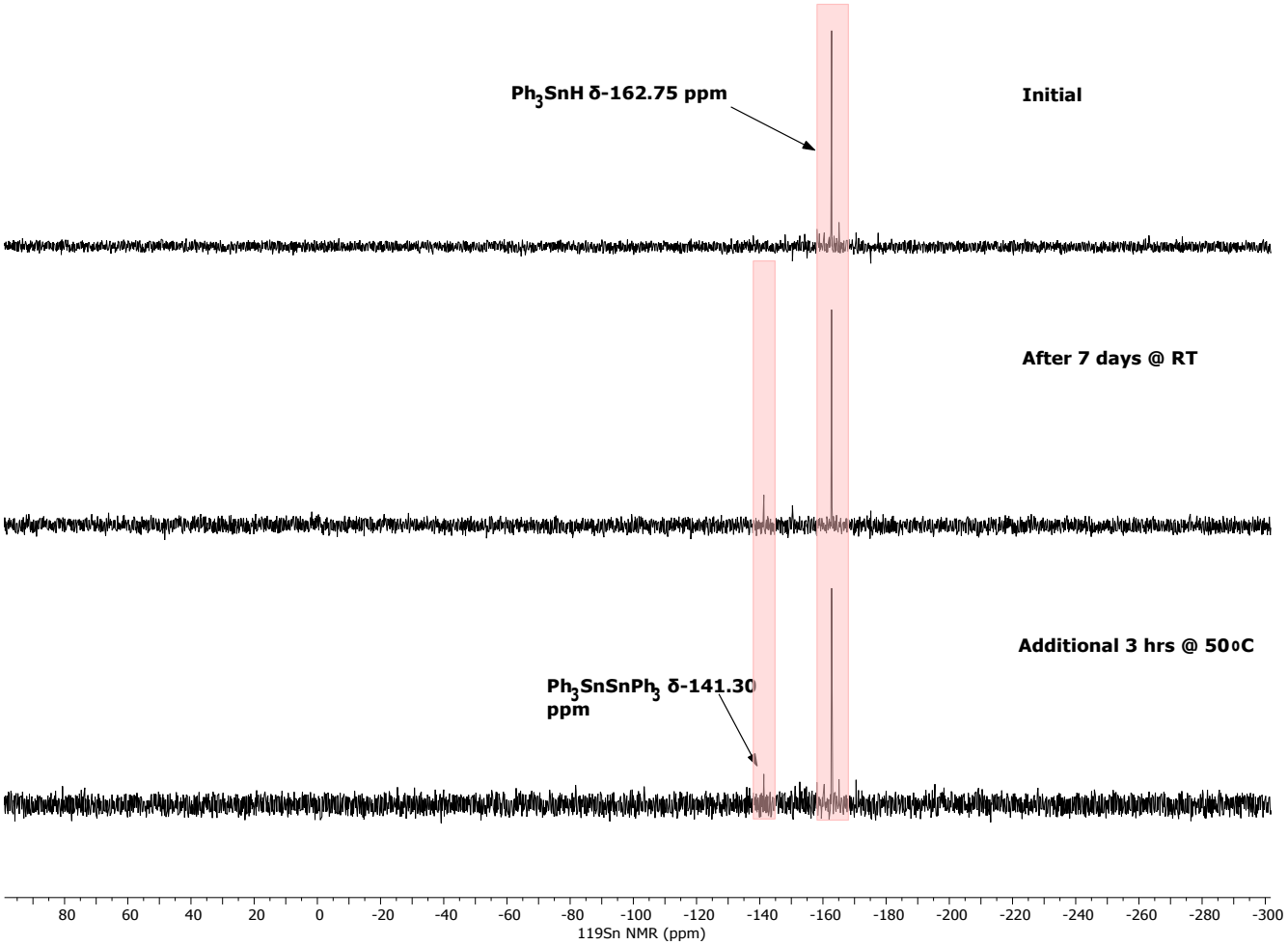

*Figure S15. Stacked ^{119}Sn(decoupled) NMR spectra of Ph_3SnH with **1** (1 eq.) and Mes_3P (1 eq.) in C_6D_6 at ambient temperature over time.*

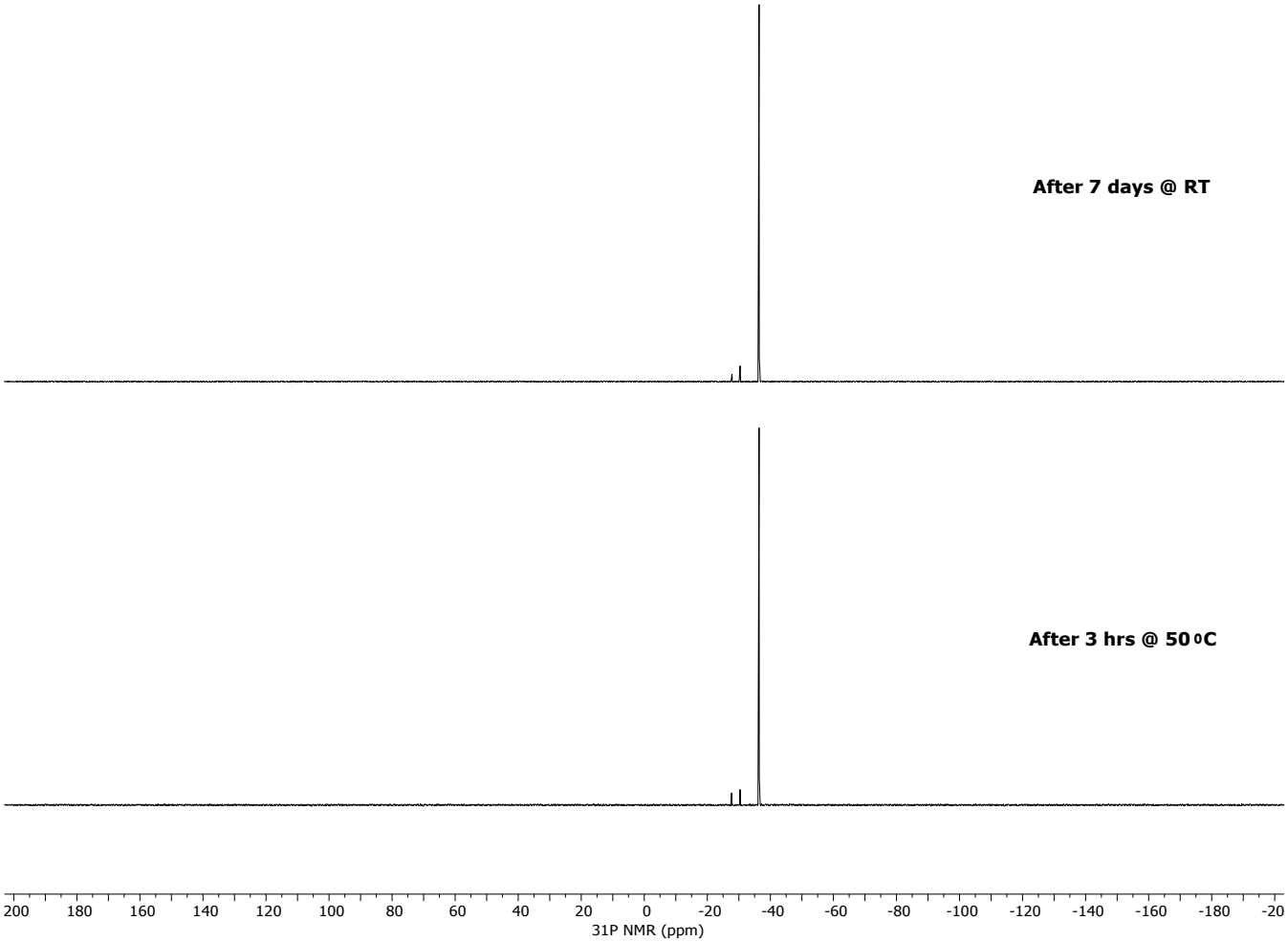

*Figure S16. Stacked ^{31}P(decoupled) NMR spectra of Ph_3SnH with **1** (1 eq.) and Mes_3P (1 eq.) in C_6D_6 at ambient temperature over time.*

In the glovebox, Ph_3SnH (15.0 mg, 0.043 mmol) and **1** (11.6 mg, 0.021 mmol) were massed out into separate 5 mL scintillation vial, and each were dissolved in C_6D_6 (0.3 mL). The two solutions were combined, then transferred to a J-young tap NMR spectrum tube. The NMR spectrum tube was promptly sealed. The reaction was monitored by ^{1}H and ^{119}Sn NMR spectrum overtime; and heated as necessary. The reaction was deemed complete upon either no observable progression or complete conversion.

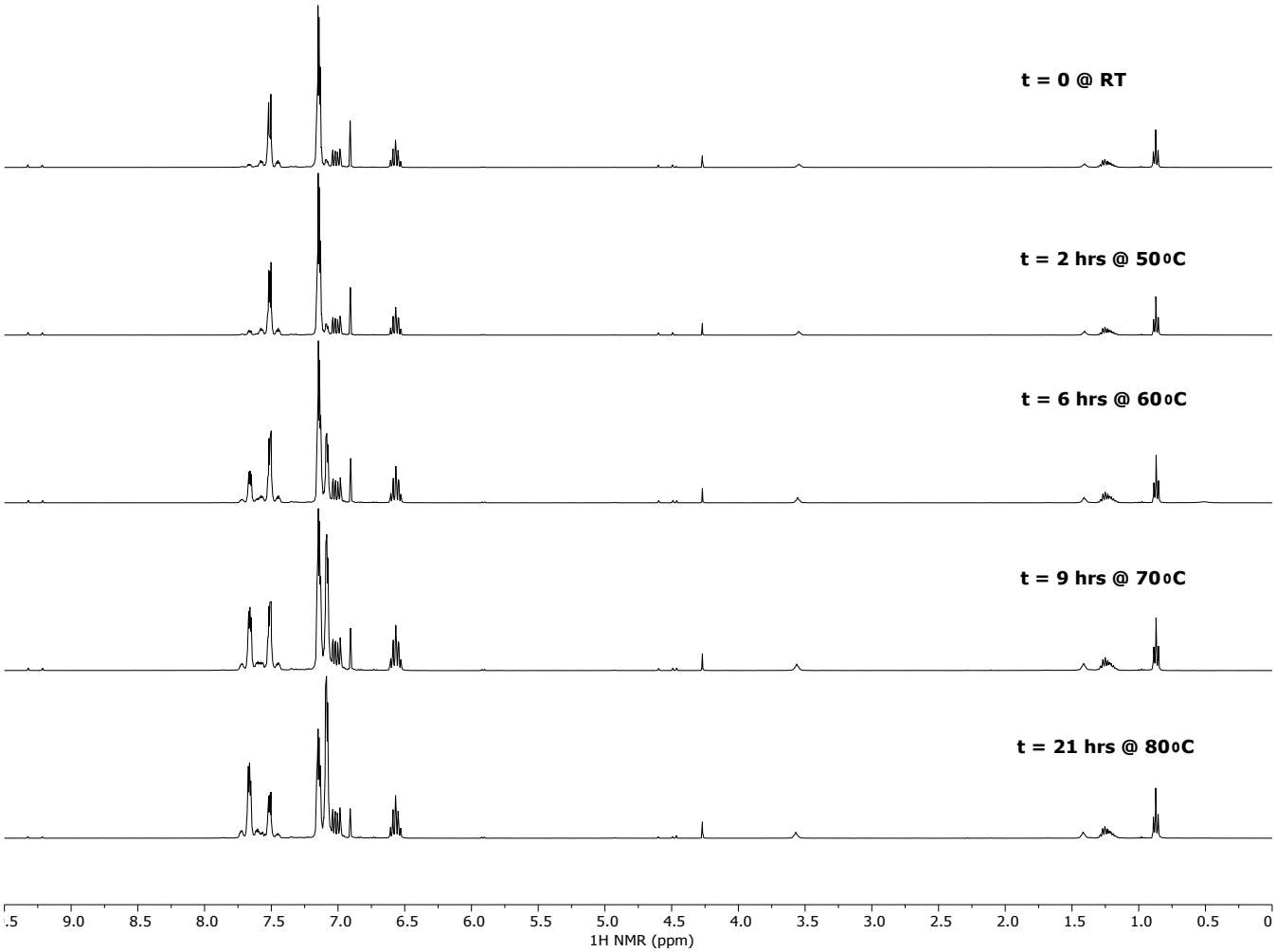

*Figure S17. Stacked ^{1}H NMR spectra of Ph_3SnH with **1** (1 eq.) in C_6D_6 with increasing temperature over time.*

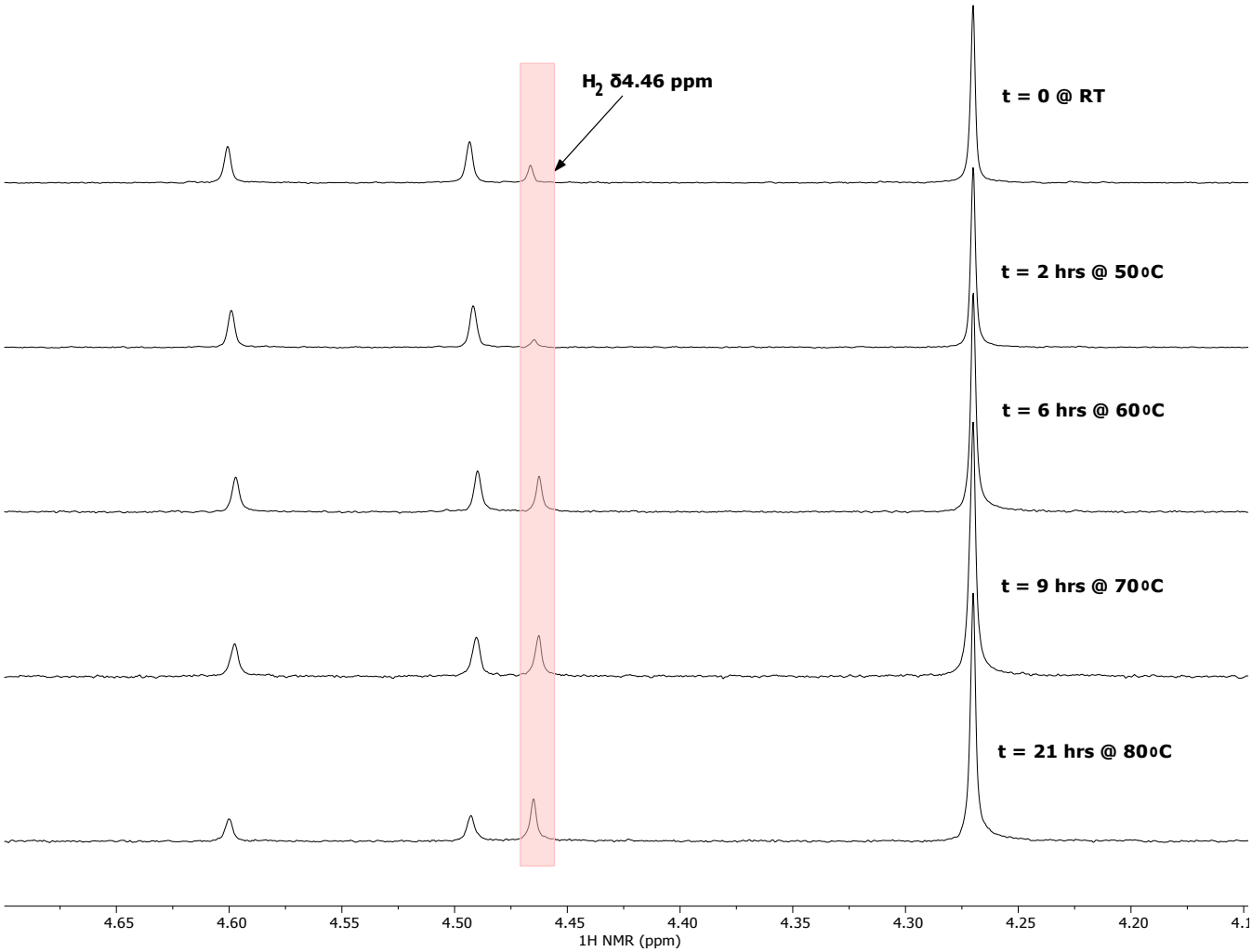

*Figure S18. Stacked ^{1}H NMR spectra of Ph_3SnH with **1** (1 eq.) in C_6D_6 with increasing temperature over time; expanded region.*

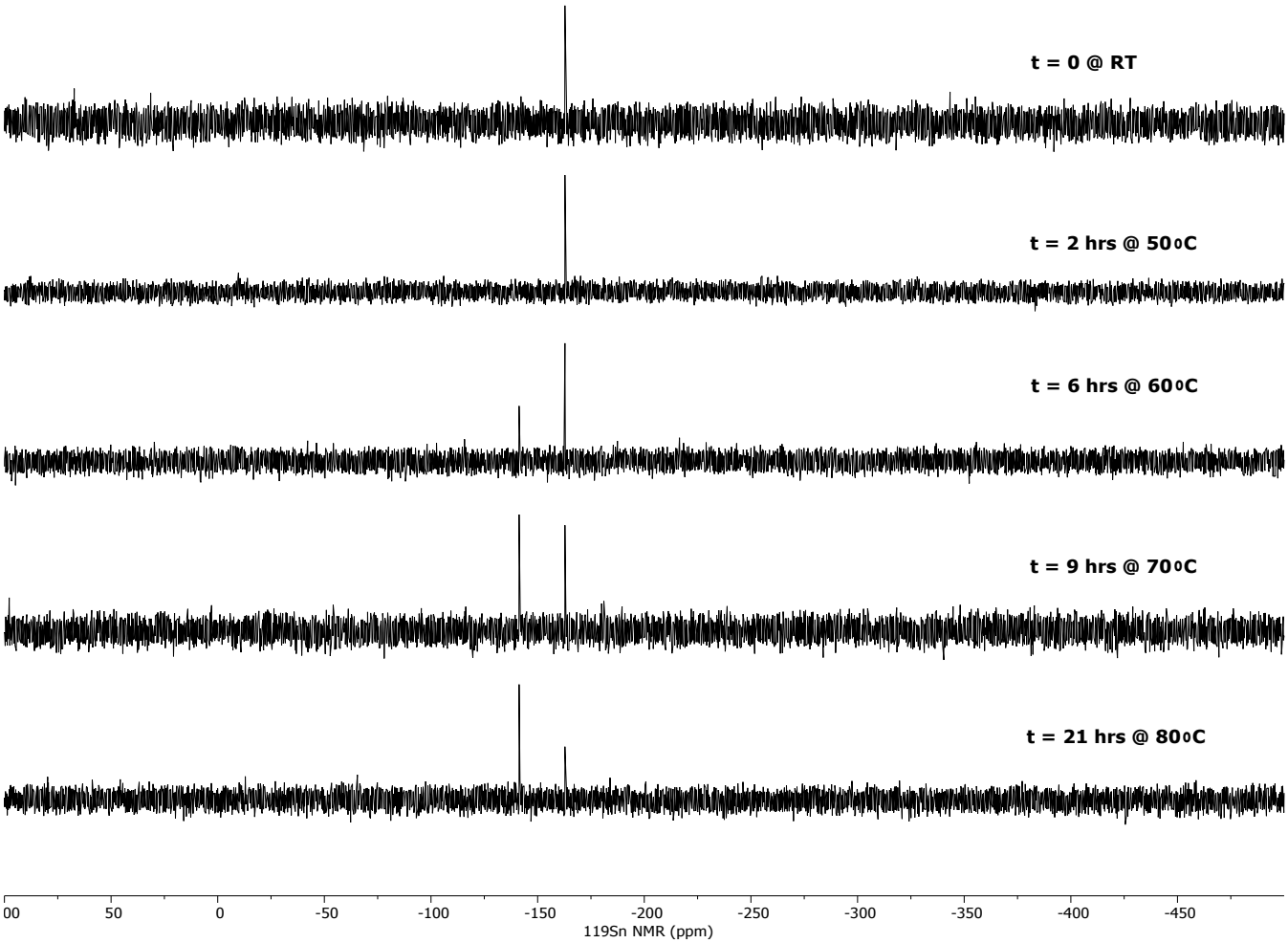

*Figure S19. Stacked ^{119}Sn(decoupled) NMR spectra of Ph_3SnH with **1** (1 eq.) in C_6D_6 with increasing temperature over time.*

5 Control Experiments

General Procedure: The control substrate (10 mol%) in C_6D_6 (0.2 mL) was addded to a solution of Ph_3SnH (106.0 mg, 0.30 mmol) or Bu_3SnH (87.3 g, 0.30 mmol) , in C_6D_6 (0.4 mL), in a J-Young tapped NMR tube. The NMR tube was sealed and monitored from room tempeature to 50 °C overtime.

