

Electronic Supporting Information for

Cyclooctatetraenyl calcium and strontium amido complexes

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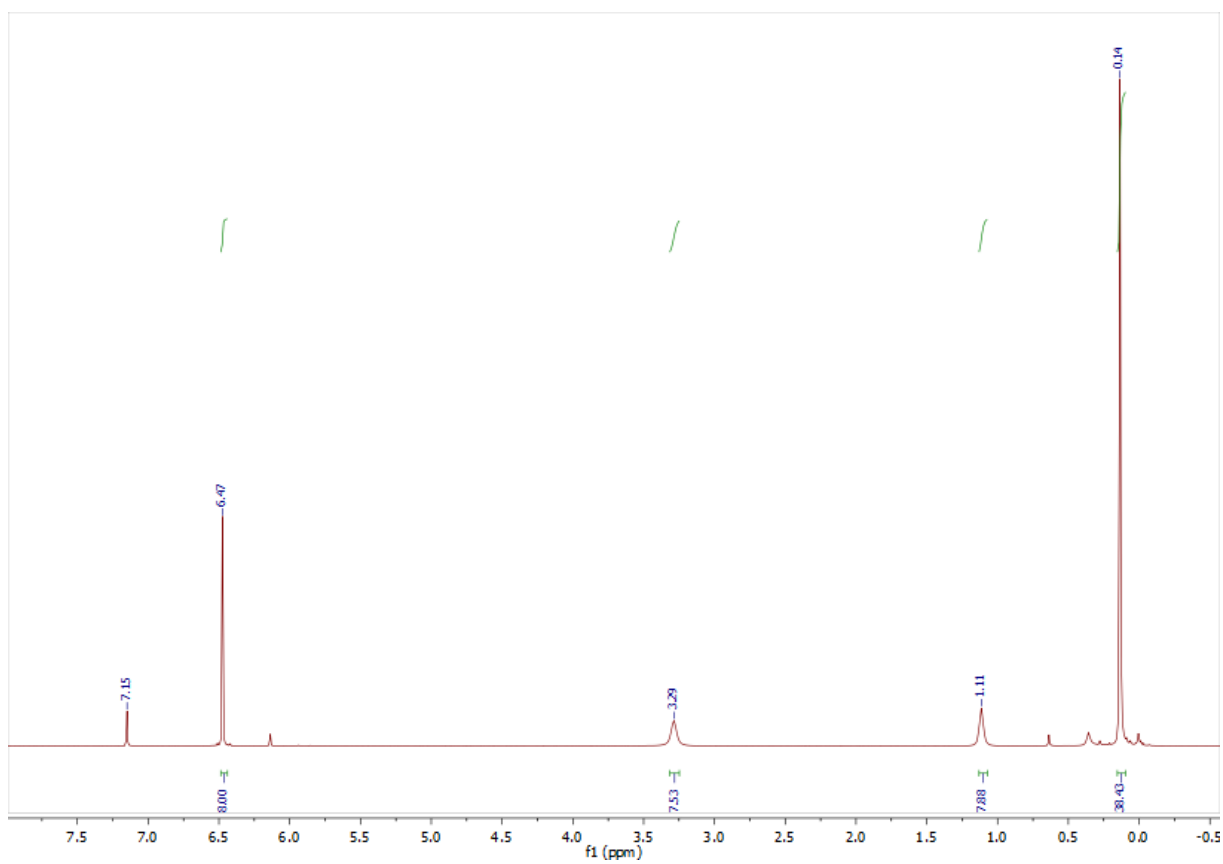
