

## **Supporting Information**

# **Monocationic bis-alkyl and bis-allyl yttrium complexes, synthesis, $^{89}\text{Y}$ NMR characterization, ethylene or isoprene polymerization and modelling**

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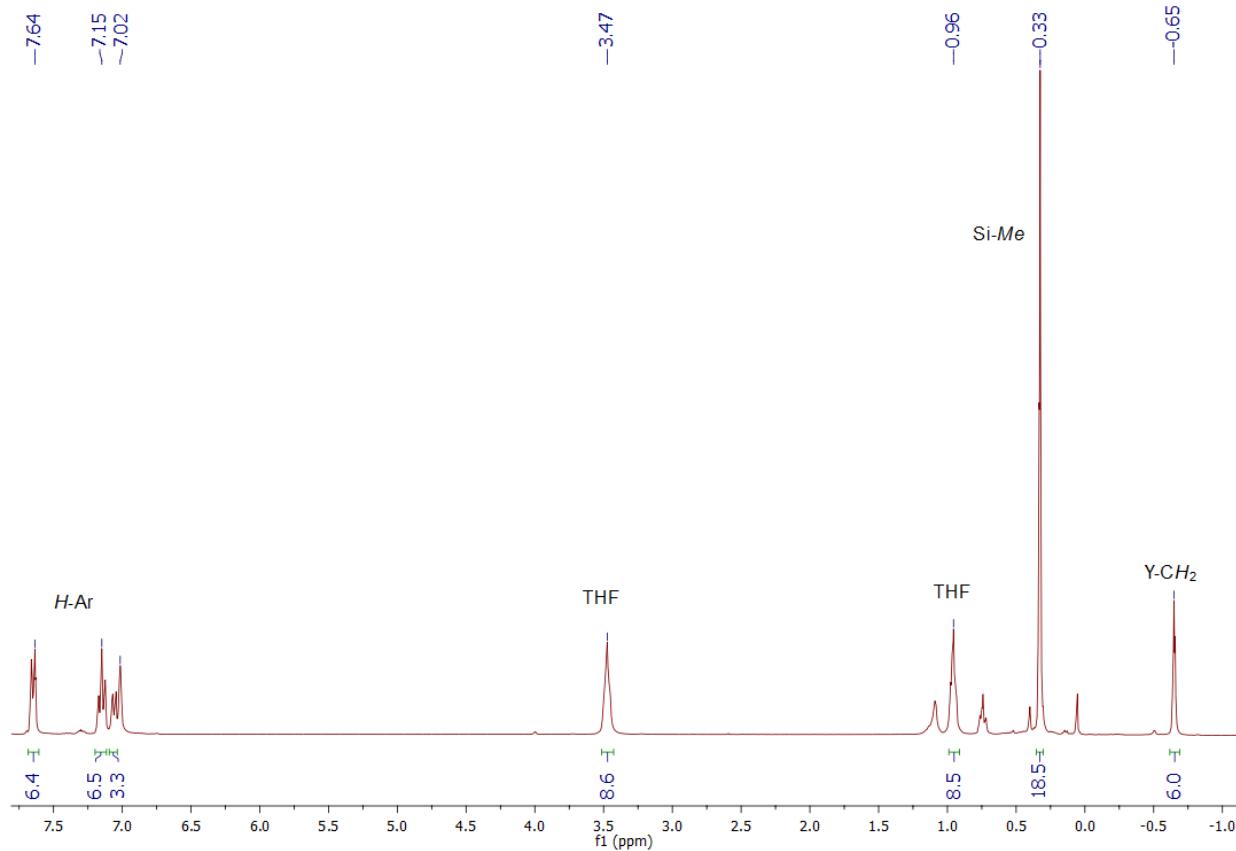
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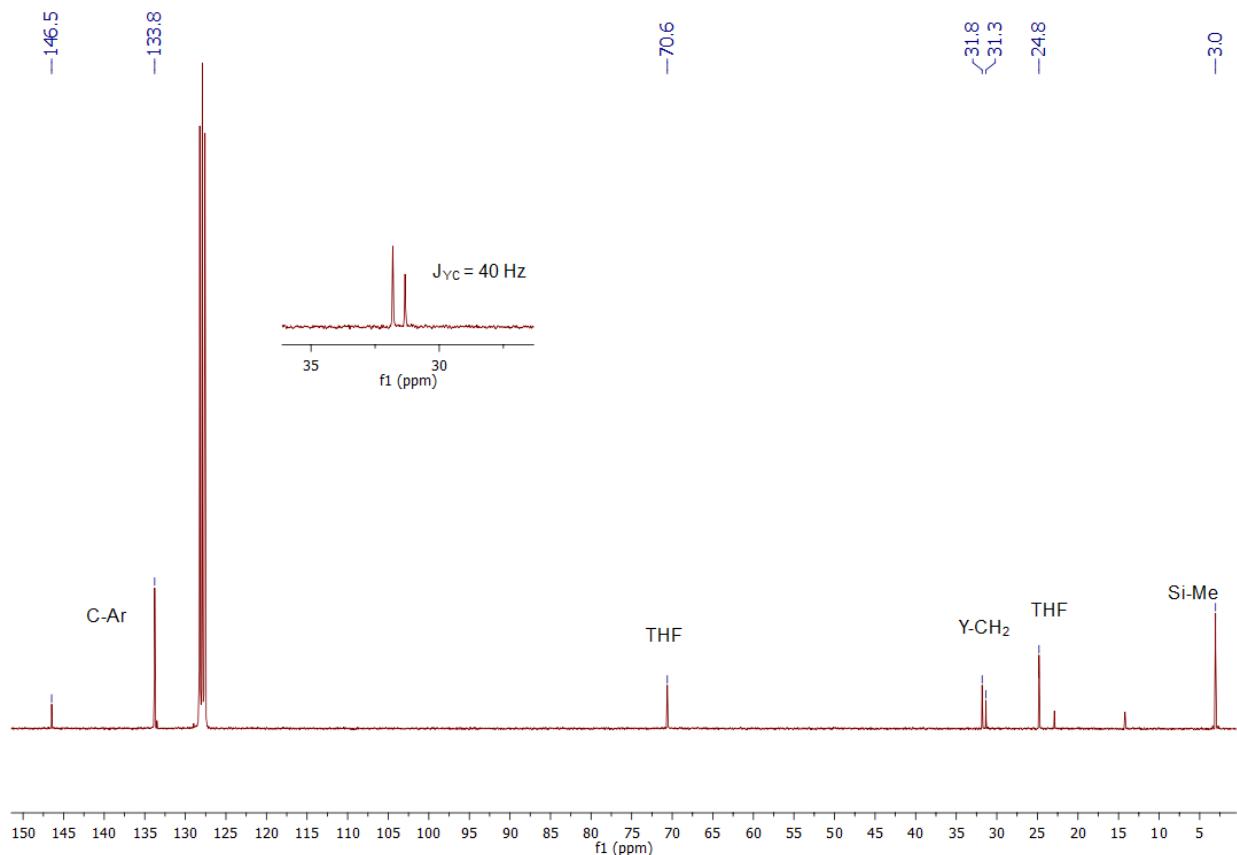
<sup>d</sup> Manufacture Michelin, 23 places Carmes Déchaux, F-63000 Clermont-Ferrand, France

Figure S1. $^1\text{H}$ NMR spectrum of $\text{Y}(\text{CH}_2\text{SiMe}_2\text{Ph})_3(\text{THF})_2$ (1a) in $\text{C}_6\text{D}_6$ at 298 K.	3
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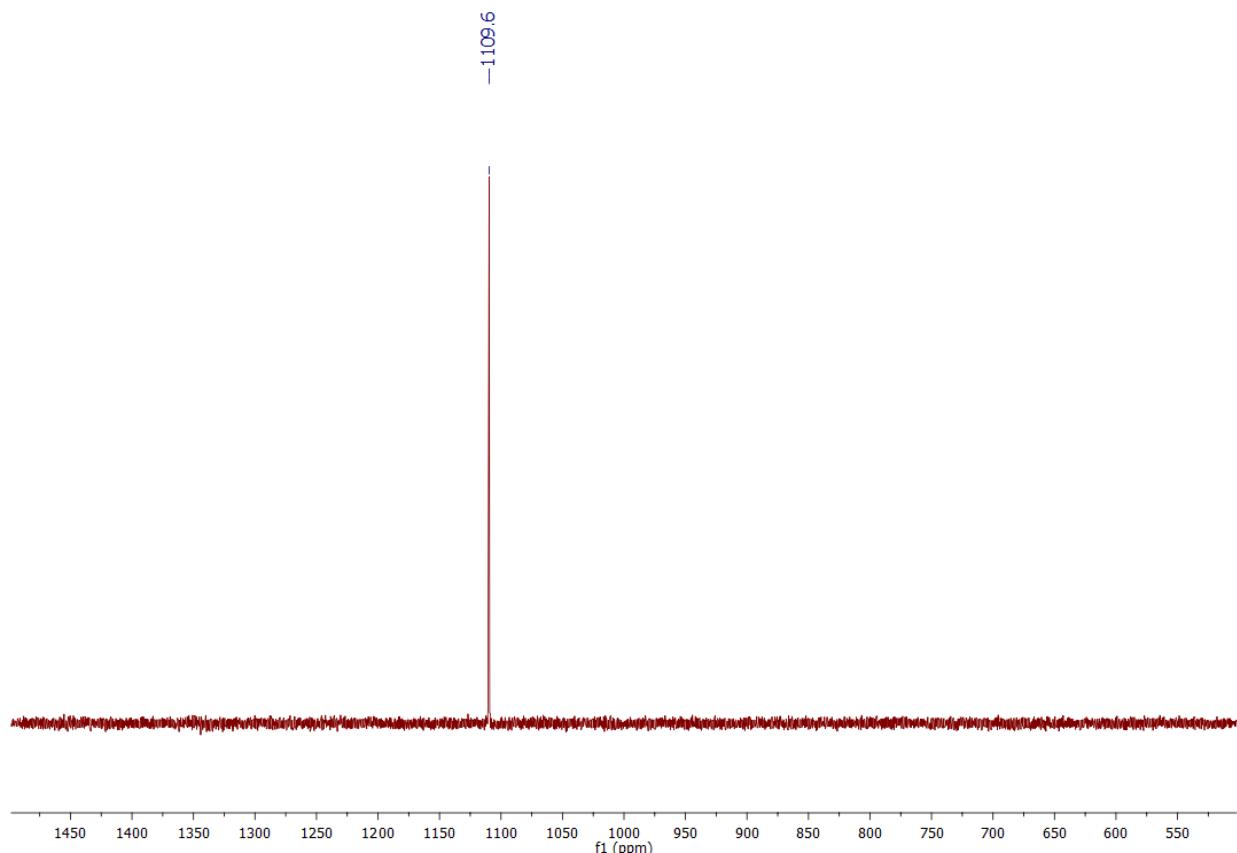
## NMR Spectra



