Supplementary Information for

Alkali and Alkaline Earth Metal Complexes Ligated by an Acetyl substituted Cyclopentadienyl Ligand

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Table of contents

1. Crystallographic data

Compound	**1**	**2**	**3**
Formula	$C_{26}H_{45}NaO_3Si$	$C_{22}H_{37}KO_2Si$	$C_{44}H_{74}Ca_2I_2O_4Si_2$
$D_{calc.}$/ g cm^{-3}	1.083	1.096	1.160
μ/mm^{-1}	0.121	0.282	1.278
Formula Weight	456.70	400.70	1057.17
Colour	clear colourless	colorless	yellow
Shape	plate	plate	block
Size/mm^3	0.30×0.16×0.07	0.33×0.20×0.10	0.33×0.29×0.28
T/K	100	100	220
Crystal System	monoclinic	orthorhombic	monoclinic
Flack parameter		0.03(4)	
Space Group	$P2_1/c$	$P2_12_12_1$	$P2_1/n$
a/Å	8.1123(16)	10.287(2)	9.4746(4)
b/Å	14.126(3)	11.429(2)	14.9924(8)
c/Å	24.766(5)	20.495(4)	21.7467(8)
β/°	99.36(3)		101.490(3)
V/Å^3	2800.4(10)	2409.6(8)	3027.1(2)
Z	4	4	2
Z'	1	1	0.5
Wavelength/Å	0.71073	0.71073	0.71073
Radiation type	Mo Kα	Mo Kα	MoKα
Θ_{min}/°	1.665	1.987	1.911
Θ_{max}/°	26.088	26.104	26.125
Measured Refl.	12871	19379	14525
Independent Refl.	5468	4731	5910
Reflections Used	2890	3955	3630
R_{int}	0.1124	0.0584	0.0286
Parameters	287	242	251
Restraints	40	0	0
Largest Peak	0.955	0.337	0.587
Deepest Hole	-0.997	-0.342	-0.779
GooF	1.003	0.993	0.975
wR_2 (all data)	0.2846	0.0913	0.1181
wR_2	0.2343	0.0872	0.1089
R_1 (all data)	0.1644	0.0503	0.0636
R_1	0.0931	0.0380	0.0392

Figure S1: Molecular structure of **1** in the solid-state structure. Hydrogen atoms and solvent molecules are omitted for clarity. Thermal ellipsoids are drawn to encompass 50 % probability.

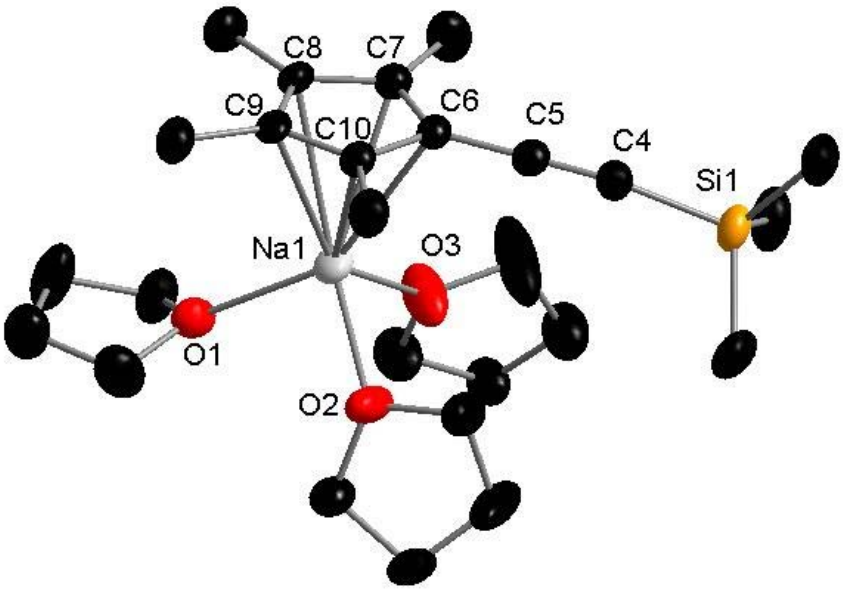


Figure S2: Molecular structure of **2** in the solid-state structure. Hydrogen atoms and solvent molecules are omitted for clarity. Thermal ellipsoids are drawn to encompass 50 % probability.