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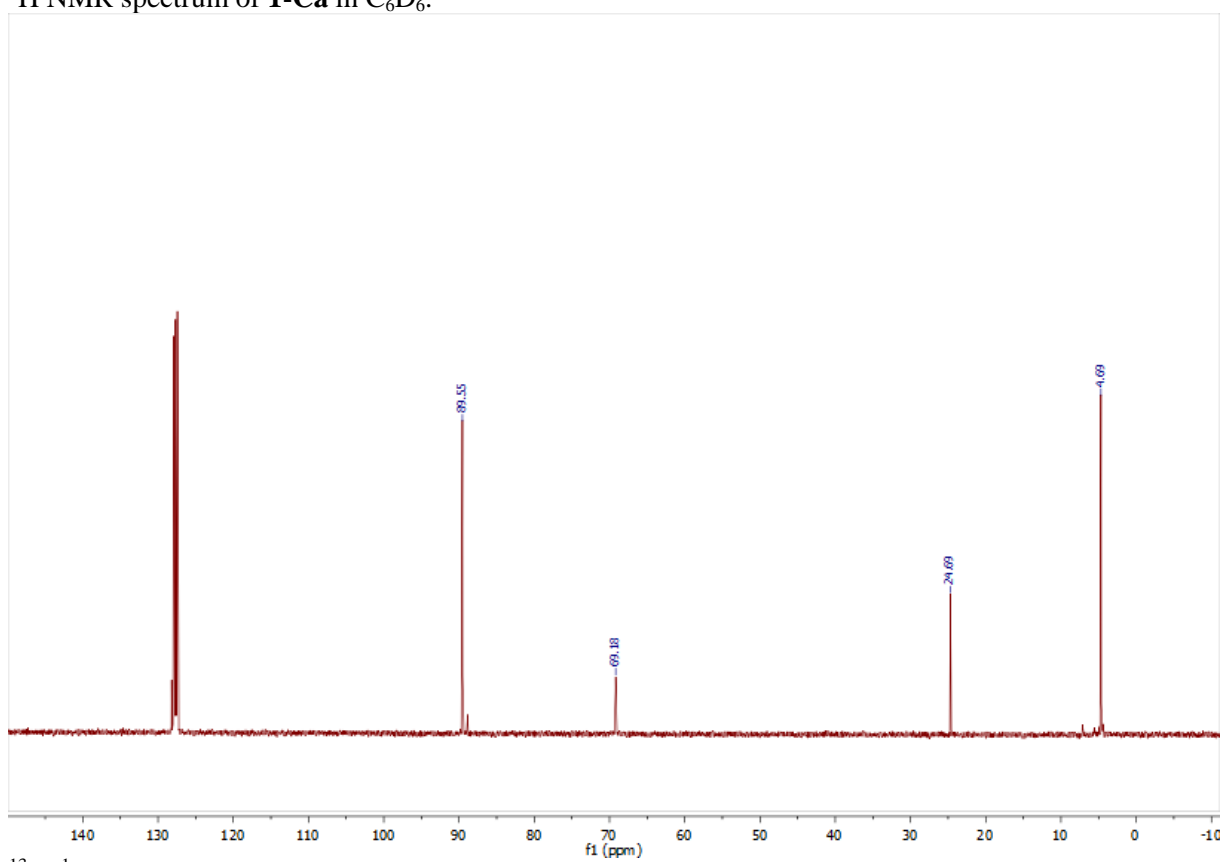
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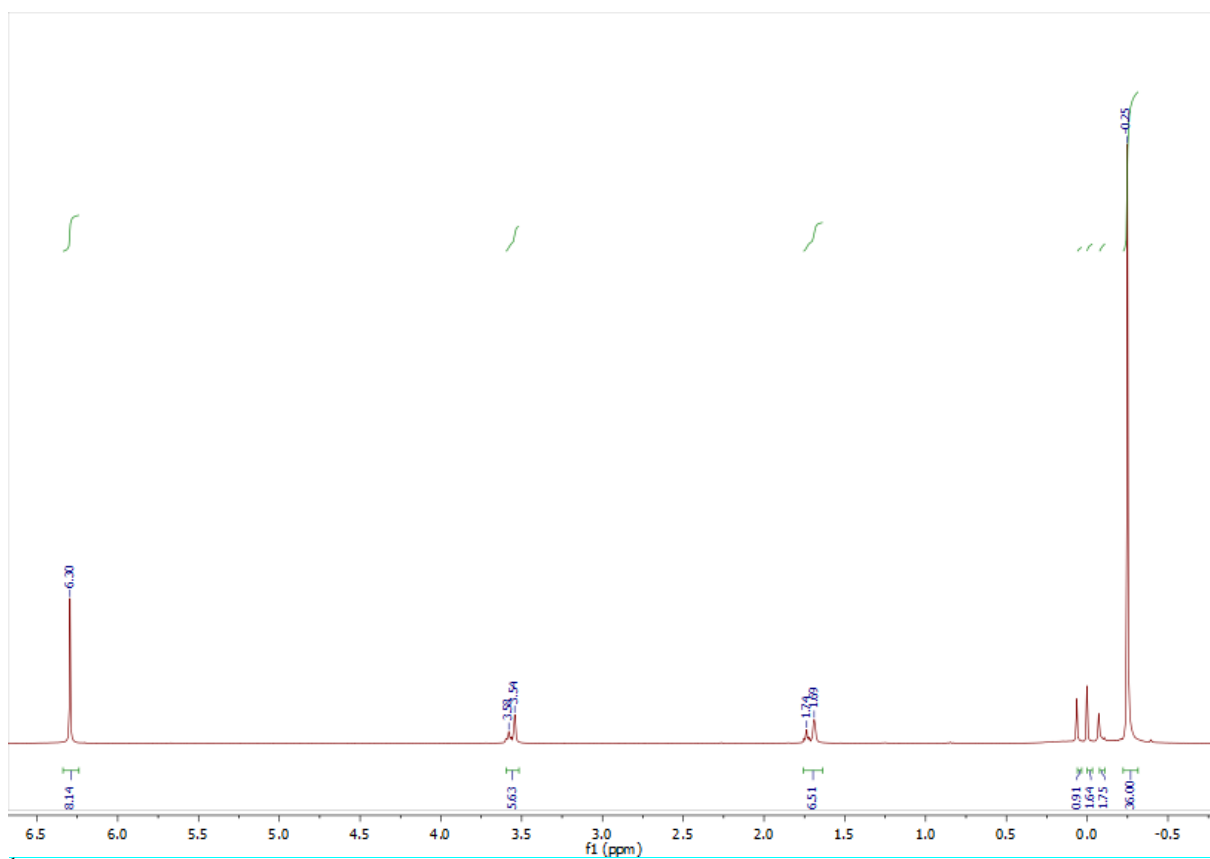
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¹ H and ¹³ C{ ¹ H} NMR spectra of 1-Sr in thf-d ₈ .	S3
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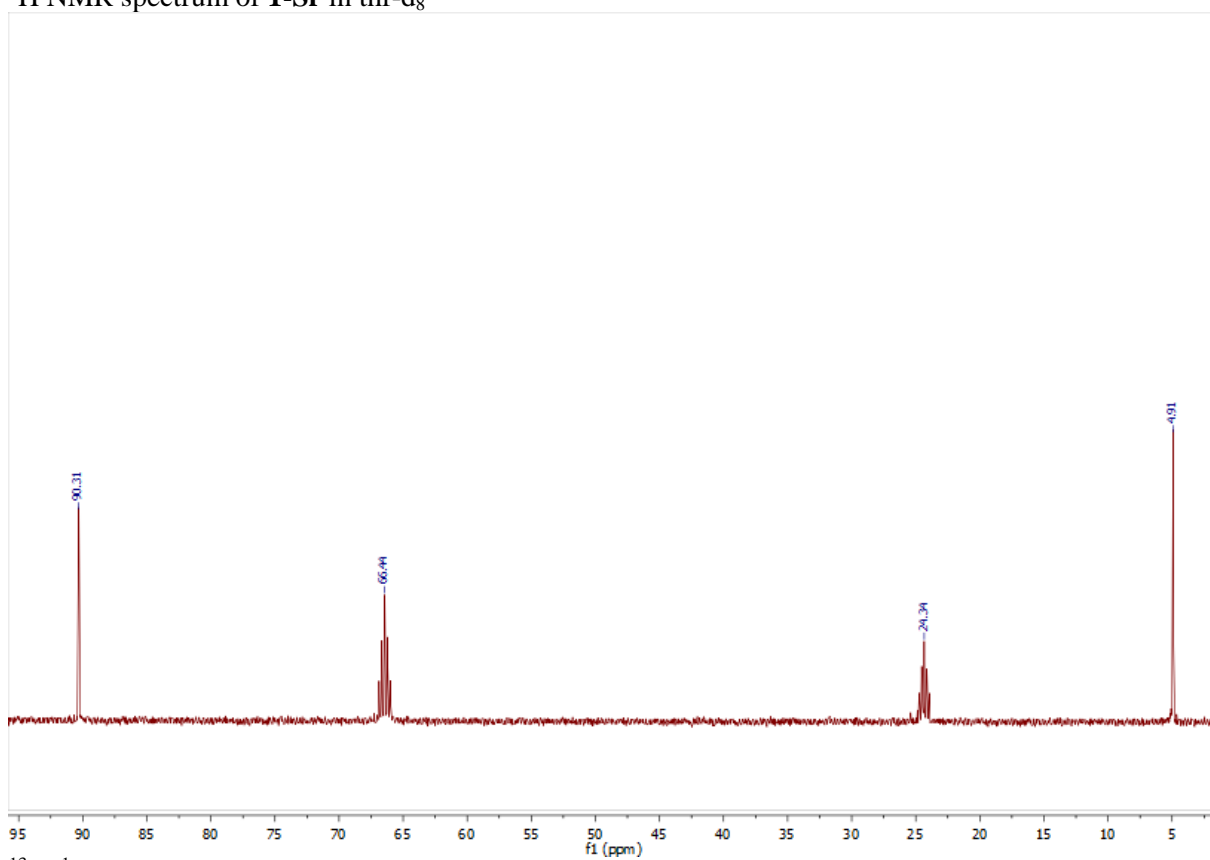
^1H NMR spectrum of **1-Ca** in C_6D_6 .