N-Methylphenothiazine

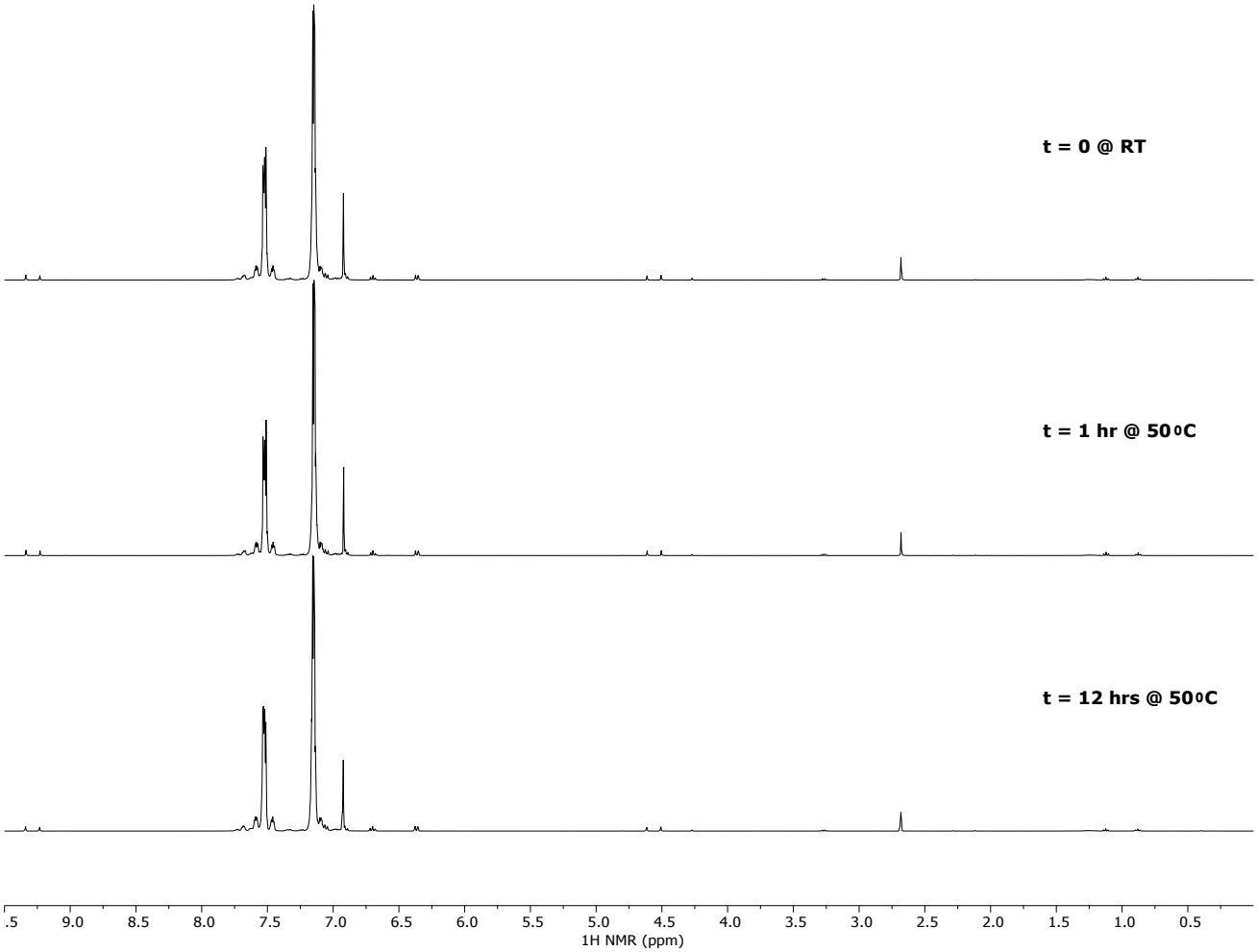

Figure S20. Stacked ^1H NMR spectra of Ph_3SnH with N-methylphenothiazine (10 mol%) in C_6D_6 at 50 °C over time.

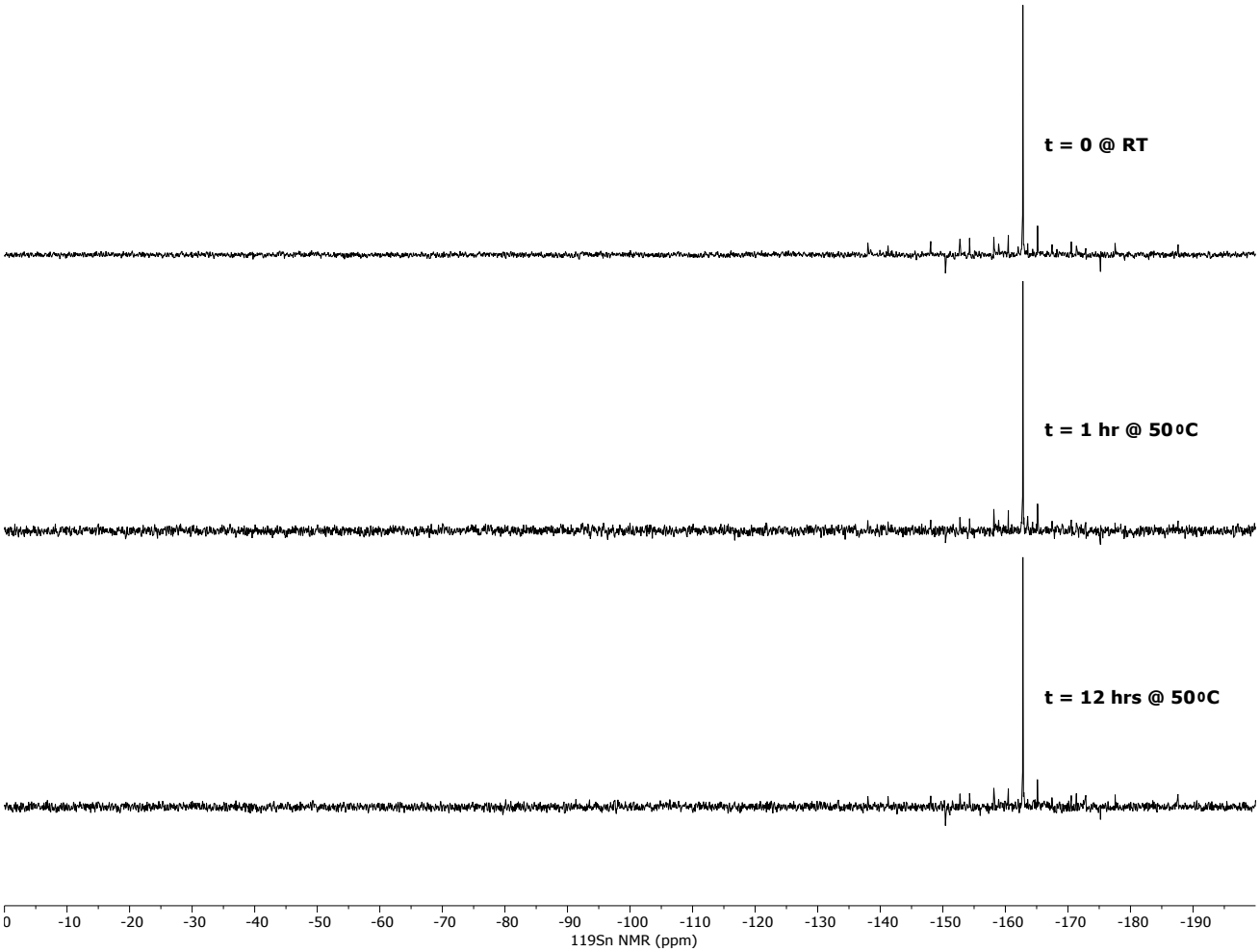

Figure S21. Stacked ^{119}Sn(decoupled) NMR spectra of Ph_3SnH with N-methylphenothiazine (10 mol%) in C_6D_6 at 50 °C over time.

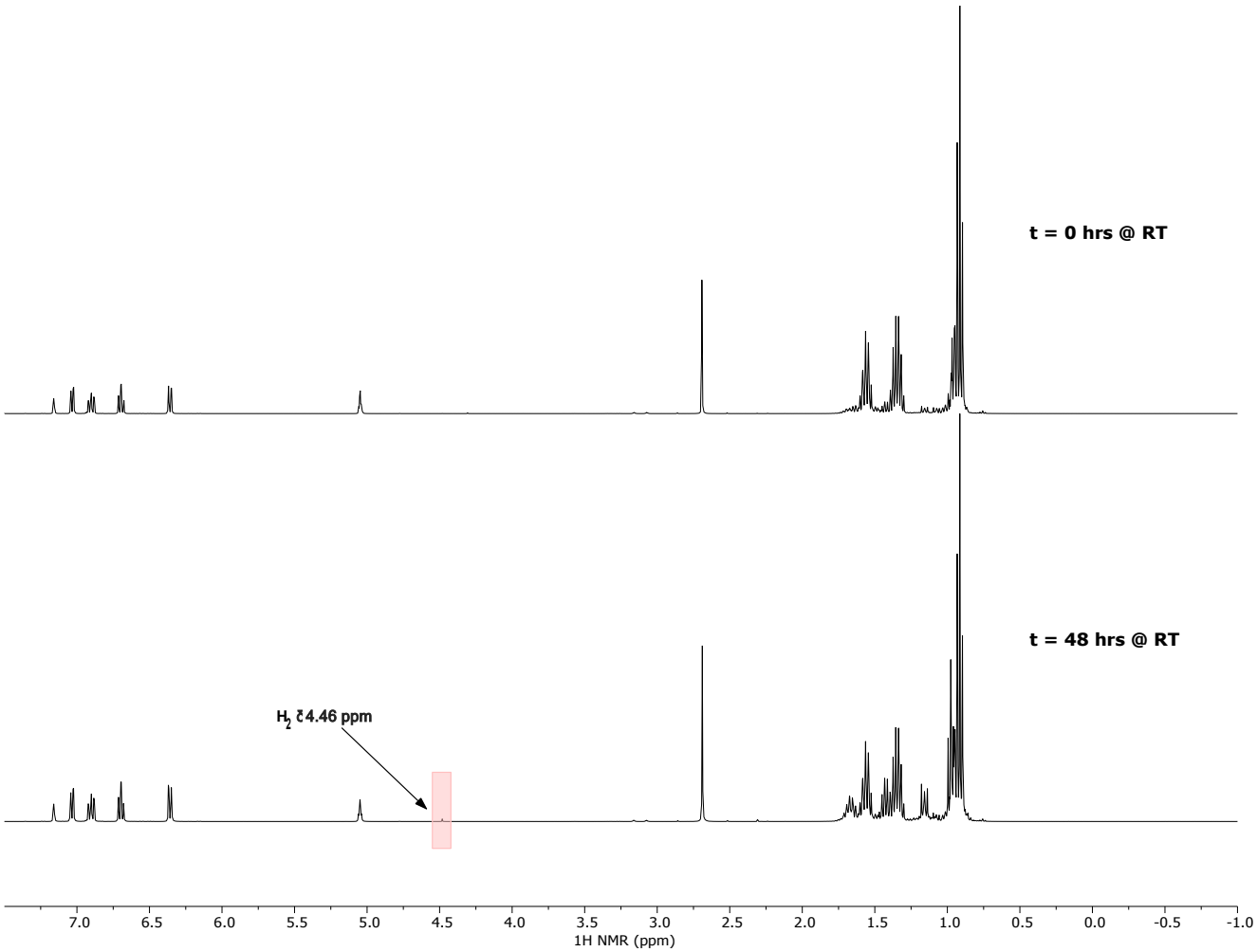

Figure S22. Stacked ^1H NMR spectra of Bu_3SnH with N-methylphenothiazine (10 mol%) in C_6D_6 at room temperature.

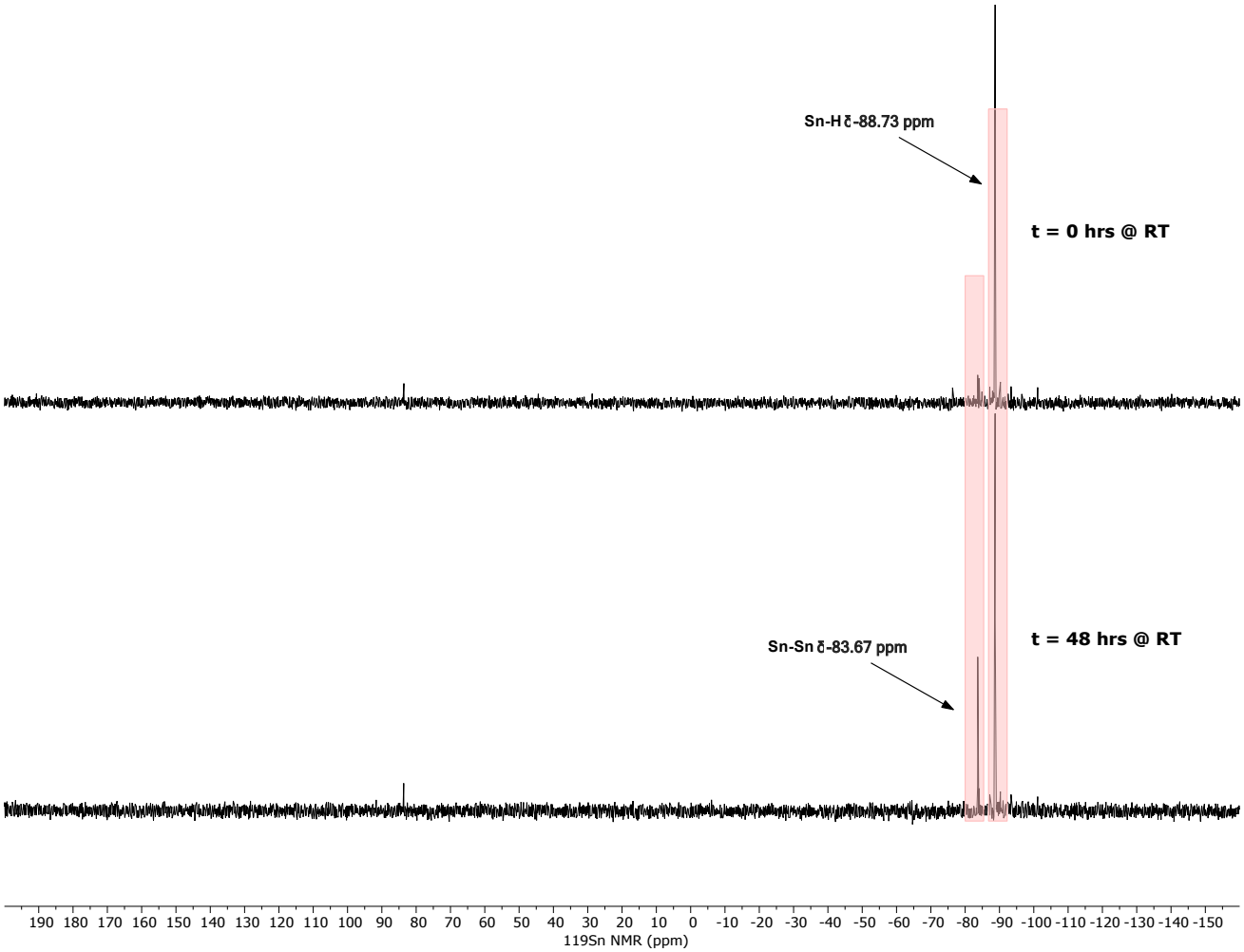

Figure S23. Stacked ^{119}Sn(decoupled) NMR spectra of Bu_3SnH with N-methylphenothiazine (10 mol%) in C_6D_6 at room temperature.