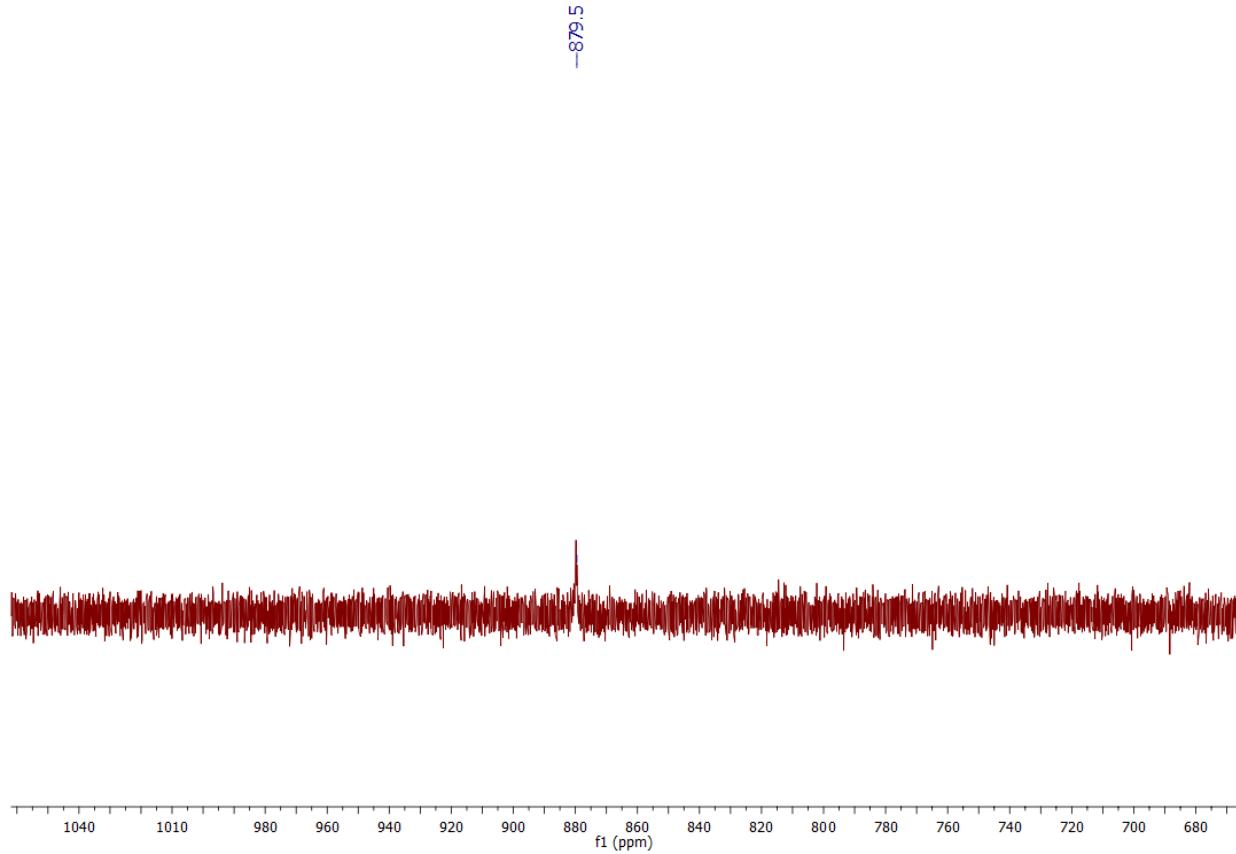
**Figure S1.**  $^1\text{H}$  NMR spectrum of  $\text{Y}(\text{CH}_2\text{SiMe}_2\text{Ph})_3(\text{THF})_2$  (**1a**) in  $\text{C}_6\text{D}_6$  at 298 K.



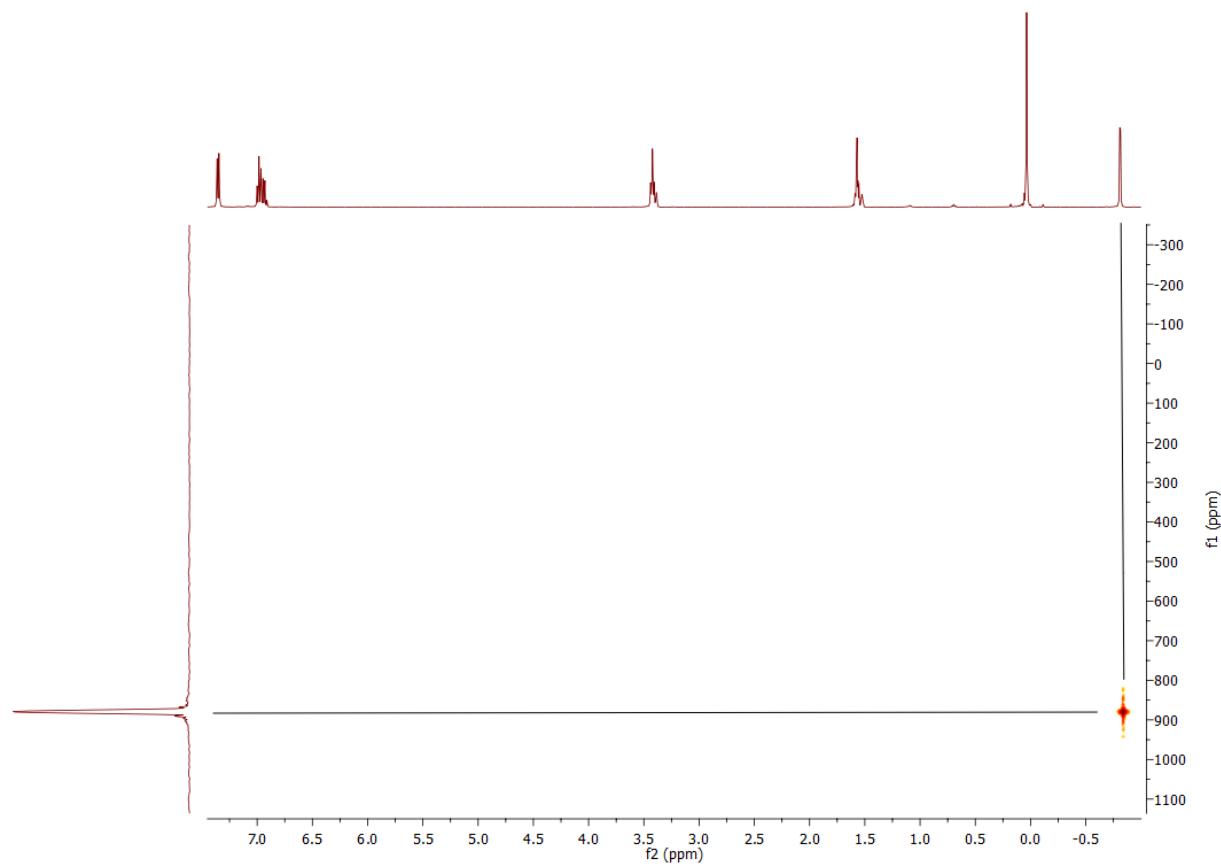
**Figure S2.**  $^{13}\text{C}-\{{}^1\text{H}\}$  NMR spectrum of  $\text{Y}(\text{CH}_2\text{SiMe}_2\text{Ph})_3(\text{THF})_2$  (**1a**) in  $\text{C}_6\text{D}_6$  at 298 K.



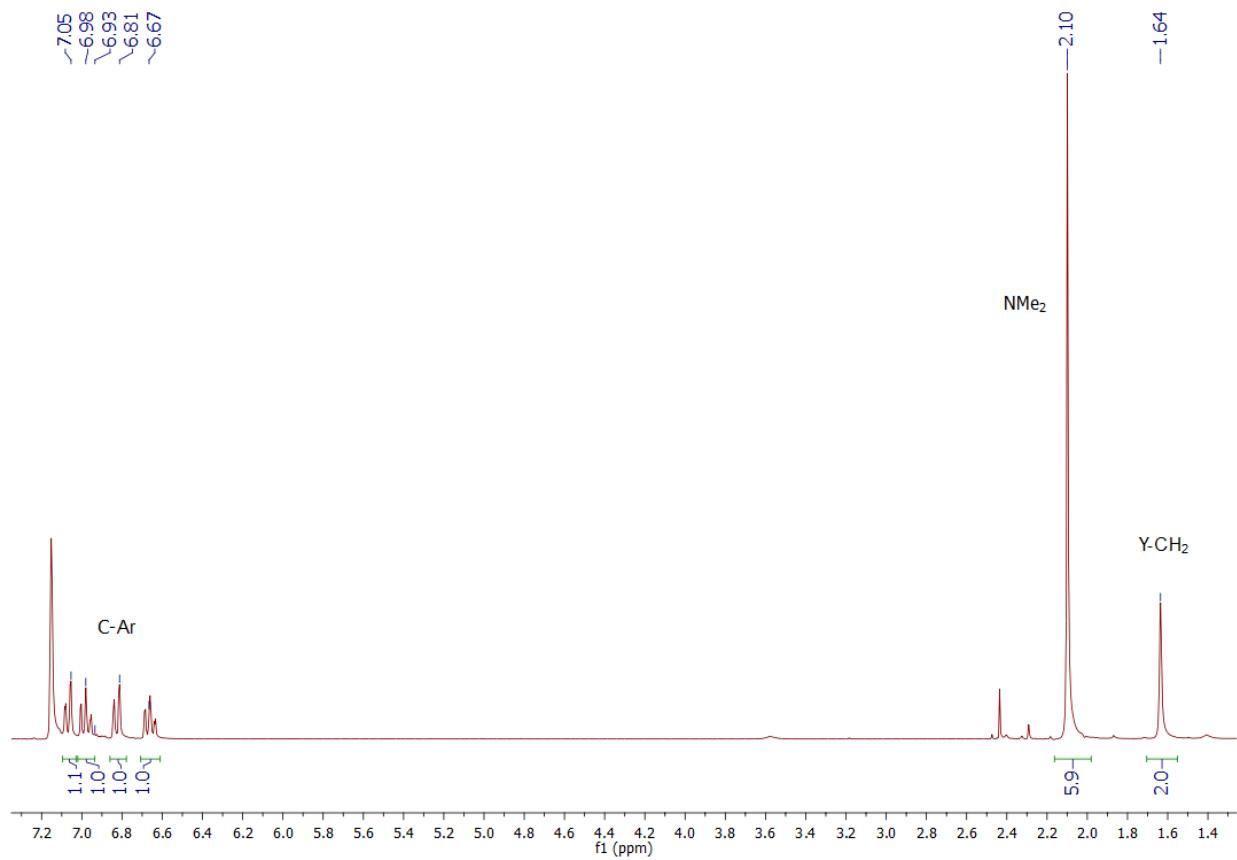
**Figure S3.** <sup>89</sup>Y INEPT spectrum of  $\text{Y}(\text{CH}_2\text{SiMe}_2\text{Ph})_3(\text{THF})_2$  (**1a**) in  $\text{C}_6\text{D}_6$  at 298 K.