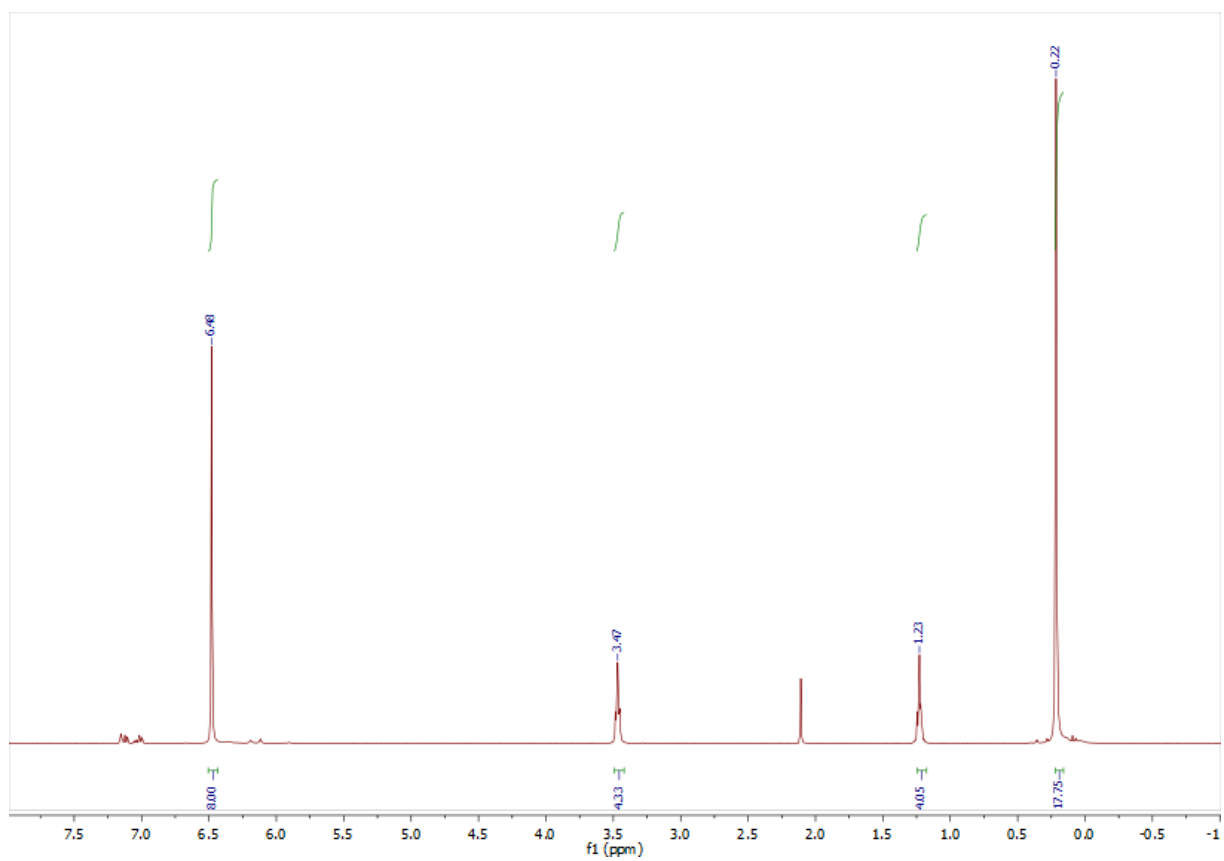
$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **1-Ca** in C_6D_6 .



