Supporting Information to Accompany

Dimethylsilyl Bis(amidinate) Actinide Complexes: Synthesis and Reactivity Towards Oxygen Containing Substrates. †

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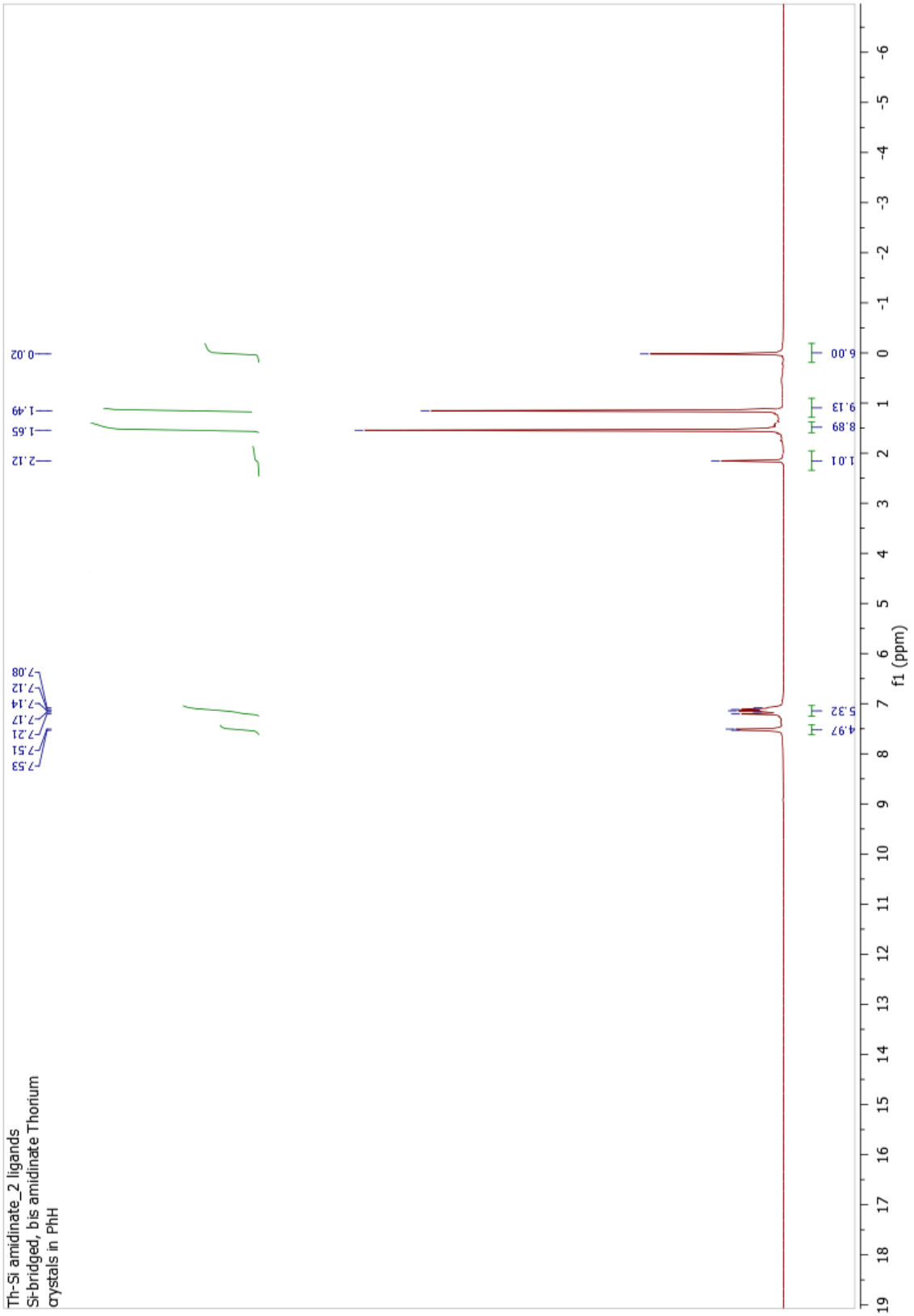
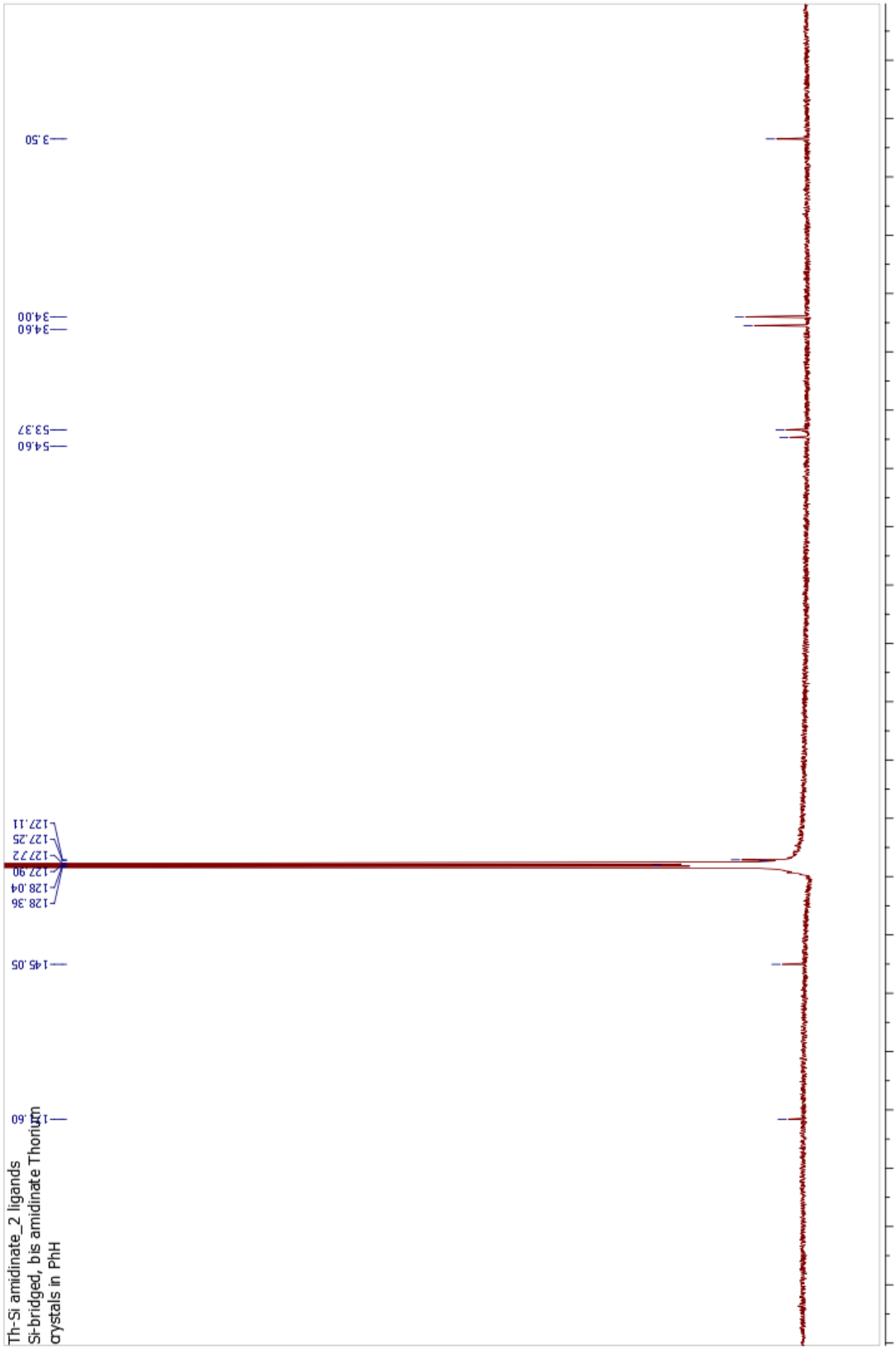
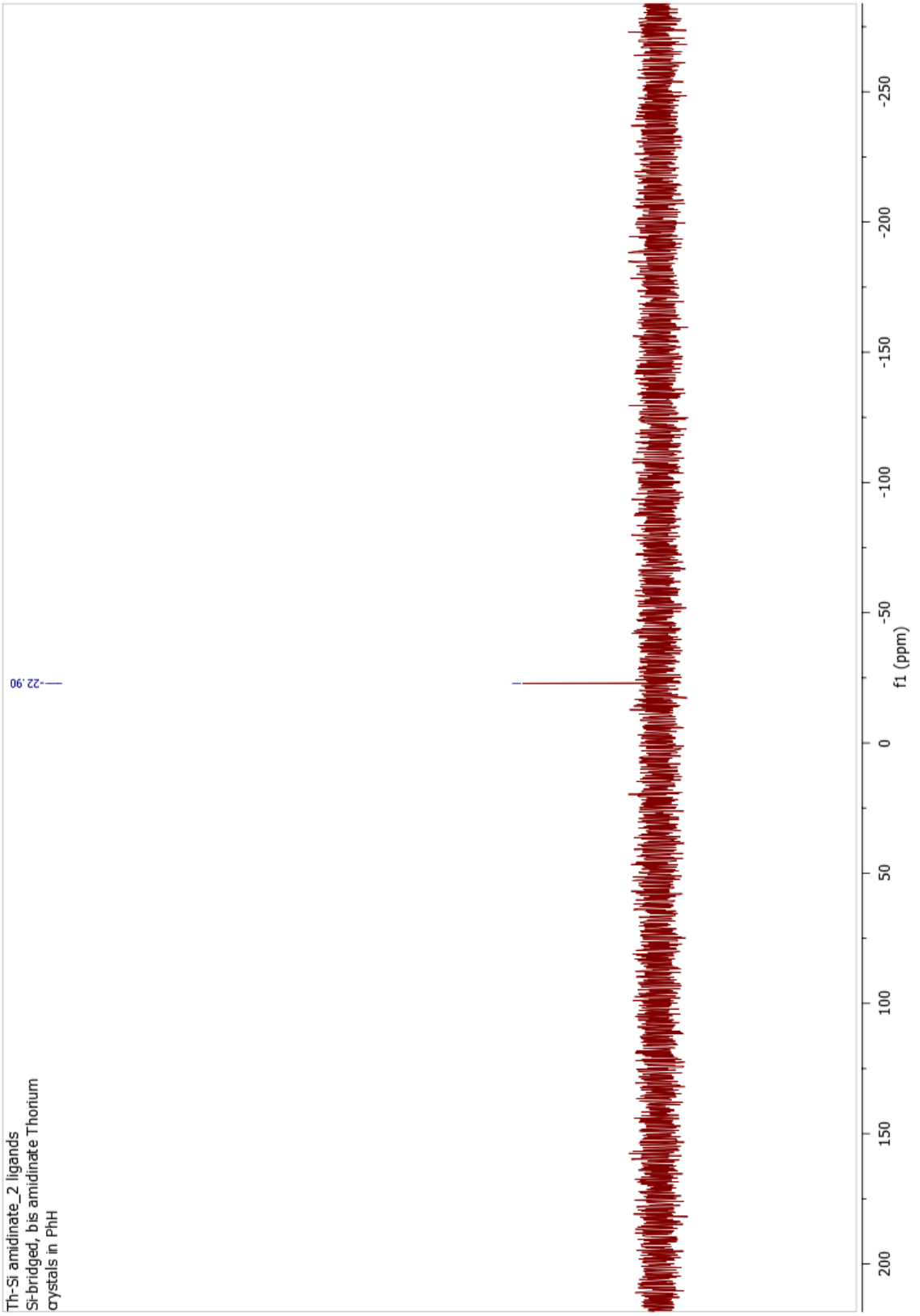


