

Supporting Information for

Transmetallation Reactions of a Scandium Complex Supported by a Ferrocene Diamide Ligand

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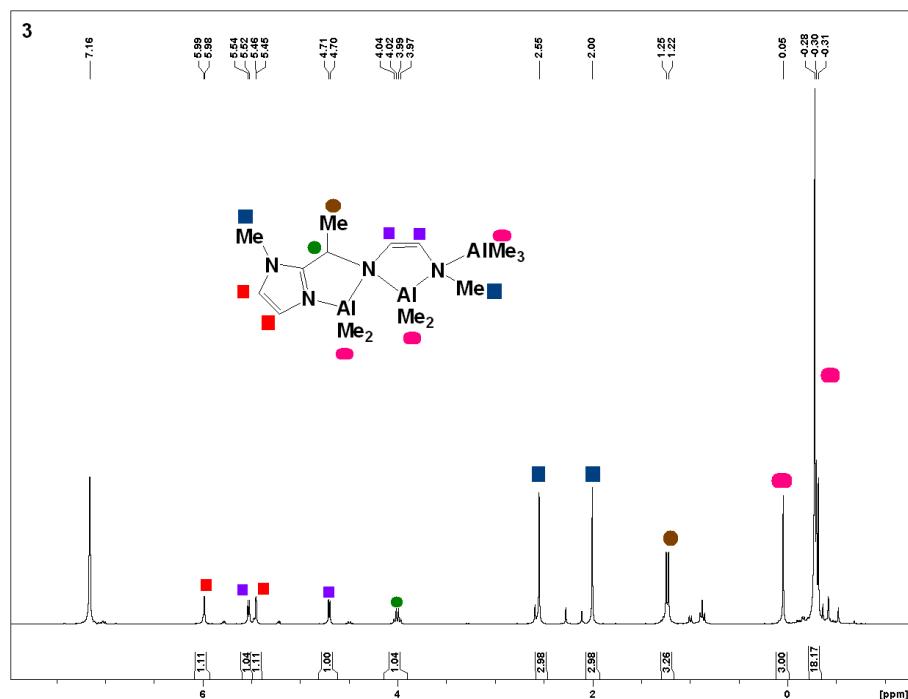
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NMR Spectra

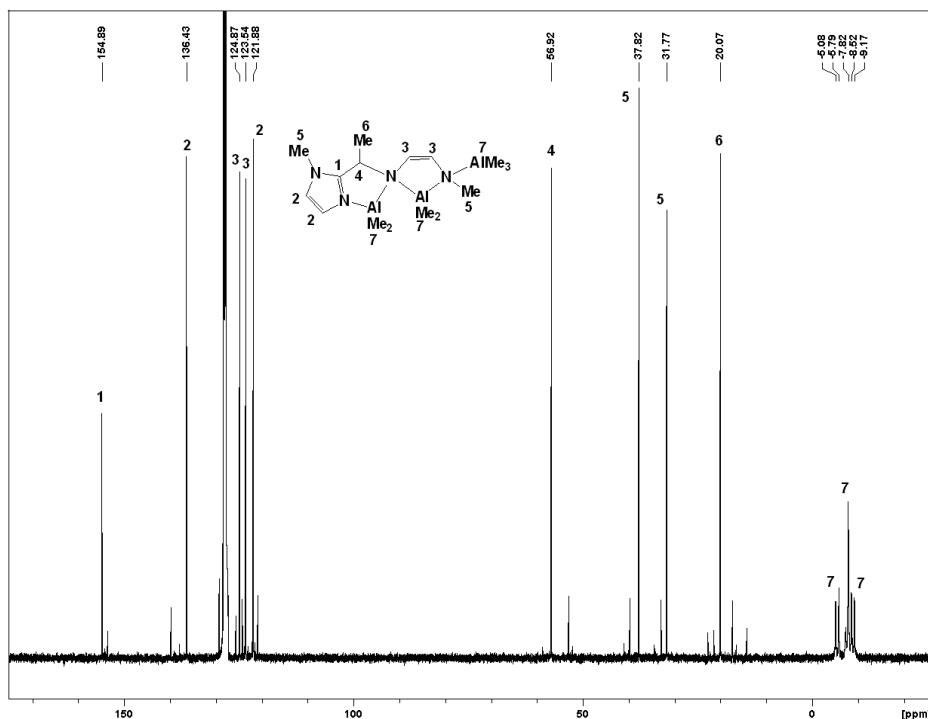
3

Note: The small peaks always appear in both the ^1H and the ^{13}C NMR spectra of **3**. As mentioned in the article, they likely correspond to a form of **3** with two aluminum fragments. Solvent peaks for toluene and hexanes are also present.

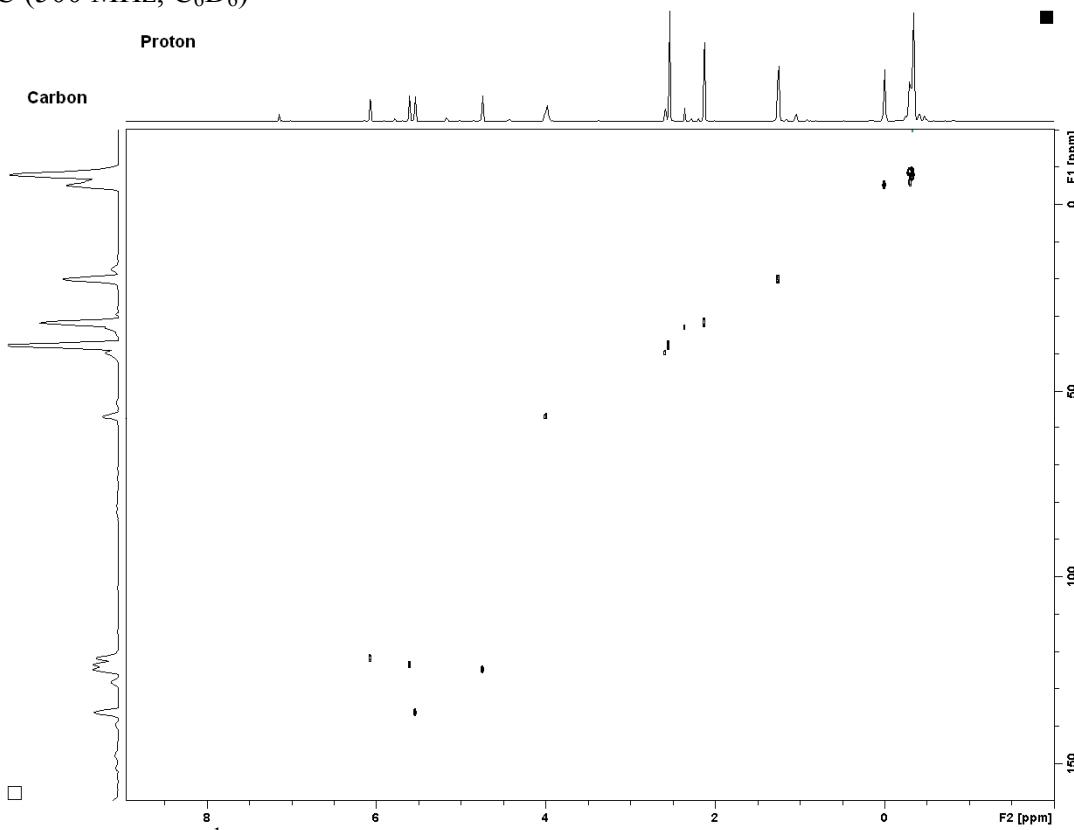
^1H NMR (300 MHz, C_6D_6)