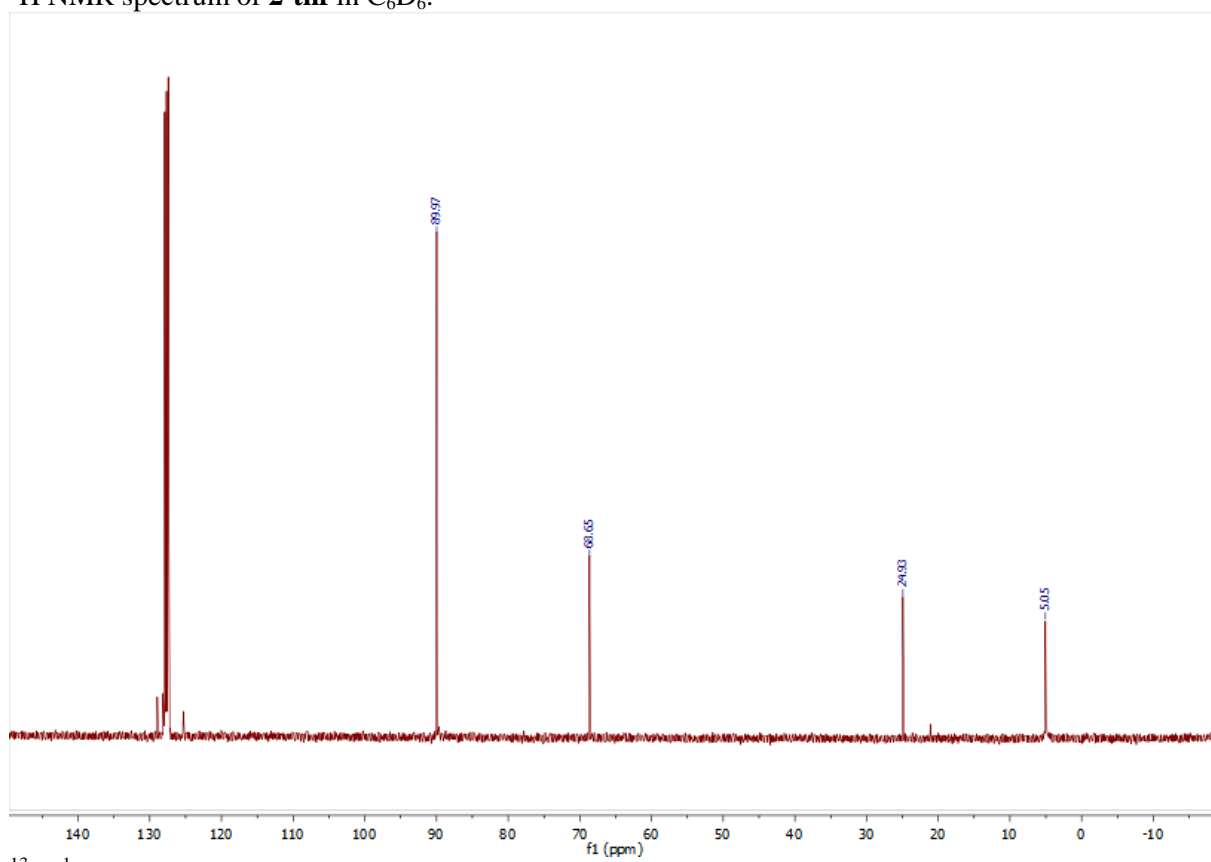
^1H NMR spectrum of **1-Sr** in thf-d_8



$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **1-Sr** in thf-d_8 .