1.2. ^{13}C-NMR Spectrum of Complex **2**

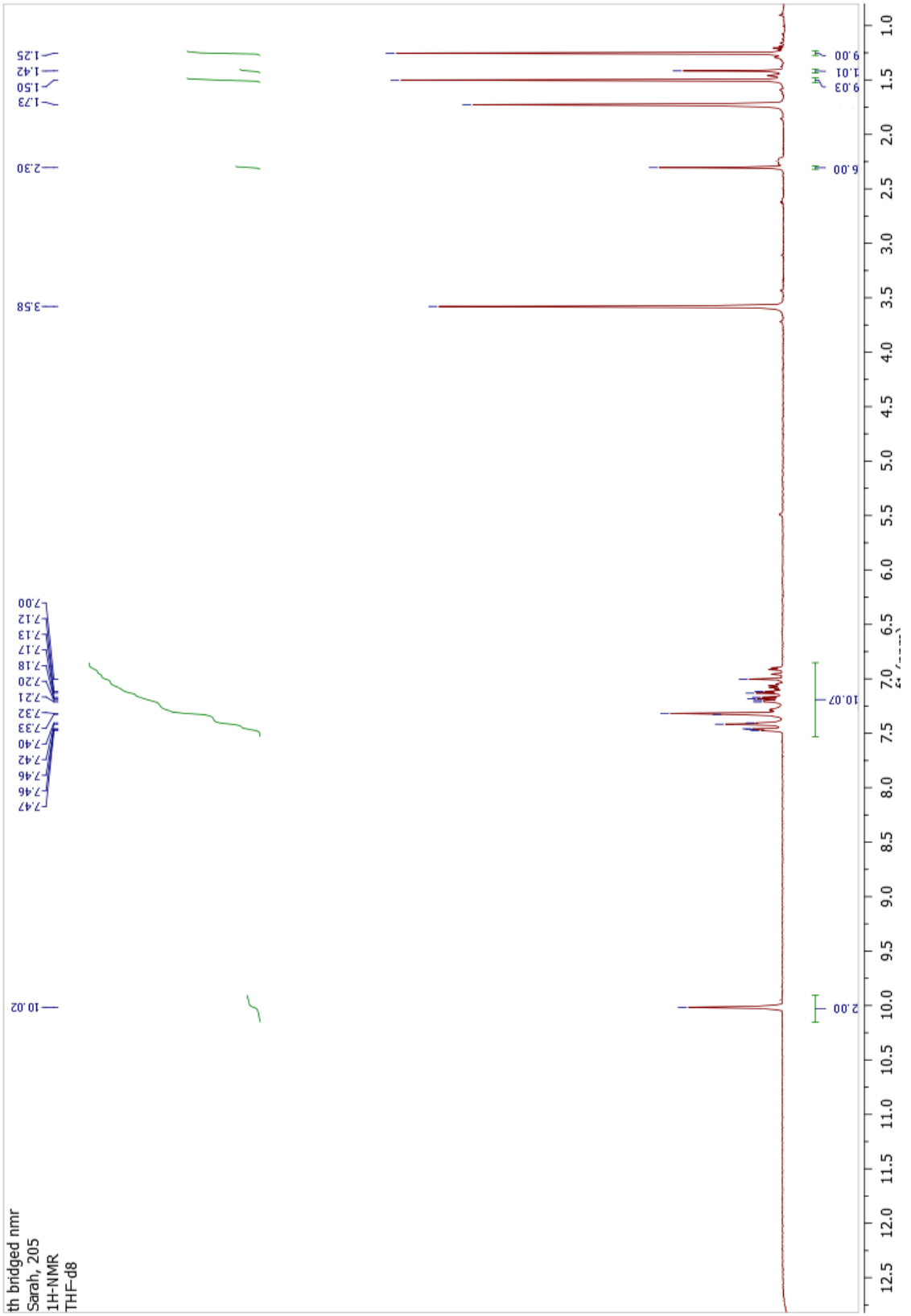


1.3. ^{29}Si-NMR Spectrum of Complex **2**

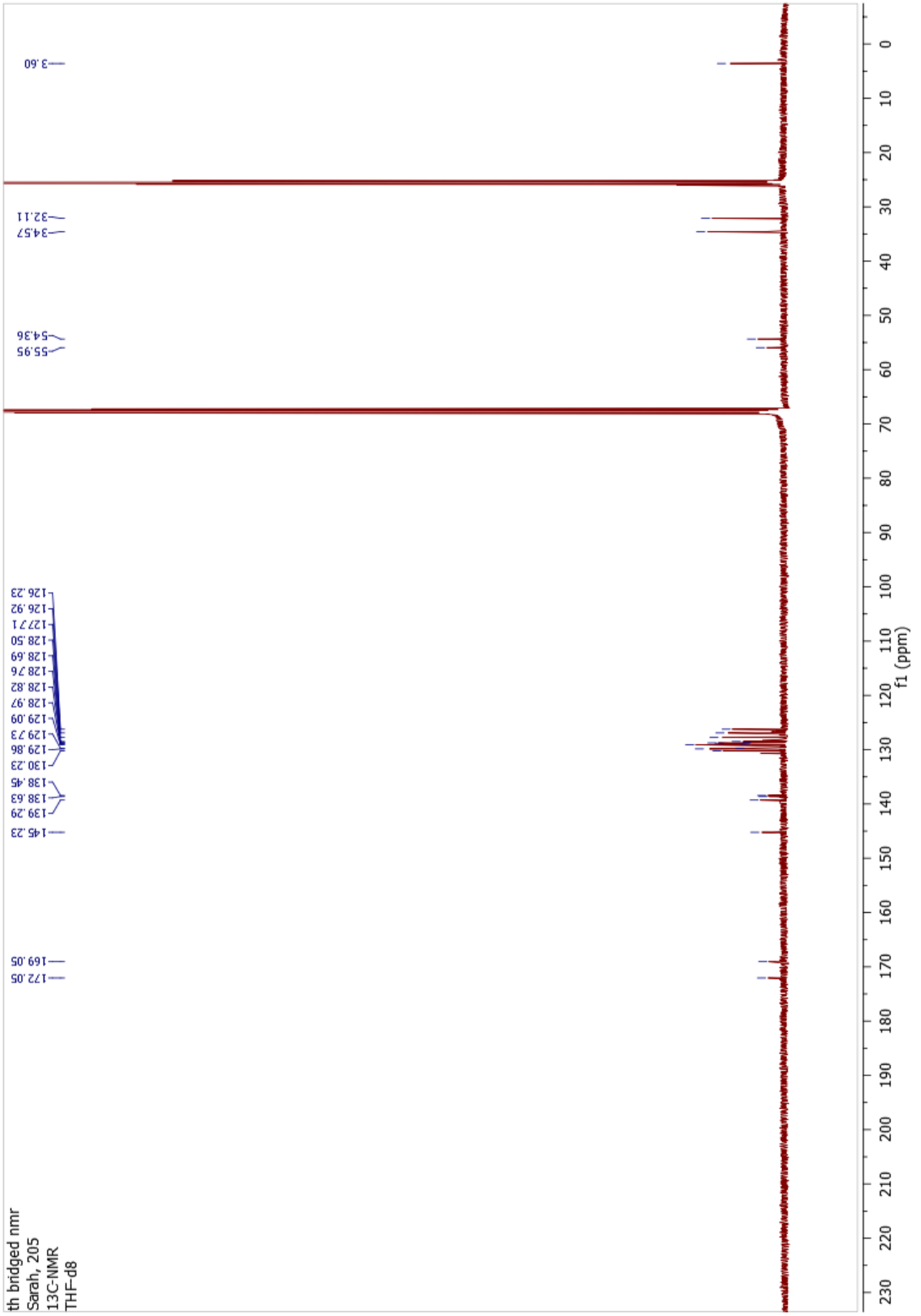


2. Spectroscopic Data for Complex **3**

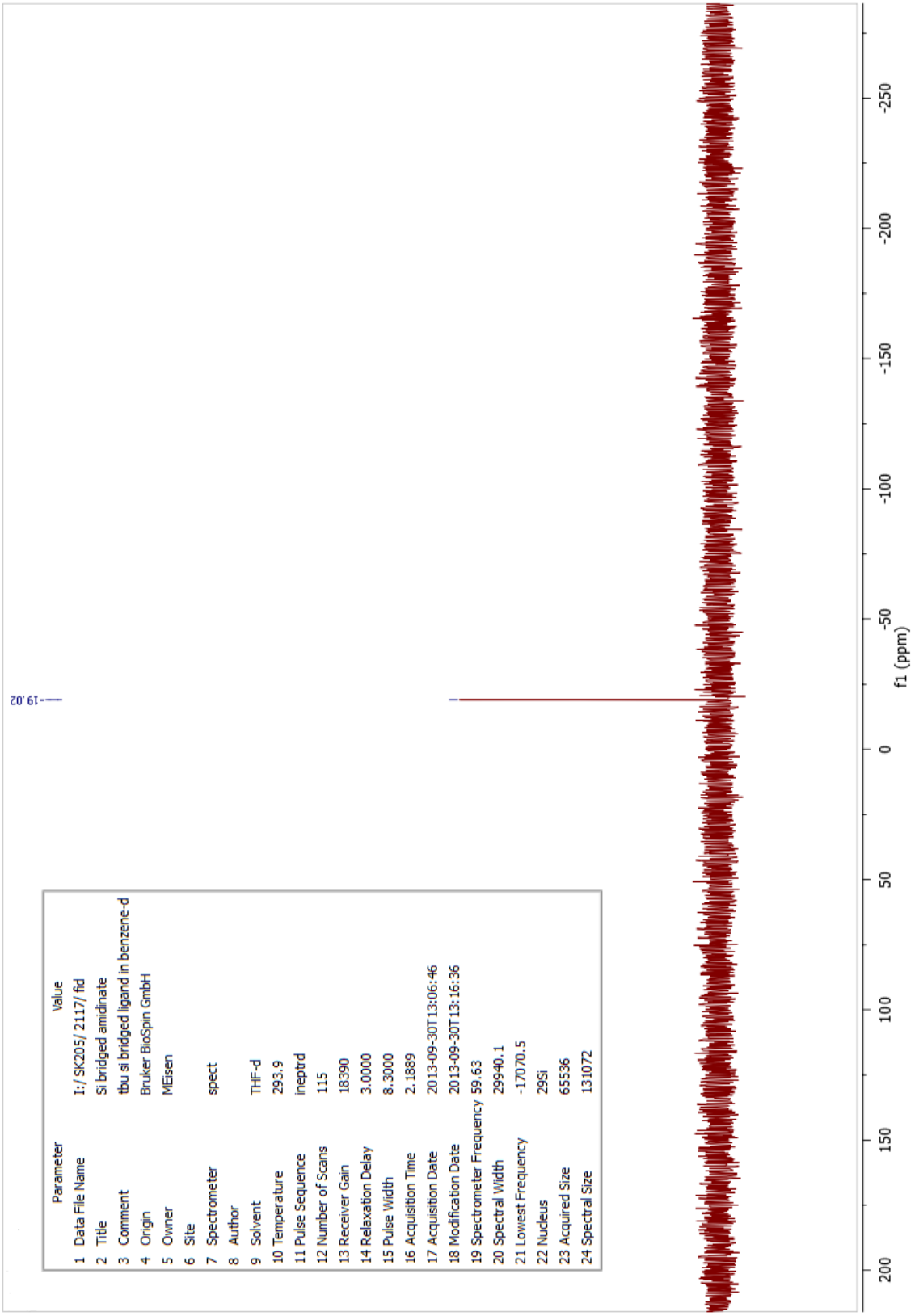
2.1. ^{1}H-NMR Spectrum of Complex **3**