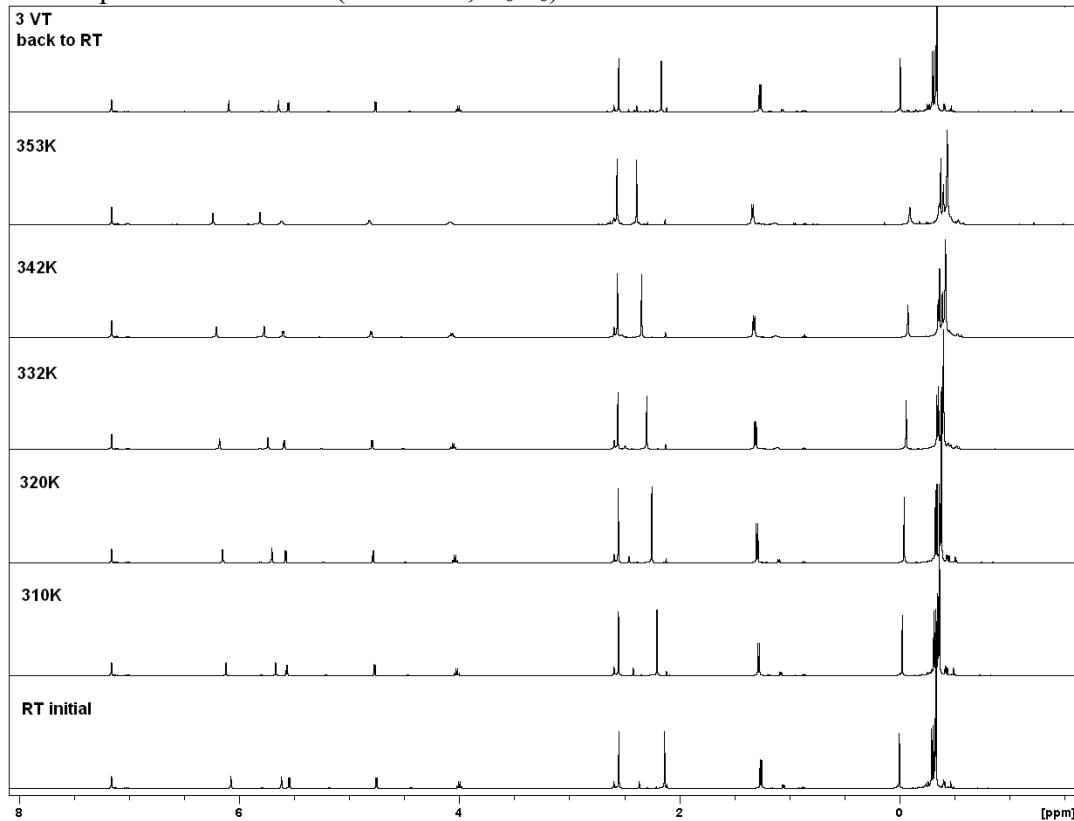
^{13}C NMR (126 MHz, C_6D_6)



HMQC (500 MHz, C₆D₆)



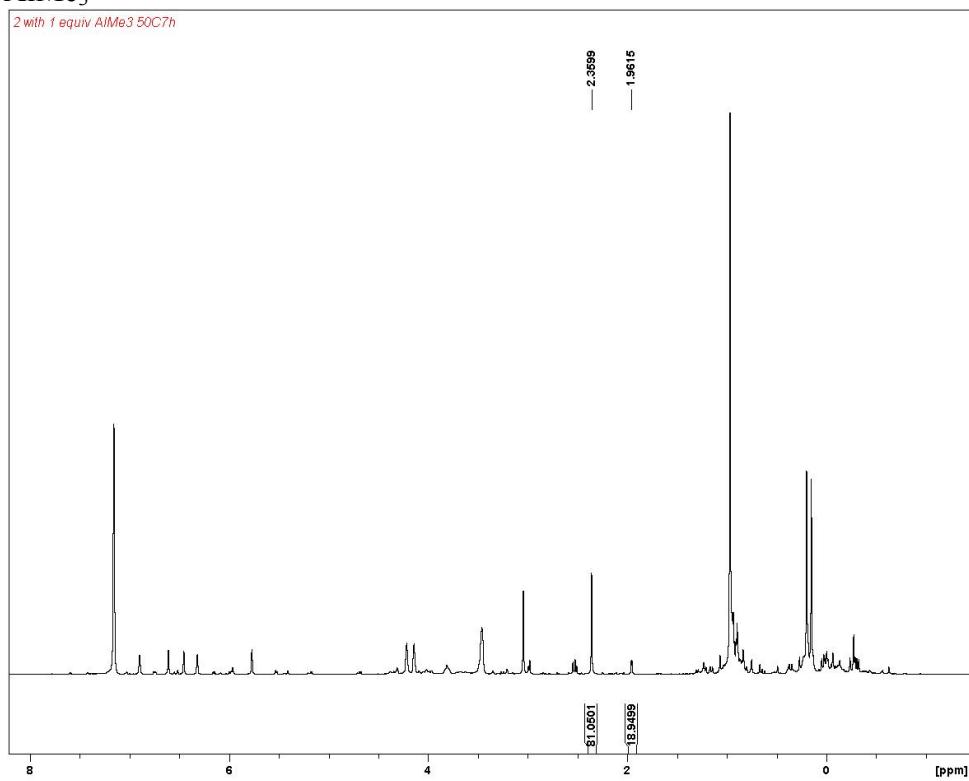
Variable-Temperature ¹H NMR (500 MHz, C₆D₆)



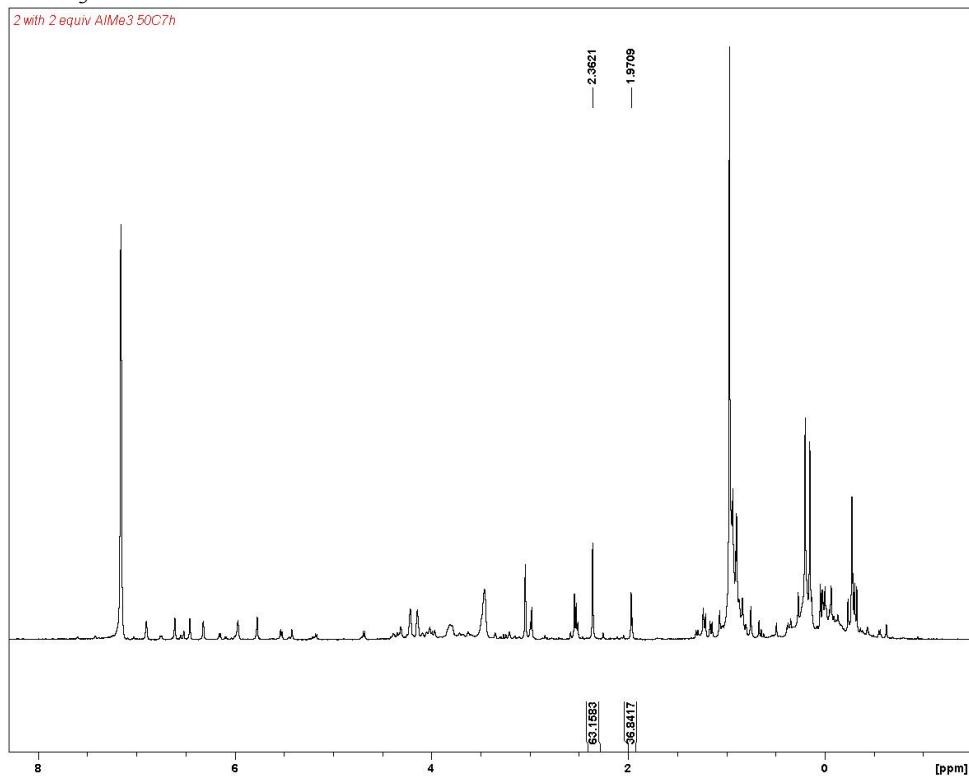
Reaction of 2 with a sub-stoichiometric amount of AlMe₃

¹H NMR (300 MHz or 500 MHz, C₆D₆)