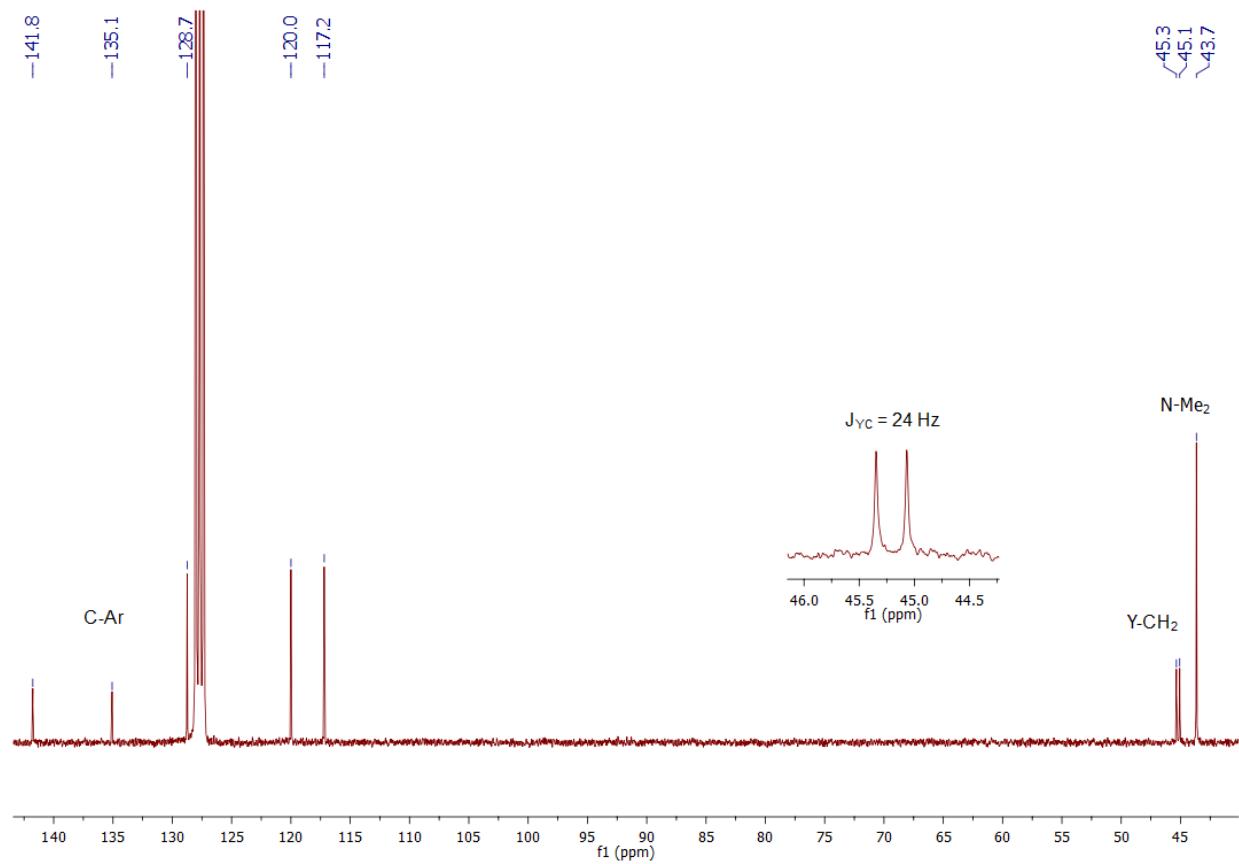
**Figure S4.** <sup>89</sup>Y INEPT spectrum of  $\text{Y}(\text{CH}_2\text{SiMe}_2\text{Ph})_3(\text{THF})_2$  (**1a**) complex in  $\text{THF}-d_8$  at 298 K.



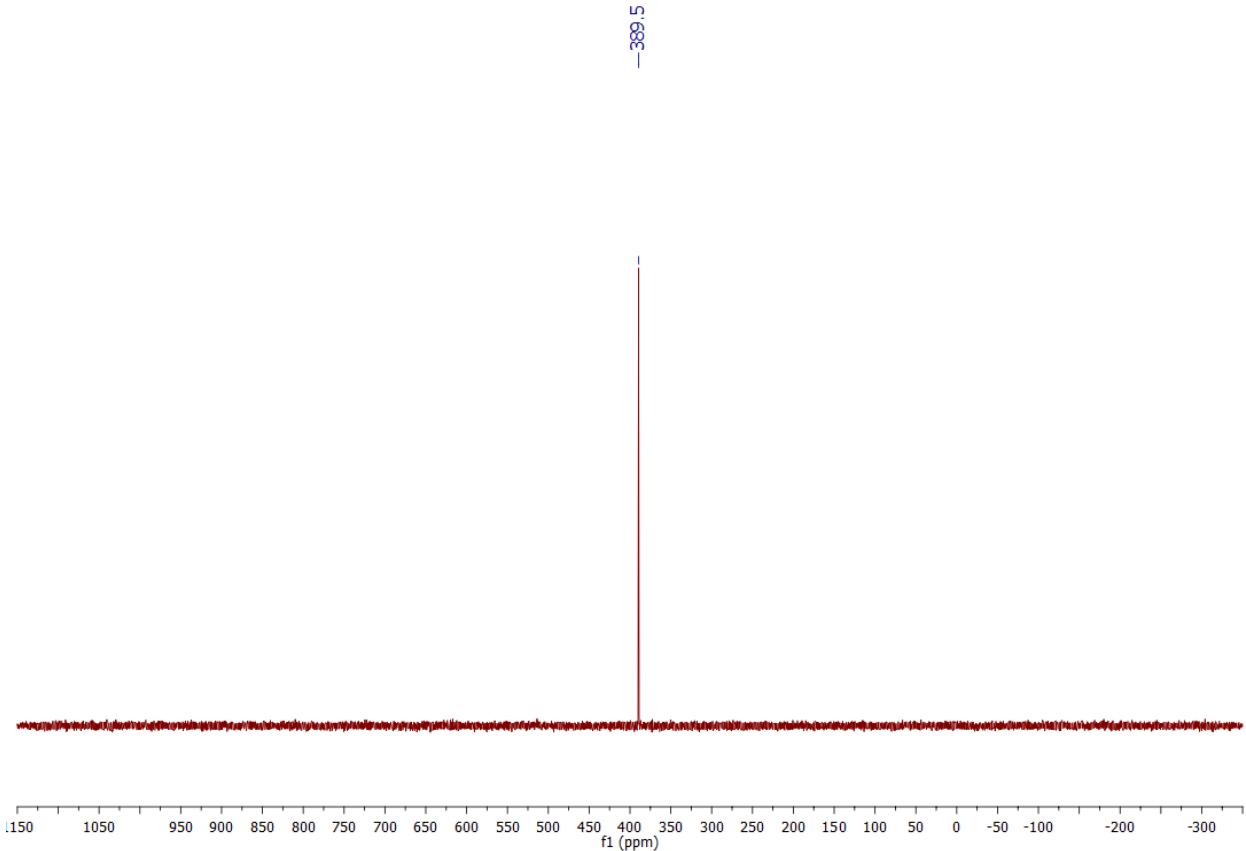
**Figure S5.** 2D <sup>1</sup>H-<sup>89</sup>Y HMBC NMR spectrum of  $\text{Y}(\text{CH}_2\text{SiMe}_2\text{Ph})_3(\text{THF})_2$  (**1a**) in  $\text{THF}-d_8$  at 298 K.



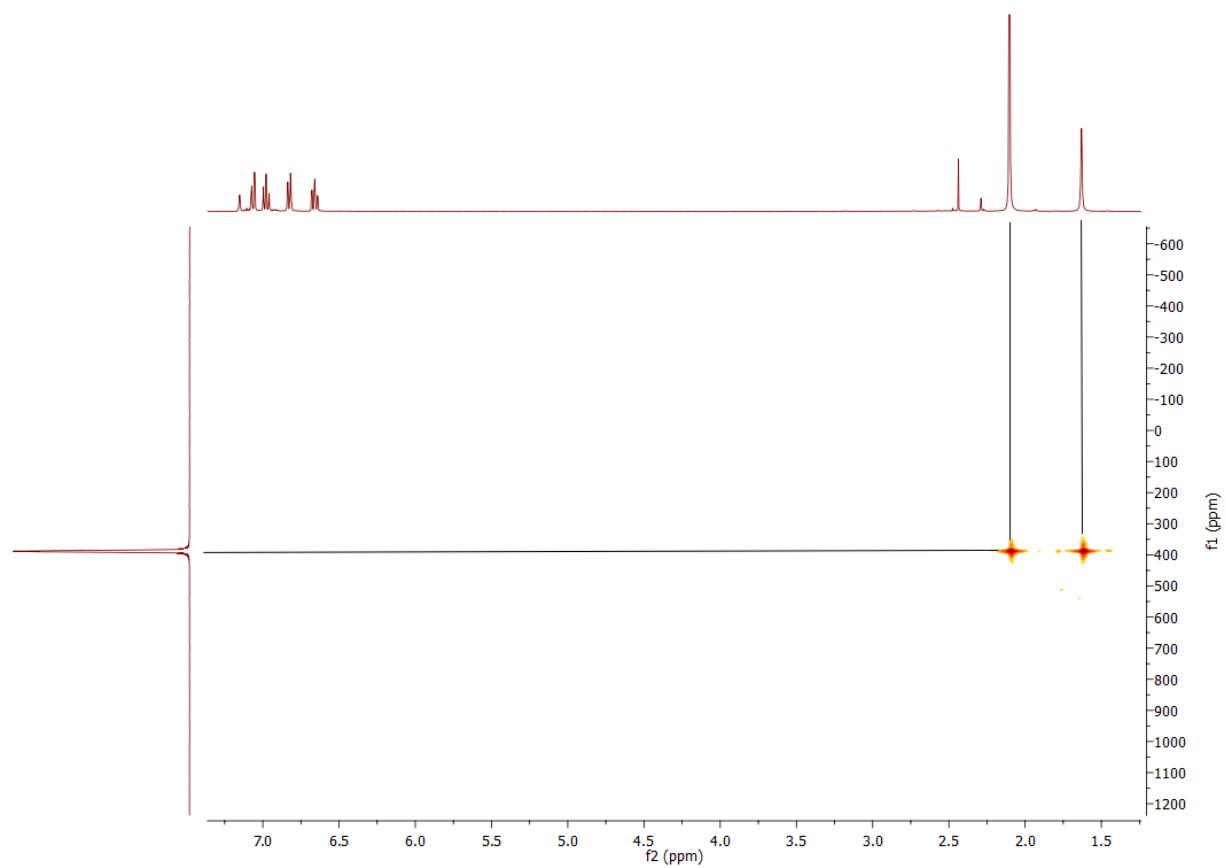
**Figure S6.**  $^1\text{H}$  NMR spectrum of  $\text{Y}(\text{CH}_2\text{C}_6\text{H}_4\text{NMe}_2)_3$  (**1b**) in  $\text{C}_6\text{D}_6$  at 298 K.