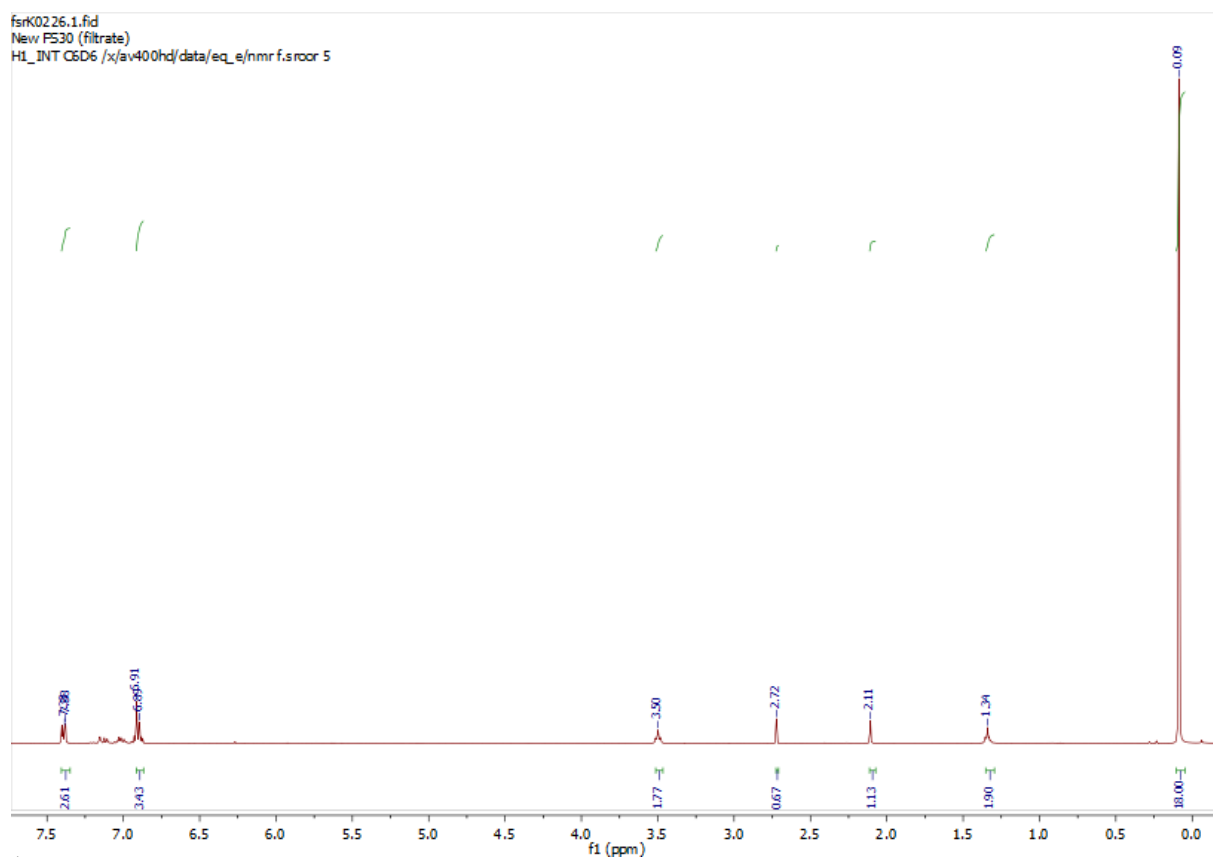


^1H NMR spectrum of **2-thf** in C_6D_6 .