2.2. ^{13}C-NMR Spectrum of Complex **3**

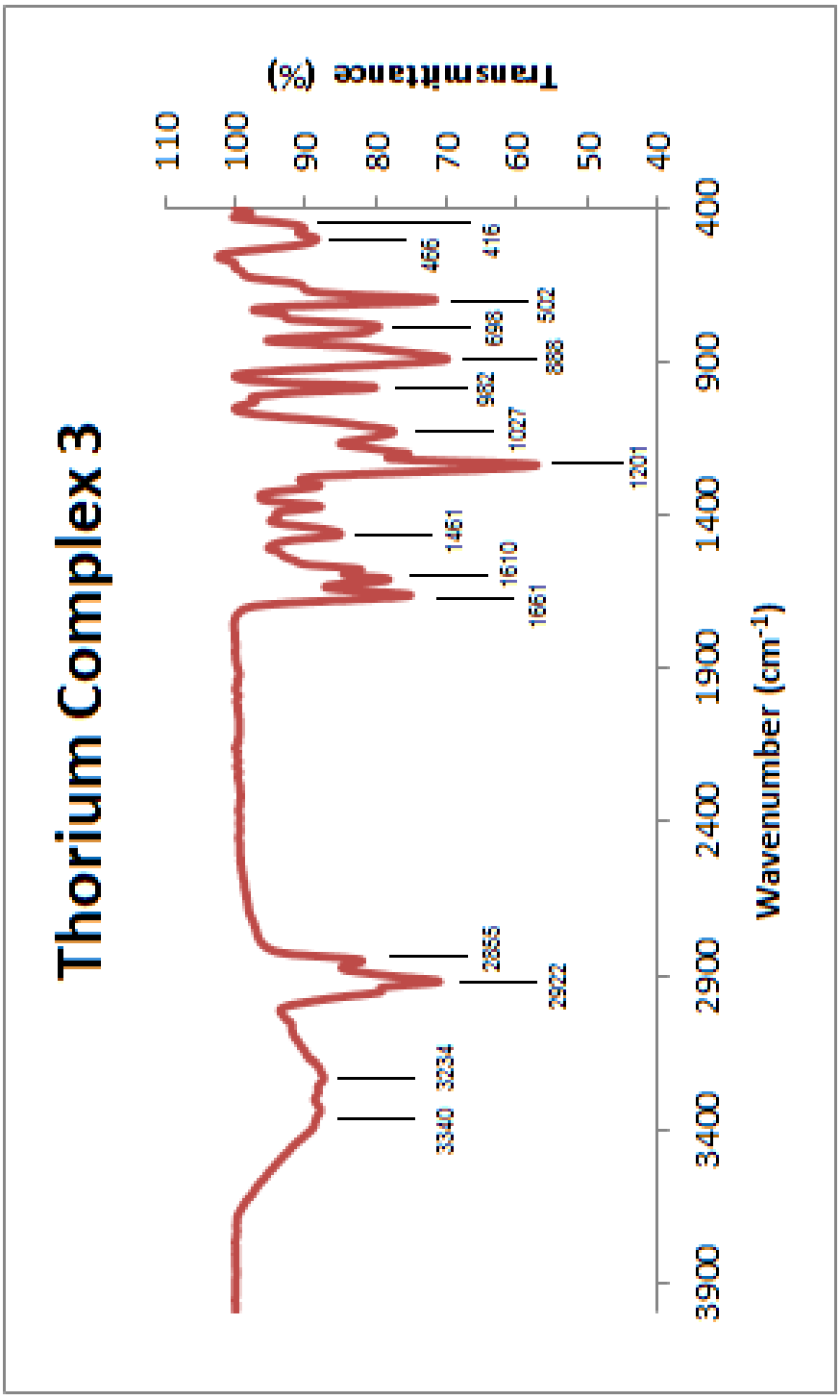


2.3. ^{29}Si-NMR Spectrum of Complex **3**

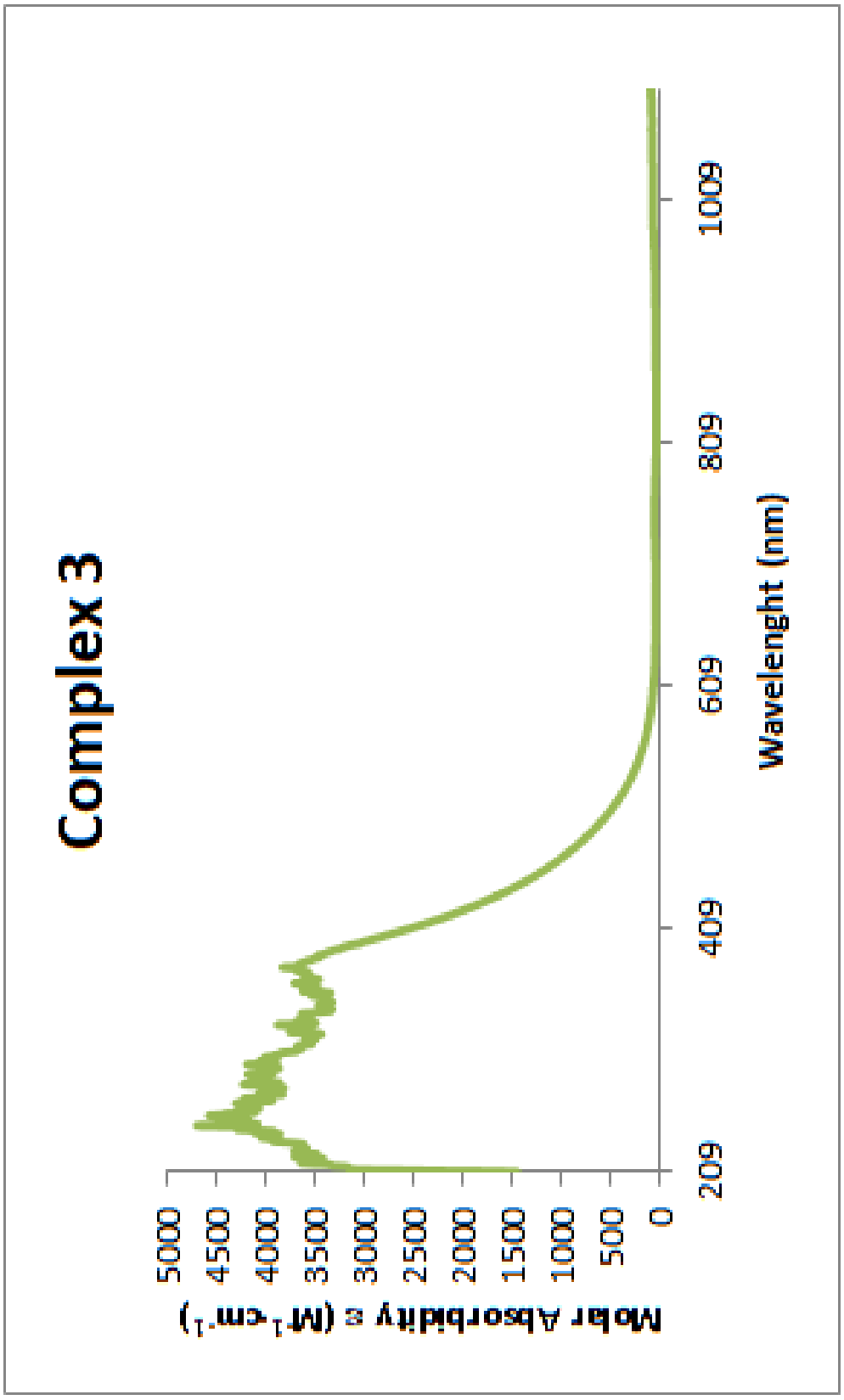


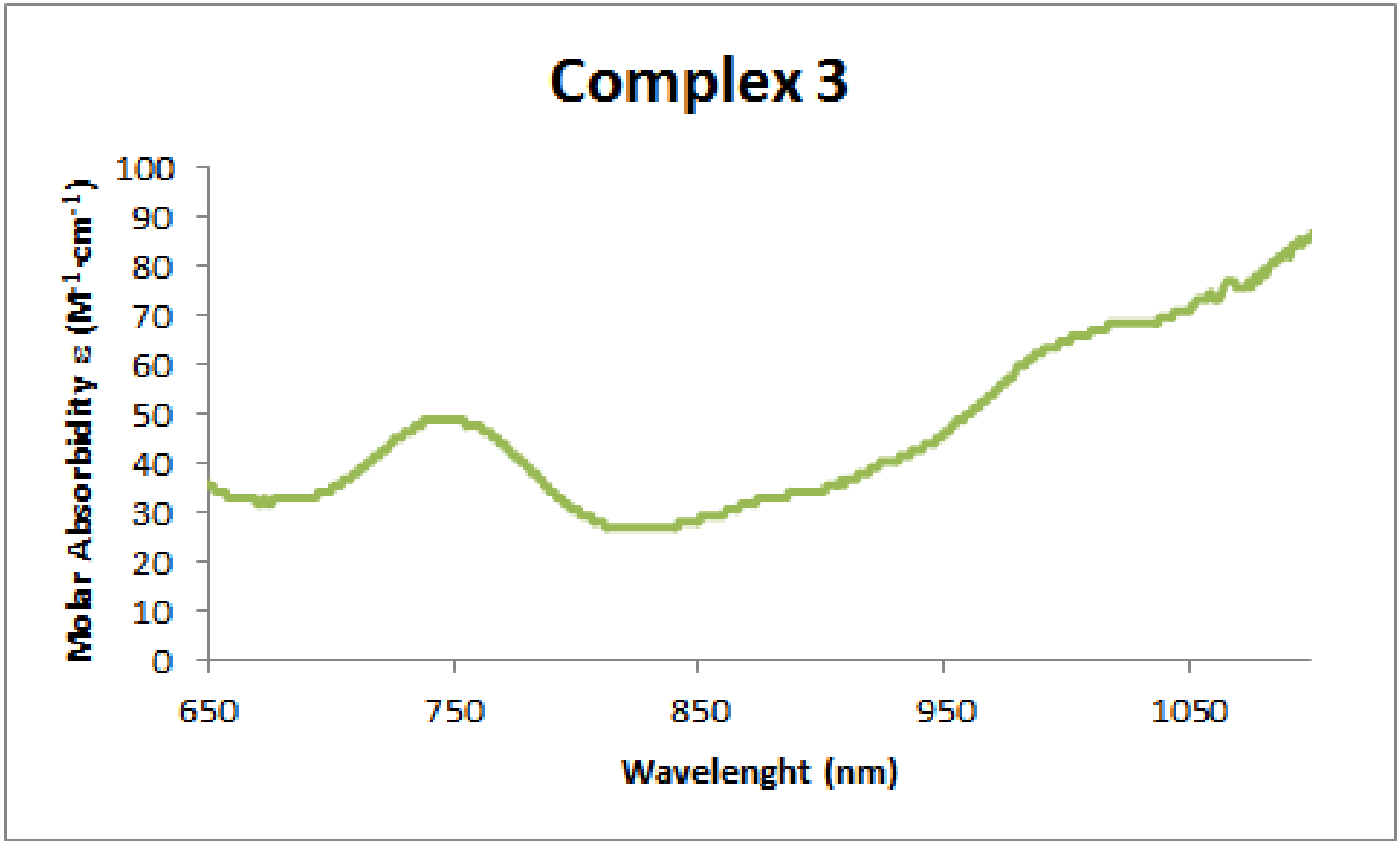
Parameter	Value
1 Data File Name	I:/ SK205/ 2117/ fid
2 Title	Si bridged amidinate
3 Comment	tbu si bridged ligand in benzene-d
4 Origin	Bruker BioSpin GmbH
5 Owner	MEisen
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	THF-d
10 Temperature	293.9
11 Pulse Sequence	ineptrd
12 Number of Scans	115
13 Receiver Gain	18390
14 Relaxation Delay	3.0000
15 Pulse Width	8.3000
16 Acquisition Time	2.1889
17 Acquisition Date	2013-09-30T13:06:46
18 Modification Date	2013-09-30T13:16:36
19 Spectrometer Frequency	59.63
20 Spectral Width	29940.1
21 Lowest Frequency	-17070.5
22 Nucleus	29Si
23 Acquired Size	65536
24 Spectral Size	131072