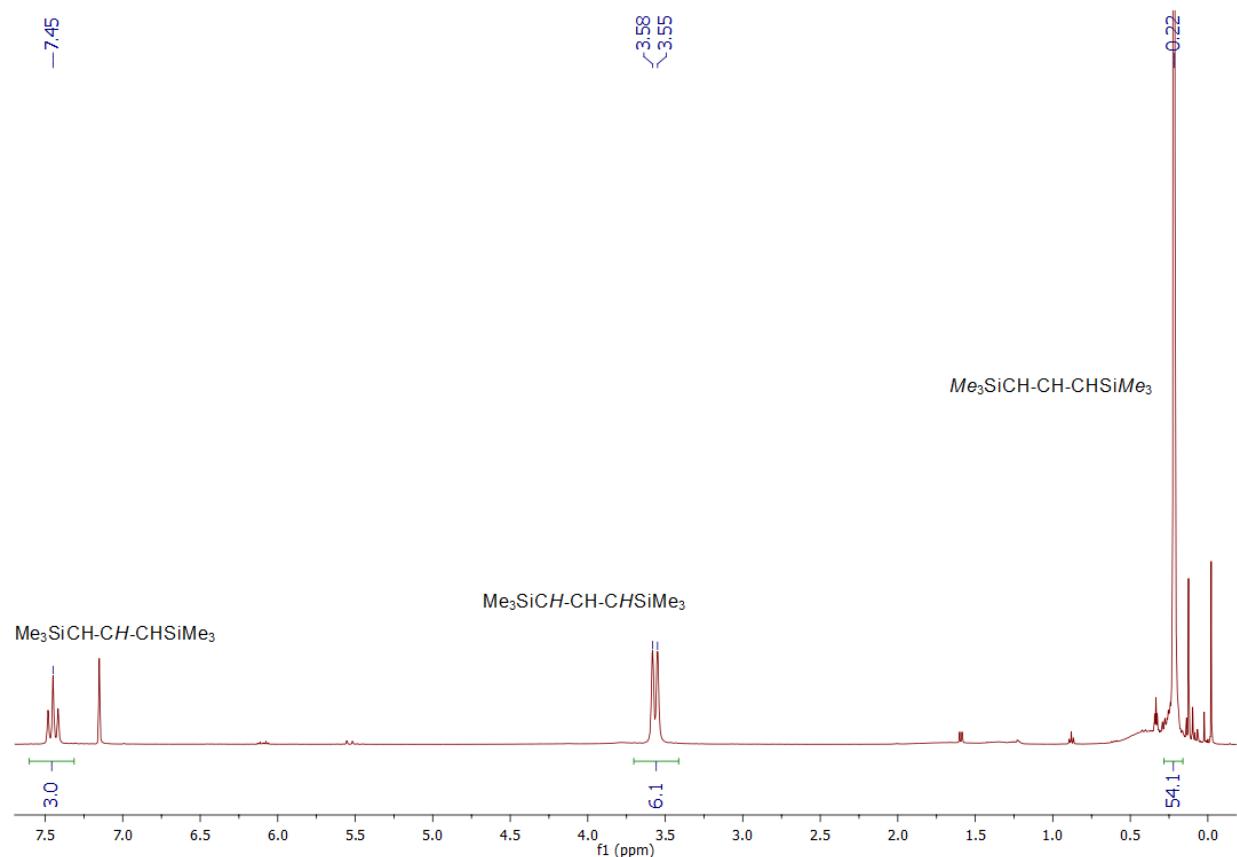
**Figure S7.**  $^{13}\text{C}$ - $\{{}^1\text{H}\}$  NMR spectrum of  $\text{Y}(\text{CH}_2\text{C}_6\text{H}_4\text{NMe}_2)_3$  (**1b**) in  $\text{C}_6\text{D}_6$  at 298 K.



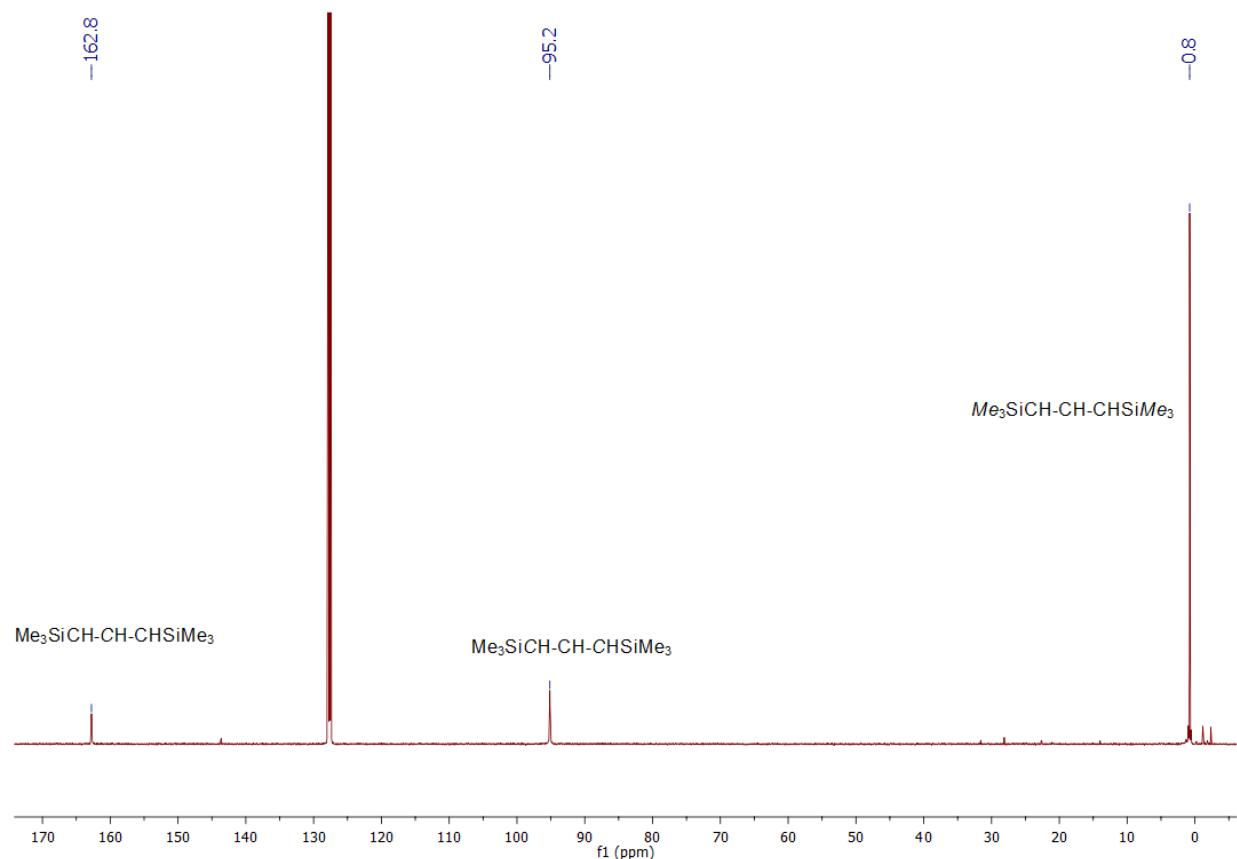
**Figure S8.** <sup>89</sup>Y INEPT spectrum of  $\text{Y}(\text{CH}_2\text{C}_6\text{H}_4\text{NMe}_2)_3$  (**1b**) in  $\text{C}_6\text{D}_6$  at 298 K.



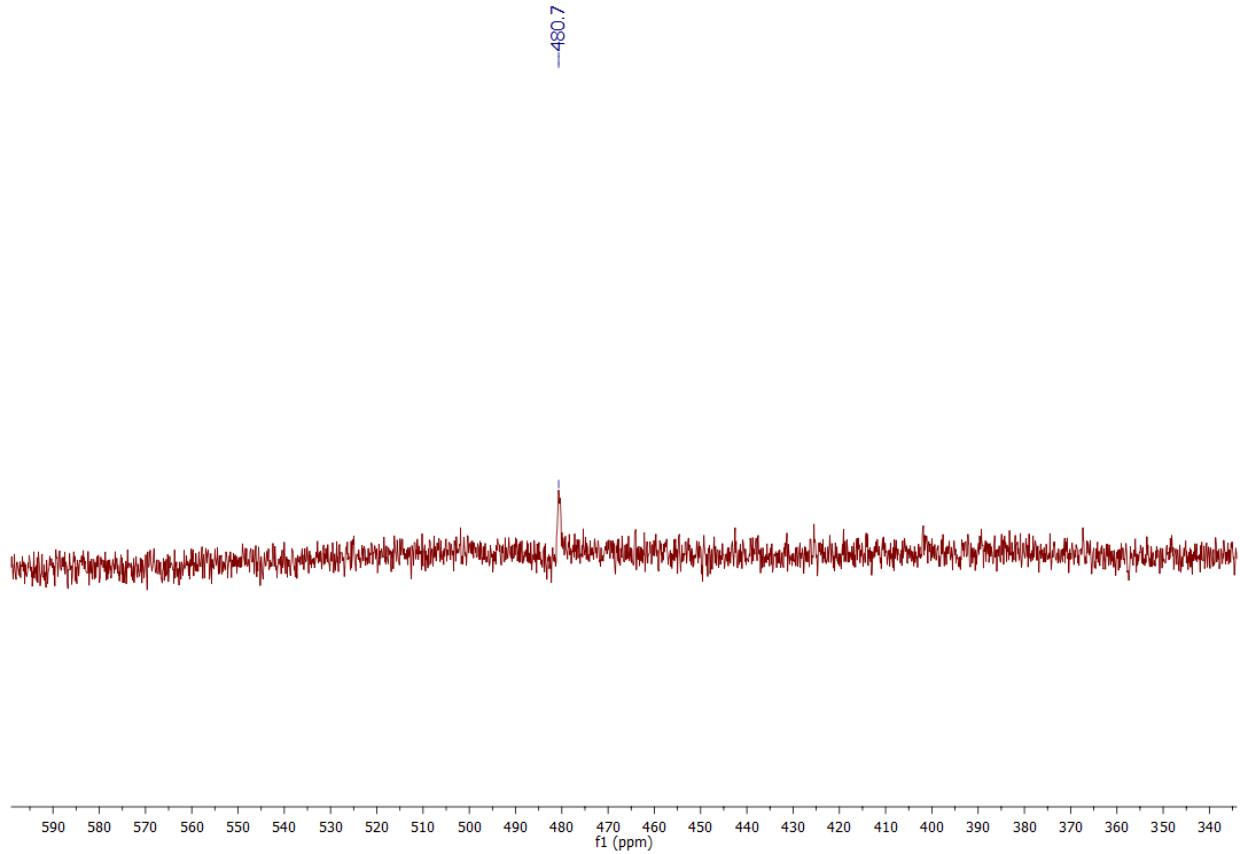
**Figure S9.** 2D <sup>1</sup>H-<sup>89</sup>Y HMBC NMR spectrum of  $\text{Y}(\text{CH}_2\text{C}_6\text{H}_4\text{NMe}_2)_3$  (**1b**) complex in  $\text{C}_6\text{D}_6$  at 298 K.