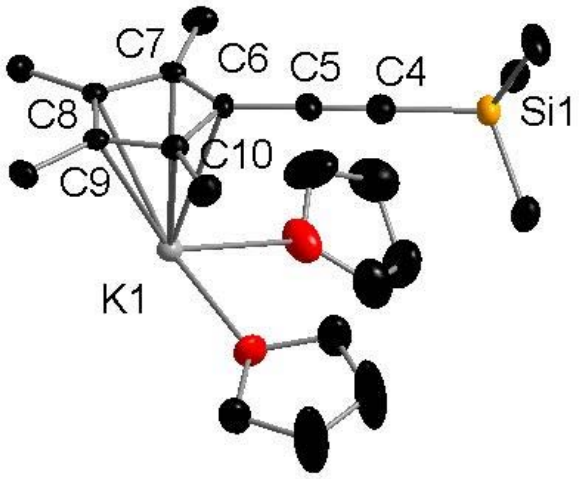
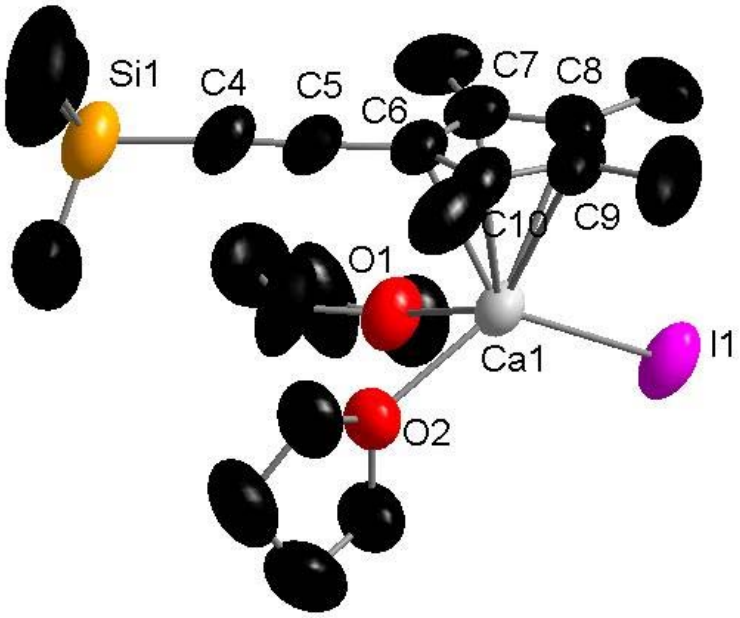


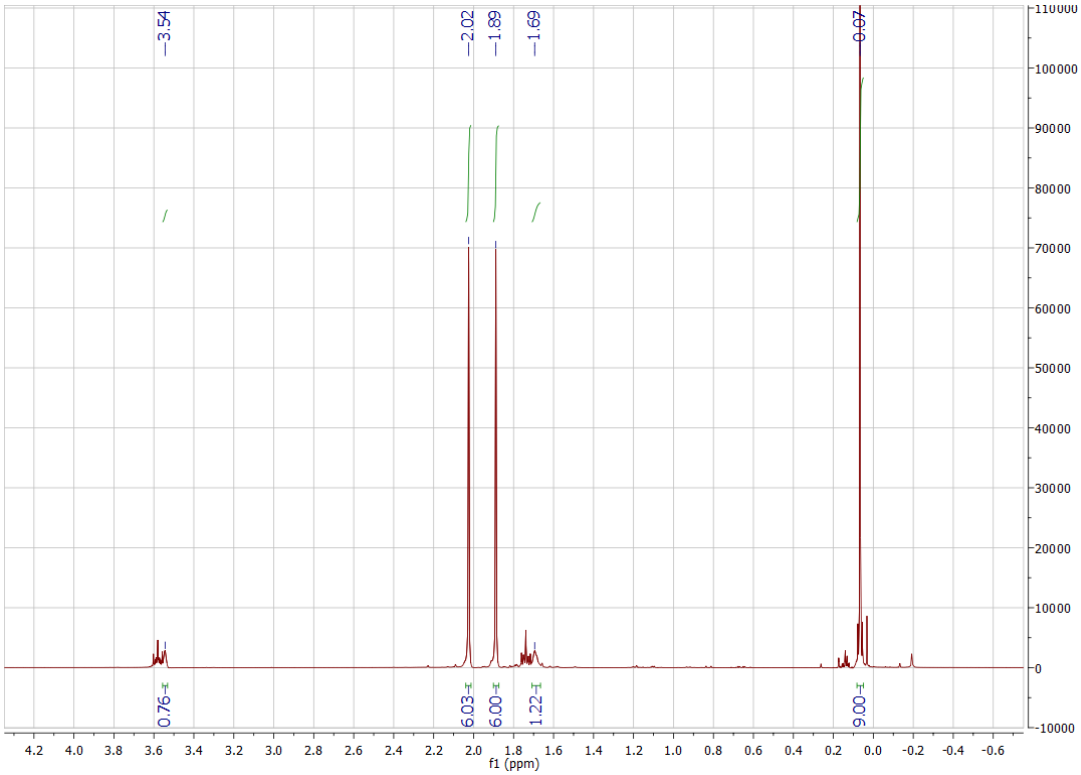
Figure S3: Molecular structure of **3** in the solid-state structure. Hydrogen atoms and solvent molecules are omitted for clarity. Thermal ellipsoids are drawn to encompass 50 % probability.