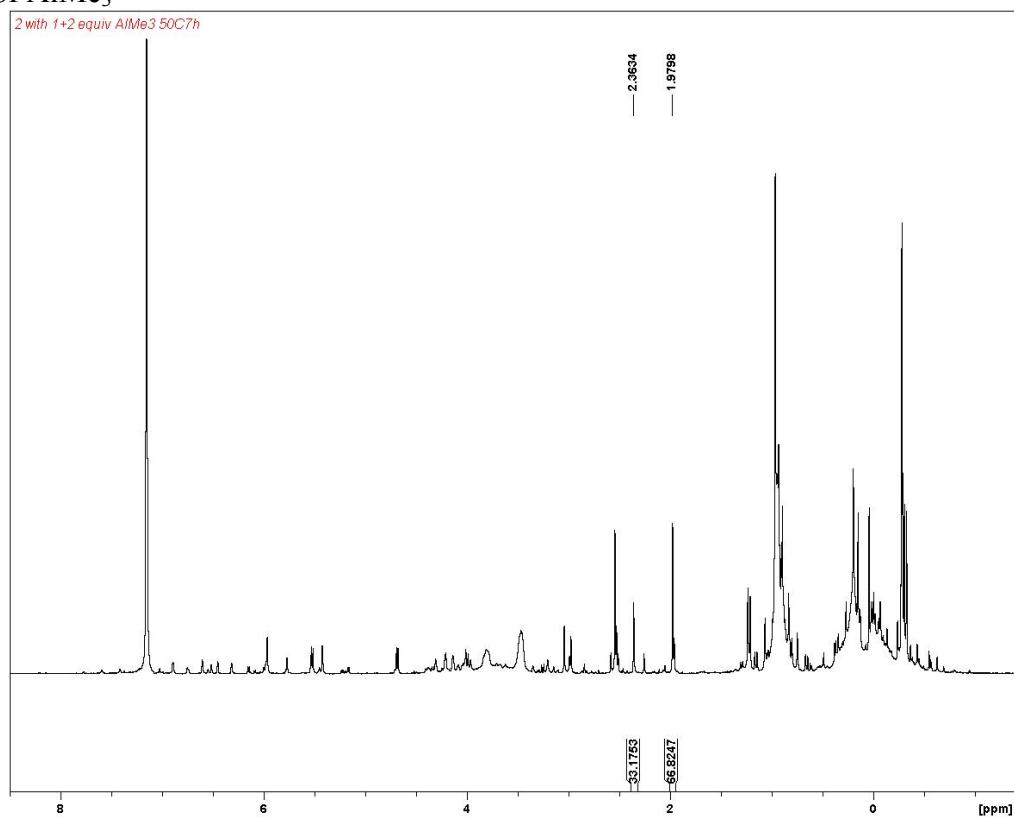
1 equiv of AlMe₃



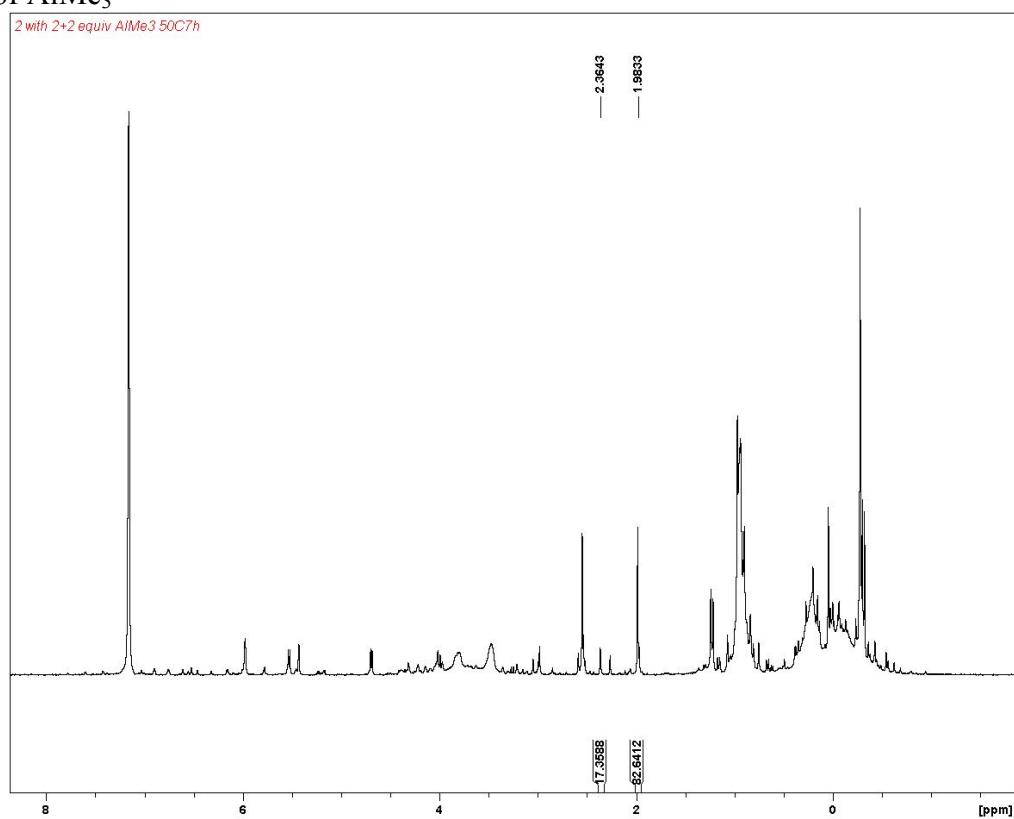
2 equiv of AlMe₃



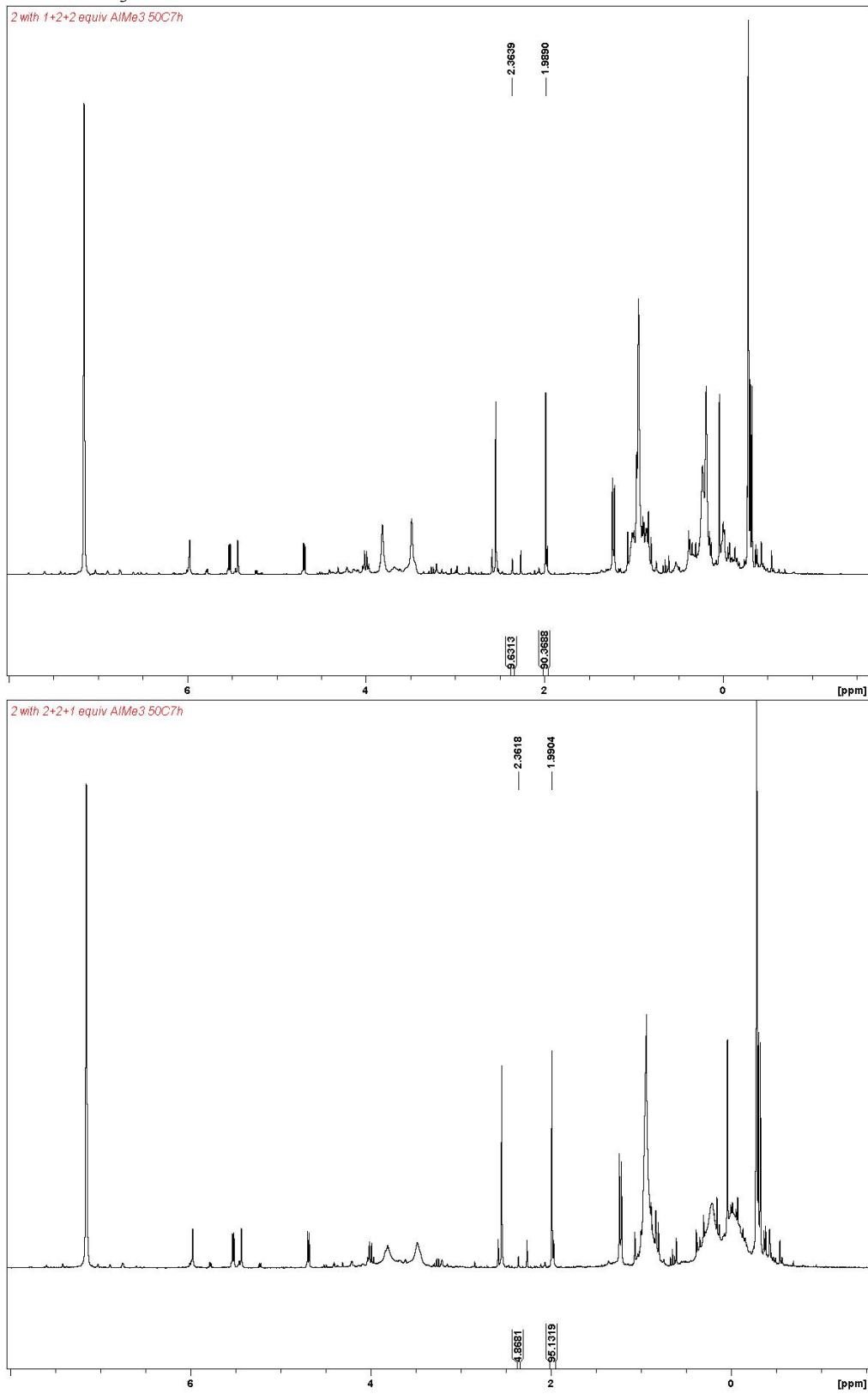
3 equiv of AlMe₃



4 equiv of AlMe₃



5 equivalents AlMe₃

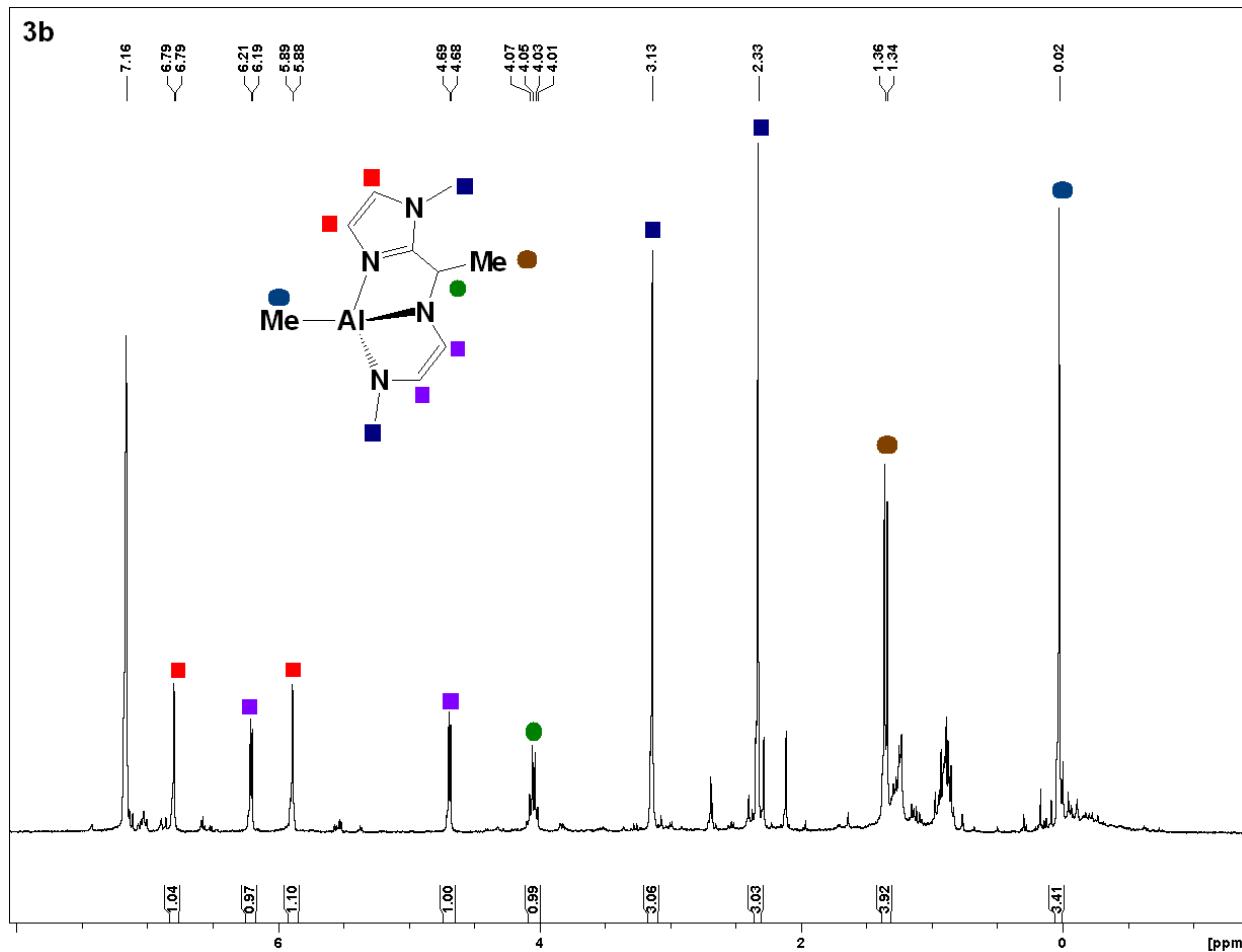


Note: The conversion percentage showed by integration was not exactly 20, 40, 60, 80, and 100%, likely due to a measuring error.

3b