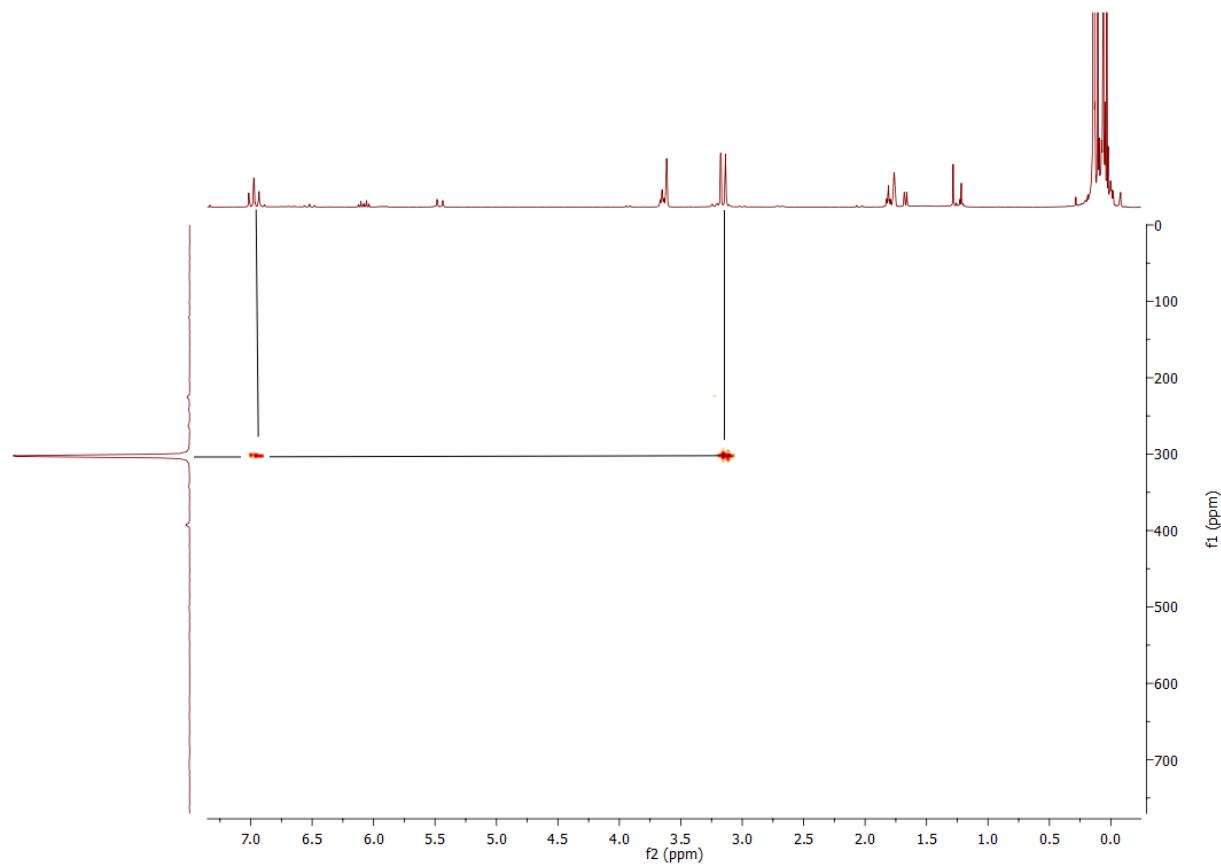
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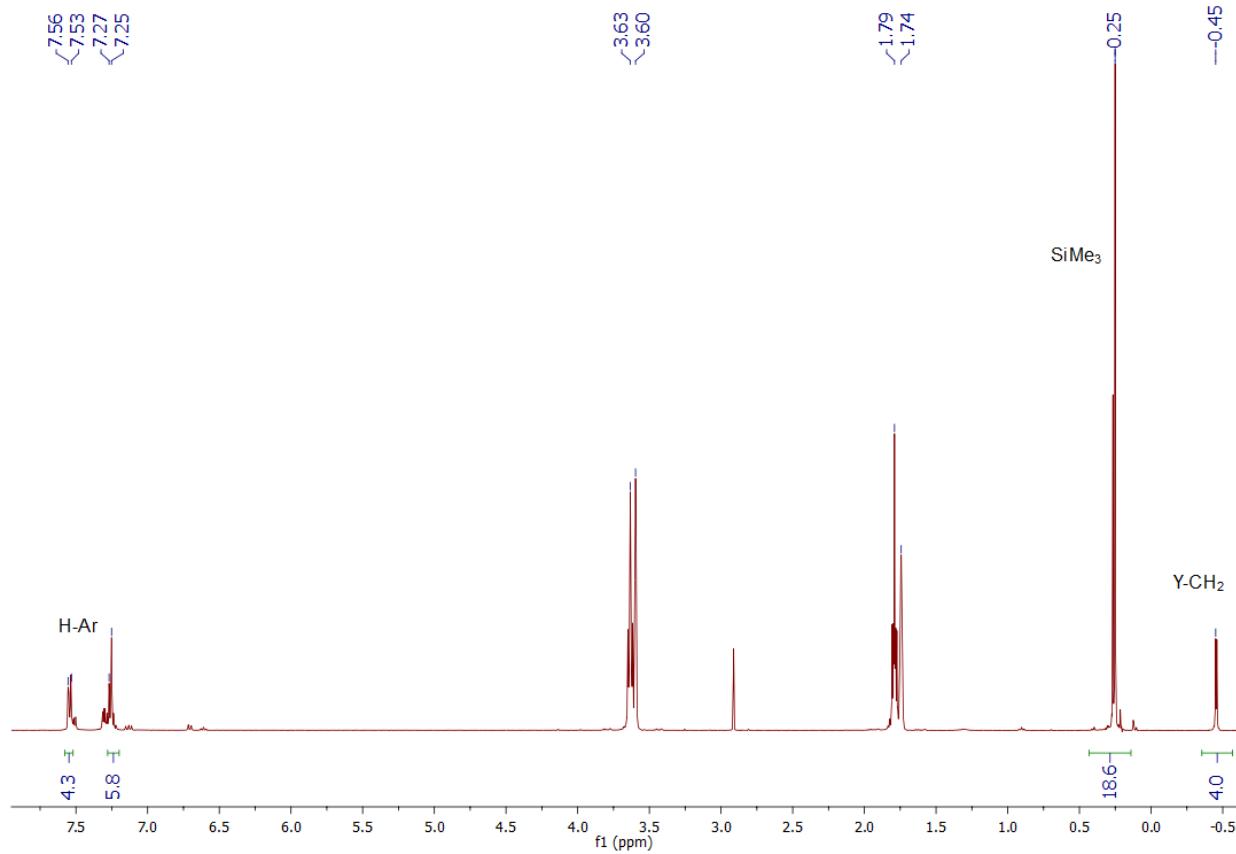
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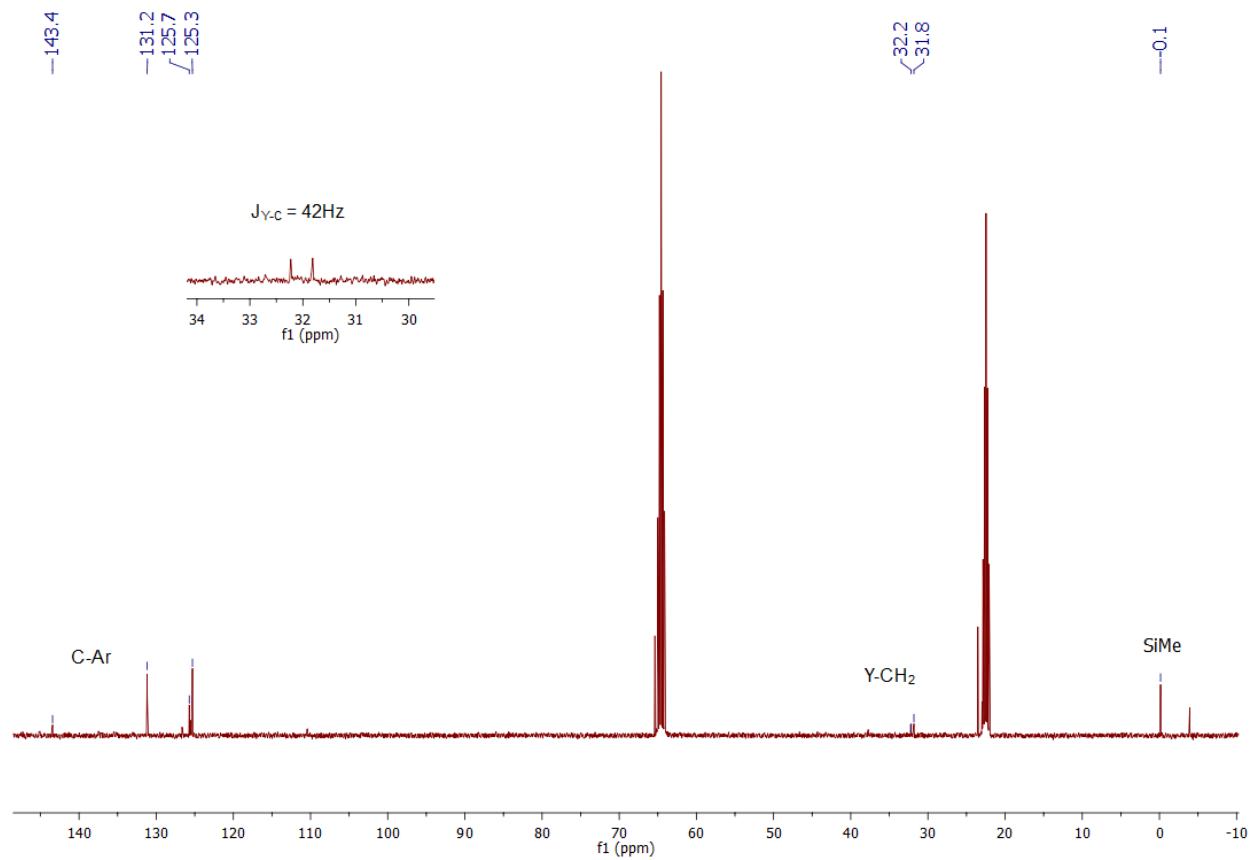
**Figure S12.** <sup>89</sup>Y INEPT spectrum of Y[1,3-(SiMe<sub>3</sub>)<sub>2</sub>C<sub>3</sub>H<sub>3</sub>]<sub>3</sub> (**1c**) complex in C<sub>6</sub>D<sub>6</sub> at 298 K.



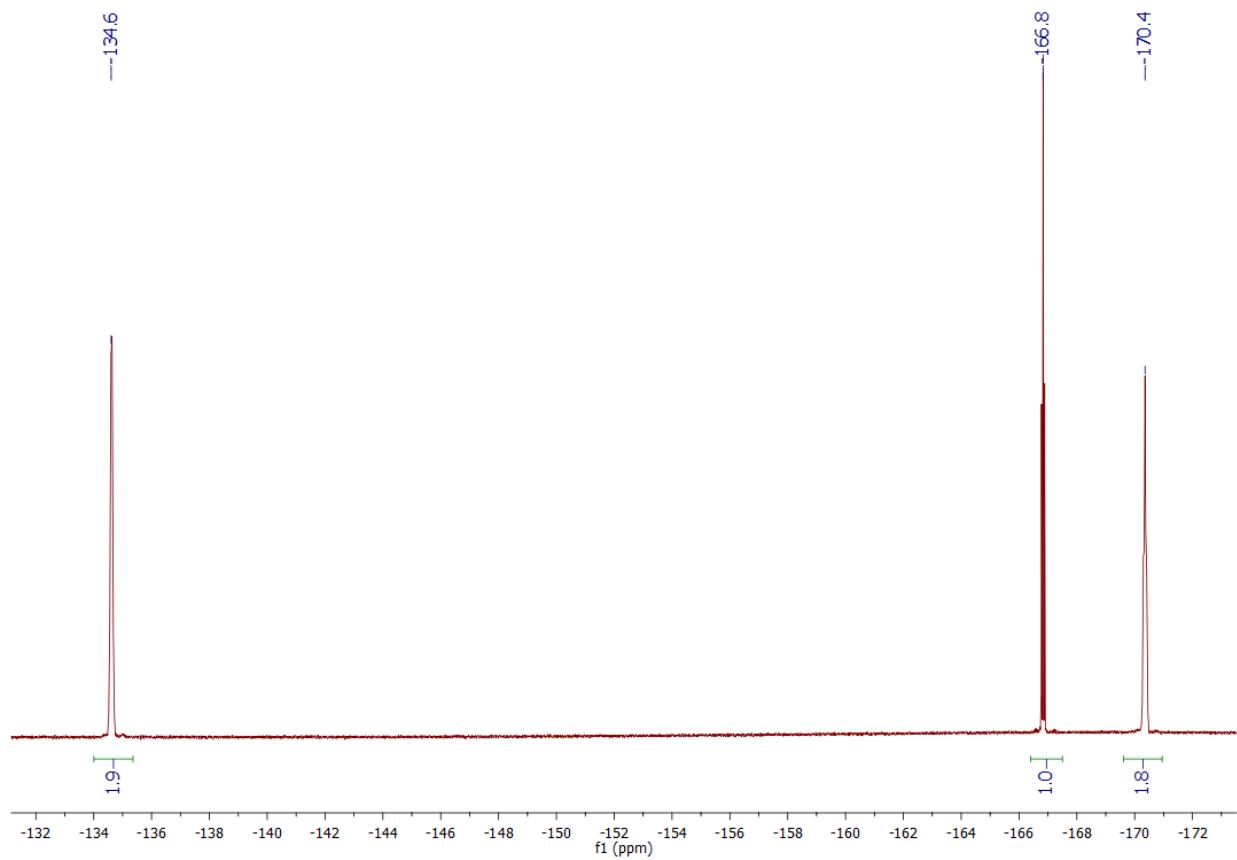
**Figure S13.** 2D <sup>1</sup>H-<sup>89</sup>Y HMBC NMR spectrum of Y[1,3-(SiMe<sub>3</sub>)<sub>2</sub>C<sub>3</sub>H<sub>3</sub>]<sub>3</sub> (**1c**) in THF-*d*<sub>8</sub> at 298 K.