2.4. Infrared absorption Spectrum of Complex **3.**



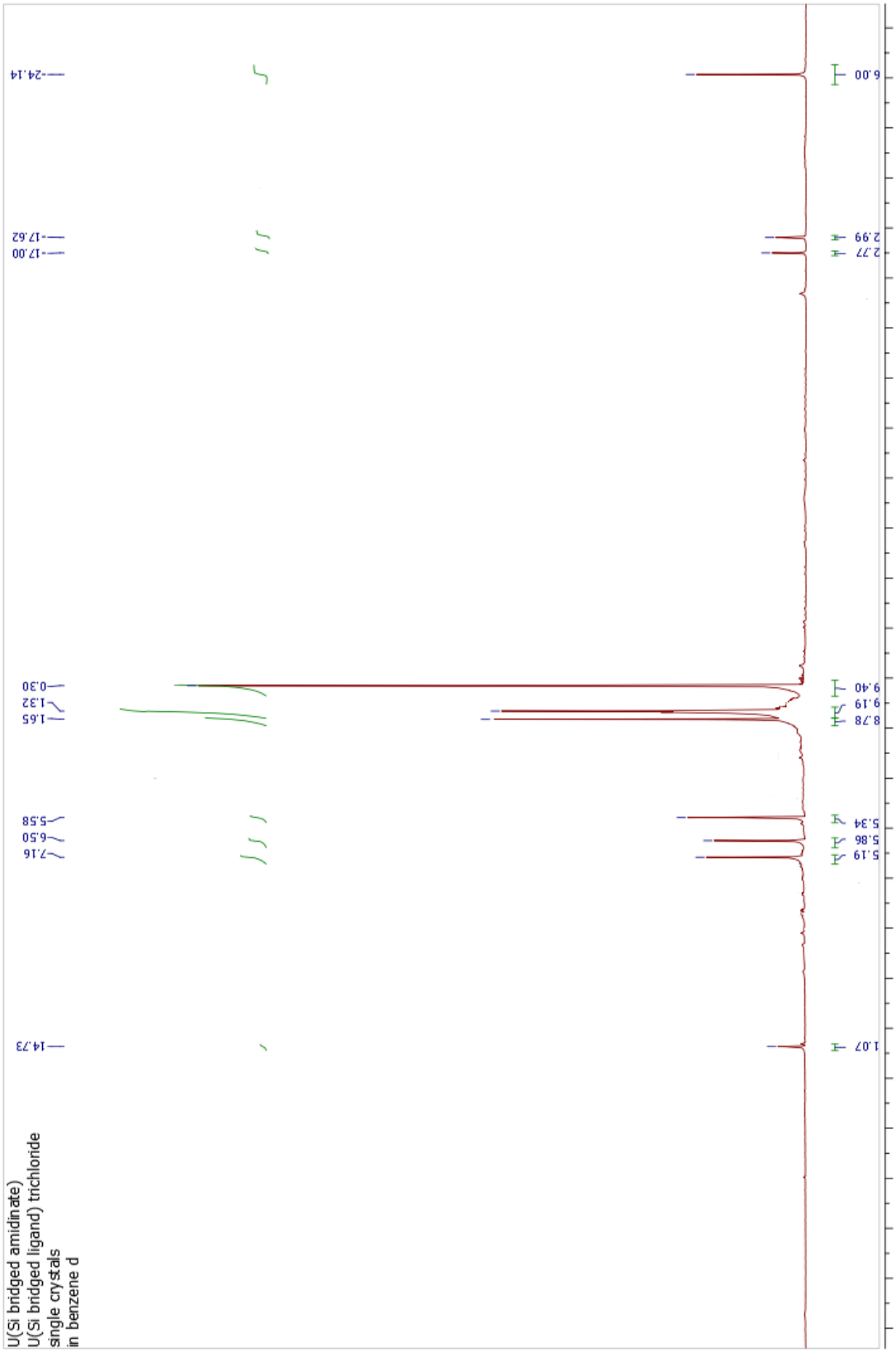
2.5. UV Vis Spectrum of Complex **3**



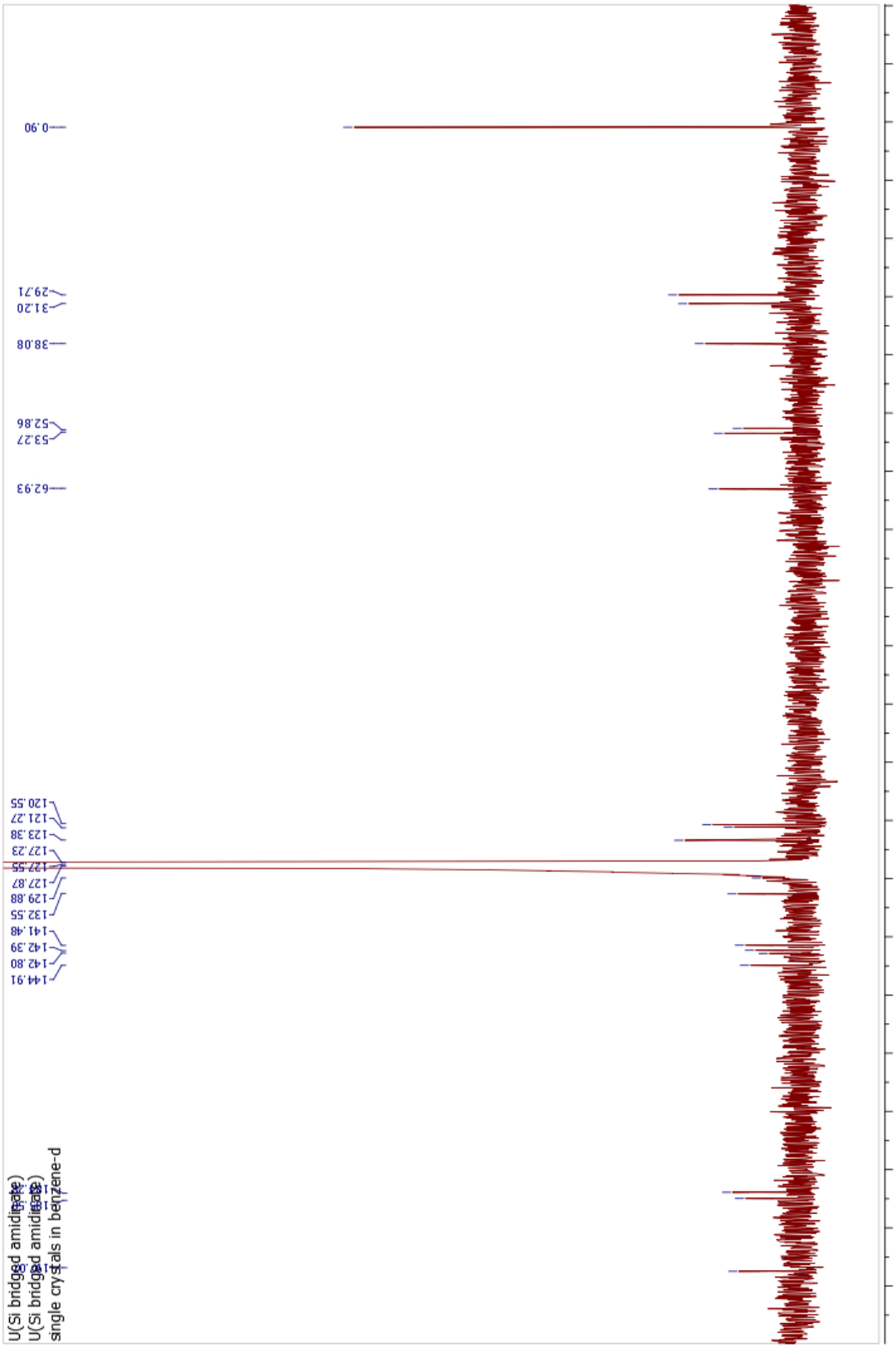

Complex 3
Molar Absorbidity ε (M-1·cm-1)