Ph_3SnH in the Dark at Reaction Temperatures

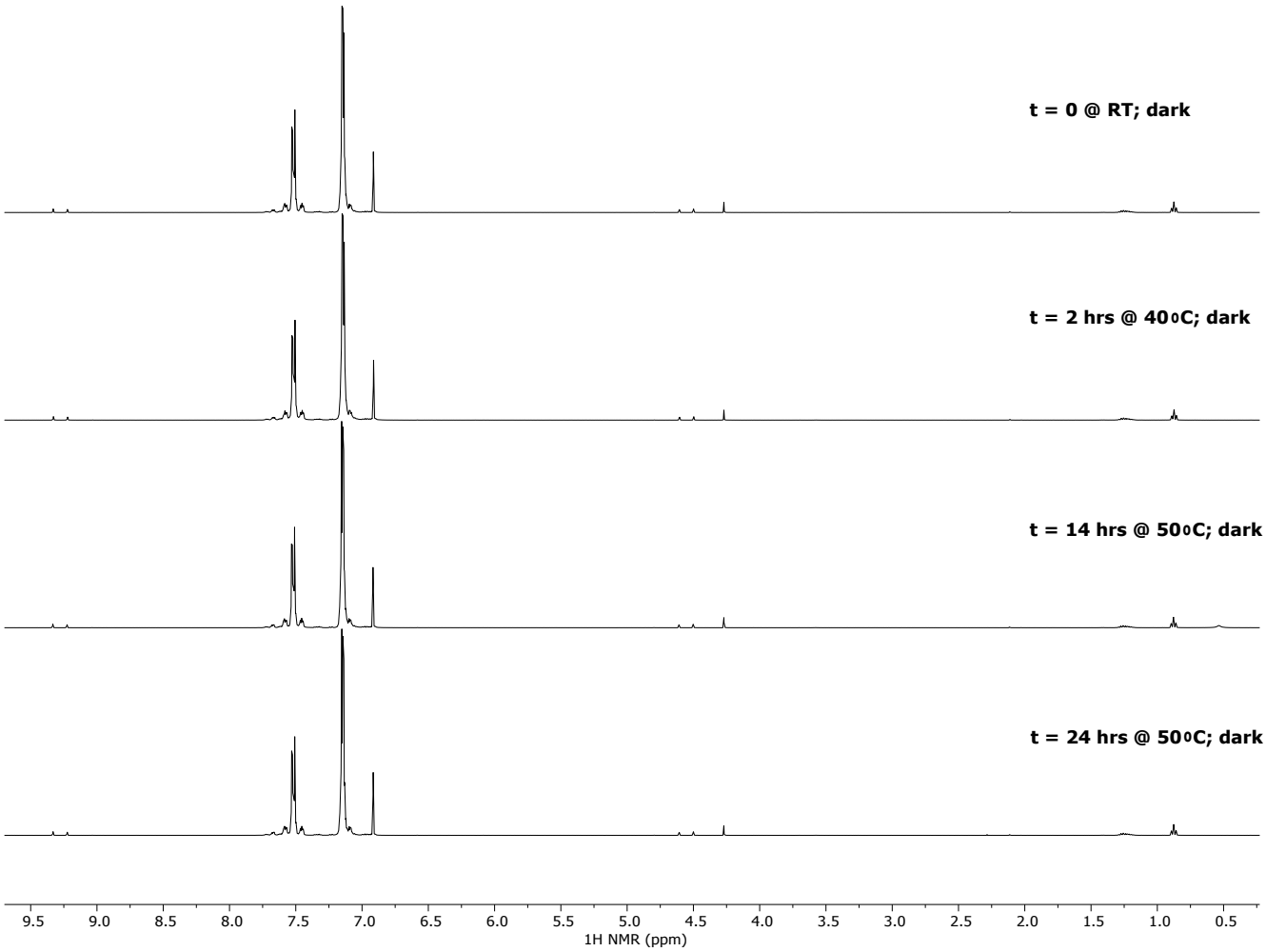

Figure S24. Stacked ^1H NMR spectra of Ph_3SnH in C_6D_6 at 50 °C over time.

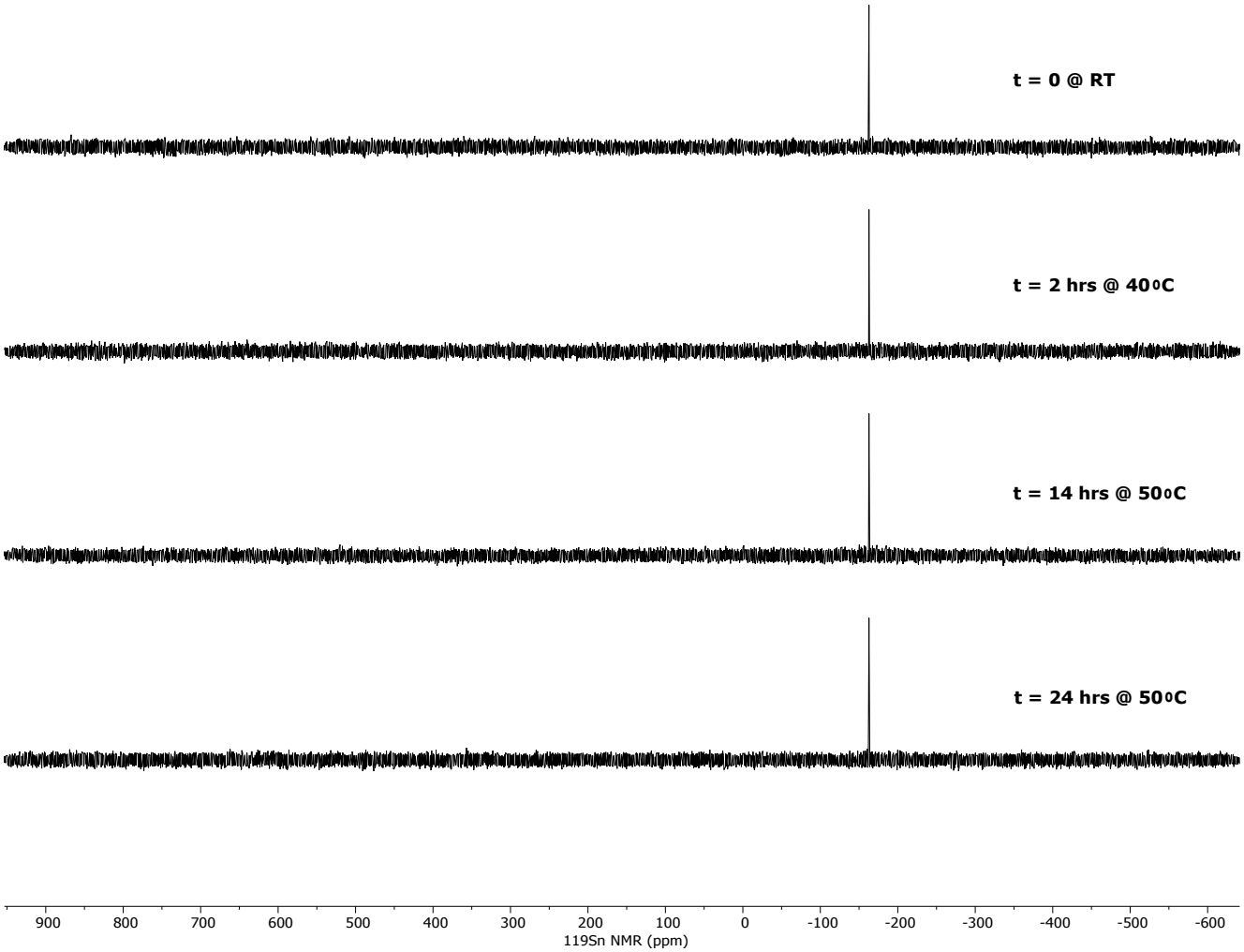

Figure S25. Stacked ^{119}Sn(decoupled) NMR spectra of Ph_3SnH in C_6D_6 at 50 °C over time.

Mes$_2$BPtz as a Catalyst

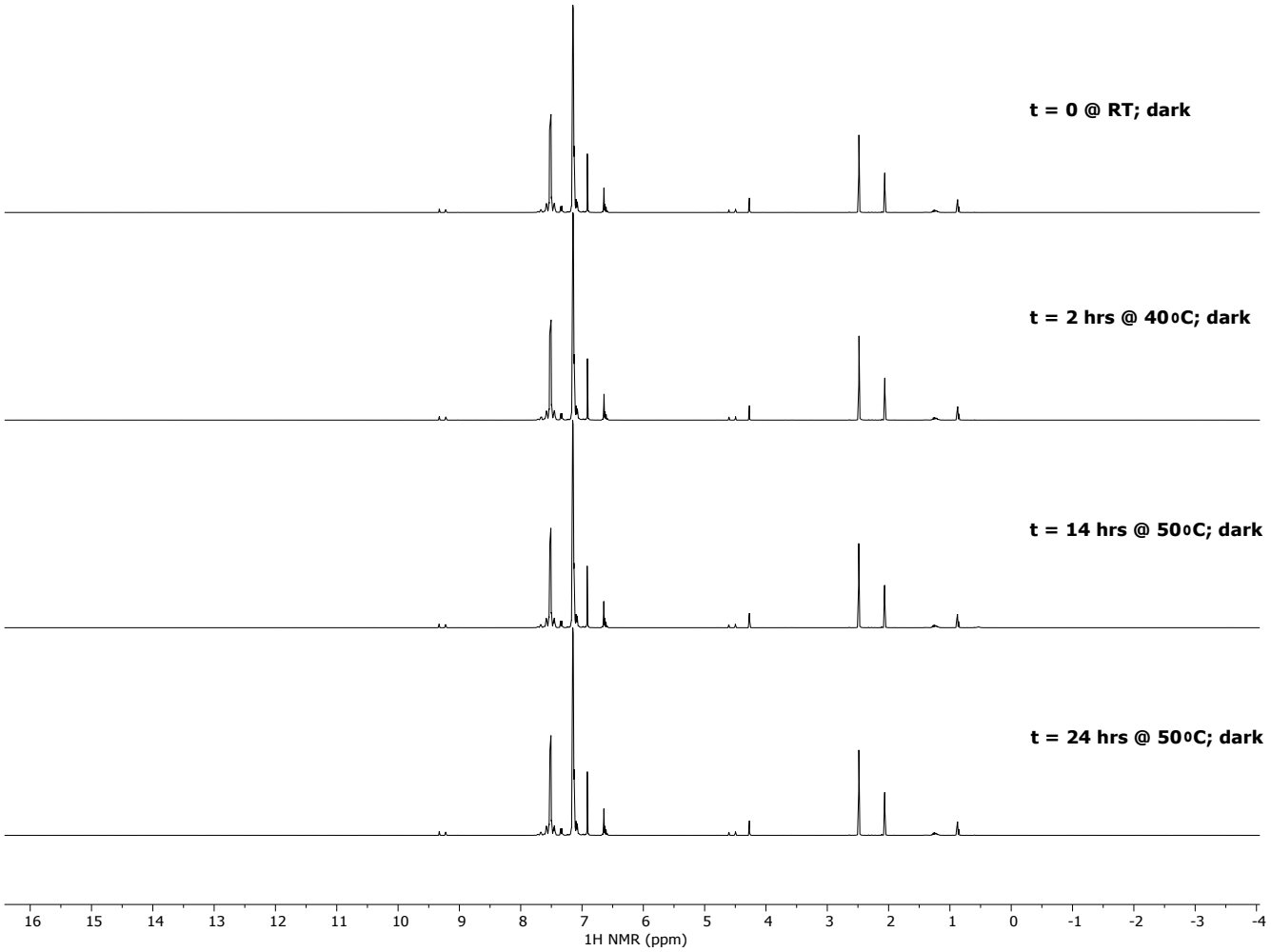

Figure S26. Stacked ^{1}H NMR spectra of Ph_3SnH with N-dimesitylboryl-phenothiazine (10 mol%) in C_6D_6 at 50 ºC over time.

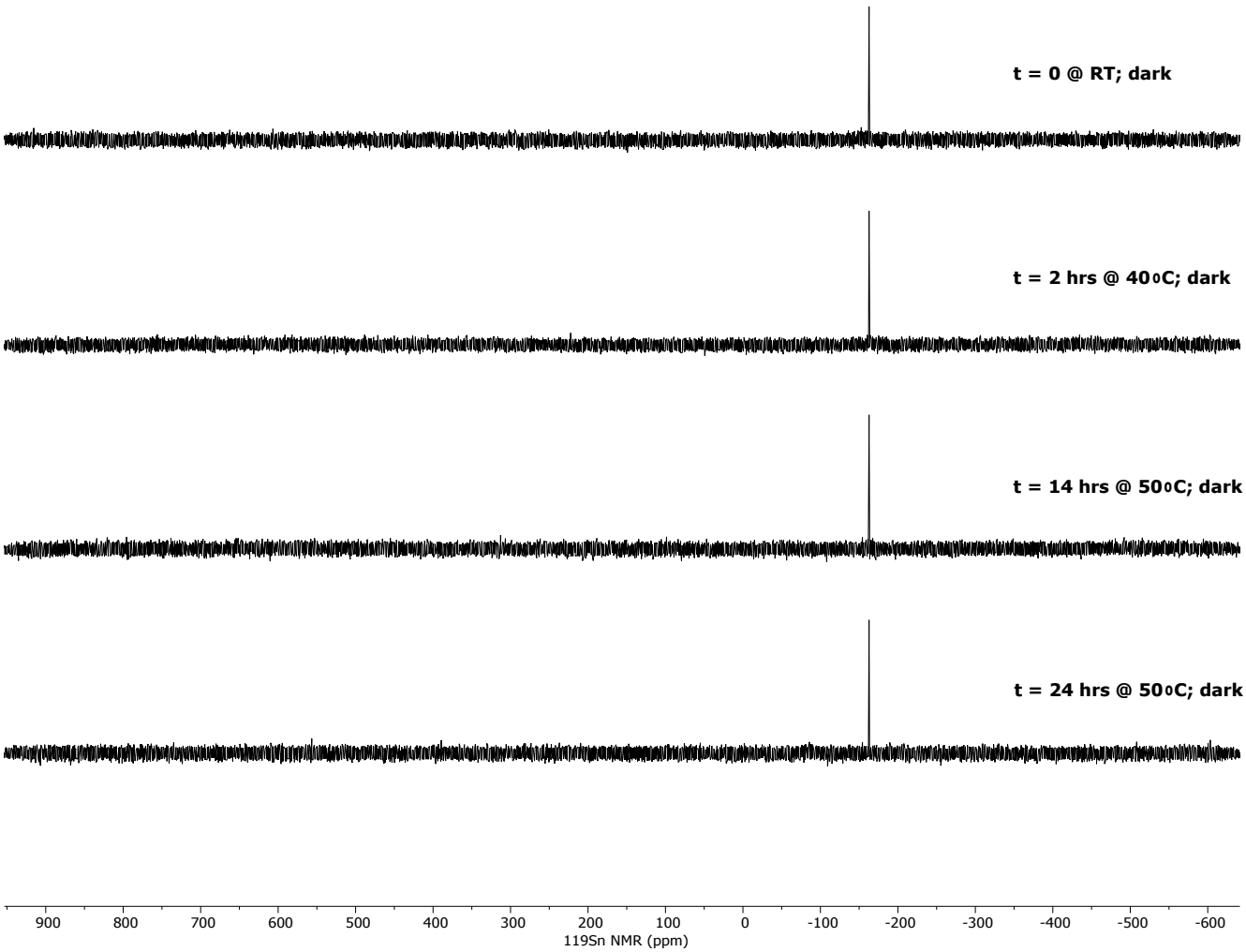

Figure S27. Stacked ^{119}Sn(decoupled) NMR spectra of Ph_3SnH with N-dimesitylboryl-phenothiazine (10 mol%) in C_6D_6 at 50 ^oC over time.

Control Experiment Between $B(C_6F_5)_3$ and Ph_3SnH

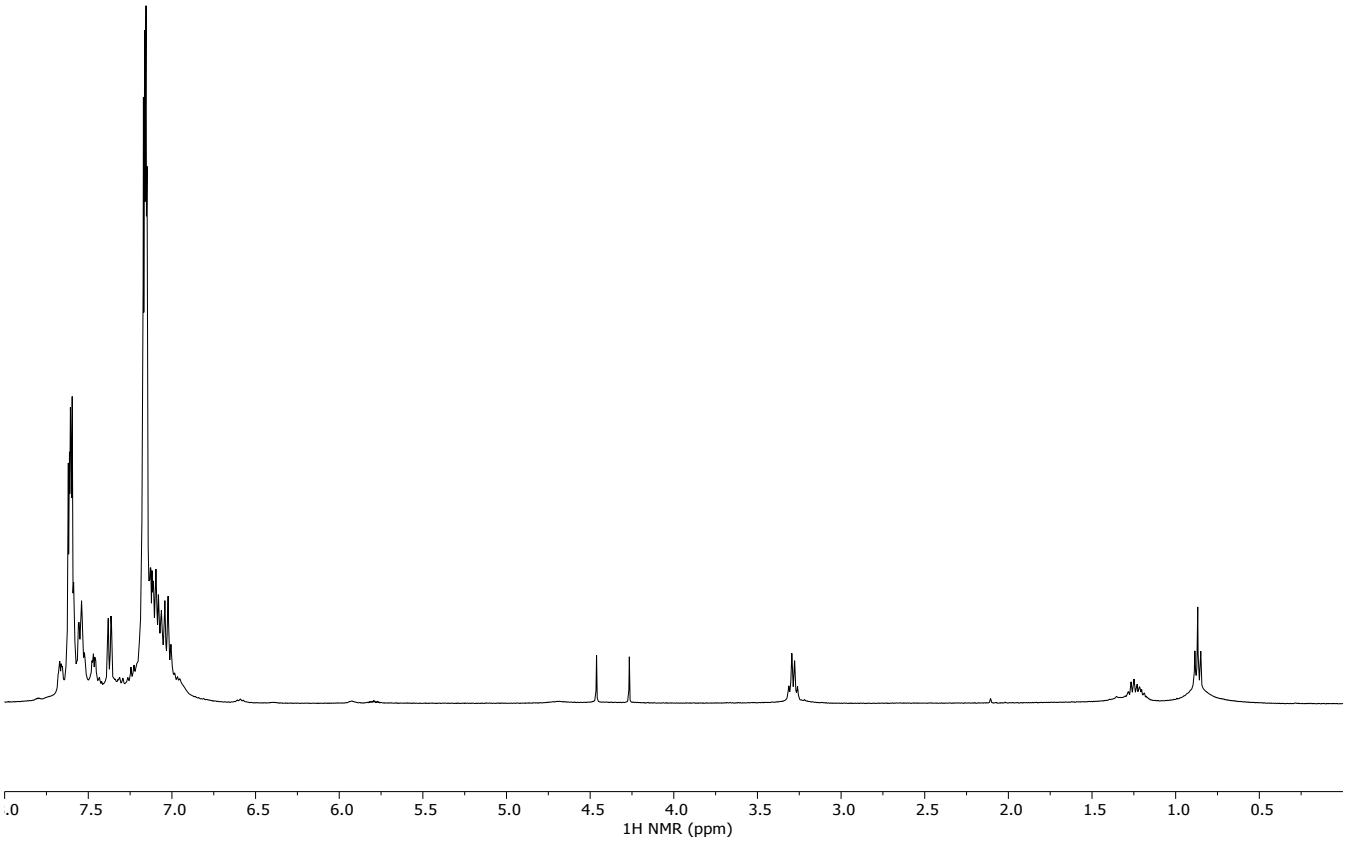

Figure S28. Stacked ^1H NMR spectra of Ph_3SnH with $B(C_6F_5)_3$ (1 eq.) in C_6D_6 at 50 °C over time.