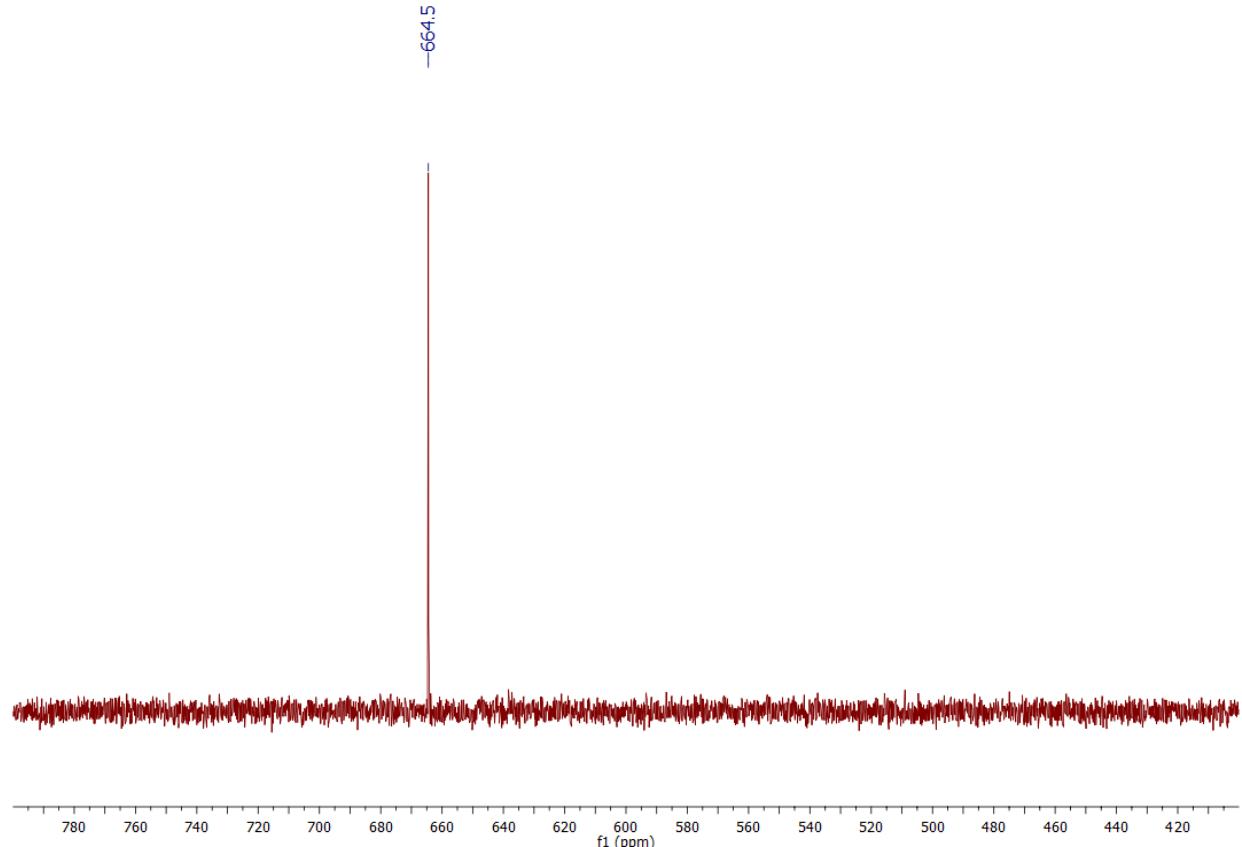
**Figure S14.**  $^1\text{H}$  NMR spectrum of  $[\text{Y}(\text{CH}_2\text{SiMe}_2\text{Ph})_2(\text{THF})_4][\text{B}(\text{C}_6\text{F}_5)_4]$  (**2a**) in  $\text{THF}-d_8$  at 298 K.