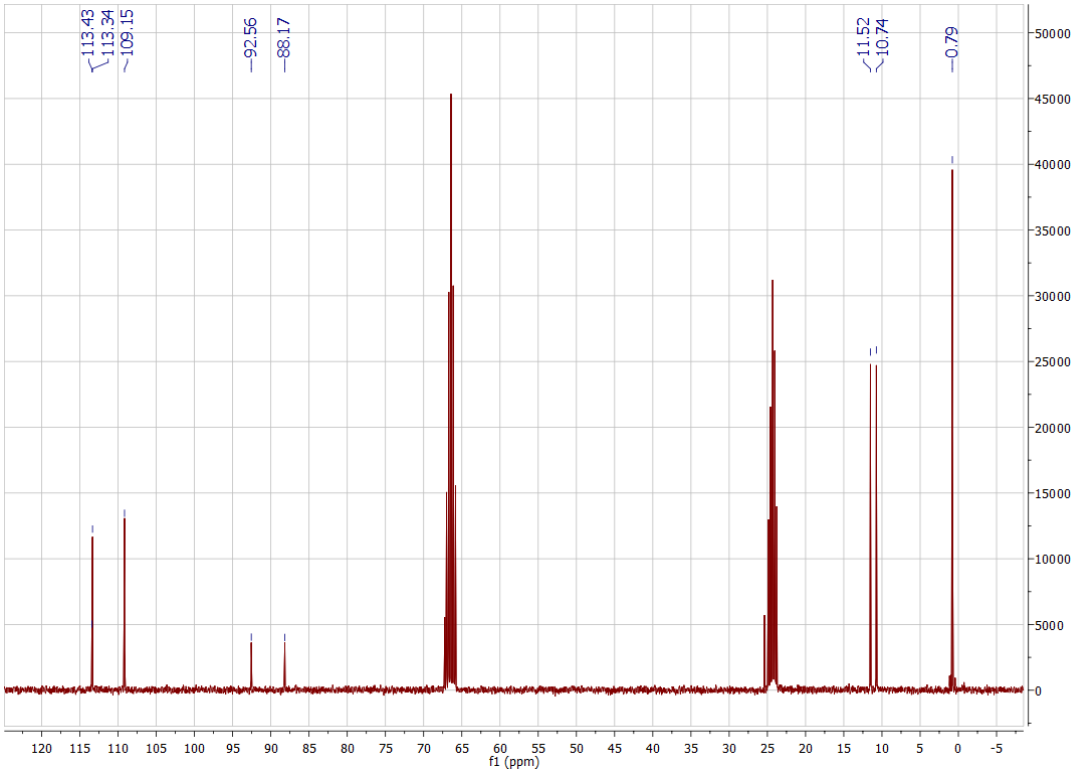
2. NMR Spectra

2.1 [NaCpMe$_4$(C≡CSiMe$_3$)(THF)$_3$] (**1**)

^{1}H NMR (298K, 300 MHz, THF-D$_8$)