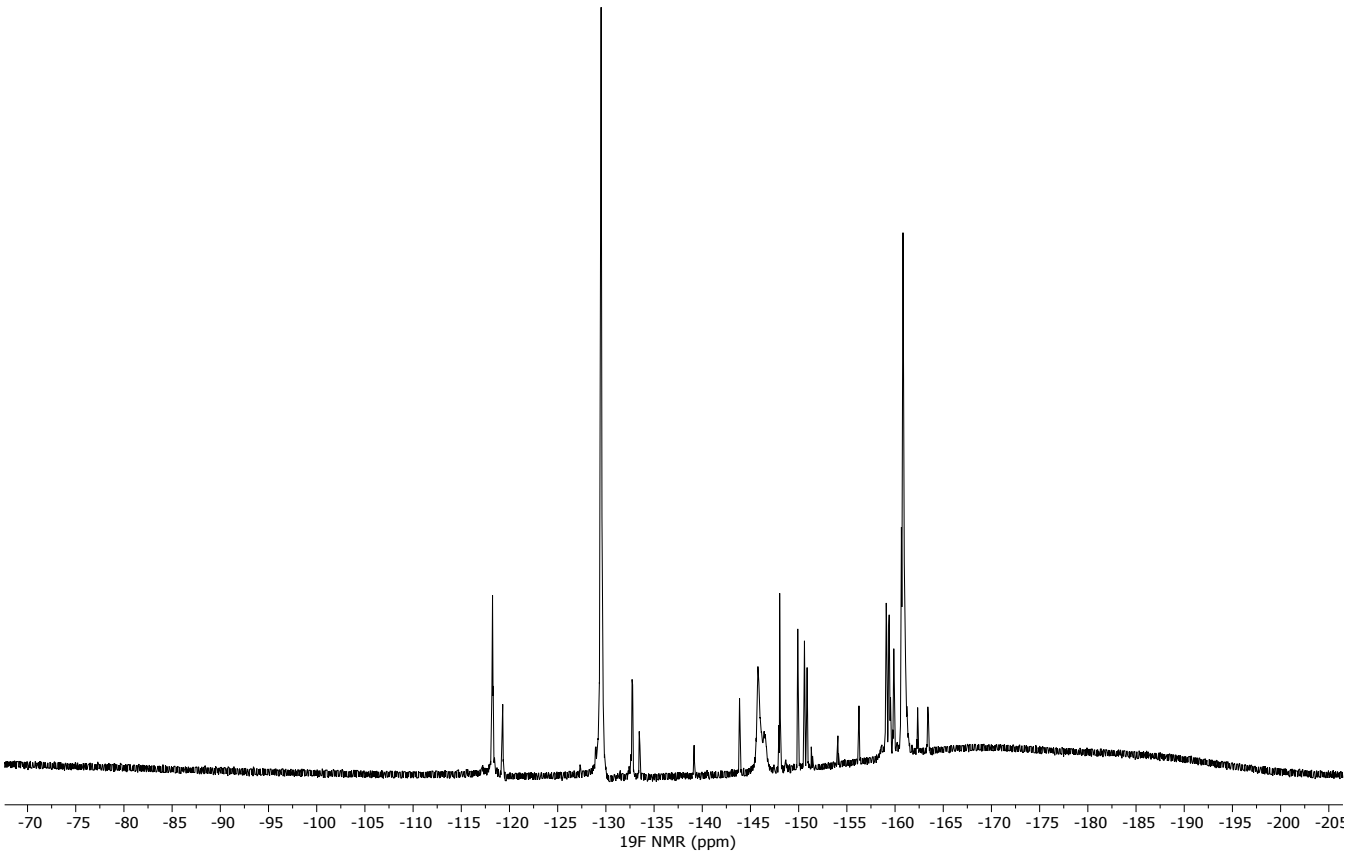

Figure S29. Stacked ^{19}F(decoupled) NMR spectra of Ph_3SnH with $B(C_6F_5)_3$ (1 eq.) in C_6D_6 at 50 °C over time.

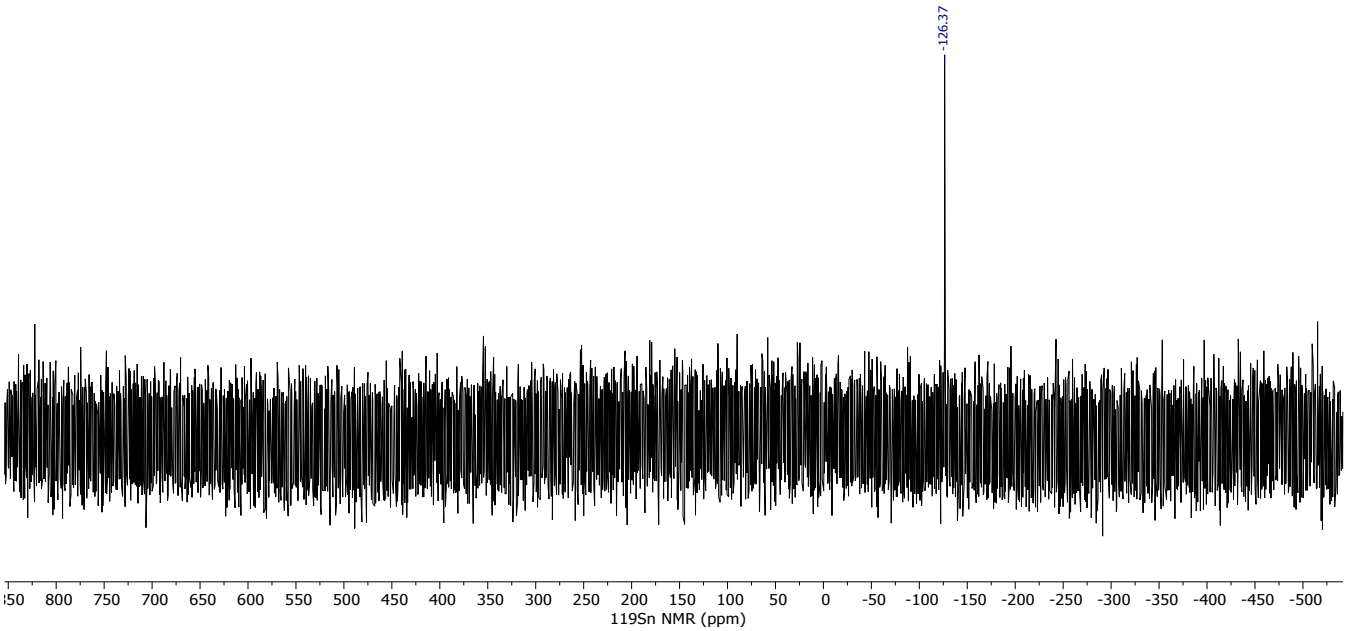

Figure S30. Stacked ^{119}Sn(decoupled) NMR spectra of Ph_3SnH with $B(C_6F_5)_3$ (1 eq.) in C_6D_6 at 50 ^oC over time.

Control Experiment Between $HB(C_6F_5)_2$ and Ph_3SnH

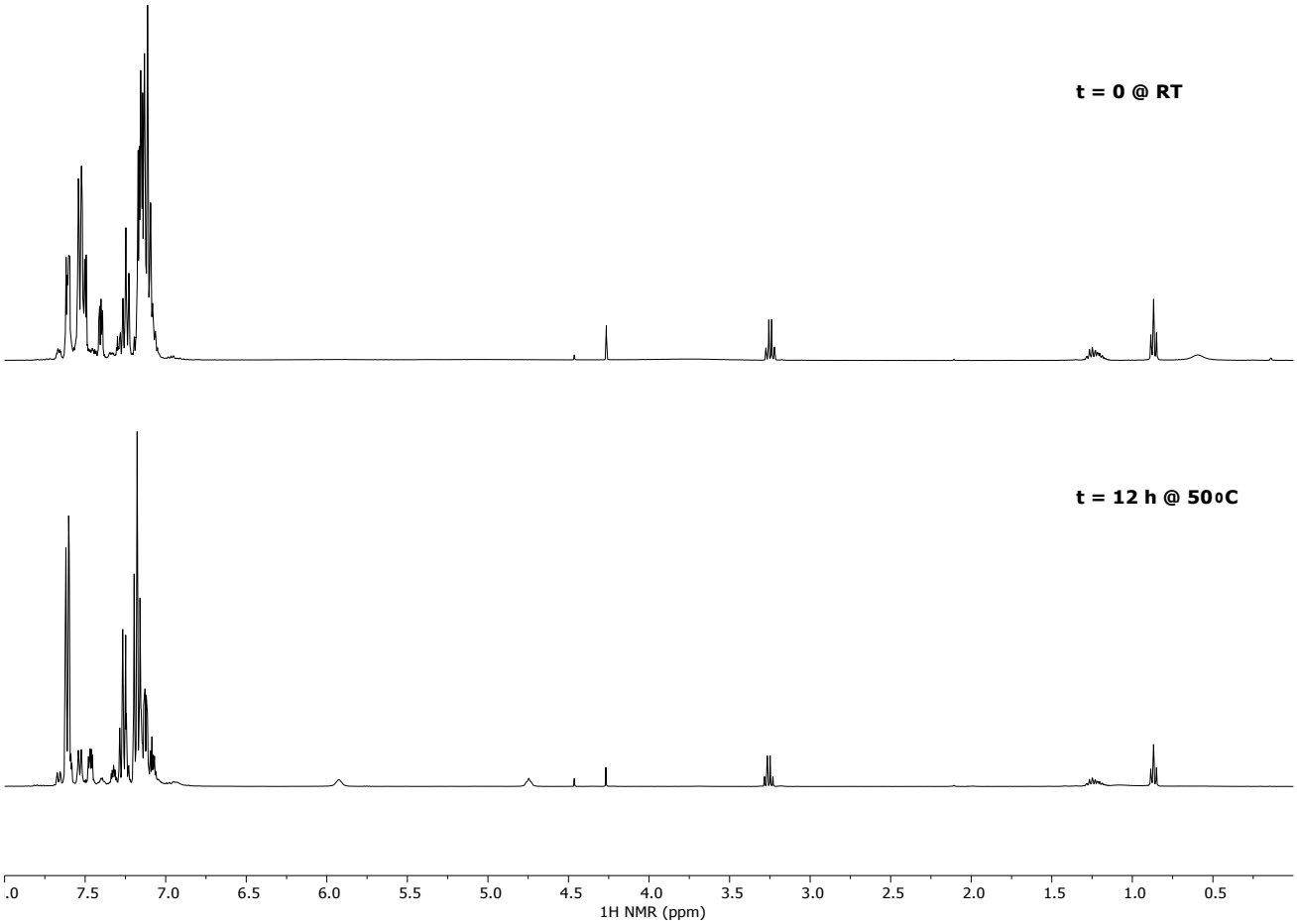

Figure S31. Stacked ^1H NMR spectra of Ph_3SnH with $HB(C_6F_5)_2$ (1 eq.) in C_6D_6 at 50 °C over time.

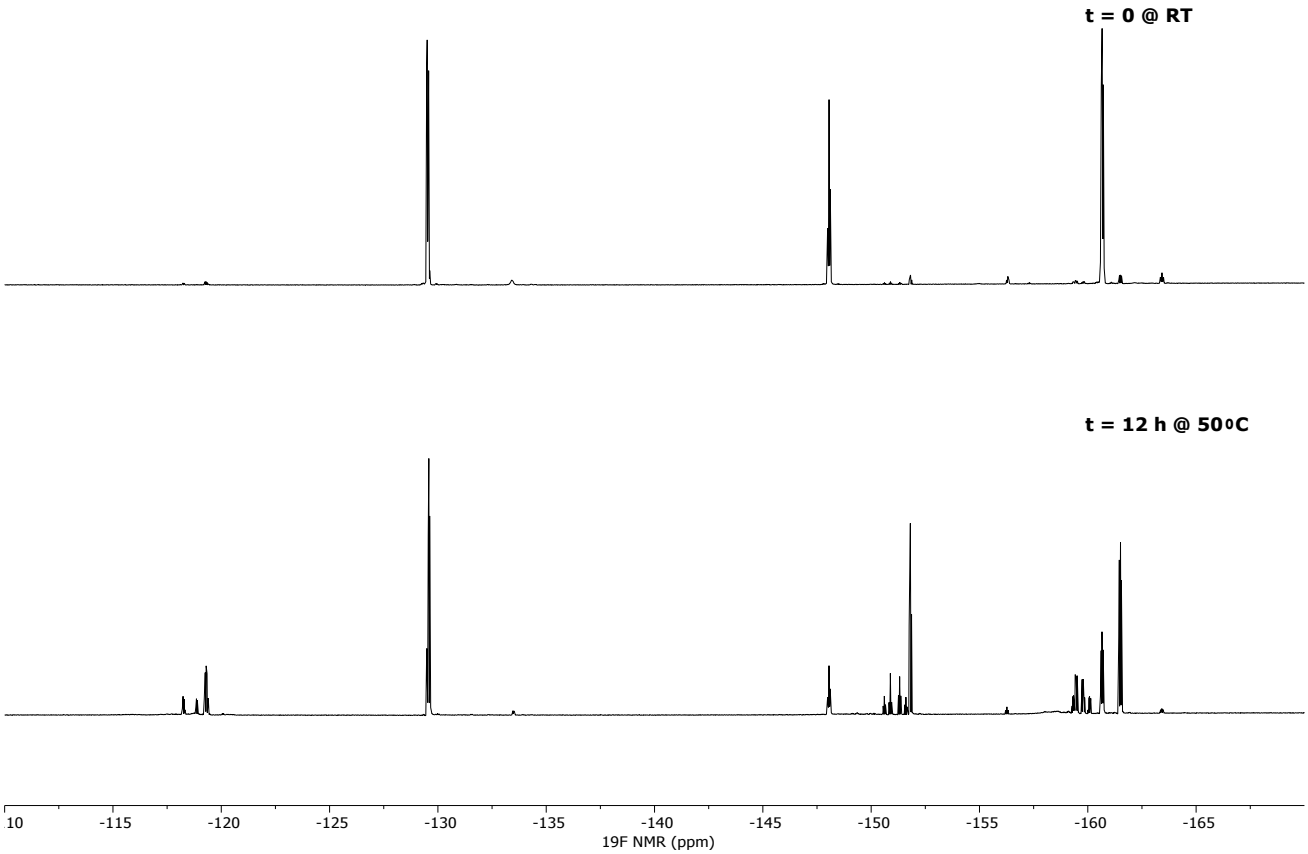

Figure S32. Stacked ^{19}F NMR spectra of Ph_3SnH with $HB(C_6F_5)_2$ (1 eq.) in C_6D_6 at 50 °C over time.

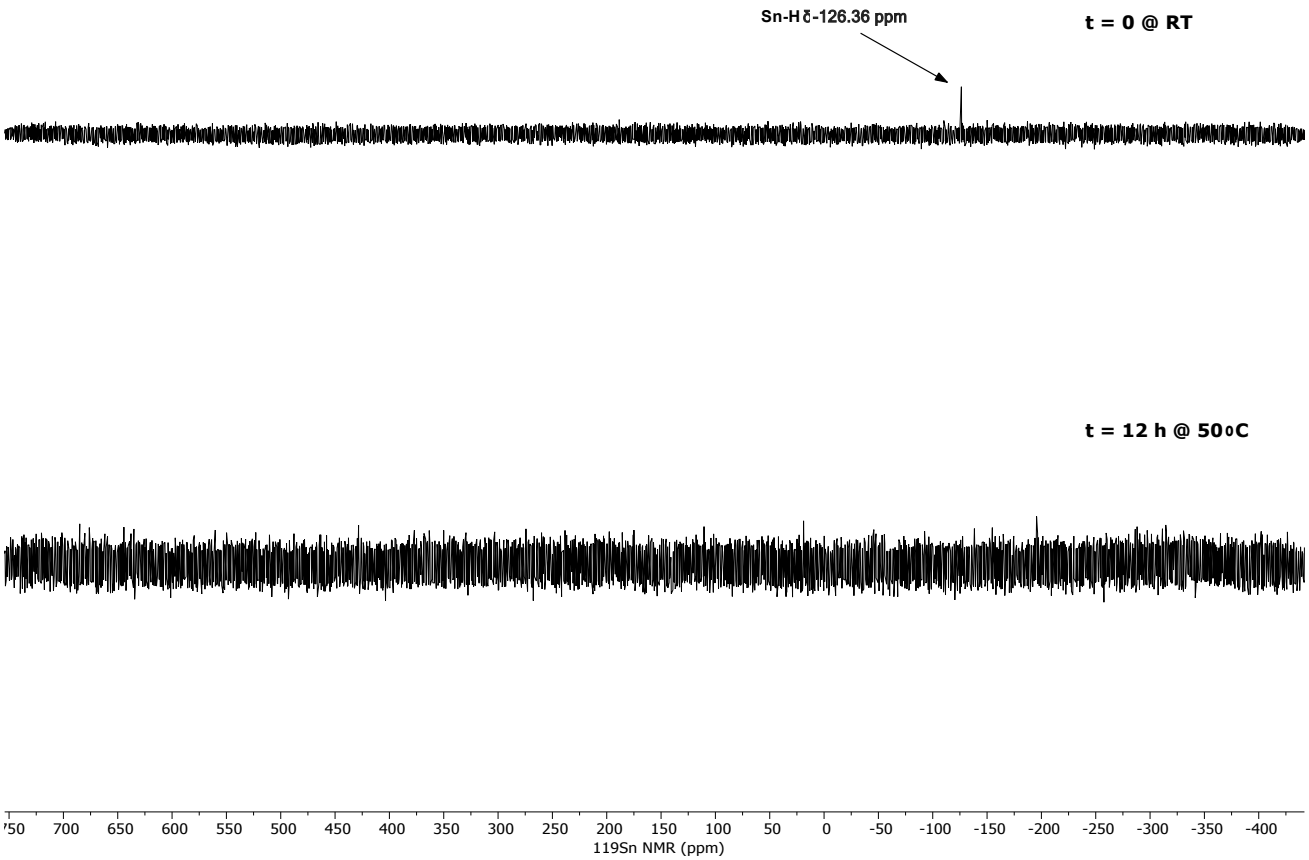

Figure S33. Stacked ^{119}Sn NMR spectra of Ph_3SnH with $HB(C_6F_5)_2$ (1 eq.) in C_6D_6 at 50 °C over time.

*Metallic Sn was observed to preciptate as a grey insoluble powder, hence no signal was observed after 12 h at 50 °C.