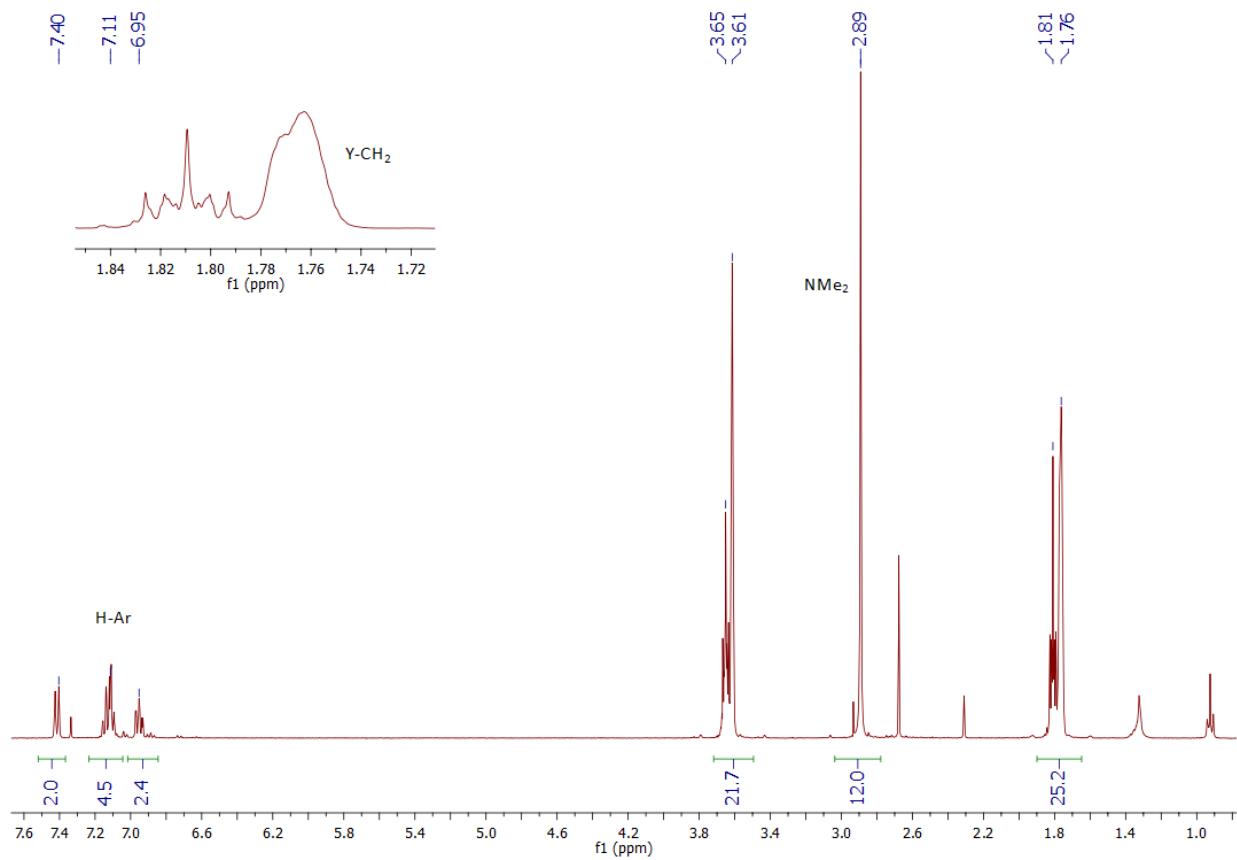
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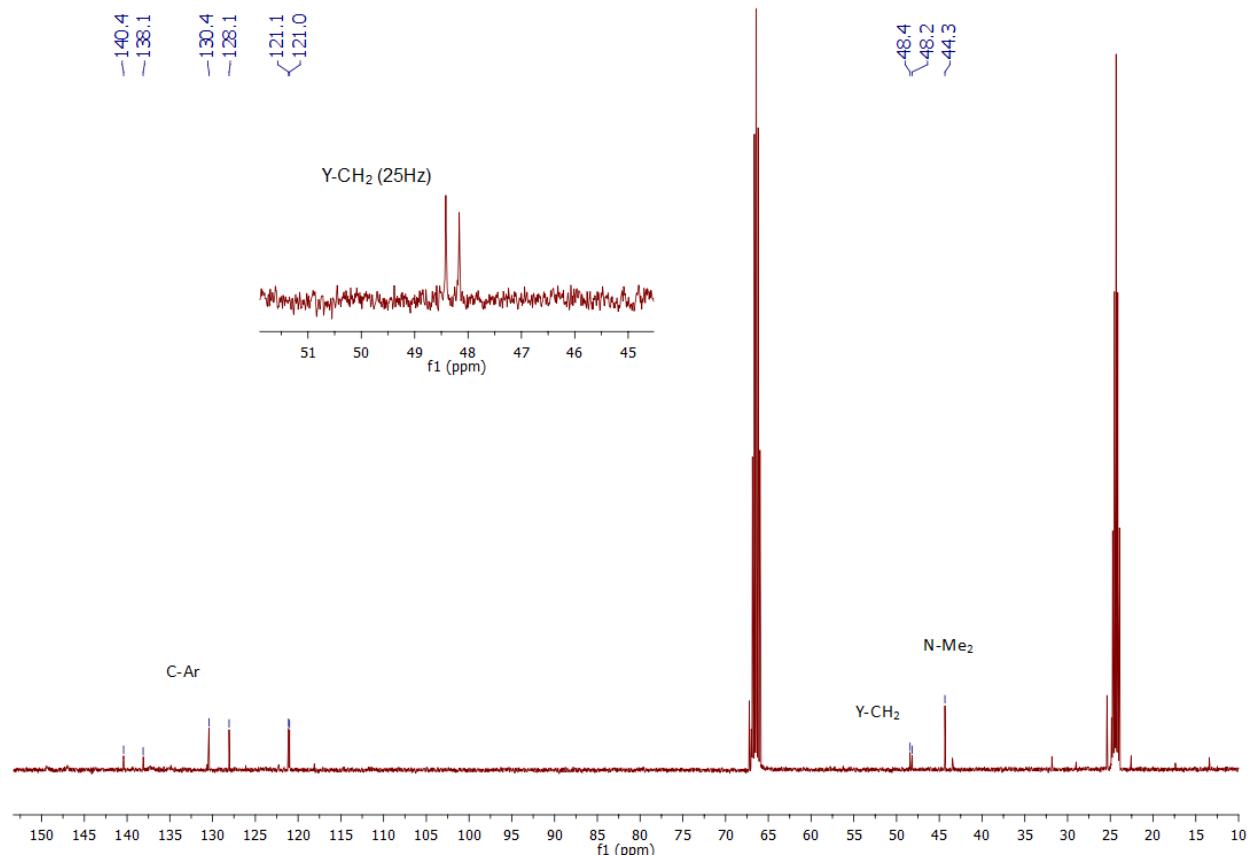
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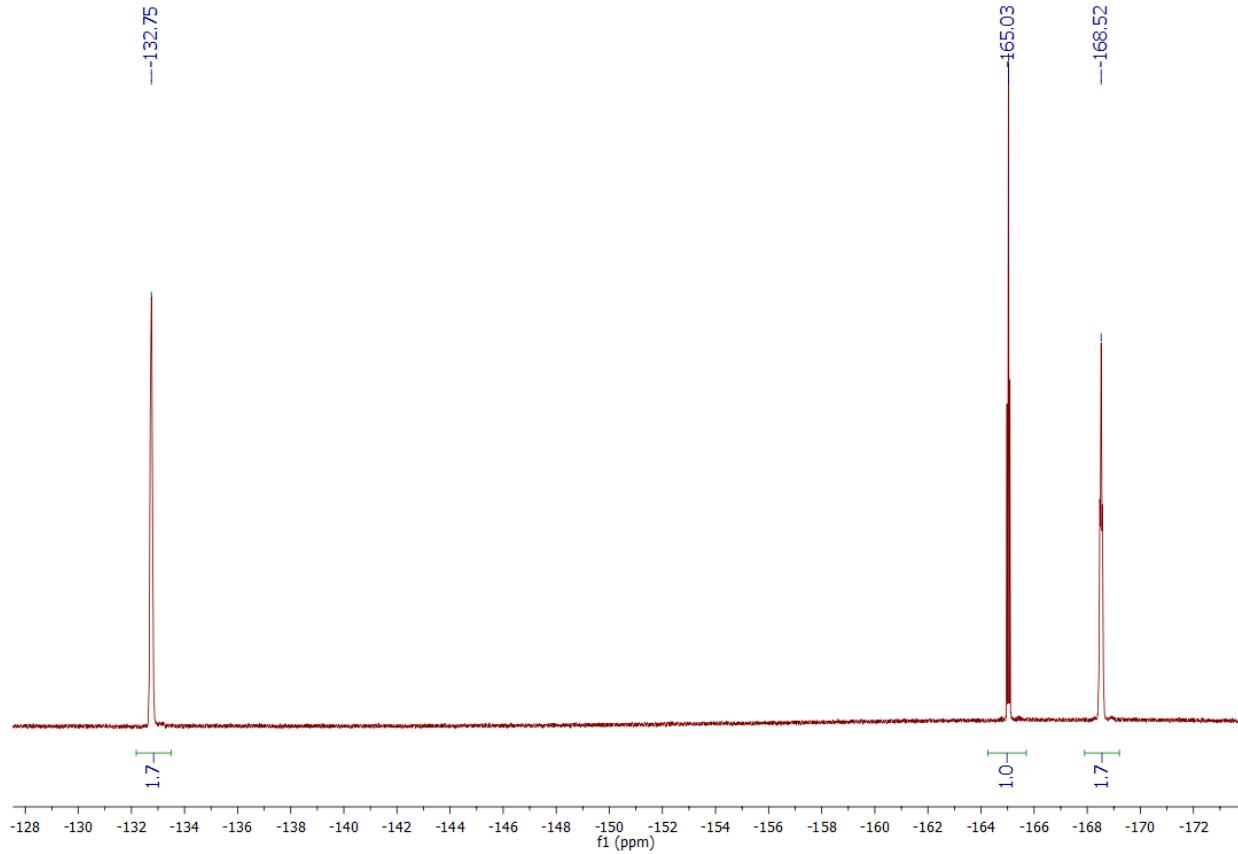
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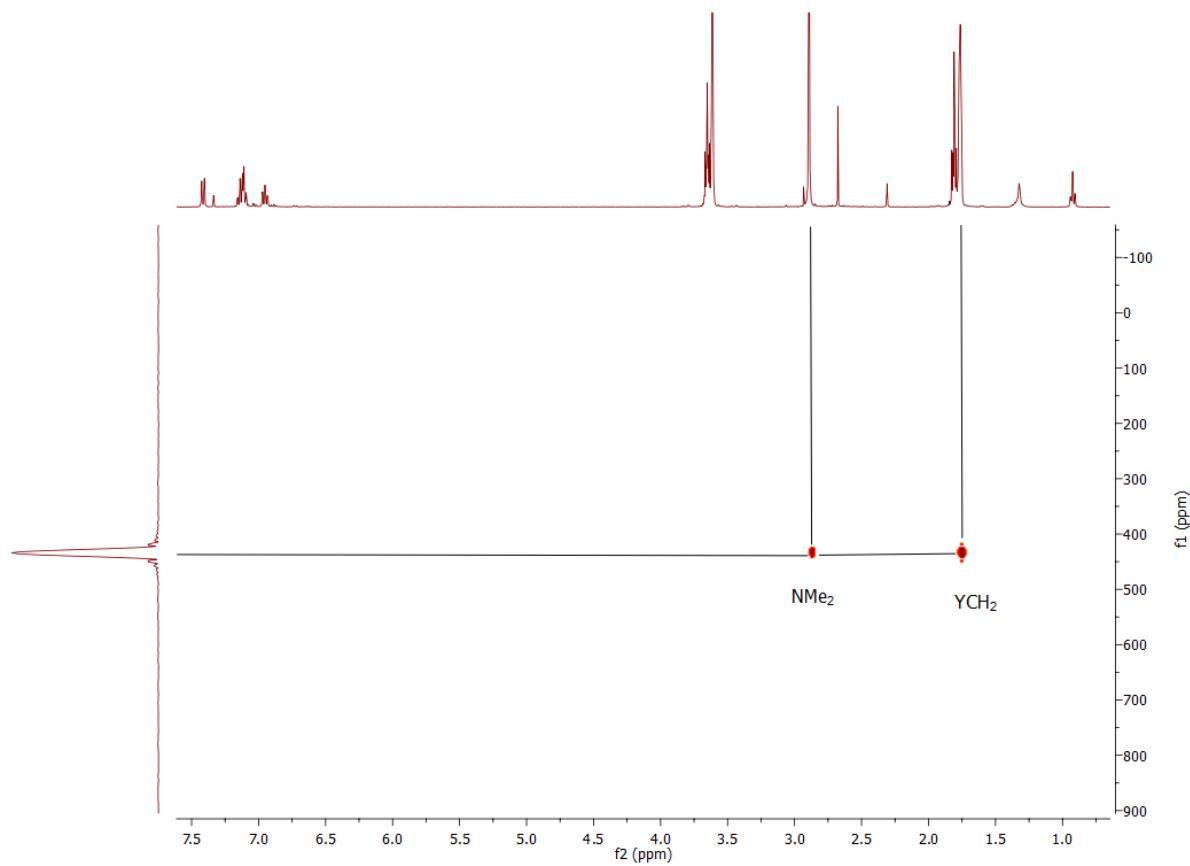
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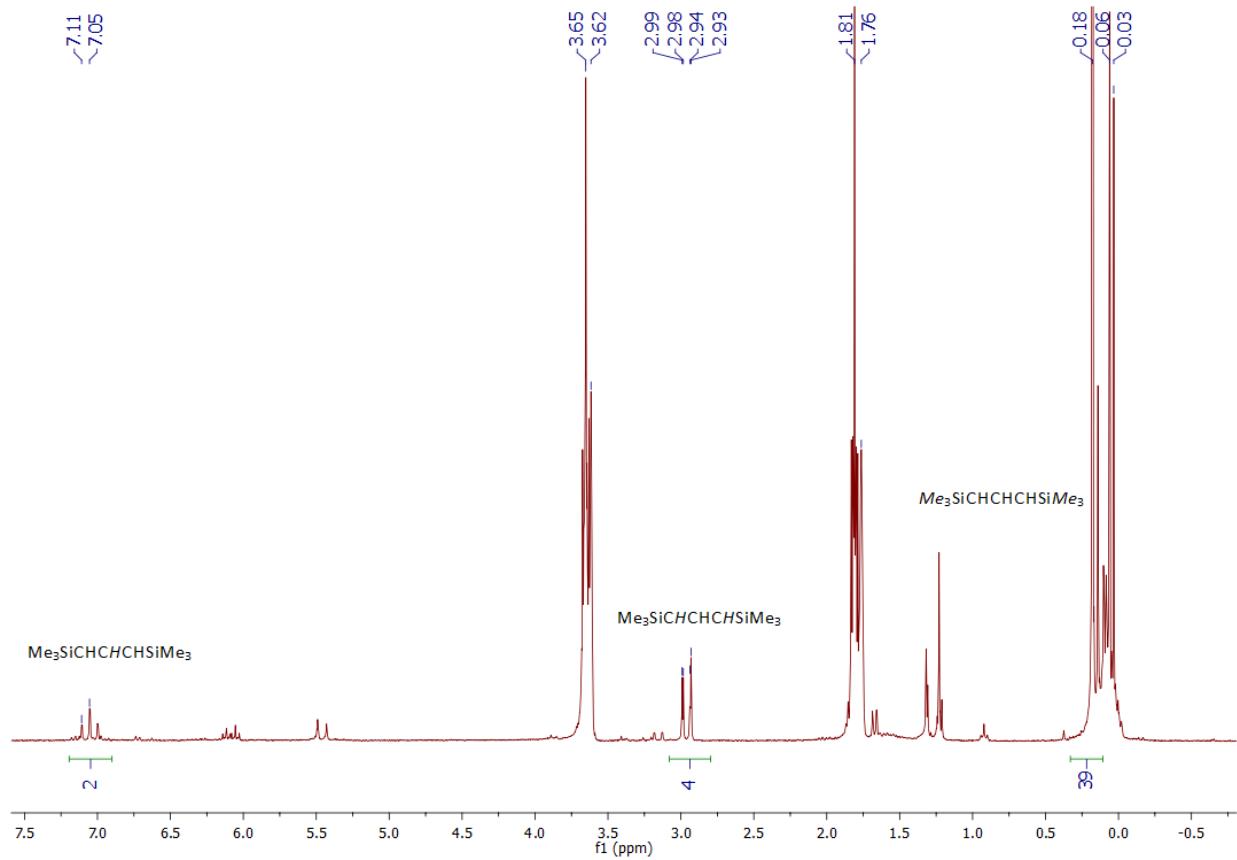
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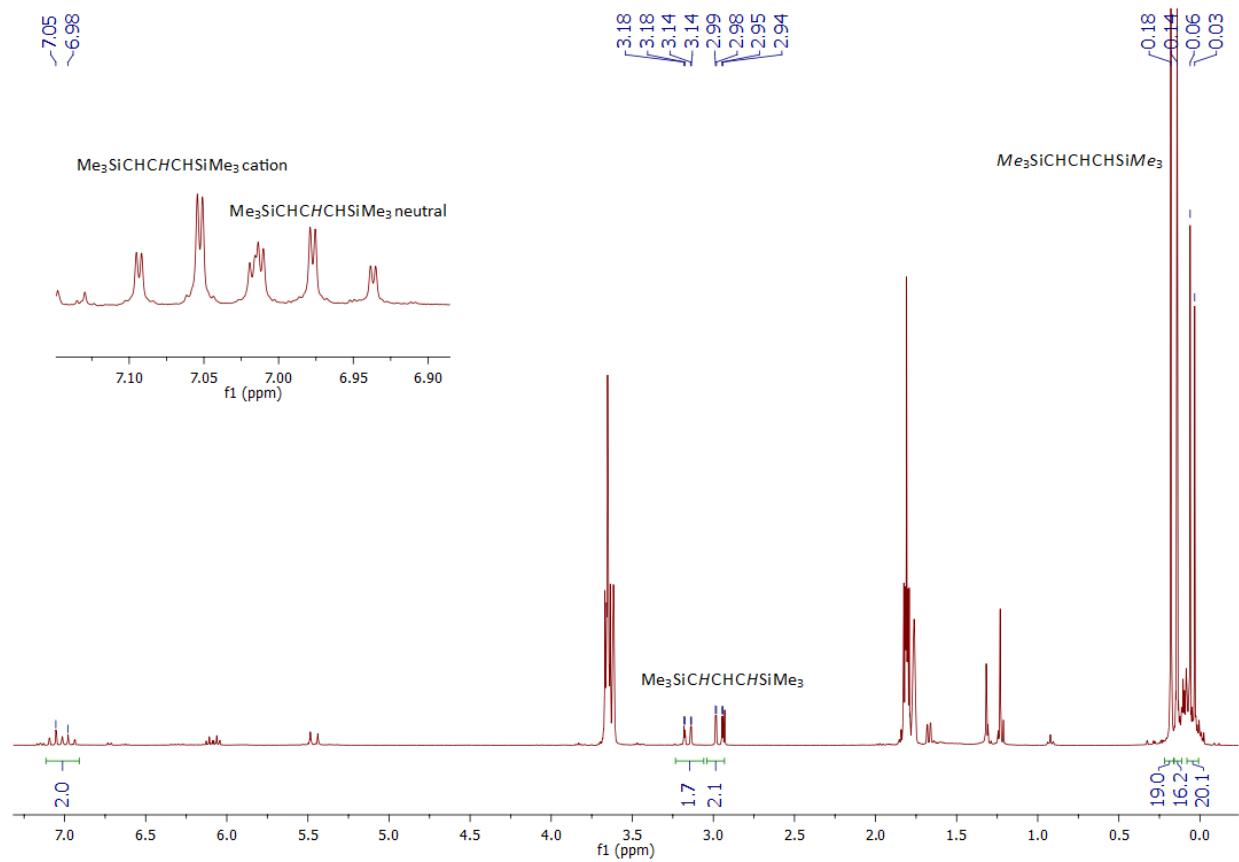
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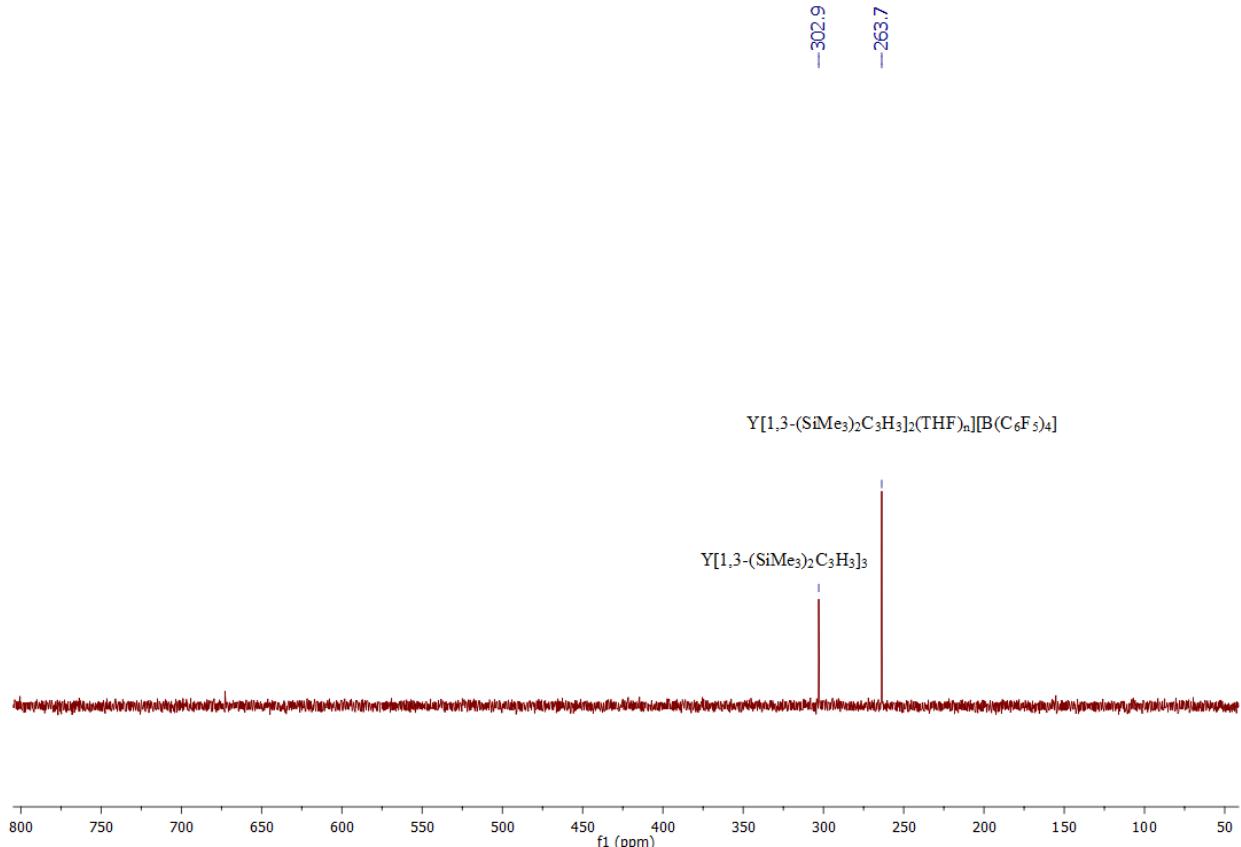
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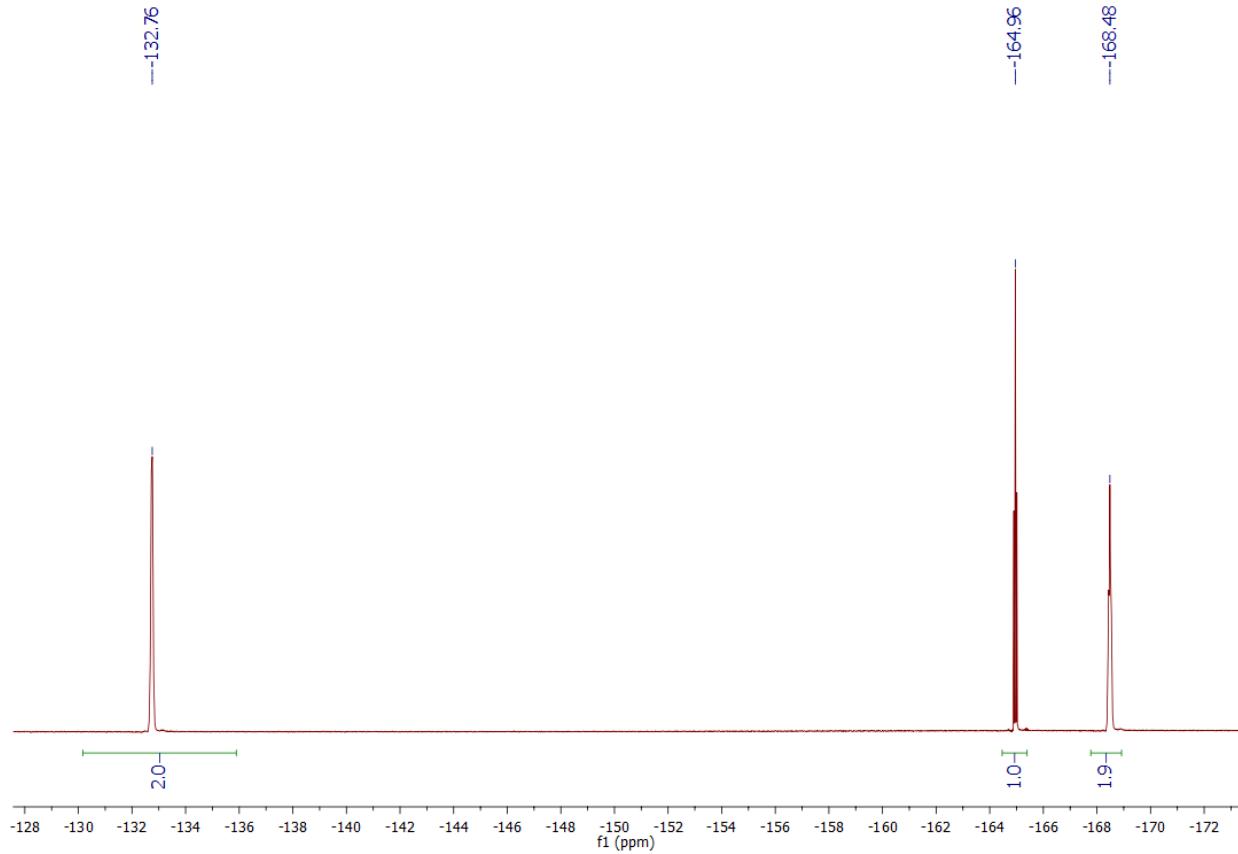