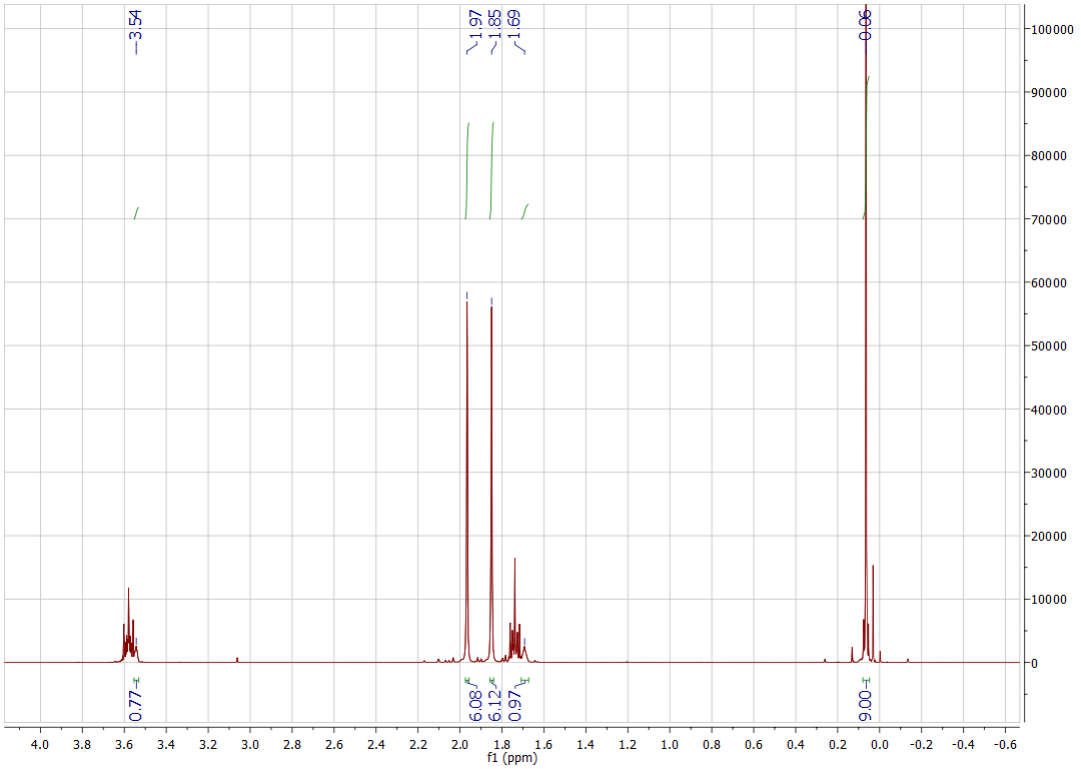


^{13}C{^{1}H} NMR (298K, 75 MHz, THF-D$_8$)