6 Catalytic Dehydrocoupling Experiments

General Catalytic Procedure: In the glovebox, R_3SnH (0.25 mmol) was massed out into a 5 mL scintillation vial and dissolved in C_6D_6 (0.4 mL). Compound **1** (5-10 mol%) was massed out into a separate vial and dissolved in C_6D_6 (0.2 mL). The solution of R_3SnH was transferred to a J-young tap NMR spectrum tube, followed by the careful addition of the solution of **1**. The NMR spectrum tube was promptly sealed. The reaction was monitored by ^{1}H and ^{119}Sn NMR spectrum overtime at specific time intervals (ie. 0 hour, 3 hours 6 hours, etc); and heated as necessary. The reaction was deemed complete upon either no observable progression or complete conversion.

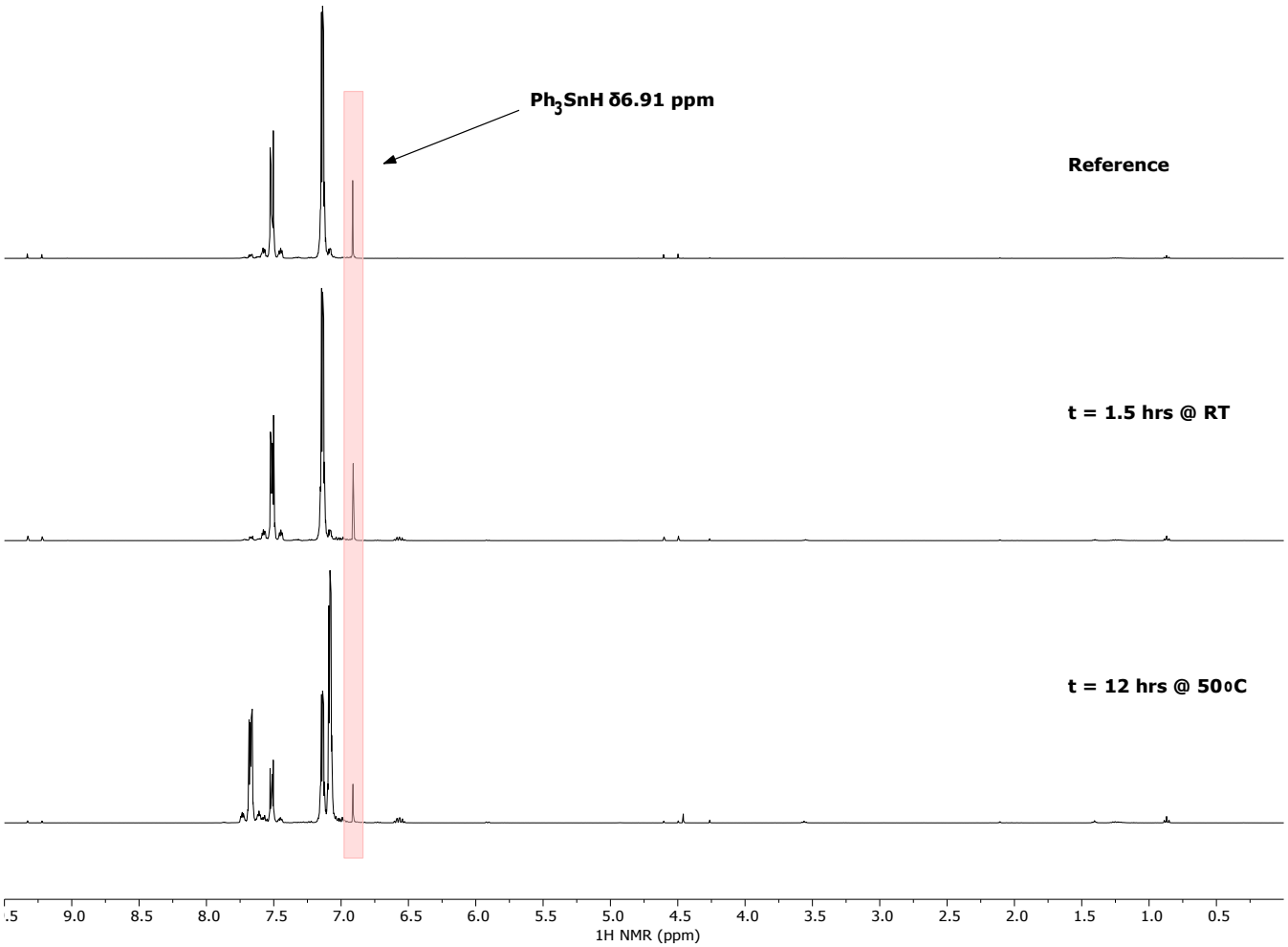

*Figure S34. Stacked ^{1}H NMR spectra of Ph_3SnH with **1** (5 mol%) in C_6D_6 with increasing temperature over time.*

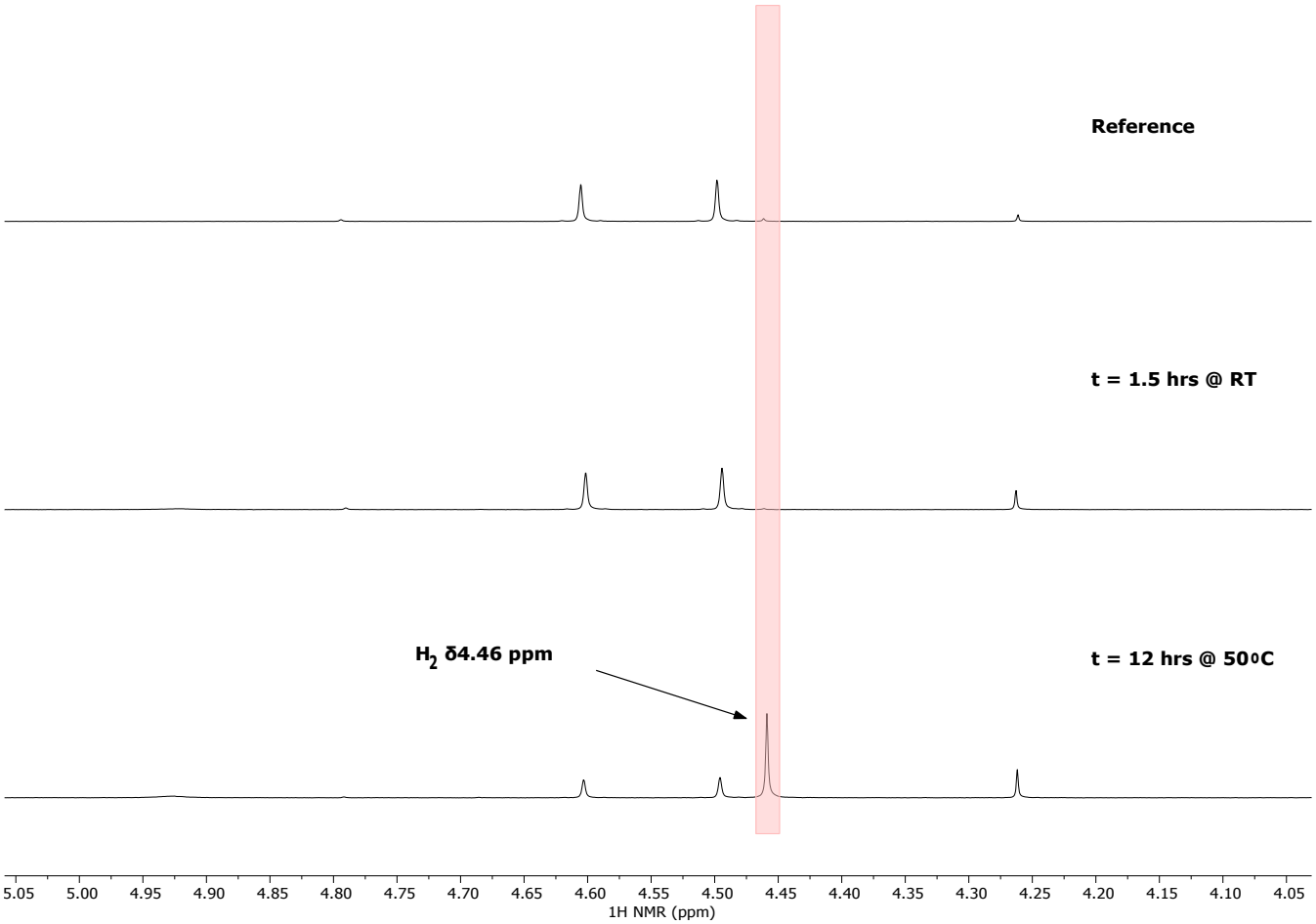

*Figure S35. Stacked ^{1}H NMR spectra of Ph_3SnH with **1** (5 mol%) in C_6D_6 with increasing temperature over time; expanded region.*

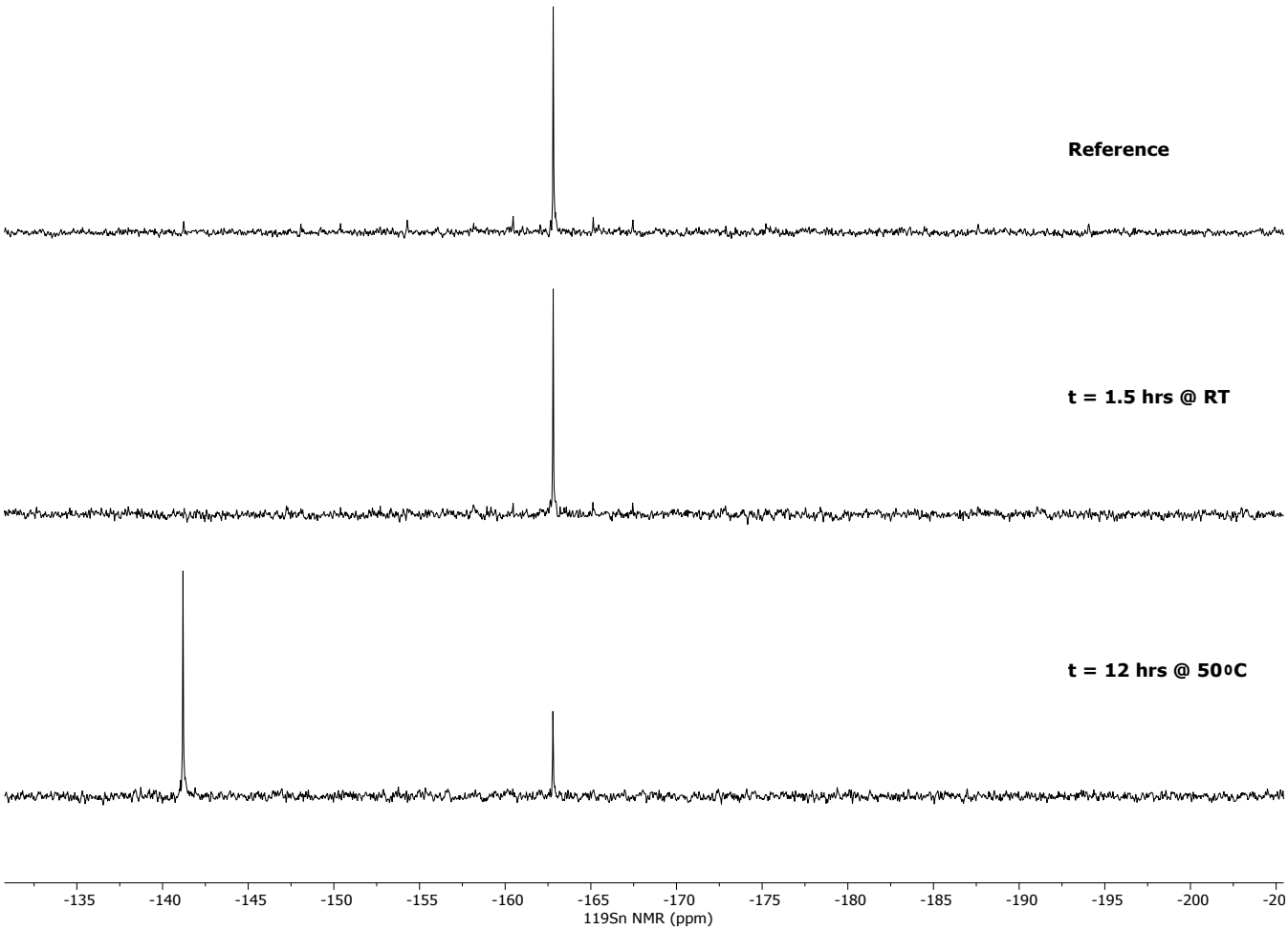

*Figure S36. Stacked ^{119}Sn(decoupled) NMR spectra of Ph_3SnH with **1** (5 mol%) in C_6D_6 with increasing temperature over time.*

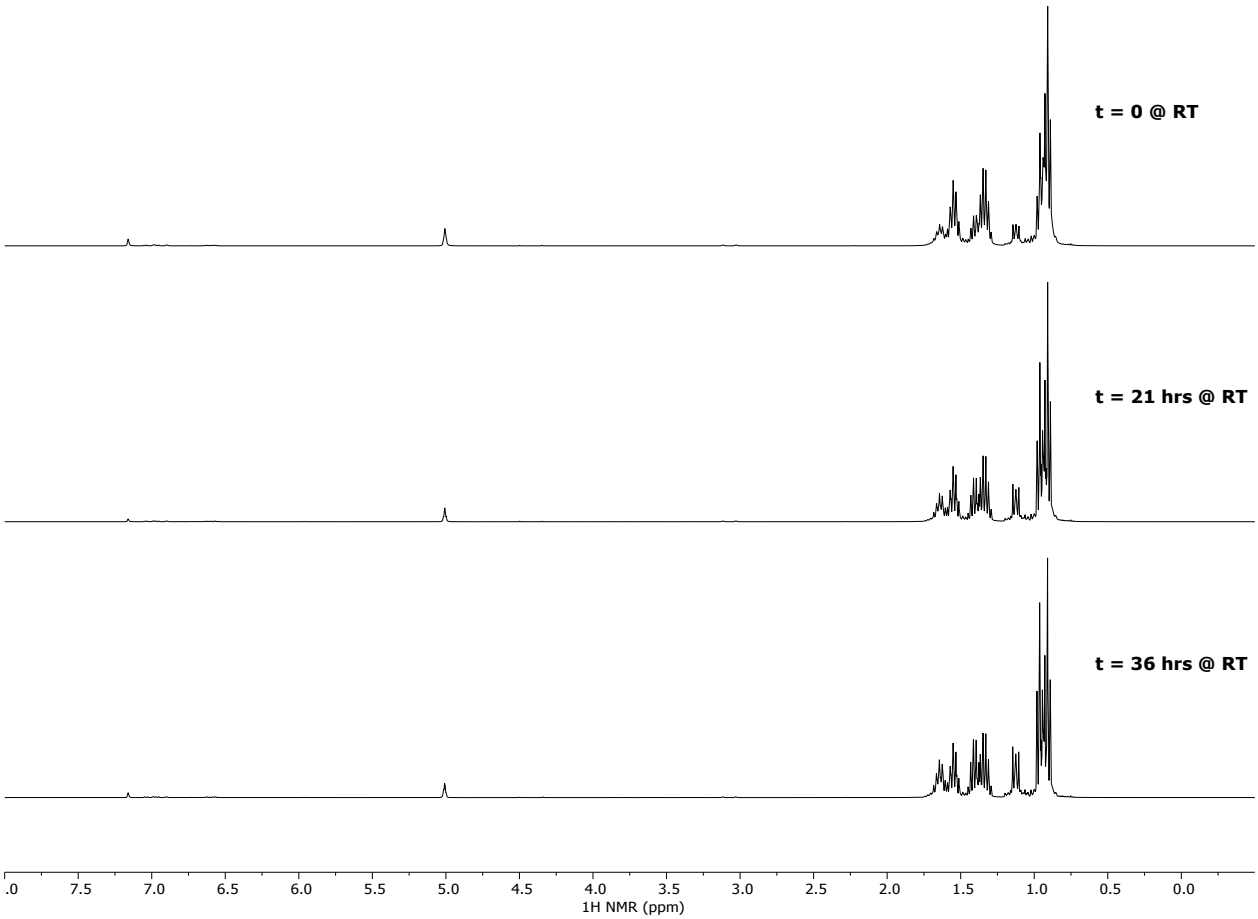

*Figure S37. Stacked ^{1}H NMR spectra of Bu_3SnH with **1** (5 mol%) in C_6D_6 at room temperature over time.*

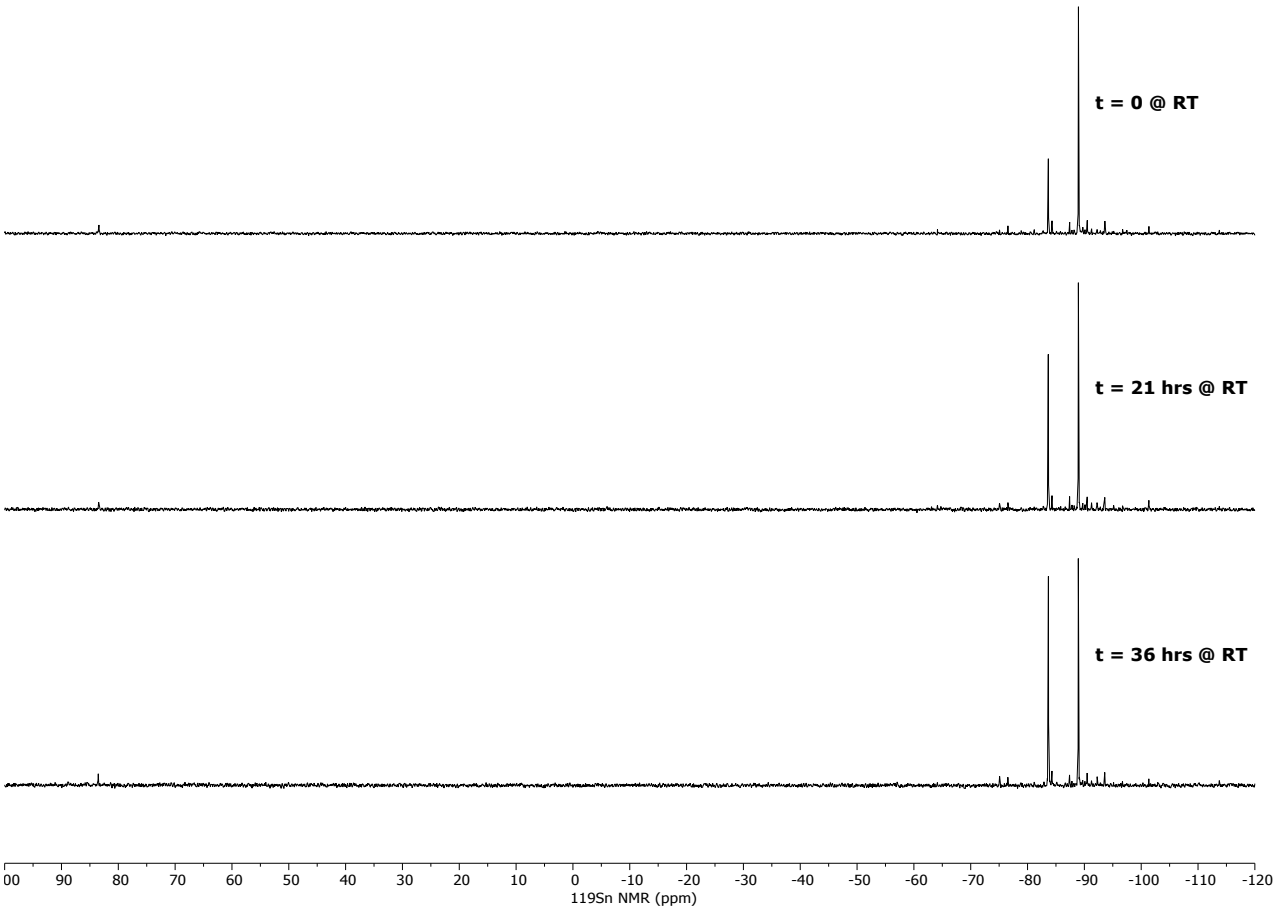

*Figure S38. Stacked ^{119}Sn(decoupled) NMR spectra of Bu_3SnH with **1** (5 mol%) in C_6D_6 at room temperature over time.*