100
90
80
70
60
50
40
30
20
10
0
650
750
850
950
1050
Wavelenght (nm)

3. Spectroscopic Data for Complex **4**

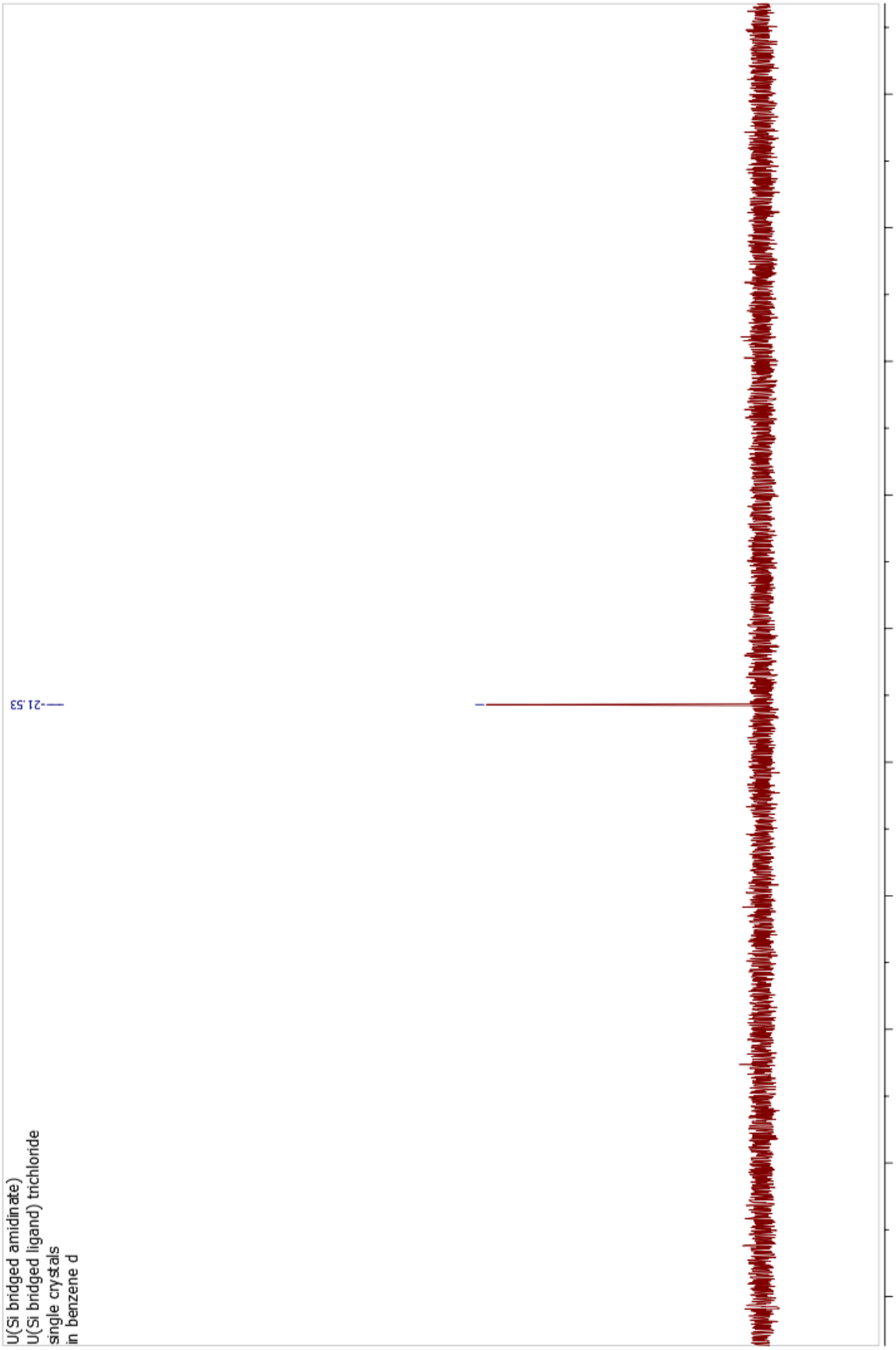
3.1. ^{1}H-NMR Spectrum of Complex **4**