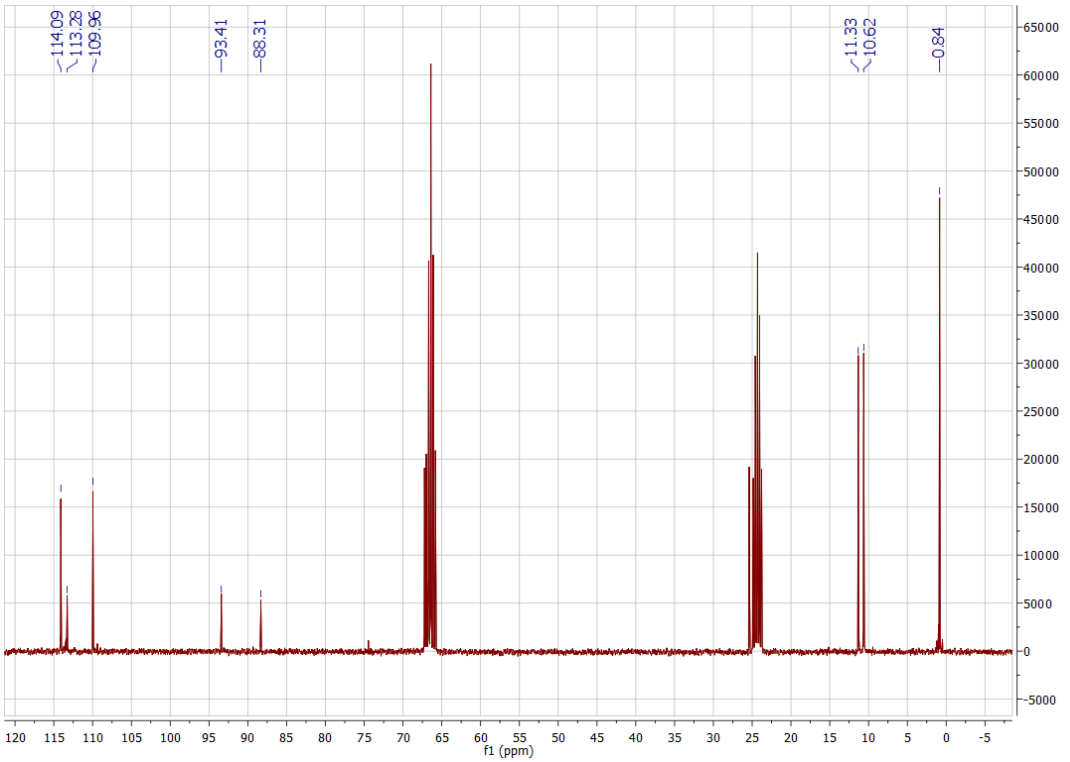


2.2 $[KCpMe_4(C{\equiv}CSiMe_3)(THF)_2]_n$ (**2**)

^1H NMR (298K, 300 MHz, THF-D_8)

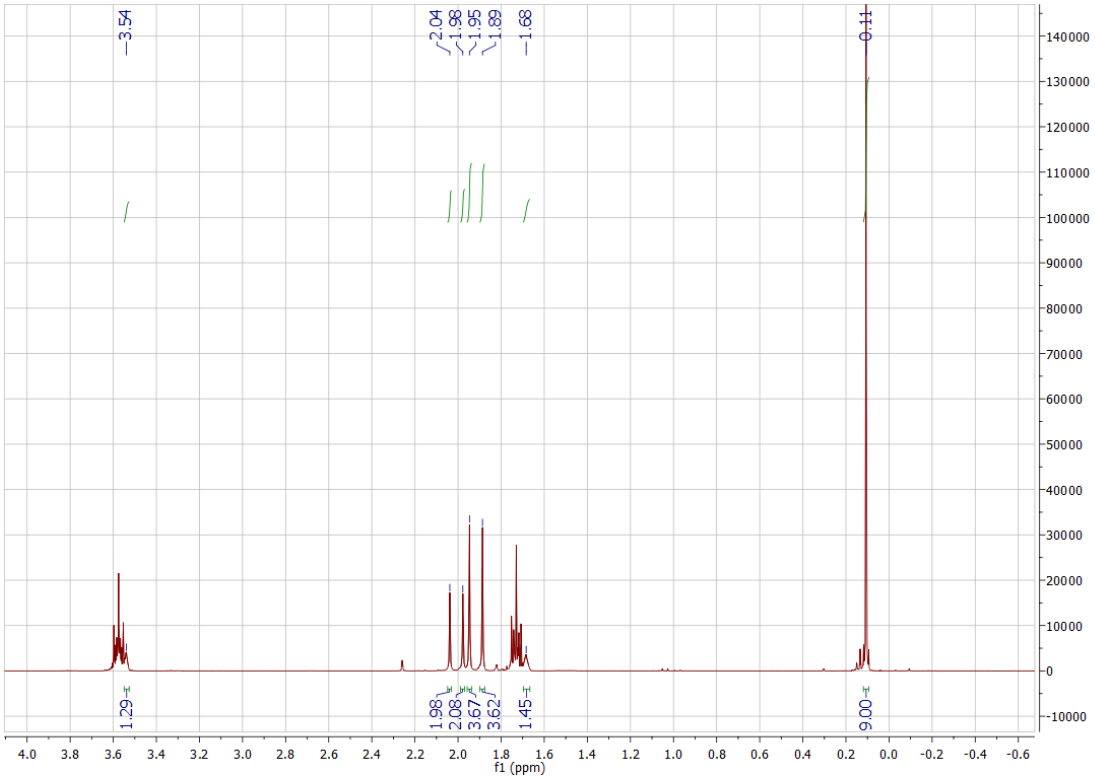


$^{13}C\{^1H\}$ NMR (298K, 75 MHz, THF-D_8)