**Figure S22.**  $^1\text{H}$  NMR spectrum of  $[\text{Y}[1,3-(\text{SiMe}_3)_2\text{C}_3\text{H}_3]_2(\text{THF})_n][\text{B}(\text{C}_6\text{F}_5)_4]$  (**2c**) in  $\text{THF}-d_8$  at 298 K.



**Figure S23.** <sup>1</sup>H NMR spectrum of [Y[1,3-(SiMe<sub>3</sub>)<sub>2</sub>C<sub>3</sub>H<sub>3</sub>]<sub>2</sub>(THF)<sub>n</sub>][B(C<sub>6</sub>F<sub>5</sub>)<sub>4</sub>] (**2c**) after 12 h in THF-*d*<sub>8</sub> at 298 K.



**Figure S24.**  $^{89}\text{Y}$  INEPT NMR spectrum of  $\text{Y}[1,3-(\text{SiMe}_3)_2\text{C}_3\text{H}_3]_2(\text{THF})_n[\text{B}(\text{C}_6\text{F}_5)_4]$  (**2c**) after 12 h in  $\text{THF}-d_8$  at 298 K.



**Figure S25.**  ${}^{19}\text{F}$  NMR spectrum of  $[\text{Y}[1,3-(\text{SiMe}_3)_2\text{C}_3\text{H}_3]_2(\text{THF})_n][\text{B}(\text{C}_6\text{F}_5)_4]$  (**2c**) after 12 h in  $\text{THF}-d_8$  at 298 K.