¹H NMR (300 MHz, C₆D₆)

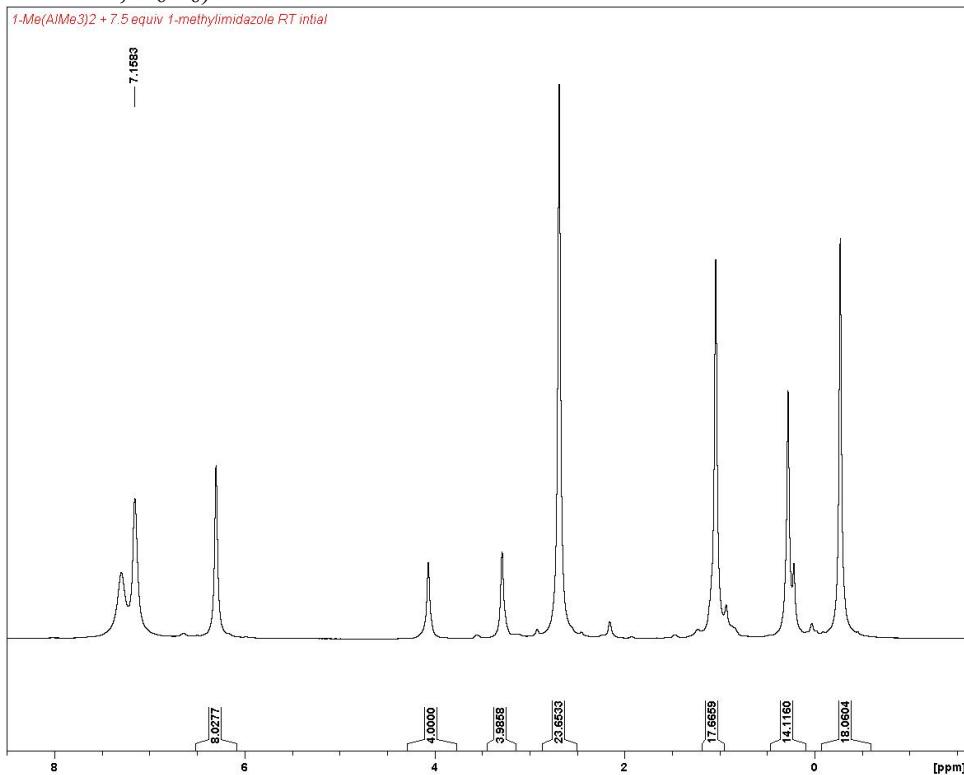
Note: **3b** is not very soluble in C₆D₆ (the spectrum shown is for a saturated sample); solvent peaks for toluene and hexanes as well as peaks for some impurities are also present.



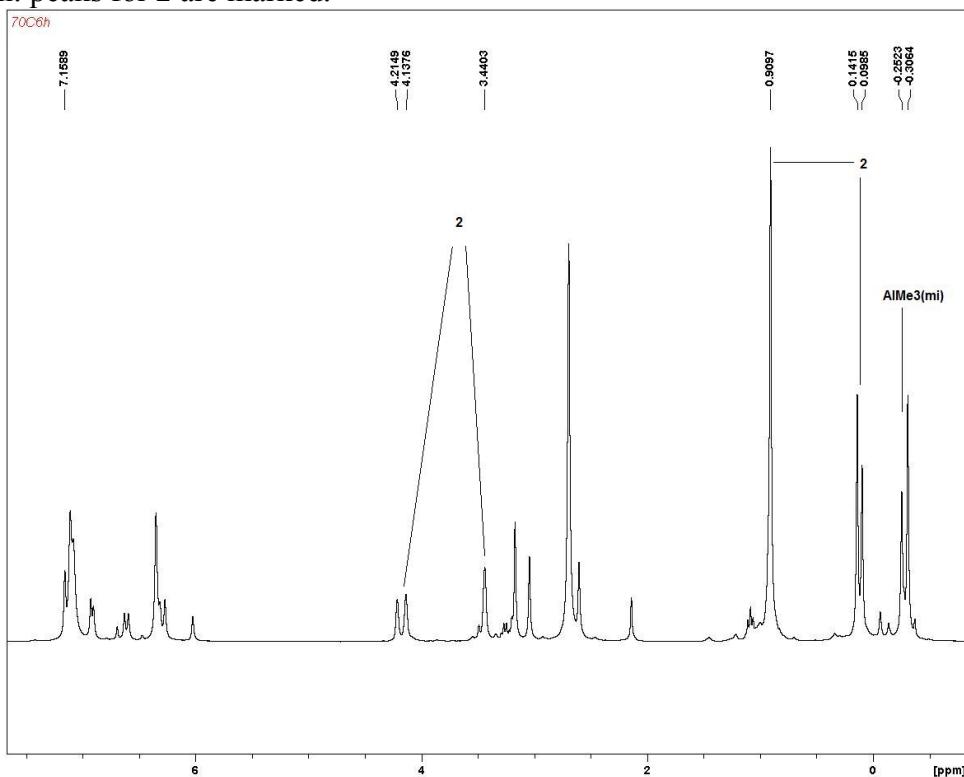
Reaction of 1-Me(AlMe₃)₂ with 1-methylimidazole

Note: Initially, **1-Me(mi)_x** and AlMe₃(mi) were formed.