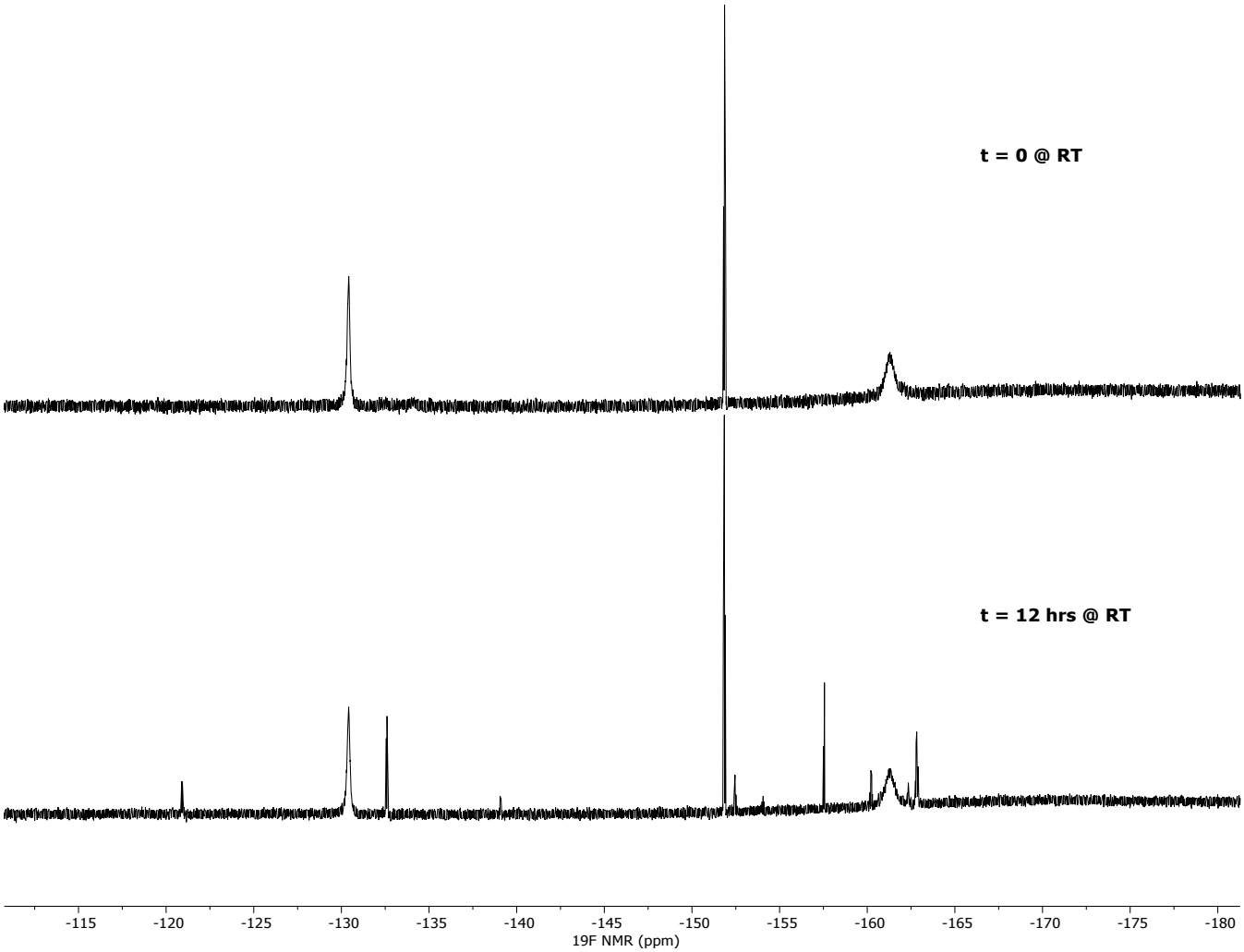

*Figure S39. Stacked ^{19}F NMR spectra of Bu_3SnH with **1** (5 mol%) in C_6D_6 at room temperature over time.*

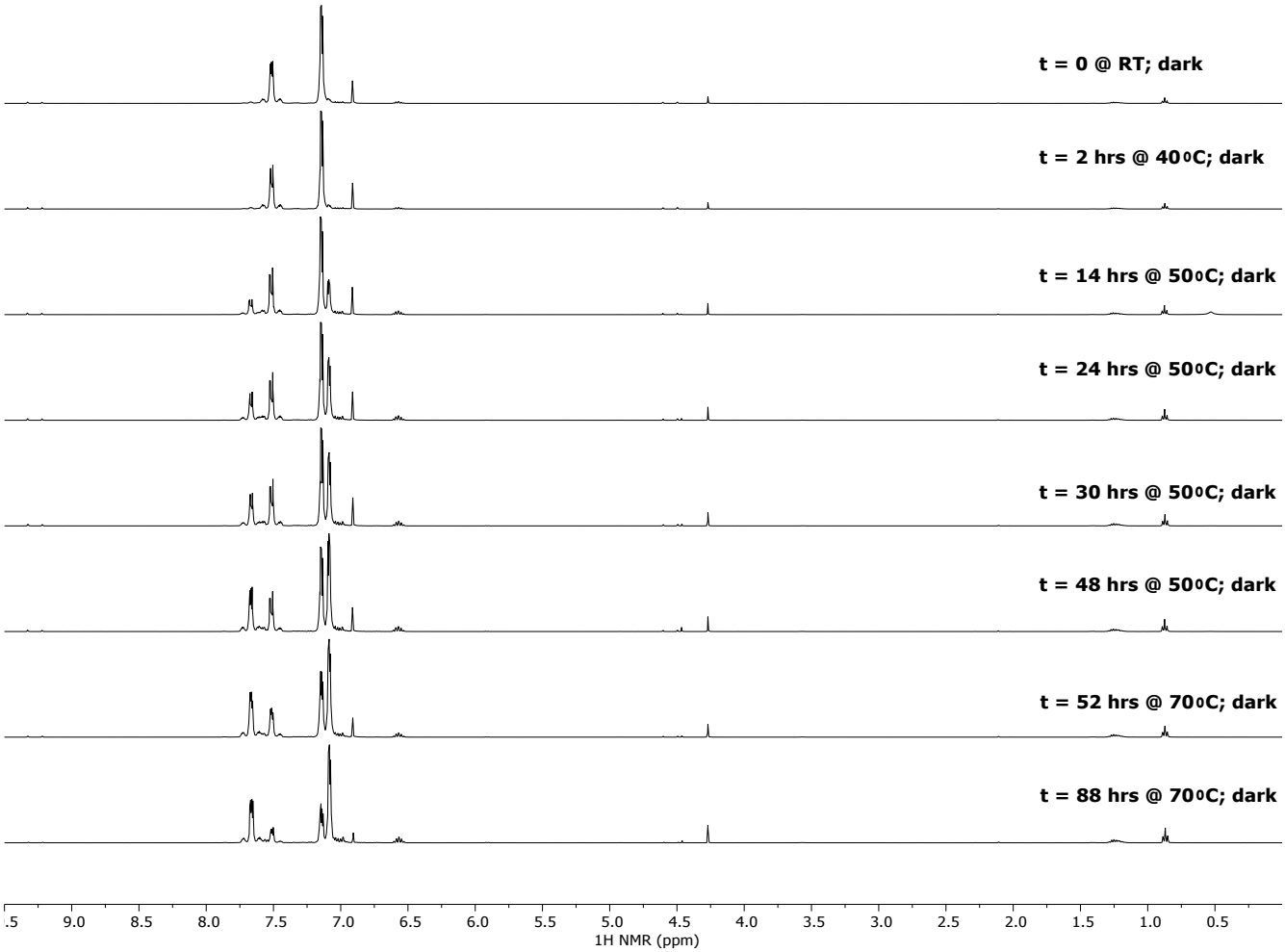

*Figure S40. Stacked ^{1}H NMR spectra of Ph_3SnH with **1** (10 mol%) in C_6D_6, in the dark, with increasing temperature.*

*The J-Young NMR tubes used were wrapped in aluminium foil as a control to observe whether the reaction was promoted via homolytic cleavage by ambient light; a common property of organotin compounds.

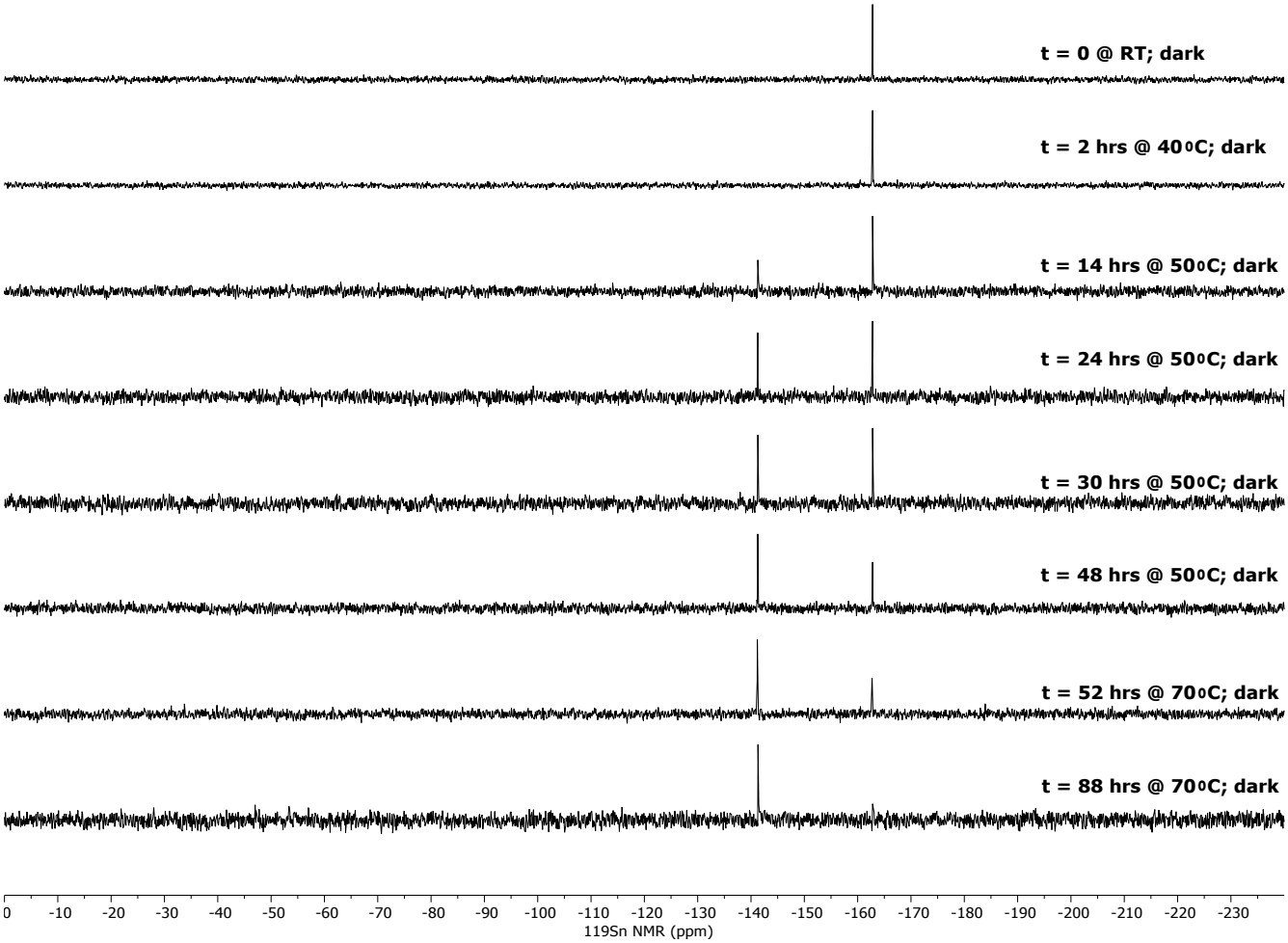

*Figure S41. Stacked ^{119}Sn(decoupled) NMR spectra of Ph_3SnH with **1** (10 mol%) in C_6D_6, in the dark, with increasing temperature.*

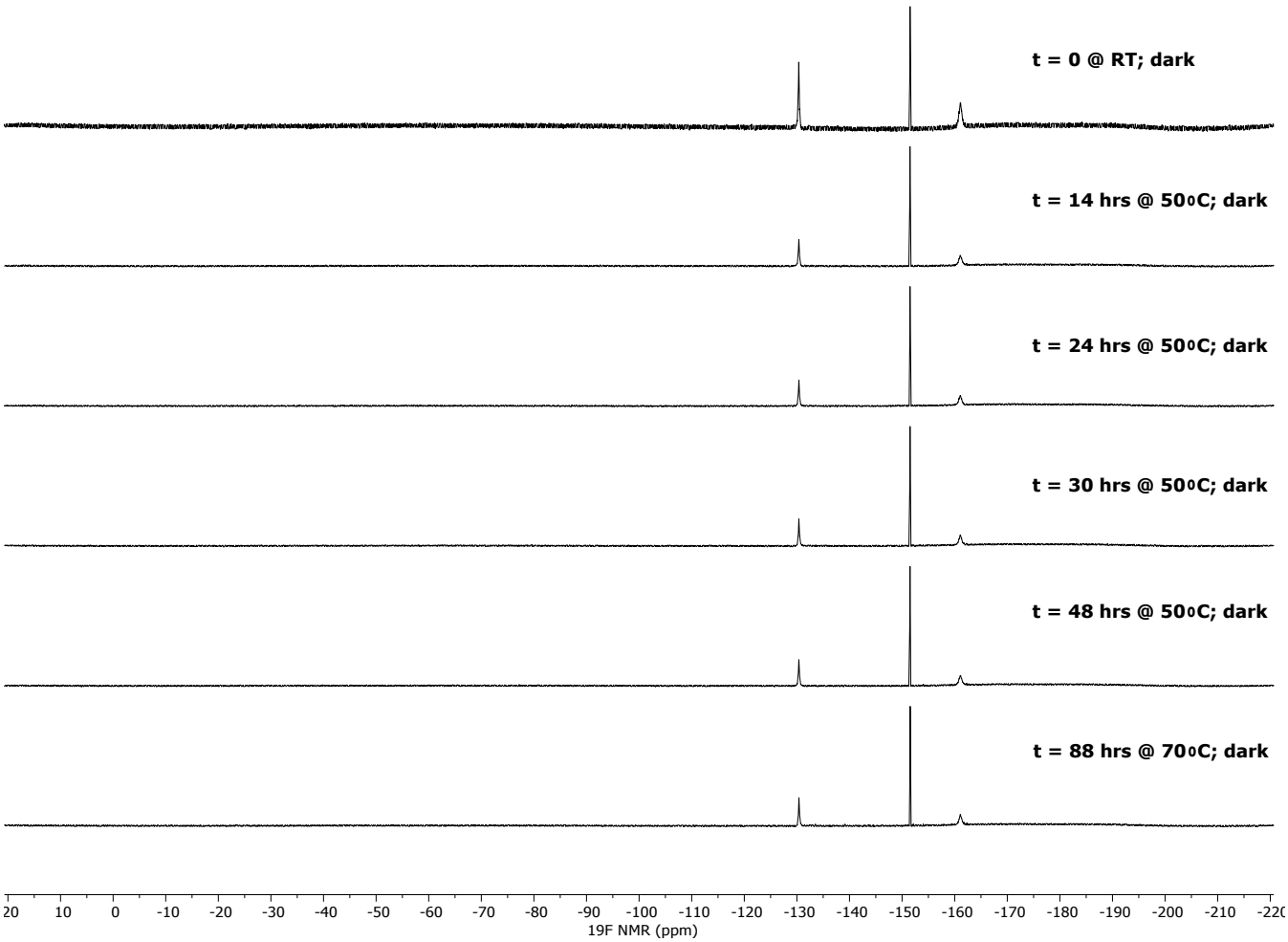

*Figure S42. Stacked ^{19}F NMR spectra of Ph_3SnH with **1** (10 mol%) in C_6D_6, in the dark, with increasing temperature.*

7 X-ray Diffraction (XRD) Analysis

*Table S1. Crystal Data and Structure Refinement of **1**.*

	1
Identification Code	Jnb017_0ma_a
Empirical Formula	$C_{24}H_8B_1F_{10}N_1S_1$
Formula Weight	543.18
Temperature	173(2) K
Wavelength	0.71073 Å
Crystal System	triclinic
Space Group	P-1
Unit Cell Dimensions	a = 9.7033(4) Å; α = 99.0980(1) b = 10.0984(4) Å; β = 107.0960(1) c = 11.5708(4) Å; γ = 98.3520(1)
Volume	1047.75(7)
Z	2
Density (calculated)	1.722
Absorption Coefficient	0.258
F(000)	540
Crystal Size	0.4 x 0.4 x 0.2 mm3
Theta range for data collection	5.47 – 93.342
Index Ranges	-19<=h<=19, -20<=k<=20, -23<=l<=23
Reflections Collected	125982
Independent Reflections	18699
Completeness to theta = 25.242 °	0.994
Absorption Correction	N/A
Max. and min. Transmission	0.902, 0.950
Refinement Method	Full-matrix least-squares on F^2
Data / Restraints / Parameters	18699 / 0 / 366
Goodness-of-fit on F^2	1.068
Final R Indices [I>2sigma(I)]	R1 = 0.0970 wR2 = 0.2010
R Indices (all data)	R1 = 0.1575 wR2 = 0.2497
Extinction coefficient	N/A
Largest diff. peak and hole ($e.Å^{-3}$)	1.05; -0.86

Table S2. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for JNB017_0ma_a. U_{eq} is defined as 1/3 of the trace of the orthogonalized UIJ tensor.