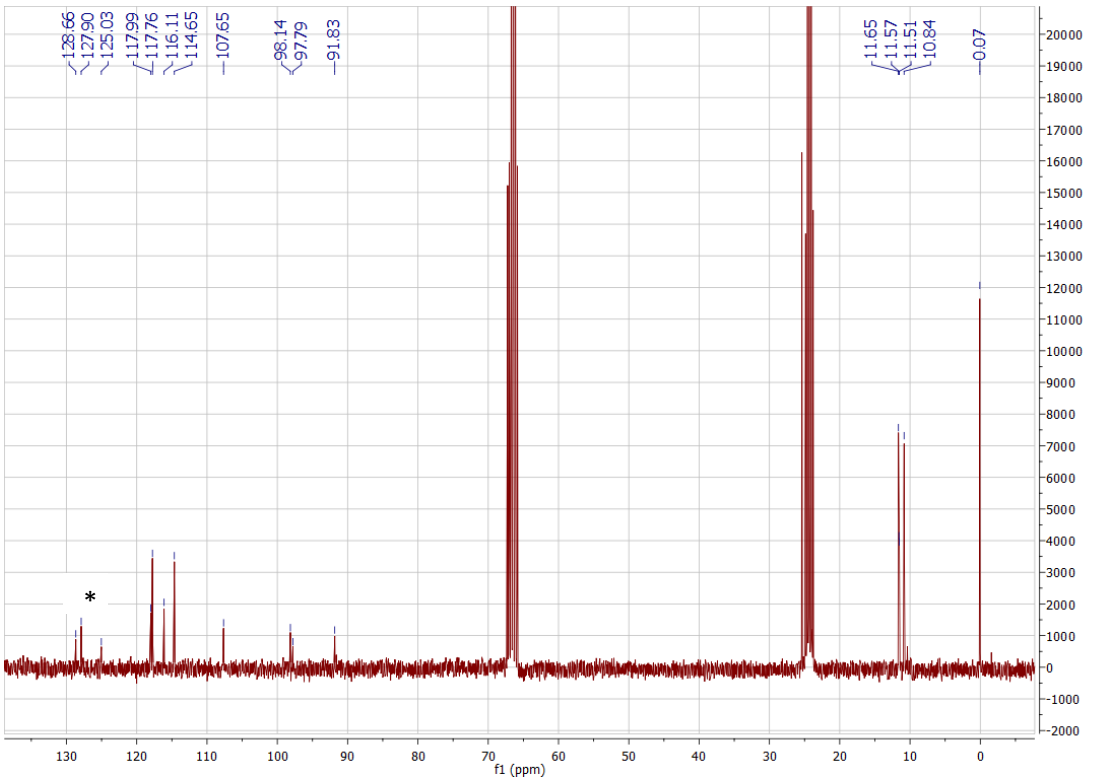


2.3 $[CpMe_4(C{\equiv}CSiMe_3)CaI(THF)_2]_2$ (**3**)

^1H NMR (298K, 300 MHz, THF-D_8)



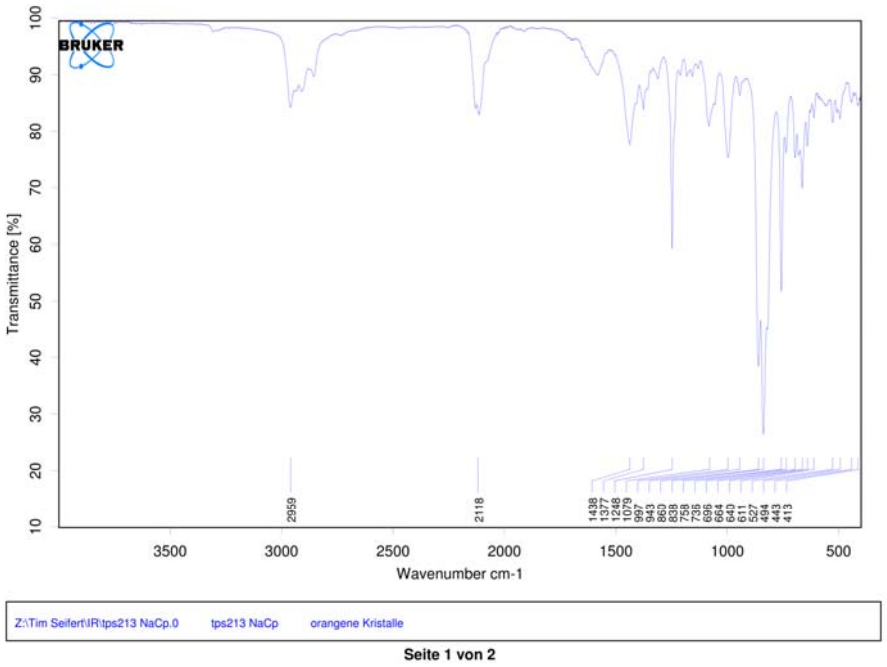
$^{13}C\{^1H\}$ NMR (298K, 75 MHz, THF-D_8)