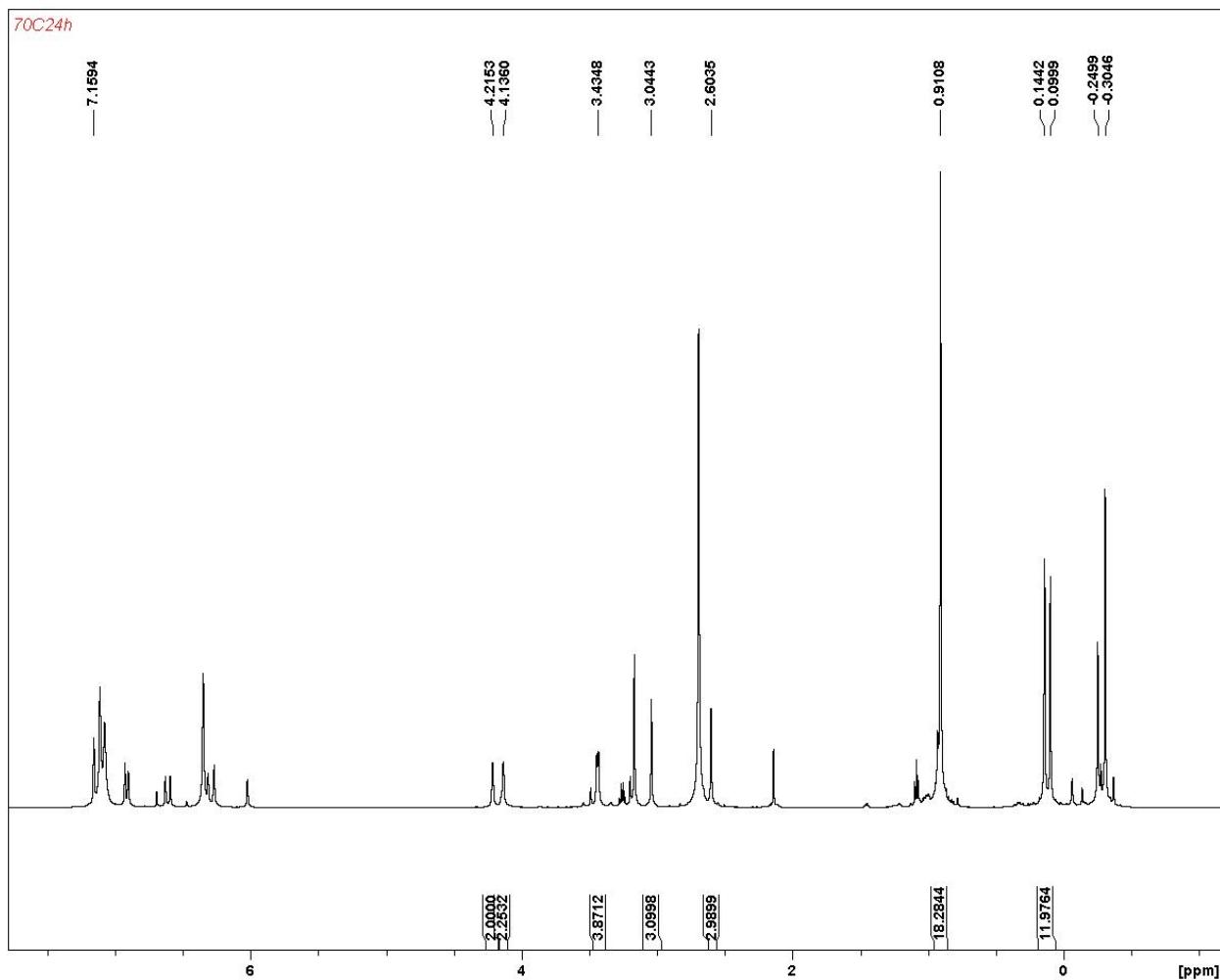
¹H NMR (300 MHz, C₆D₆)



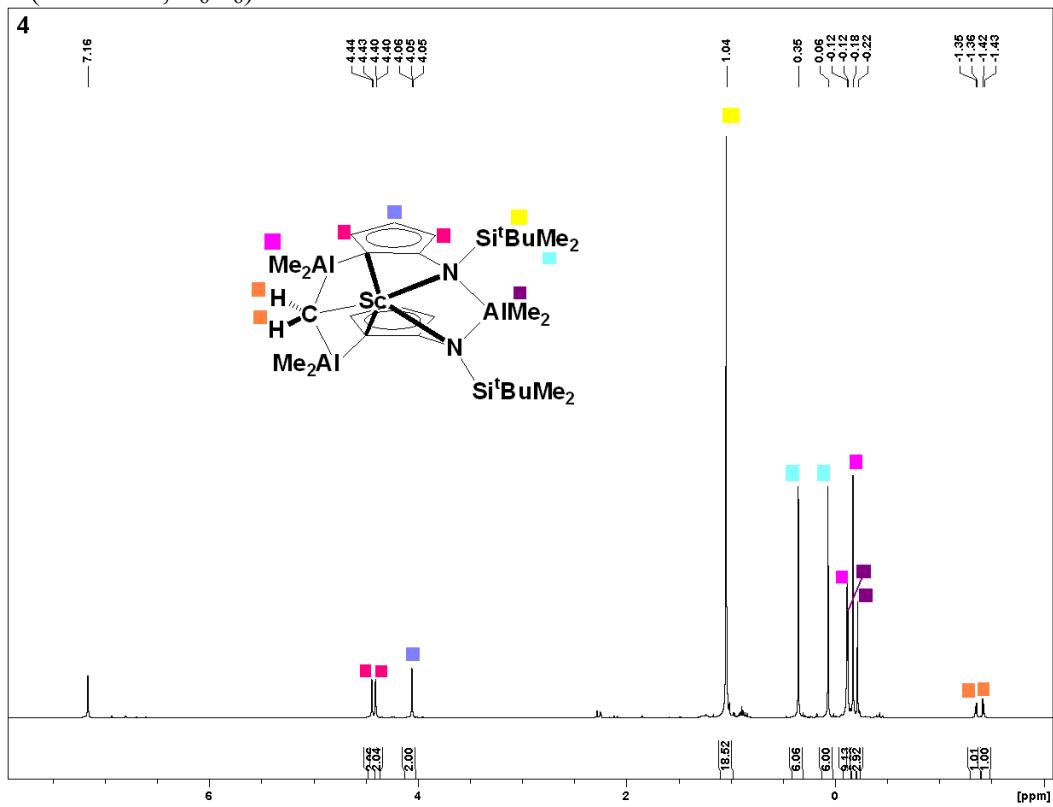
70 °C 6 h: peaks for **2** are marked.



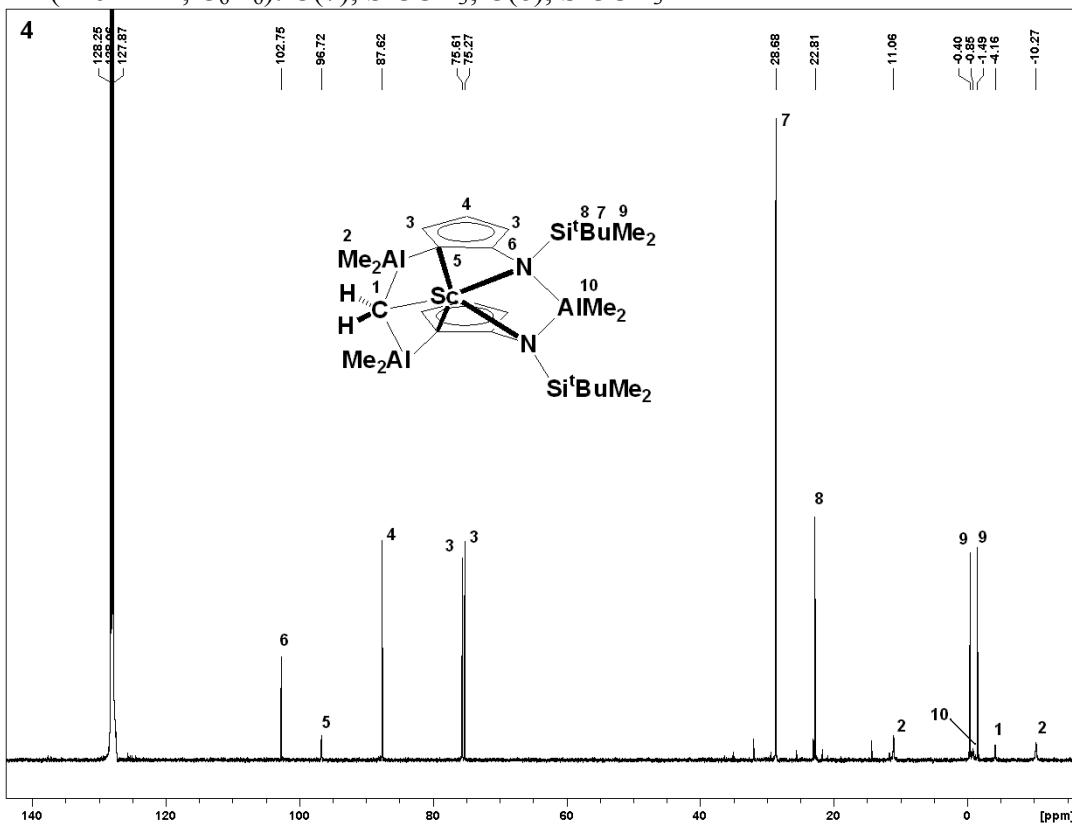
70 °C 24 h: All peaks belonging to compound **2** were confirmed by their chemical shifts as well as their relative integration.