Atom	***x***	***y***	***z***	**U(eq)**
S001	4224.6(4)	10408.5(4)	3334.5(3)	23.17(7)
F00A	9861.4(16)	5034.1(16)	2663.4(15)	49.5(4)
F00B	11499.1(14)	7072.9(17)	4653.7(16)	49.8(4)
F002	7347.5(11)	8982.1(10)	4479.5(10)	26.88(18)
F003	4564.9(12)	6896.6(10)	4570.3(9)	26.57(18)
F004	2276.8(14)	2128.5(10)	1167.4(10)	32.1(2)
F005	1643.3(13)	2469.2(11)	3316.7(11)	32.2(2)

F006	6986.7(14)	4964.3(12)	1612.2(10)	32.7(2)
F007	3931.6(14)	4192.3(11)	666.3(9)	30.4(2)
F008	10197.5(12)	8971.2(12)	5605.3(11)	32.6(2)
F009	2833.3(13)	4838.2(11)	5038.3(10)	29.2(2)
N00C	4729.6(12)	7927.0(10)	1922.2(10)	16.42(15)
C00D	5586.5(14)	9170.7(12)	1831.2(11)	17.46(18)
C00E	3116.5(15)	4688.0(13)	3966.9(12)	19.60(19)
C00F	4310.7(14)	5619.2(12)	2604.8(11)	16.90(17)
C00G	3996.2(14)	5731.7(12)	3706.7(11)	17.62(18)
C00H	7942.6(15)	8014.9(13)	3991.3(13)	19.78(19)
C00I	3711.5(16)	4381.7(13)	1769.6(12)	19.60(19)
C00J	6504.1(17)	9147.2(14)	1107.9(14)	22.3(2)
C00K	7072.2(14)	7007.0(12)	2966.0(12)	17.98(18)
C00L	5453.6(15)	10409.0(13)	2474.1(13)	19.81(19)
C00M	2100.8(16)	6933.1(14)	789.8(13)	22.0(2)
C00N	2821.1(15)	9064.4(13)	2313.6(12)	19.80(19)
C00O	3194.1(14)	7958.9(12)	1664.8(11)	17.49(17)
C00P	2527.2(16)	3474.6(13)	3098.4(13)	21.0(2)
C00Q	2834.9(16)	3306.1(13)	1999.9(12)	20.9(2)
C00R	7766.0(17)	6004.5(15)	2567.8(13)	22.6(2)
C00S	9418.6(16)	8031.5(15)	4584.2(14)	23.8(2)
C00T	6297.0(19)	11634.3(14)	2433.3(16)	26.3(3)
C00U	1340.1(17)	9094.8(16)	2140.8(16)	26.1(3)
C00V	629.7(17)	6971.6(17)	618.4(17)	28.5(3)
C00W	252.3(18)	8039.8(18)	1305.5(18)	29.6(3)
C00X	7351(2)	10369.6(17)	1072.7(17)	29.0(3)
C00Y	9241.8(19)	6012.5(18)	3110.5(18)	29.9(3)
C00Z	10071.0(18)	7037.2(19)	4122.3(18)	30.0(3)
C010	7260(2)	11603.7(17)	1745.8(18)	30.7(3)
B11	5344.7(16)	6889.7(14)	2418.2(13)	16.9(2)

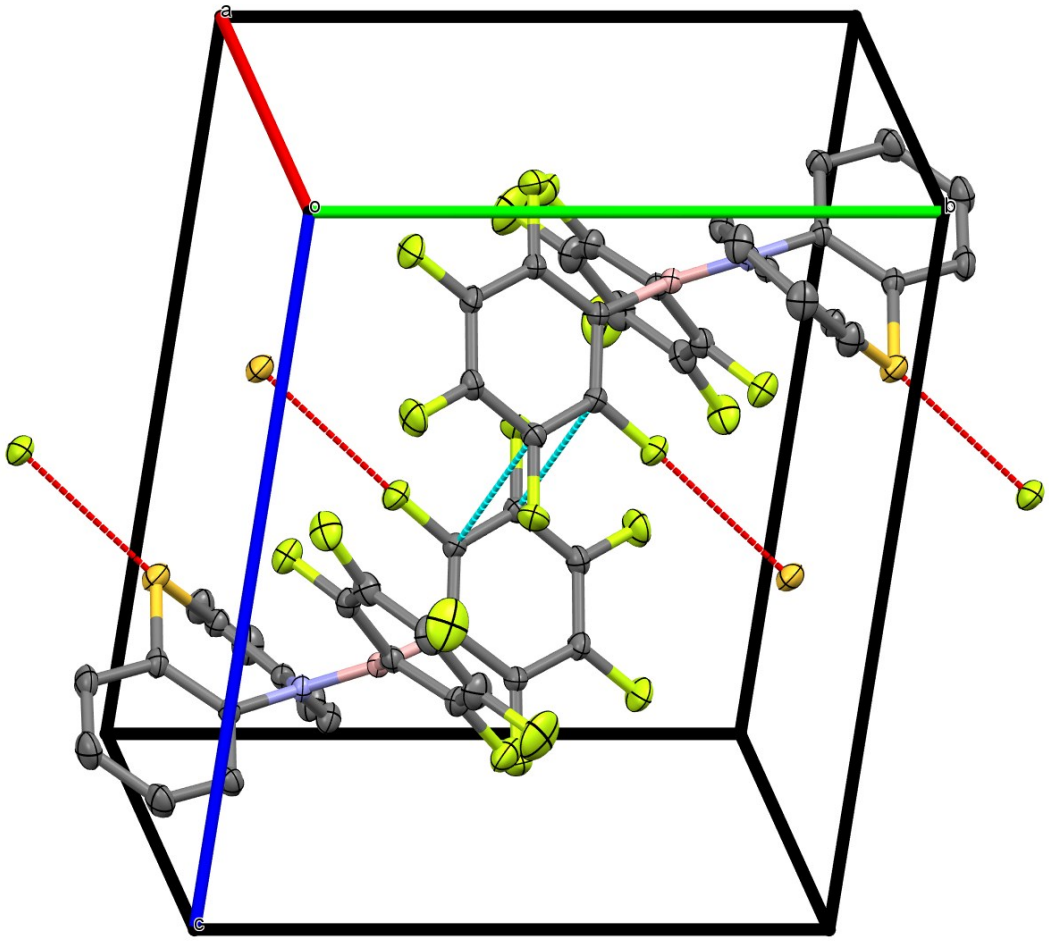

*Figure S43. Packed unit cell of **1** with significant contacts highlighted. Thermal ellipsoids are drawn at the 50% probability level. Hydrogen atoms are omitted for clarity. B: pink, B: black, N: blue, F: yellow-green, S: yellow.*

8 Computations

Given below are the cartesian coordinates in Å of the optimized structures and transition state structures obtained from quantum chemistry calculations. Also given are the PCM corrected Gibbs energies, dispersion corrections, and zero point energies of the structures. The energies are in the unit of Hartree.

8.1 Structures for Figure 2 in the main text

Structures of this section are obtained by optimizations and transition state searches using CAM-B3LYP functional, DEF2-SVP basis set, D3 dispersion correction, and PCM solvent model.

$HSnMe_3$: G(Solv) = -334.4257696, dispersion correction = -0.008460456, ZPE = 0.11477442
$HSnMe_3$ coordinates:

Sn	-0.11245400	0.04748000	-0.17049500
C	-1.01600600	1.79126800	-1.05896800
C	-0.92939700	-1.83583200	-0.82182000
C	1.99496400	0.01571400	-0.61204400
H	-0.54747500	2.68134500	-0.61511300
H	-0.39129600	-2.64169800	-0.30314500
H	2.48359700	-0.80313300	-0.06742700
H	-2.09387500	1.82317600	-0.84405200
H	-0.79175300	-1.96806600	-1.90497700
H	2.14873000	-0.14183100	-1.68988400
H	-0.86196400	1.81619600	-2.14729700
H	-1.99816200	-1.92162800	-0.57915600
H	2.47113500	0.96151900	-0.31853100
H	-0.35604600	0.17549200	1.53291200

Sn_2Me_6: G(Solv) = -667.69250615, dispersion correction = -0.023574506, ZPE = 0.21658855
Sn_2Me_6 coordinates:

Sn	-2.58292200	0.41843300	0.36979400
Sn	0.16461000	0.26821500	0.39582400
C	0.92712600	2.28005800	0.60910900
H	2.00302800	2.35075900	0.39176600
H	0.74166700	2.63113200	1.63498700
H	0.38645500	2.94265900	-0.08092100
C	-3.17970300	0.48844100	-1.70766000
H	-4.25925100	0.32987000	-1.84287800
H	-2.63503600	-0.27754400	-2.27583300
H	-2.90636700	1.47210300	-2.11758400
C	0.79090000	-0.56718300	-1.50079900
H	0.14270500	-1.41329800	-1.76664400
H	1.83251300	-0.91994100	-1.48416800
H	0.68487300	0.20178000	-2.27957300
C	-3.36633900	-1.35602900	1.33640500
H	-2.74930500	-1.59301000	2.21423300
H	-3.29348700	-2.19704800	0.63183400
H	-4.41096700	-1.24937300	1.66212400
C	0.81634200	-0.95900000	2.05322700
H	0.71764400	-0.38548400	2.98671000
H	1.85935100	-1.29025300	1.94396800
H	0.17748800	-1.85004900	2.12768700
C	-3.19791400	2.27762700	1.28914900
H	-2.61268500	3.08748200	0.82998900
H	-2.98918500	2.27555200	2.36908200
H	-4.26601200	2.48178600	1.12588300

H_2: G(Solv) = -1.16346598, dispersion correction = -0.000051553, ZPE = 0.00994098
H_2 coordinates:

H	0.000000	0.000000	0.381891
H	0.000000	0.000000	-0.381891

$B(PFP)_2$-$NS(Ph)_2$: G(solv) = -2393.19944119, dispersion correction = -0.066005798, ZPE = 0.27872243
$B(PFP)_2$-$NS(Ph)_2$ coordinates:

F	0.30169600	2.56959700	1.55742400
F	1.35728600	5.00627200	1.17359100
F	2.35105700	5.68771300	-1.27114900
F	2.34210800	3.88138200	-3.28726800
F	1.24279700	1.45151400	-2.91494400
F	-1.14470100	-1.24297700	-2.55374500
F	-4.63400900	2.45817300	-0.67913200
F	-2.09985500	2.43068700	0.23336200
N	0.42445000	-0.56478500	0.10962300
C	1.76895200	-0.70241200	0.58631700
C	2.29376800	0.13365500	1.56766000
H	1.67063000	0.91882600	1.99099800
C	3.59718900	-0.06118000	2.01707600
C	4.36484600	-1.10536400	1.50487200
C	3.83483200	-1.95860700	0.54136700
H	4.41910300	-2.79421900	0.15216100
C	2.53336200	-1.76152500	0.08510000
C	-1.55835900	-1.81801200	0.87362700
H	-1.95289200	-0.90945900	1.32930700
C	-0.33186700	-1.77856400	0.21874700
C	0.74303500	1.92529200	-0.66511200
C	0.80155900	2.86610100	0.35398500
C	1.34054100	4.13334400	0.17734600
C	1.85293600	4.47972000	-1.06810800
C	1.83771300	3.55609600	-2.10676500
C	1.28083100	2.30206700	-1.88907800
C	-1.53991900	0.58427700	-1.12094500
C	-1.98184700	-0.32574500	-2.07710100
C	-3.28523300	-0.32663100	-2.55955200
C	-3.77440100	1.55905400	-1.13669300
C	-2.46234500	1.52851400	-0.68235300
B	-0.07627100	0.57752800	-0.52301200
H	4.00564100	0.59727800	2.78561100
H	5.37418300	-1.28174900	1.88213100
S	1.80307400	-2.87021500	-1.09236500
C	-2.27207600	-3.01128600	0.93599500
C	0.20221200	-2.94466100	-0.33817400
F	-3.68427900	-1.21342700	-3.46205300
C	-4.18448700	0.61649200	-2.07337700
H	-3.23494200	-3.03945300	1.44867500
C	-1.75356900	-4.16682200	0.35518200
C	-0.51448600	-4.13777200	-0.27770400
F	-5.43411100	0.61564400	-2.50216000
H	-2.30969400	-5.10394600	0.41799300
H	-0.09010800	-5.04121100	-0.71957800

$B(\cdots H)(PFP)_2$-$N(\cdots SnMe3)S(Ph)_2$ TS1: G(solv) = -2727.58704224, dispersion correction = --0.097956779, ZPE = 0.39814719
$B(\cdots H)(PFP)_2$-$N(\cdots SnMe3)S(Ph)_2$ TS1 coordinates:

F	-1.05514700	-2.74242300	0.98371400
F	-2.83240900	-3.54324000	2.79654100
F	-4.62702600	-1.79682700	3.83841300
F	-4.62550600	0.79773500	2.99310600
F	-2.87087700	1.62227400	1.17522900
C	-1.86172800	-0.51737200	0.99676200
C	-1.91078600	-1.83371500	1.45135800

C	-2.82481300	-2.27646100	2.40167300
C	-3.74707900	-1.38521300	2.93496400
C	-3.74345700	-0.06552100	2.50318400
C	-2.81308900	0.33550100	1.54998200
F	-2.45687100	1.84130300	-1.84106200
F	-1.64439200	-3.03793700	-4.05036100
F	-0.71430800	-2.54941000	-1.61341100
F	-3.49065800	1.28594800	-4.21777600
F	-3.04167400	-1.12117400	-5.39823000
C	-1.50155700	-0.32366400	-1.61439400
C	-2.24257000	0.61119800	-2.33038600
C	-2.78037700	0.35873000	-3.58799900
C	-1.85649400	-1.85054400	-3.49748400
C	-1.37199300	-1.56775000	-2.22766600
C	-2.56828300	-0.87632600	-4.18539500
B	-0.84931700	0.00069000	-0.16394600
H	-0.88921800	1.25863700	-0.07359900
N	0.66914000	-0.45778300	0.00326900
C	1.41345200	-0.86714300	-1.14414000
C	1.33038000	-0.12303900	-2.32644700
C	1.98226100	-0.50218400	-3.49469600
C	2.79944000	-1.62716700	-3.50027000
C	2.92861500	-2.36390800	-2.32926400
C	2.22794000	-2.00983500	-1.17579400
H	0.69939700	0.75898700	-2.35915000
H	3.55674800	-3.25658500	-2.30533600
H	1.83326300	0.09021200	-4.39928300
H	3.32623200	-1.94178100	-4.40290200
S	2.30156100	-3.12663300	0.18192800
C	0.72222300	-0.17466300	2.43121400
C	1.10677100	-0.88853200	1.28946500
C	1.13524200	-0.53698700	3.70869400
C	1.92263700	-2.01124200	1.49012100
C	1.98711200	-1.62275700	3.88214600
C	2.37792800	-2.34971200	2.76446300
H	0.78406800	0.04369100	4.56360000
H	2.34433400	-1.91684100	4.87104000
H	3.03005600	-3.21842200	2.87315500
H	0.05022500	0.67404100	2.33186600
Sn	0.94197000	2.22103500	0.13537400
C	0.08779100	3.17789100	1.85222400
C	0.61821200	3.17295300	-1.75330600
C	3.00199000	1.74855500	0.46490800
H	0.60343200	2.82762000	2.75500000
H	-0.41654300	3.03327900	-2.08824300
H	3.23754300	0.71221600	0.19858500
H	-0.98627200	2.96598400	1.92040400
H	1.31736800	2.78170600	-2.50102400
H	3.59216100	2.42376000	-0.16950600
H	0.24642700	4.26168100	1.74672200
H	0.81651400	4.24620600	-1.61064100
H	3.24458900	1.93141400	1.51951700

$B(H)(PFP)_2$-N(SnMe3)$S(Ph)_2$: G(solv) = -2727.59663449, dispersion correction = -0.098170103, ZPE = 0.39920378
$B(H)(PFP)_2$-N(SnMe3)$S(Ph)_2$ coordinates:

F	-2.35172300	-2.84769600	-0.31390400
F	-4.19680500	-3.79456400	1.34503800
F	-4.93948700	-2.36609600	3.54214900
F	-3.74238300	0.03260500	4.04455500
F	-2.00124000	1.04240500	2.34721600
C	-2.09020800	-0.84098600	0.90729100

C	-2.70384400	-2.07663400	0.71220500
C	-3.65946700	-2.60289400	1.57527900
C	-4.03688200	-1.88242200	2.70234700
C	-3.44542800	-0.65142900	2.94638800
C	-2.52098700	-0.15427100	2.03828900
F	-2.32086800	1.83719000	-1.68289400
F	-0.98598000	-2.59319900	-4.48528400
F	-0.32399500	-2.43784300	-1.90310100
F	-2.94413600	1.67670000	-4.25824400
F	-2.28179700	-0.52347400	-5.69853500
C	-1.34353700	-0.32318200	-1.64677100
C	-1.99484700	0.70817700	-2.31967800
C	-2.32139400	0.65935900	-3.66962300
C	-1.31862900	-1.51496800	-3.78490900
C	-1.00526100	-1.41772400	-2.43380100
C	-1.97953400	-0.46368900	-4.40838500
B	-1.00631600	-0.13964600	-0.07155200
H	-1.10406100	1.03144400	0.18238300
N	0.61398300	-0.47946500	0.23754500
C	1.39203600	0.14687900	-0.84764400
C	1.05927500	1.45665200	-1.22669200
C	1.72503600	2.12868400	-2.24103900
C	2.78053900	1.51452200	-2.90856300
C	3.12783100	0.22433500	-2.55283800
C	2.43564200	-0.46749300	-1.54903900
H	0.22544100	1.95318400	-0.74188900
H	3.94298600	-0.28737700	-3.06888700
H	1.39017000	3.12780700	-2.52605900
H	3.32397000	2.02988800	-3.70165800
S	2.97740300	-2.11676800	-1.31735200
C	0.29208500	-2.42906300	1.69910900
C	0.96504800	-1.85444200	0.61508800
C	0.60010100	-3.68823300	2.19627500
C	1.99422600	-2.61371600	0.04329600
C	1.63038600	-4.42349100	1.62266100
C	2.31384100	-3.87845700	0.54857300
H	0.03510100	-4.08041500	3.04271100
H	1.91579800	-5.40105100	2.01573900
H	3.12690900	-4.43506000	0.07723500
H	-0.49058500	-1.86678100	2.19029200
Sn	1.28087100	0.70843400	2.08914400
C	0.51870500	-0.10740900	3.91370700
C	0.72190200	2.75854700	1.91765100
C	3.36631300	0.30310600	1.91266300
H	0.82472100	-1.14966500	4.05555400
H	-0.36966000	2.85369100	1.94153600
H	3.73480000	0.56873700	0.91426500
H	-0.56916900	-0.00318000	3.98806200
H	1.13257200	3.23088300	1.01917000
H	3.89369700	0.91416900	2.65766600
H	0.98348900	0.50737500	4.69921800
H	1.15164200	3.25064600	2.80240000
H	3.56612900	-0.75715700	2.11566400