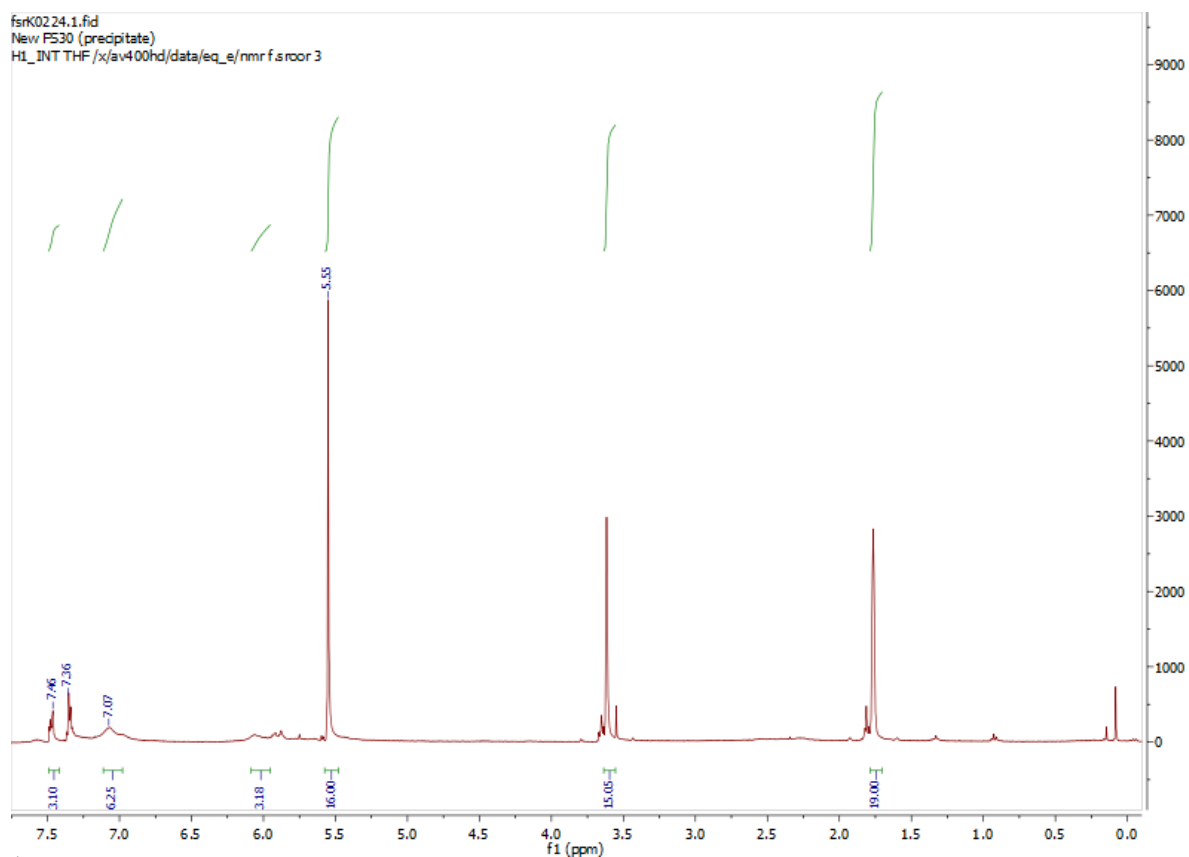


$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **2-thf** in C_6D_6 .