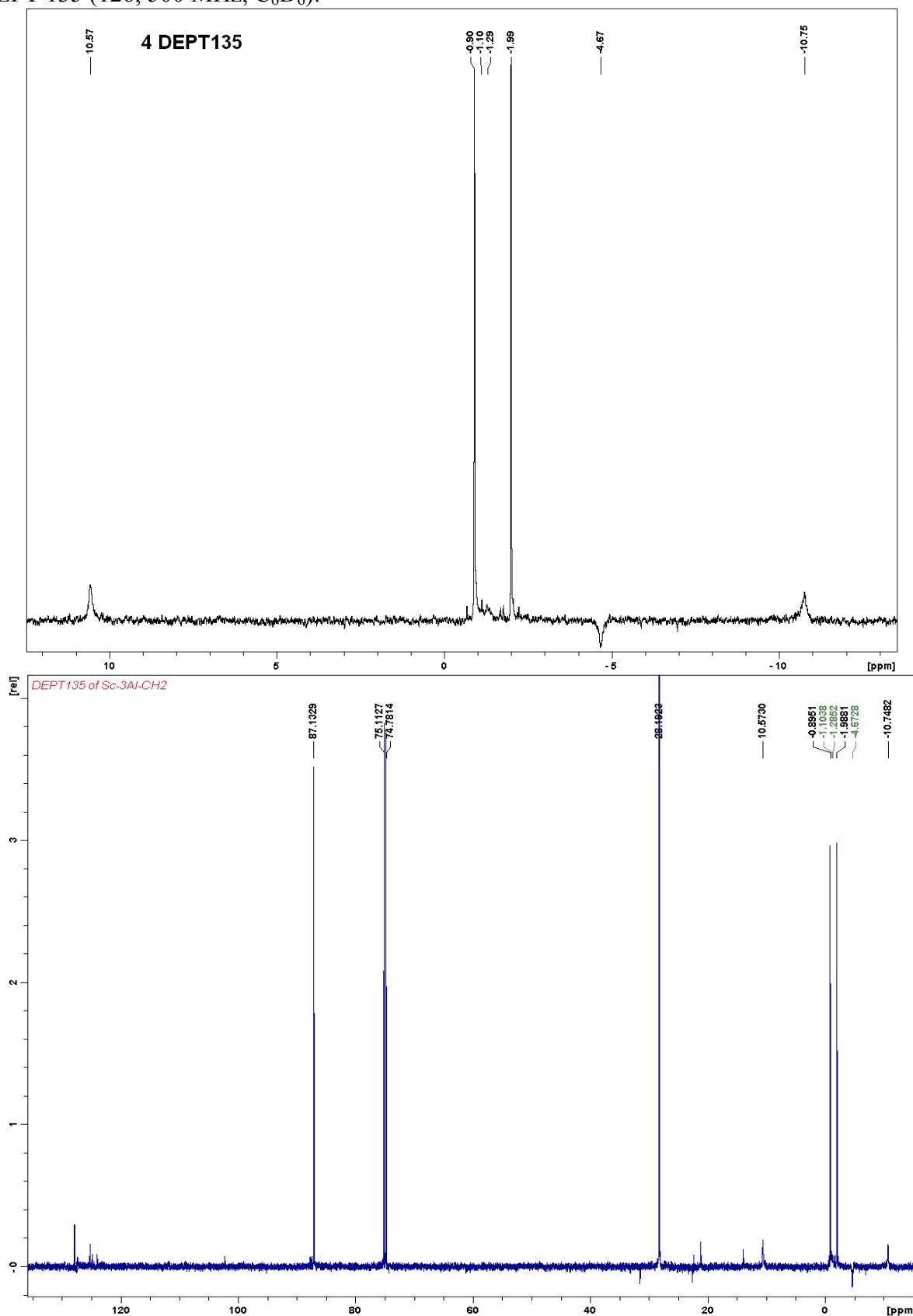
4
 ^1H NMR (500 MHz, C_6D_6)



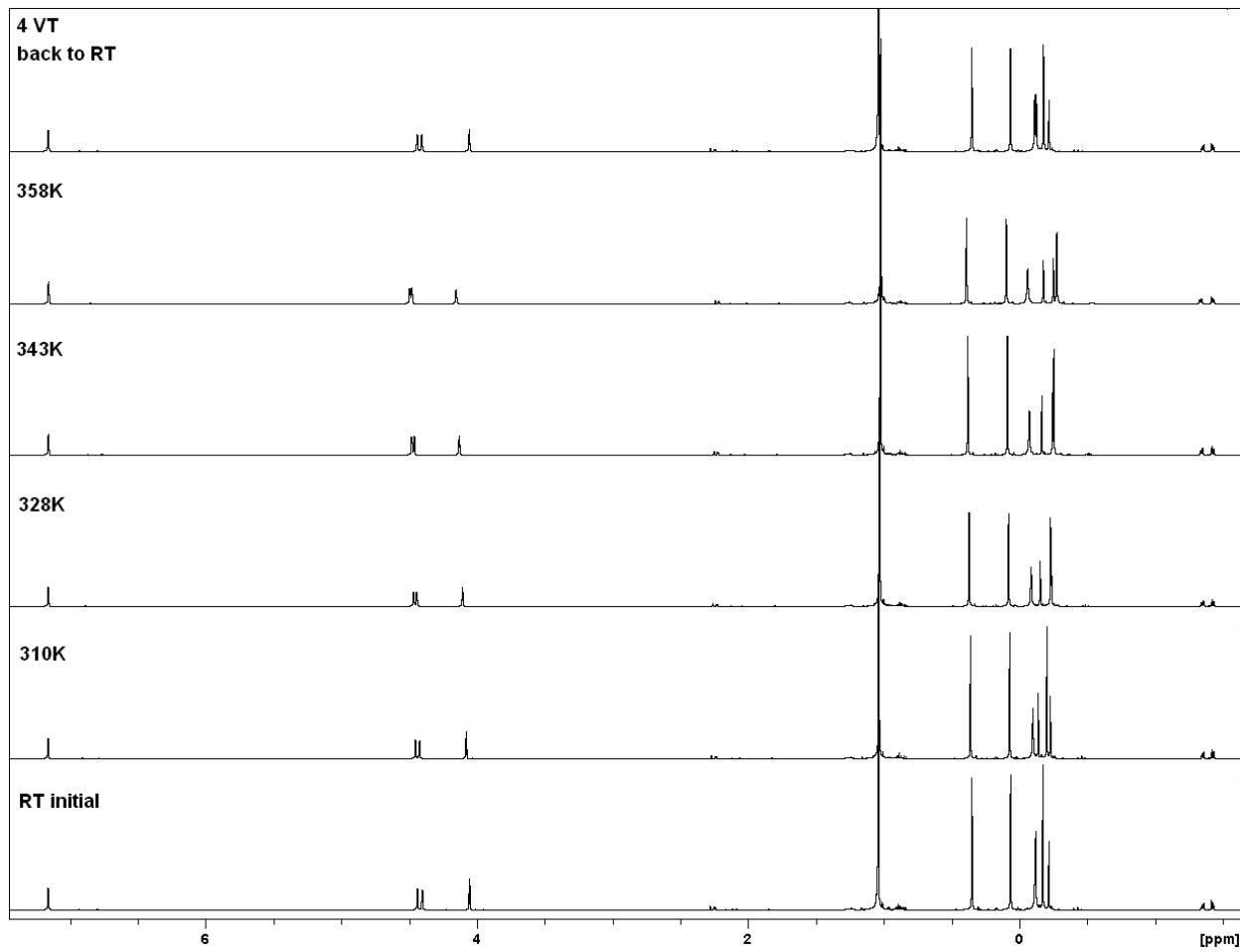
^{13}C NMR (126 MHz, C_6D_6): C(7), SiCCH_3 ; C(8), SiCCH_3



DEPT 135 (126, 500 MHz, C₆D₆):