B(H)$(PFP)_2$-N(···H···SnMe3···SnMe3)$S(Ph)_2$ TS2: G(solv) = -3061.96734849, dispersion correction = -0.126860383, ZPE = 0.51412294

B(H)$(PFP)_2$-N(···H···SnMe3···SnMe3)$S(Ph)_2$ TS2 coordinates:

B	-3.05566000	1.03206100	0.04029200
H	-3.05612800	2.07419700	0.63535300
N	-1.62228200	1.00928100	-0.76717800
Sn	1.59973500	1.81662700	-0.11540000

C	2.74607900	3.63492900	-0.20445200
C	1.75447300	1.11409100	-2.13567800
C	2.38241600	0.46403300	1.35691900
H	2.23737200	4.37248500	-0.83670100
H	2.72882900	1.48347500	-2.48768700
H	2.82498900	-0.39988800	0.84282000
H	3.68813800	3.34295600	-0.69283300
H	0.97131900	1.52326000	-2.78085000
H	3.15076900	0.97983600	1.94765000
H	2.96965700	4.07663500	0.77288300
H	1.73249300	0.01918400	-2.17667600
H	1.59276100	0.11166300	2.03033700
Sn	-0.36092500	3.40478400	1.67434900
C	0.17787800	5.34861400	0.91376400
C	0.90426100	2.88798600	3.32863100
C	-2.36861000	3.61874900	2.40261300
H	0.04806500	5.42251000	-0.17322600
H	0.69615700	1.86671100	3.67194300
H	-2.75538700	2.67946700	2.80728600
H	1.21307500	5.59687000	1.17579800
H	0.65096000	3.59064200	4.13579400
H	-2.28655200	4.36720800	3.20586200
H	-0.49313500	6.06899700	1.40127600
H	1.96955500	2.99408100	3.08668800
H	-3.04374600	3.98822600	1.62314000
H	-0.50246300	1.80607900	0.15883800
C	-4.20234400	1.12599900	-1.10555800
C	-4.88762600	2.30938900	-1.34828000
F	-4.78314100	3.34946200	-0.51103200
C	-5.66870600	2.51143700	-2.48300100
F	-6.28993800	3.66996000	-2.69318700
C	-5.77963100	1.49573400	-3.42125400
F	-6.50226500	1.68929200	-4.51859200
C	-5.12401700	0.28652700	-3.20948900
F	-5.18757900	-0.68059500	-4.11822200
C	-4.38430200	0.12399200	-2.04868700
F	-3.77676300	-1.05387000	-1.86921300
C	-3.25870300	-0.12689600	1.16753900
C	-2.42654900	-0.21281100	2.27910500
F	-1.37004400	0.62662700	2.39926700
C	-2.55674500	-1.13590700	3.30526700
F	-1.68231900	-1.17226900	4.30521600
C	-3.62352800	-2.02439500	3.28064900
F	-3.76578300	-2.92391000	4.24322200
C	-4.53067400	-1.94517200	2.23437500
F	-5.58811000	-2.74470200	2.20321200
C	-4.33741200	-1.01192600	1.21756800
F	-5.28813900	-1.00958900	0.28544300
C	-1.64058500	1.97402100	-1.82955300
C	-1.76433600	3.32999100	-1.50253800
H	-1.95634200	3.61340400	-0.47230100
C	-1.73630900	4.32888900	-2.46686300
H	-1.84193200	5.37011000	-2.15546900
C	-1.59280700	3.99279600	-3.80753600
H	-1.55765300	4.76418300	-4.57787200
C	-1.50531500	2.65319100	-4.16083900
H	-1.39884700	2.36262100	-5.20845100
C	-1.54613100	1.64982500	-3.19124700
C	-1.00707000	-0.25502400	-1.05528300
C	-0.89732800	-0.81252500	-2.33871600
S	-1.54305000	-0.01463100	-3.76816600
C	-0.24872400	-2.03082900	-2.53616700
H	-0.15730600	-2.42516300	-3.55085200

C	0.29515800	-2.73098000	-1.46741400
H	0.79935000	-3.68355800	-1.63922900
C	0.21099500	-2.18610600	-0.19280000
H	0.65240900	-2.70127300	0.66165700
C	-0.41834200	-0.96094300	-0.00234600
H	-0.43959700	-0.52670400	0.98941600

$B(H)(PFP)_2$-$N(H)S(Ph)_2$: G(Solv) = -2394.36519048, dispersion correction = -0.070636090, ZPE = 0.30124993
$B(H)(PFP)_2$-$N(H)S(Ph)_2$ coordinates:

F	-3.49866800	-2.13697400	-0.83991000
F	-5.02402100	-3.13432700	1.03685800
F	-4.70729000	-2.37755400	3.64324600
F	-2.79347700	-0.56155900	4.29093200
F	-1.17499200	0.42865300	2.39424100
C	-2.22091500	-0.82386300	0.68496900
C	-3.24465100	-1.72721200	0.40210800
C	-4.08367100	-2.26091300	1.37668800
C	-3.93067900	-1.87184700	2.69924200
C	-2.94906500	-0.94376600	3.03016300
C	-2.13915800	-0.44563800	2.02143800
F	-1.99131400	1.63809800	-2.48991300
F	-1.58754900	-3.53600800	-4.04575200
F	-0.98346600	-2.85996900	-1.51732200
F	-2.63217200	0.95825800	-4.99224600
F	-2.43867400	-1.64004000	-5.79149100
C	-1.41454200	-0.58103800	-1.91295200
C	-1.84496100	0.35978100	-2.84148800
C	-2.19480900	0.02807100	-4.14846100
C	-1.66273300	-2.26660700	-3.66099500
C	-1.33158500	-1.89020400	-2.36969300
C	-2.09656600	-1.29475500	-4.55832500
B	-1.21479500	-0.14340000	-0.38434400
H	-1.30244200	1.05931500	-0.28665500
N	0.38539500	-0.35506400	0.16575100
C	1.31853900	0.39892100	-0.66815200
C	1.48694200	1.75735500	-0.42116400
C	2.34389500	2.50922900	-1.21559700
C	3.01994700	1.90417500	-2.27418600
C	2.86897500	0.54401700	-2.50673400
C	2.02690600	-0.22199800	-1.69544600
H	0.93745800	2.22876500	0.39603600
H	3.42960400	0.05232100	-3.30341900
H	2.49824400	3.56650600	-0.99256200
H	3.68778900	2.48980500	-2.90752700
S	1.92992300	-1.96234600	-1.97267400
C	0.62338500	-2.11511300	1.86253400
C	0.87028600	-1.67528700	0.56571100
C	1.07592200	-3.36210500	2.27806600
C	1.59943000	-2.47290100	-0.31510800
C	1.81534900	-4.15642000	1.40747200
C	2.08392700	-3.70741900	0.11934500
H	0.85357700	-3.70569200	3.28980000
H	2.20418400	-5.12100600	1.73885800
H	2.68151000	-4.31341700	-0.56392100
H	0.08915100	-1.47331200	2.56037500
H	0.29726300	0.17424600	1.03660500

$B(\cdots H)(PFP)_2$-$N(\cdots H)S(Ph)_2$ TS3: G(Solv) = -2394.29939166,
dispersion correction = -0.072153952, ZPE = 0.29490751

$B(\cdots H)(PFP)_2$-$N(\cdots H)S(Ph)_2$ TS3 coordinates:

F	-1.79951300	-2.64666700	0.50906700

F	-2.40586000	-3.66248400	2.88190700
F	-2.16838500	-2.13809500	5.13052300
F	-1.36227000	0.45095400	4.91902900
F	-0.84572600	1.50934300	2.53962500
C	-1.27284500	-0.53027500	1.40691700
C	-1.69951300	-1.84537500	1.56465900
C	-2.00942300	-2.40072100	2.79899600
C	-1.89710300	-1.62219400	3.94357800
C	-1.49259000	-0.29770700	3.83213600
C	-1.21758500	0.22643200	2.57526600
F	-2.50613400	1.84420800	-1.18273500
F	-1.92055900	-2.68804000	-4.07886000
F	-0.69190300	-2.47974200	-1.76174300
F	-3.73352800	1.61758600	-3.54646800
F	-3.51476600	-0.69512400	-4.98652900
C	-1.50559000	-0.28879200	-1.36730800
C	-2.33065700	0.71341100	-1.87543400
C	-2.99166000	0.61567000	-3.09521300
C	-2.06751000	-1.57936300	-3.36748500
C	-1.42331800	-1.44299700	-2.14491200
C	-2.87170600	-0.55229800	-3.83903500
B	-0.69591700	-0.04306900	-0.00407700
N	0.90027400	-0.27605600	-0.11255500
C	1.50402700	-0.83430400	-1.27576200
C	1.54351200	-0.13963600	-2.48217500
C	2.09984100	-0.73157200	-3.61427400
C	2.65865600	-2.00368200	-3.53309100
C	2.64136300	-2.69520800	-2.32443100
C	2.04559900	-2.12331400	-1.20470800
H	1.11837900	0.86427400	-2.53657400
H	3.08236900	-3.69053300	-2.24641000
H	2.10957300	-0.18521600	-4.55913500
H	3.11696200	-2.46236200	-4.41111900
S	1.85931400	-3.06869300	0.28381000
C	1.87074600	0.58471600	1.97659500
C	1.62011700	-0.47567400	1.10844700
C	2.49339900	0.36079800	3.20145200
C	2.07689500	-1.75457200	1.44504400
C	2.90154500	-0.92402200	3.55203100
C	2.71382000	-1.97794300	2.66433600
H	2.67321300	1.19754400	3.87813000
H	3.39868200	-1.10710100	4.50642900
H	3.07651100	-2.97813200	2.90954700
H	1.54780400	1.58966600	1.70270700
H	-0.67911500	1.31078600	0.08403500
H	0.22209500	0.98297900	-0.08348000

8.2 Structures for Fluoride Ion Affinity calculations.

Structures of this section are obtained by optimizations using CAM-B3LYP functional, MA-DEF2-SVP basis set, and D3 dispersion correction. The calculations were carried out assuming a vacuum environment, i.e., without solvent model. The diffuse basis functions in the MA-DEF2-SVP basis set are of critical importance to give reliable FIA. Calculated enthalpies at T=298.15 K are also given in the unit of Hartree. The calculated F^- enthalpy is -99.759205502090 Hartree.

$B(PFP)_2$-$NS(Ph)_2$: H = -2393.357712278914
$B(PFP)_2$-$NS(Ph)_2$ coordinates:

F	0.116185	2.585795	1.603975
F	1.486169	4.869563	1.297870
F	2.803973	5.368806	-1.045093
F	2.713471	3.556281	-3.053882
F	1.287085	1.293094	-2.769689

F	-1.384526	-1.312630	-2.437436
F	-4.607458	2.791248	-0.980489
F	-2.193310	2.547718	0.149691
N	0.289099	-0.590736	0.162938
C	1.666200	-0.671455	0.559112
C	2.195109	0.155443	1.547990
H	1.542126	0.859444	2.060764
C	3.542164	0.061687	1.884789
C	4.351655	-0.887010	1.262927
C	3.815262	-1.755113	0.316429
H	4.431812	-2.528600	-0.144675
C	2.469011	-1.649271	-0.031374
C	-1.576194	-1.971590	1.009576
H	-2.006642	-1.096396	1.497854
C	-0.395785	-1.843043	0.288251
C	0.636121	1.868233	-0.580435
C	0.726871	2.810566	0.436434
C	1.444058	3.993141	0.303376
C	2.118737	4.247053	-0.887024
C	2.068392	3.318156	-1.920326
C	1.328698	2.153025	-1.750584
C	-1.692293	0.599641	-1.081382
C	-2.151785	-0.300424	-2.046195
C	-3.391490	-0.168311	-2.666931
C	-3.809942	1.796778	-1.342534
C	-2.558305	1.642705	-0.764186
B	-0.241756	0.549758	-0.452315
H	3.954633	0.717930	2.652792
H	5.401026	-0.981951	1.548390
S	1.721436	-2.778786	-1.179463
C	-2.197435	-3.216106	1.102326
C	0.184961	-2.966118	-0.314496
F	-3.788152	-1.038446	-3.587957
C	-4.221973	0.890977	-2.314179
H	-3.124066	-3.318919	1.668434
C	-1.627876	-4.330871	0.491276
C	-0.430550	-4.210047	-0.209011
F	-5.398561	1.045138	-2.896924
H	-2.108250	-5.306724	0.582445
H	0.036445	-5.080429	-0.673275

$B(PFP)_2F\text{-}NS(Ph)_2^-$: H = -2493.257004918438
$B(PFP)_2F\text{-}NS(Ph)_2^-$ coordinates:

F	0.626316	3.018244	1.718334
F	2.121845	4.968330	0.700160
F	2.810924	4.958732	-1.922900
F	2.048194	2.884430	-3.512212
F	0.541219	0.909409	-2.519687
F	-1.533002	-1.209444	-2.122199
F	-4.514999	3.165464	-0.981327
F	-2.285478	2.739342	0.391896
N	0.351443	-0.682947	0.200210
C	1.684791	-0.668446	0.645860
C	2.121280	0.216380	1.645713
H	1.400425	0.888390	2.105699
C	3.446566	0.217556	2.068047
C	4.355772	-0.705370	1.554113
C	3.924079	-1.634132	0.609514
H	4.608283	-2.387516	0.213106
C	2.607623	-1.604317	0.154024
C	-1.512451	-2.176380	0.753027
H	-2.021114	-1.350276	1.249431

C	-0.249077	-1.949389	0.200810
C	0.511801	1.852394	-0.345674
C	0.938125	2.928350	0.423138
C	1.717093	3.965460	-0.083985
C	2.089095	3.956974	-1.418988
C	1.695388	2.897460	-2.224061
C	0.922472	1.877775	-1.677898
C	-1.808670	0.699440	-0.731945
C	-2.235725	-0.134966	-1.763713
C	-3.400177	0.087407	-2.498911
C	-3.786249	2.074993	-1.227667
C	-2.625387	1.810802	-0.511199
B	-0.452132	0.624695	0.224037
F	-0.882663	0.888736	1.564046
H	3.761312	0.929098	2.834757
H	5.387828	-0.722077	1.910469
S	2.032588	-2.742795	-1.081863
C	-2.112564	-3.430391	0.660245
C	0.428574	-3.036744	-0.380396
F	-3.778039	-0.763944	-3.457433
C	-4.184484	1.197567	-2.225206
H	-3.107012	-3.582566	1.085317
C	-1.444795	-4.492799	0.053751
C	-0.156306	-4.296285	-0.440038
F	-5.297751	1.427662	-2.922935
H	-1.916190	-5.475039	-0.019845
H	0.395582	-5.120061	-0.897840

$B(PFP)_3$: H = -2206.069990907438
$B(PFP)_3$ coordinates:

F	2.813167	-0.502218	0.852912
F	-1.930699	-1.301038	1.658830
F	-0.649919	1.917736	1.679149
F	4.294251	-2.671394	0.410684
F	-4.601072	-1.022933	1.325271
F	0.252103	4.463080	1.565352
F	3.236832	-4.815062	-0.831771
F	-5.566842	0.241645	-0.861757
F	2.080739	5.168754	-0.297953
F	0.613517	-4.828814	-1.574932
F	-3.868084	1.290545	-2.703660
F	3.057931	3.328263	-2.030473
F	-0.893278	-2.696214	-1.125073
F	-1.207158	1.038089	-2.361760
F	2.194844	0.766817	-1.895084
C	0.888750	-1.475492	-0.141087
C	-1.486589	-0.128587	-0.333714
C	0.747653	1.259167	-0.100926
C	2.235763	-1.535489	0.249892
C	-2.388273	-0.661640	0.582085
C	0.265681	2.241806	0.761963
C	3.026209	-2.651790	0.033603
C	-3.762193	-0.526436	0.428855
C	0.717136	3.553960	0.721765
C	2.479188	-3.765925	-0.600402
C	-4.262431	0.138198	-0.688739
C	1.664523	3.918523	-0.232737
C	1.140470	-3.770577	-0.978055
C	-3.391666	0.670874	-1.633316
C	2.165024	2.967992	-1.117747
C	0.370250	-2.643409	-0.723437
C	-2.025126	0.534219	-1.433685

C	1.715344	1.655543	-1.023754
B	0.073953	-0.158189	-0.141139

$B(PFP)_3F^-$: H = -2306.001444677925
$B(PFP)_3F^-$ coordinates:

F	2.431586	-0.969819	1.714010
F	-2.429327	-1.094314	2.093318
F	-0.068297	2.587042	2.013536
F	3.941997	-2.981638	0.895489
F	-4.938608	-1.212264	1.250336
F	1.293985	4.767909	1.367481
F	3.186421	-4.508324	-1.238479
F	-5.622417	-0.334679	-1.219634
F	2.765006	4.865559	-0.903332
F	0.896242	-3.902581	-2.567535
F	-3.704260	0.713116	-2.856896
F	2.832666	2.697489	-2.560308
F	-0.647858	-1.919189	-1.769684
F	-1.183318	0.872945	-2.036896
F	1.514777	0.482096	-1.931849
C	0.780473	-1.332901	0.044186
C	-1.658219	-0.067199	0.083897
C	0.671171	1.380832	0.099564
C	1.978898	-1.674611	0.673468
C	-2.674191	-0.600652	0.877892
C	0.656758	2.528402	0.892536
C	2.794708	-2.724272	0.261865
C	-4.000197	-0.691457	0.454967
C	1.350187	3.694547	0.574729
C	2.422393	-3.495583	-0.828677
C	-4.357574	-0.245725	-0.807266
C	2.103387	3.752406	-0.588048
C	1.246106	-3.190862	-1.494764
C	-3.379650	0.288470	-1.634048
C	2.129826	2.646829	-1.424509
C	0.457674	-2.136394	-1.044637
C	-2.073326	0.374366	-1.168864
C	1.429026	1.498815	-1.066135
B	-0.083727	-0.019494	0.586429
F	-0.062315	-0.048865	1.997020

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