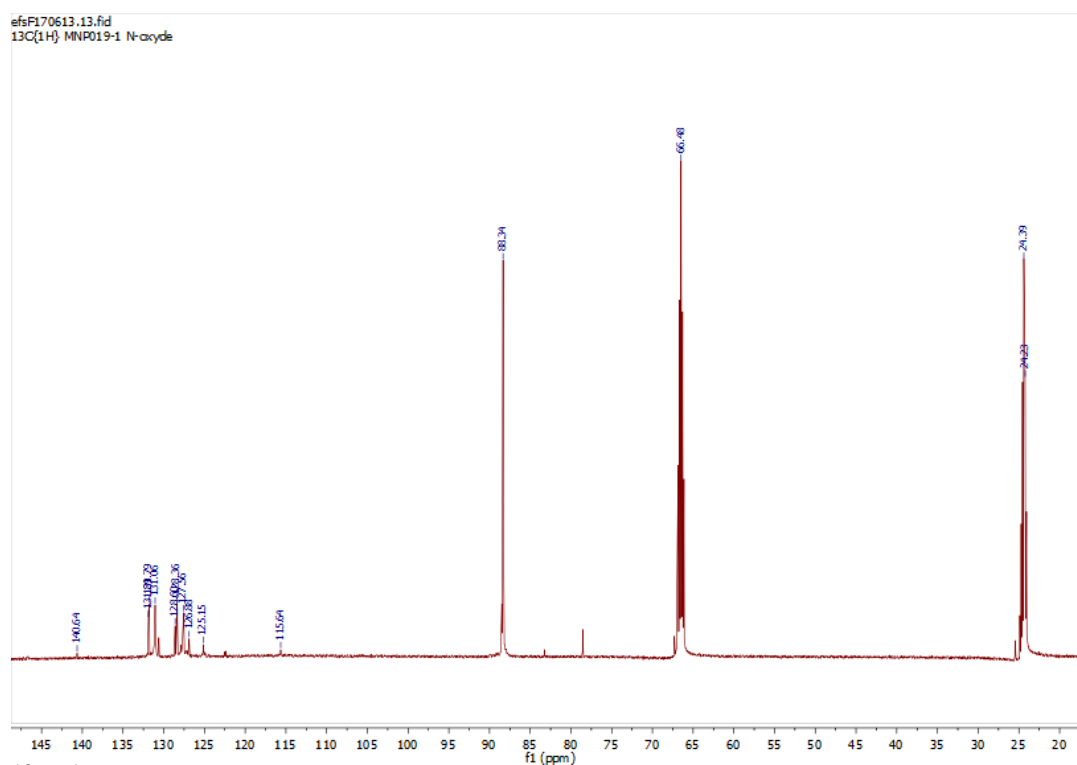
Representative spectra from the reaction of **2-thf** with $\text{PhC}\equiv\text{CH}$.



^1H NMR spectrum of the reaction mixture between **2-thf** and $\text{PhC}\equiv\text{CH}$ in C_6D_6 revealing the presence of $\text{HN}(\text{SiMe}_3)_2$ and the absence of COT containing species in solution.



^1H NMR spectrum after dissolution of compound **4** in thf-d_8 showing the absence of amido ligand, the presence of phenyl groups and COT ligand (mixture of compound **5**, purported $[\text{Ca}(\text{CPh})_2(\text{thf})_x]$, and unidentified species).



$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum after dissolution of compound **4** in thf-d_8 showing the absence of amido ligand, the presence of phenyl groups and COT ligand (mixture of compound **5**, purported $[\text{Ca}(\text{CPh})_2(\text{thf})_x]$, and unidentified species).

X-ray crystal structure of compound **3** obtained from the reaction of **2-thf** with $[\text{Sr}\{\text{N}(\text{SiMe}_3)_2\}_2]$ in toluene.

It was not possible to find a suitable crystal for good quality structure. Several trials were performed but only weakly diffracting samples (giving a low $\sin(\theta_{\text{max}})/\lambda$) or no true single crystals (not even a clear twin that can be treated) were obtained. Only a low quality structure could be obtained, refined on F2 with the help of SHELXL2016. It presents a high R factor (10.2 %) and more particularly a high residue close to K2. The ROTAX option in CRYSTALS indicated many possible twin laws but none of them helped to improve the quality of the structure.

The structural arrangement obtained is clearly polymeric when the structure of **3** (CCDC 1839572) is a discrete dimer. The metrical parameters are not significantly different in both structures.

Compound	3
Formula	$\text{C}_{40}\text{H}_{90}\text{K}_2\text{N}_4\text{Si}_8\text{Sr}_2$
Colour, shape	Colourless, block
<i>M</i>	1090.29
Crystal system	Triclinic
Space group	<i>P</i> -1
<i>a</i> /Å	10.8699 (15)
<i>b</i> /Å	11.0066 (15)
<i>c</i> /Å	12.9292 (18)
β /°	90.496 (5)
<i>V</i> /Å ³	1471.6 (4)
<i>Z</i>	1
<i>T</i> /K	100
<i>F</i> (000)	575
ρ_{calcd} /Mg m ⁻³	1.230
μ /mm ⁻¹	2.15
Crystal size /mm	0.12×0.06×0.02
Data / restraints/ parameters	4226 / 0 / 253
<i>R</i> ₁ (<i>I</i> > 2σ(<i>I</i>))	0.102
<i>wR</i> ₂	0.279
Largest diff. peak / hole	7.89 - -1.33
CCDC	1839568