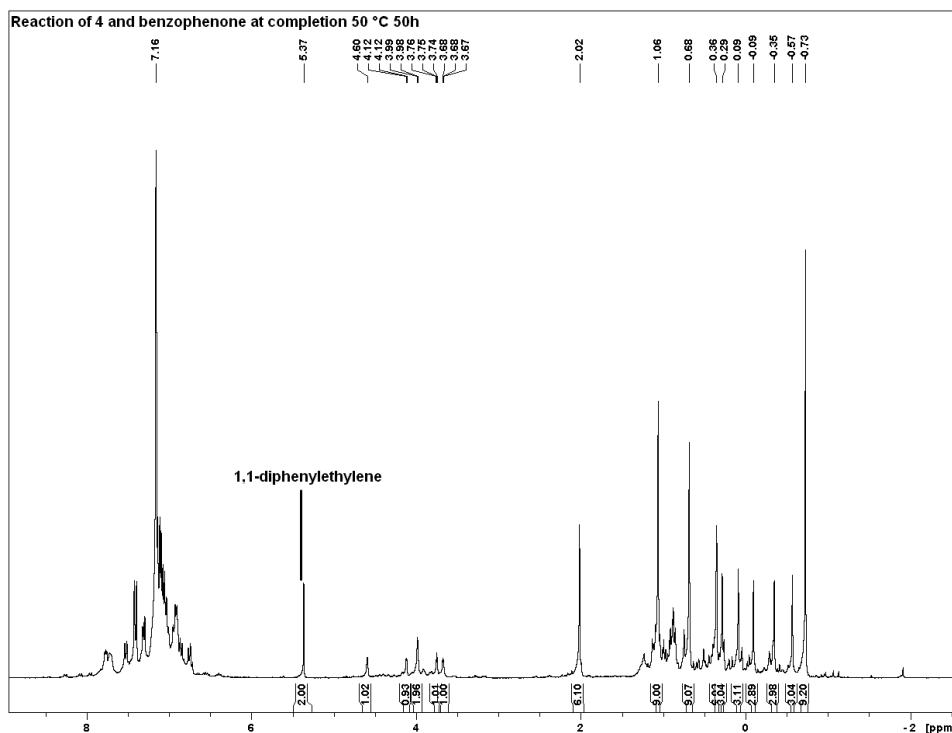
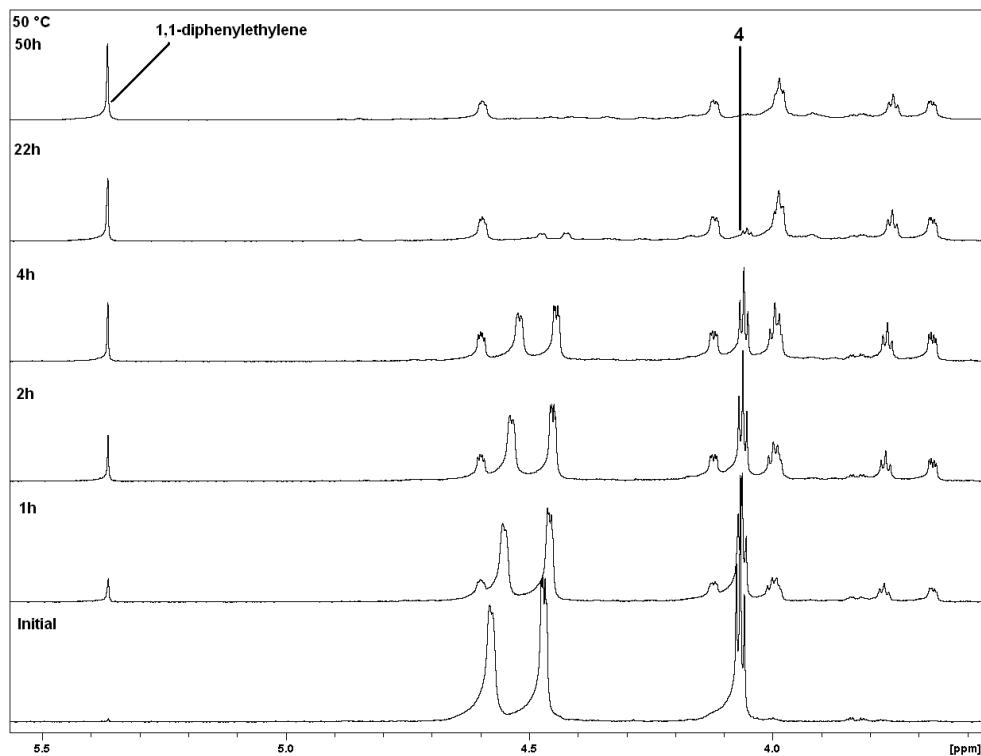


Variable-Temperature ^1H NMR (500 MHz, C_6D_6)



Reaction of 4 with benzophenone at 50 °C

¹H NMR (300 MHz, C₆D₆): When the integration of 1,1-diphenylethylene was calibrated to 1 equiv, the product containing the ferrocene diamide tetraanionic ligand also integrated to 1 equiv. This 1:1 ratio supported the formation of 1,1-diphenylethylene as resulting from transferring the methylidene group of 4.



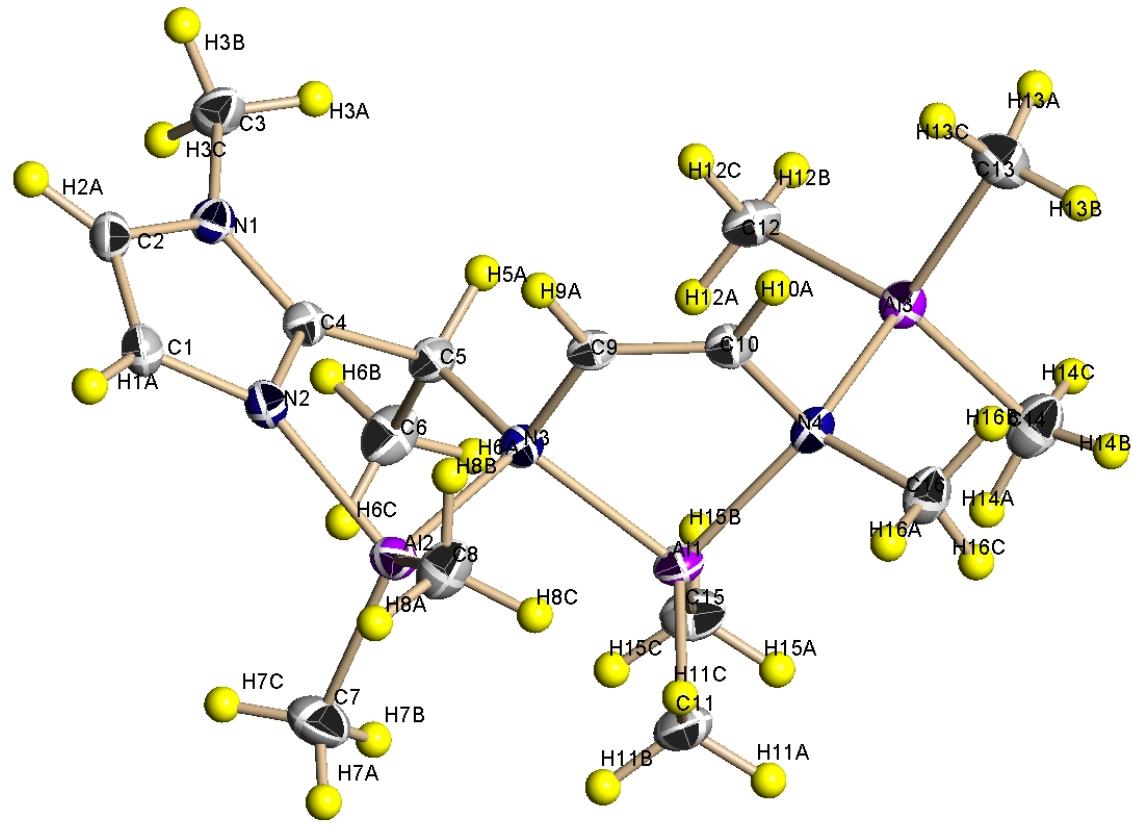


Figure SX1. Thermal-ellipsoid (50% probability) representation of **3**.