3.2. ^{13}C- NMR Spectrum of Complex **4**

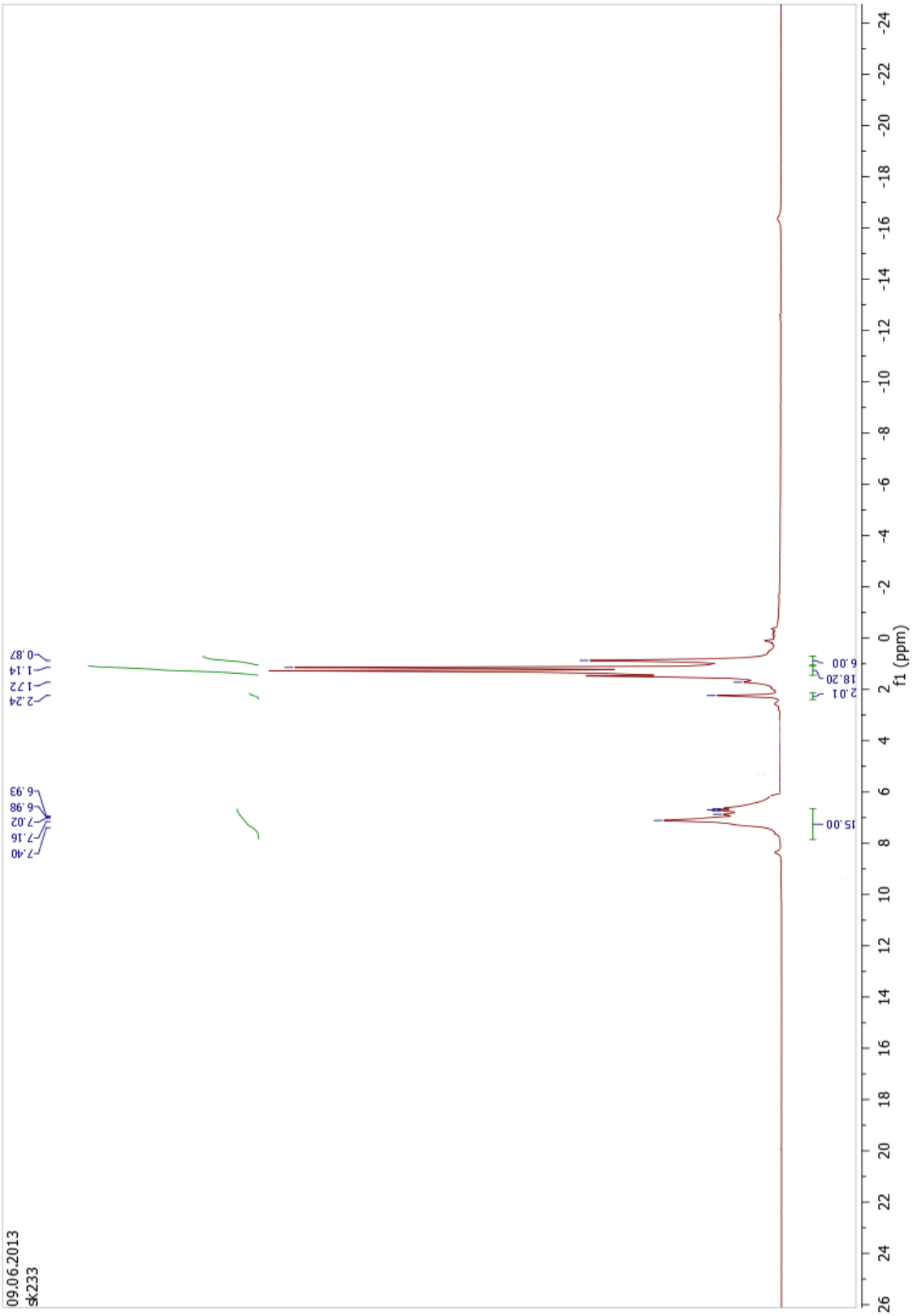


3.3. ^{29}Si-NMR Spectrum of Complex **4**

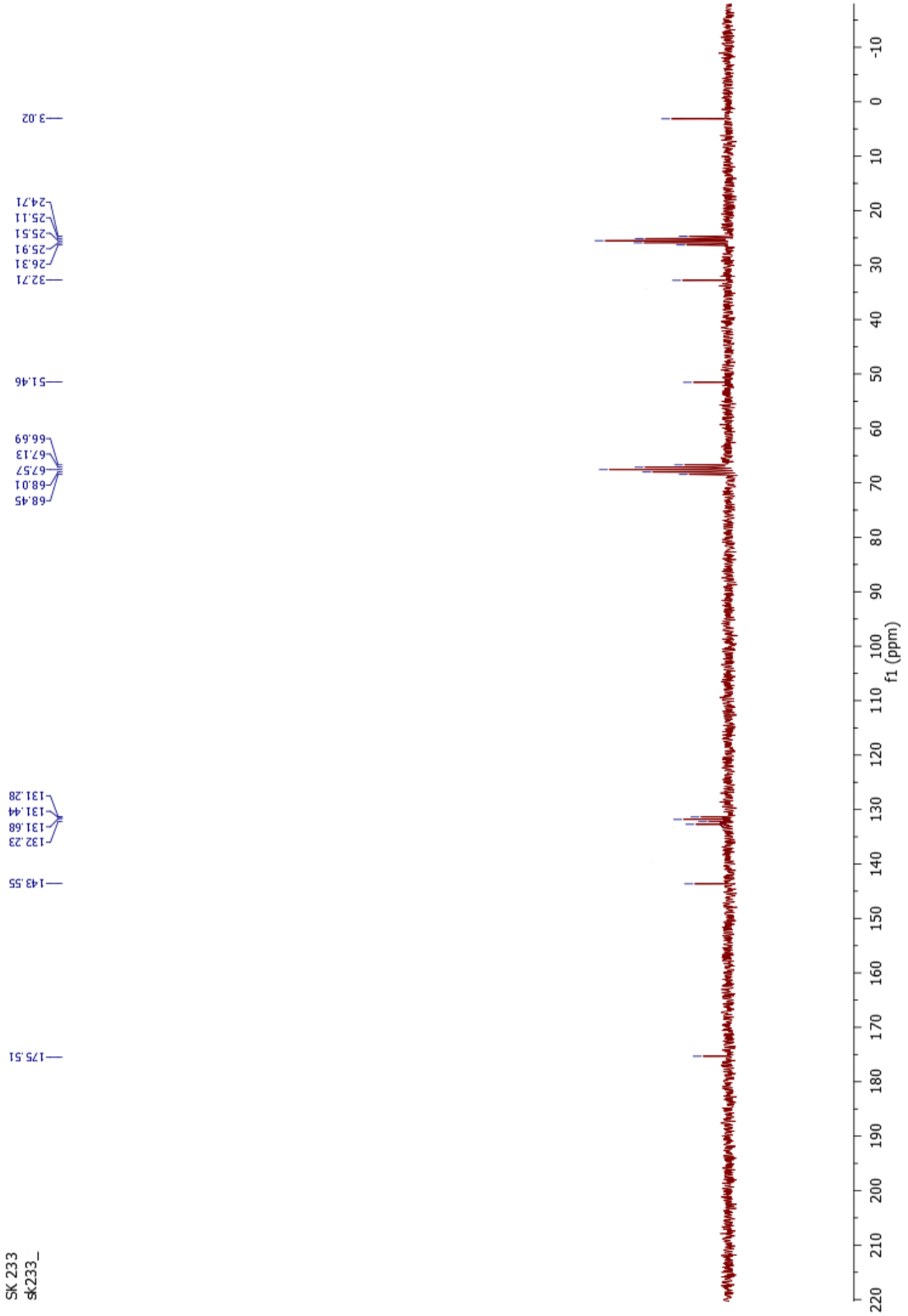


4. Spectroscopic Data for Complex **6**

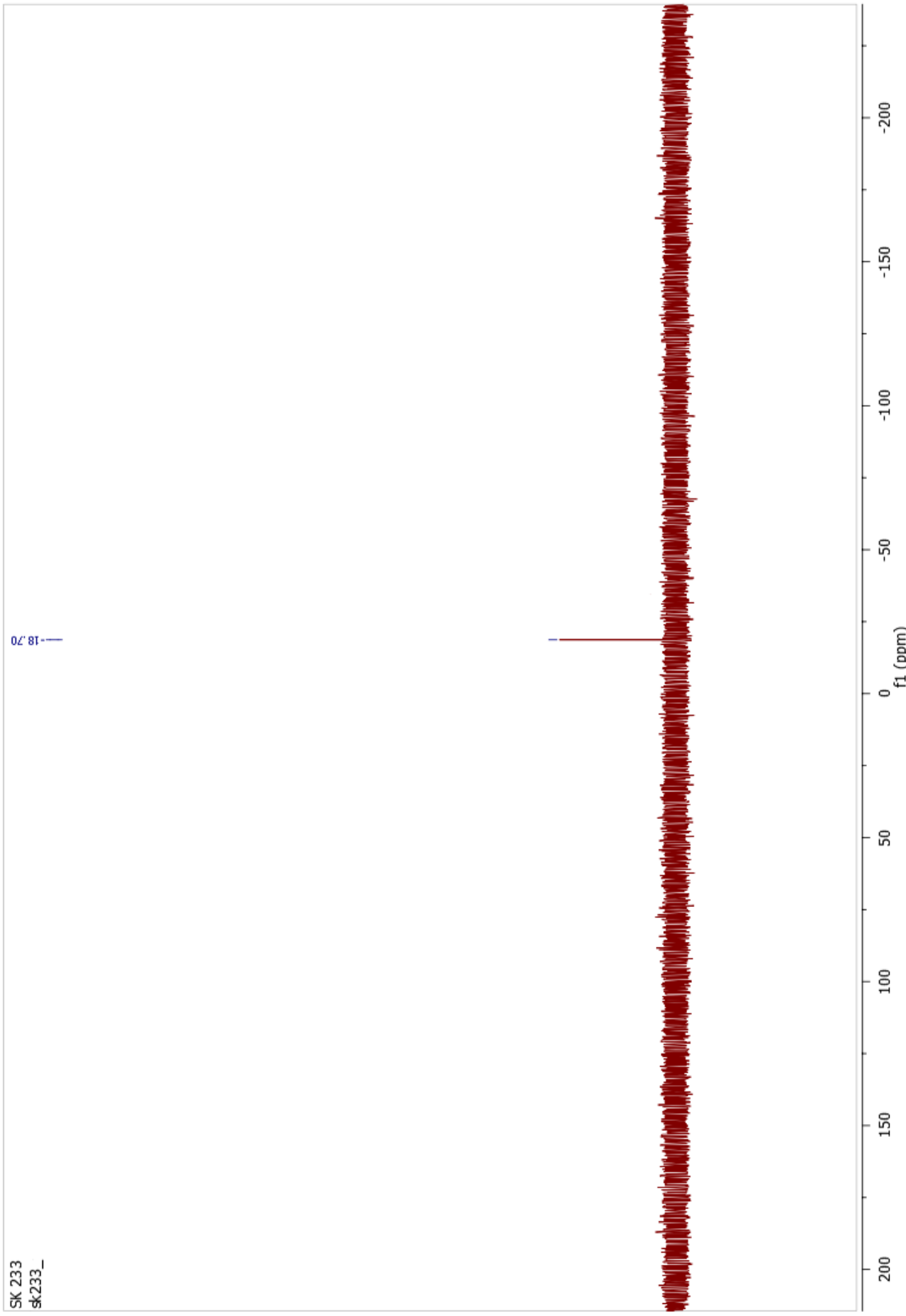
4.1. ^{1}H-NMR Spectrum of Complex **6**