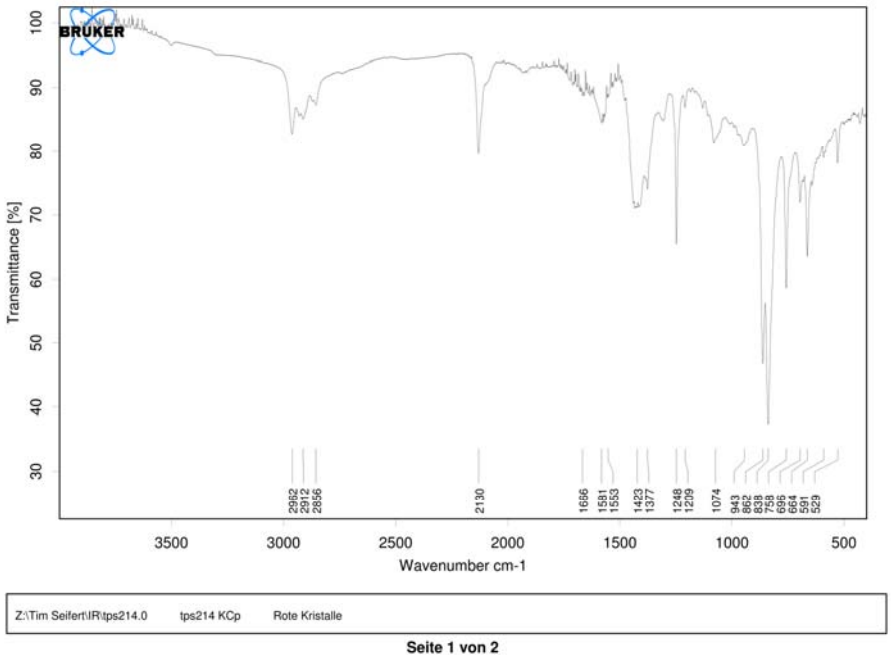
* traces of toluene

3. IR Spectra

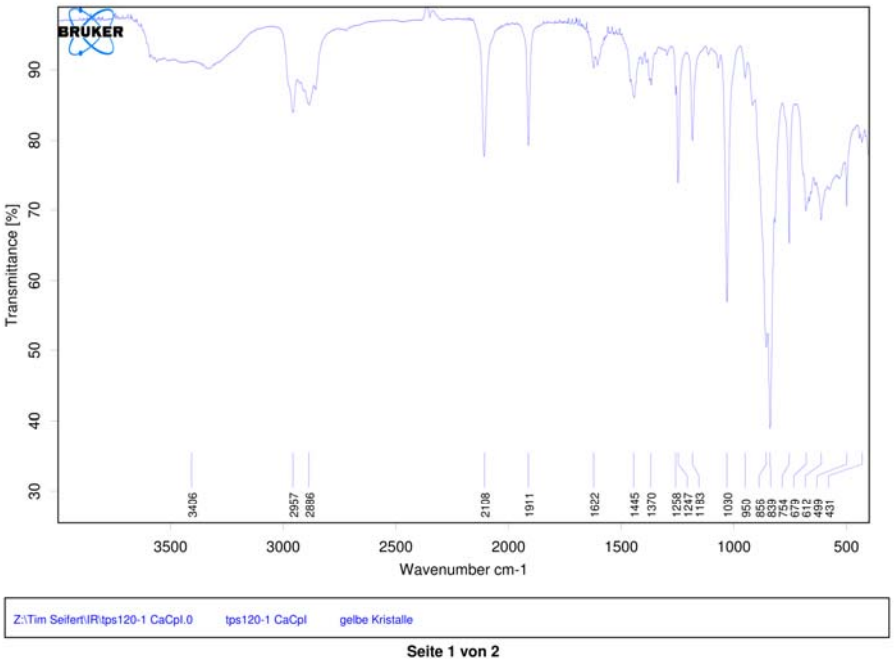
3.1 [NaCpMe$_4$(C≡CSiMe$_3$)(THF)$_3$] (**1**)



3.2 [KCpMe$_4$(C≡CSiMe$_3$)(THF)$_2$]$_n$ (**2**)



3.3 $[CpMe_4(C{\equiv}CSiMe_3)CaI(THF)_2]_2$ (**3**)



4. Mass spectra

$[CpMe_4(C{\equiv}CSiMe_3)CaI(THF)_2]_2$ (**3**)