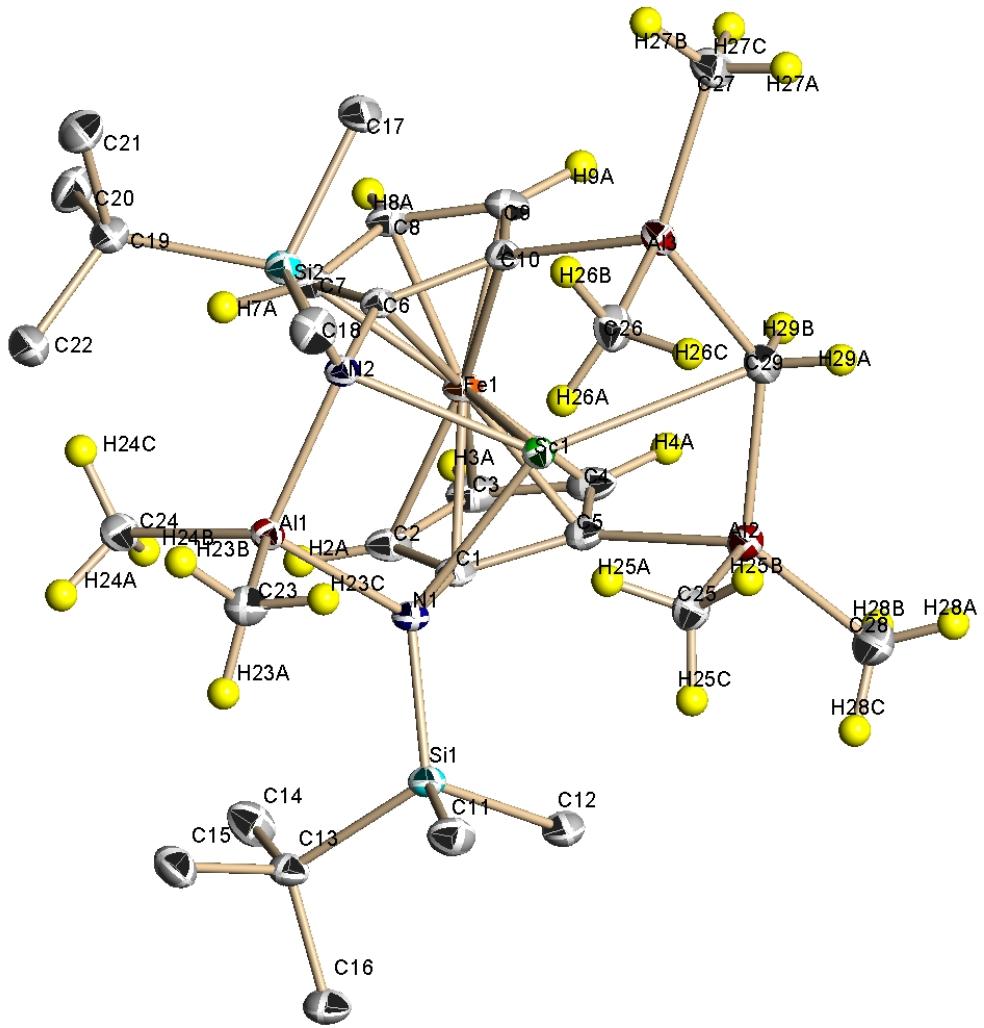


Figure SX2. Thermal-ellipsoid (50% probability) representation of **4**; irrelevant hydrogen atoms omitted for clarity.

Computational details

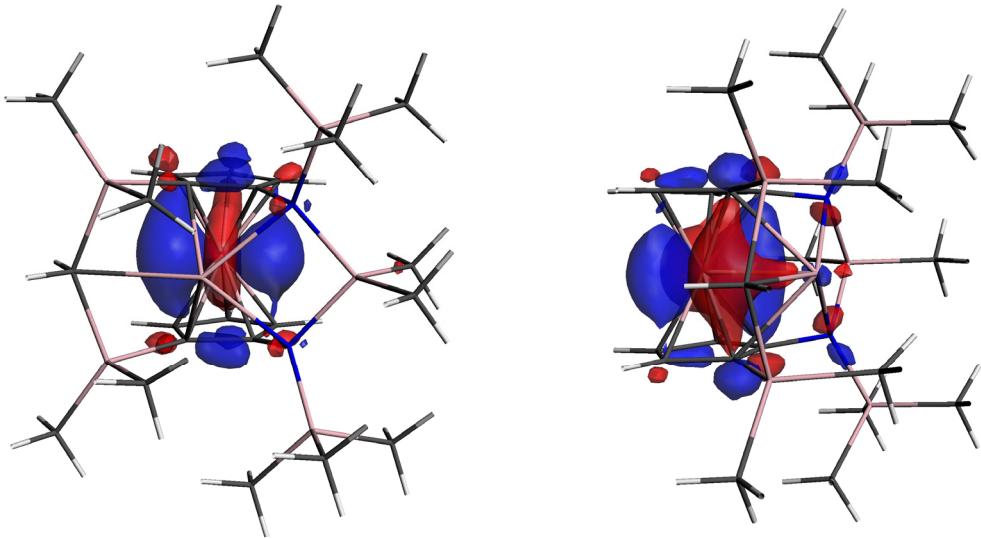


Figure SX3. HOMO (left) and HOMO-1 (right) for **4'**.

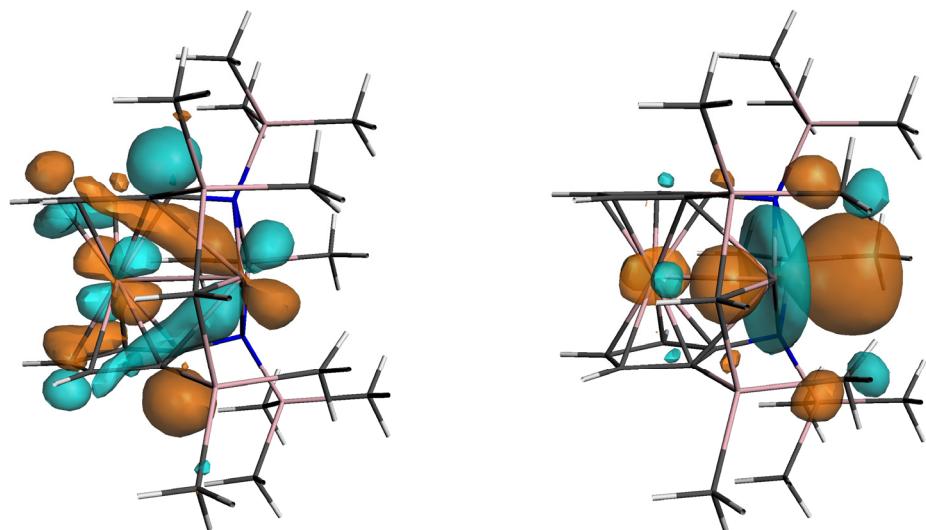


Figure SX4. LUMO (left) and LUMO+1 (right) for **4'**.

Optimized geometry for 4'

1.Sc	-0.549129	8.155330	20.803559
2.Fe	-3.154456	8.634850	21.260019
3.Al	-1.936855	5.343497	20.496124
4.Al	-0.419456	10.360925	19.269101
5.Al	0.084639	9.721267	22.905221
6.Si	-1.440192	6.452848	17.474374
7.Si	-0.568459	5.375384	23.450602
8.N	-1.704808	6.848363	19.223083
9.N	-1.290976	6.333881	22.090723
10.C	-2.648719	7.927400	19.365941
11.C	-4.076332	7.860331	19.556899
12.H	-4.676243	6.956781	19.534501
13.C	-4.547880	9.191090	19.790111
14.H	-5.581560	9.472644	19.977132
15.C	-3.419386	10.076916	19.780978
16.H	-3.469692	11.150767	19.946440
17.C	-2.215203	9.322502	19.501599
18.C	-2.188496	7.346697	22.586038
19.C	-3.617099	7.274448	22.770723
20.H	-4.227244	6.387064	22.635876
21.C	-4.074979	8.576559	23.148110
22.H	-5.106746	8.849027	23.357357
23.C	-2.947480	9.463799	23.159959
24.H	-2.991364	10.524515	23.398535
25.C	-1.747043	8.724834	22.827112
26.C	0.279037	5.736554	17.155831
27.H	1.081621	6.459365	17.355893
28.H	0.341582	5.461025	16.091029
29.H	0.474572	4.832309	17.744996
30.C	-1.693754	7.985338	16.392664
31.H	-0.989253	8.797226	16.617933
32.H	-2.711478	8.391917	16.486522
33.H	-1.542834	7.696513	15.339099
34.C	-2.736756	5.171939	16.952106
35.H	-3.758616	5.541993	17.123162
36.H	1.187217	7.836674	19.237100
37.H	1.943212	9.407409	19.125414
38.H	0.950324	8.762794	17.803190
39.H	-2.627483	4.220101	17.491860
40.C	1.503814	8.290725	22.367337
41.H	1.590430	7.509360	21.587116
42.H	1.721246	7.748630	23.298350
43.H	-2.635264	4.957271	15.876014
44.H	2.361083	8.955084	22.164489
45.C	0.473950	10.538668	24.658628
46.H	1.465186	11.020361	24.673685
47.C	-0.450628	6.422941	25.022789
48.H	0.186724	7.310215	24.905029
49.H	-0.014917	5.803711	25.825049
50.H	-1.439921	6.765390	25.362784
51.C	1.141538	4.700796	23.010917
52.H	1.879098	5.494688	22.840332
53.H	1.121402	4.048546	22.128973
54.H	1.496368	4.096751	23.860337

55.C	-1.717596	3.913565	23.824989
56.H	-2.726240	4.258283	24.099900
57.H	0.448189	9.809467	25.483188
58.H	-0.266219	11.320402	24.896729
59.C	-0.455492	11.729983	17.848840
60.H	-1.321802	3.332730	24.672937
61.H	0.502947	12.269487	17.777393
62.H	-1.232590	12.484532	18.051539
63.H	-0.671096	11.305892	16.856054
64.H	-1.814958	3.228569	22.970039
65.C	-0.044575	10.759584	21.195564
66.H	0.939598	11.271110	21.151264
67.H	-0.809569	11.526372	21.434629
68.C	-0.611020	3.924930	20.053561
69.H	-0.879123	3.432160	19.104880
70.H	-0.632333	3.130402	20.817264
71.H	0.436528	4.248003	19.959814
72.C	-3.763361	4.551653	20.626861
73.H	-3.989177	4.000509	19.696748
74.H	-4.607080	5.233468	20.805631
75.H	-3.784946	3.800205	21.436475
76.C	1.005851	8.874944	18.895858