4.2. ^{13}C-NMR Spectrum of Complex **6**

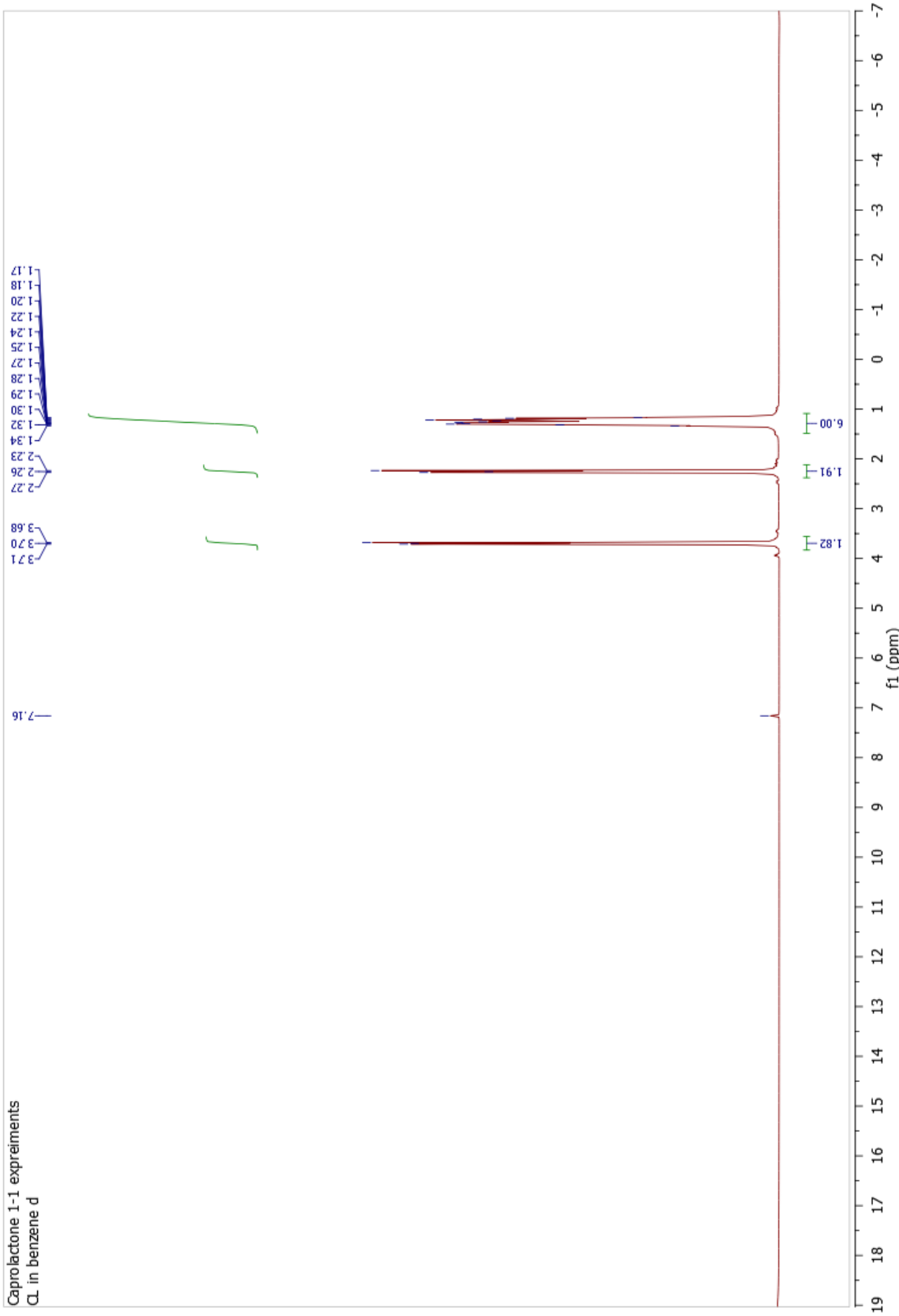


4.3. ^{29}Si-NMR Spectrum of Complex **6**

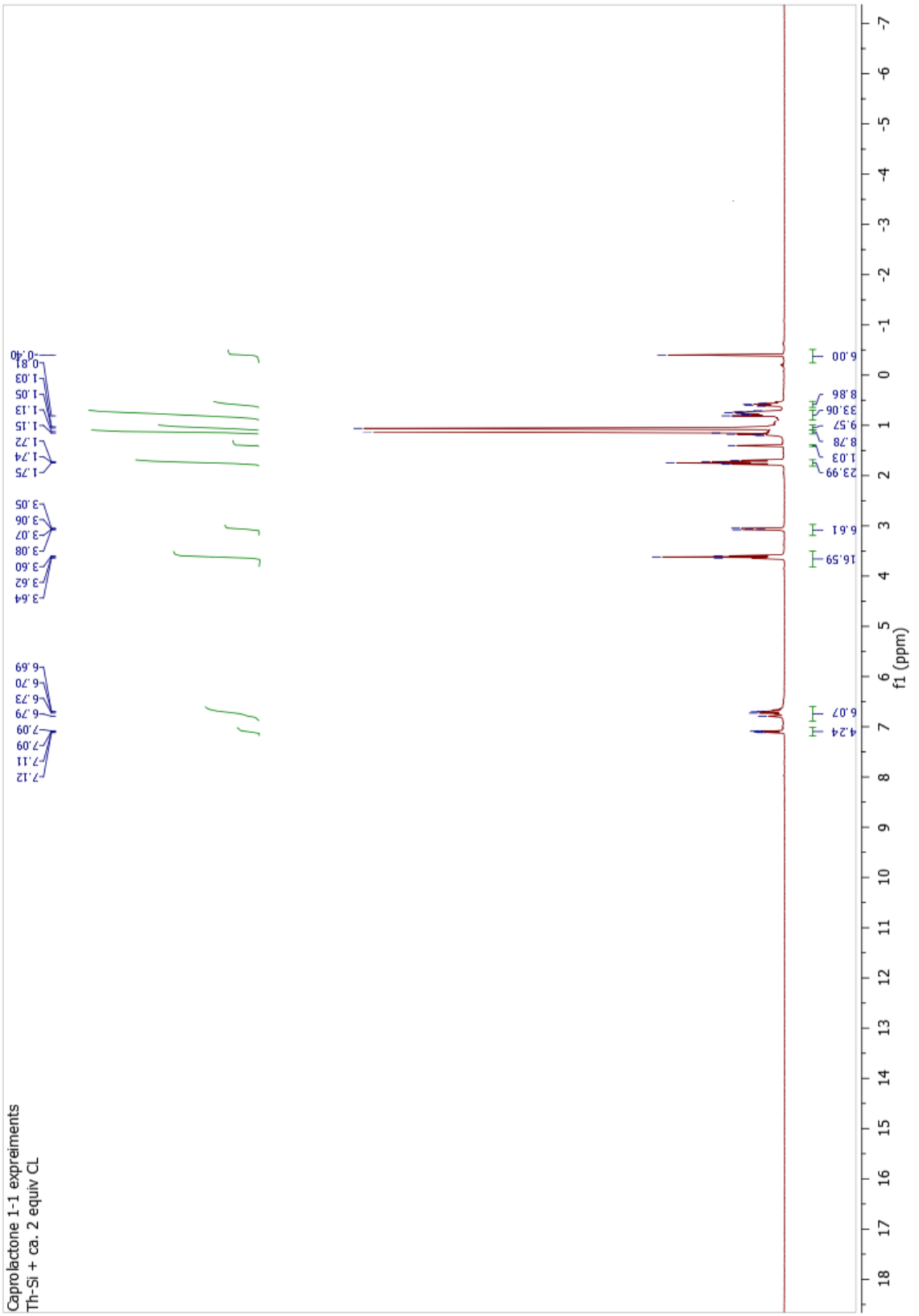


5. Spectroscopic Data for Stoichiometric Addition of ε-Caprolactone to Complex **2**

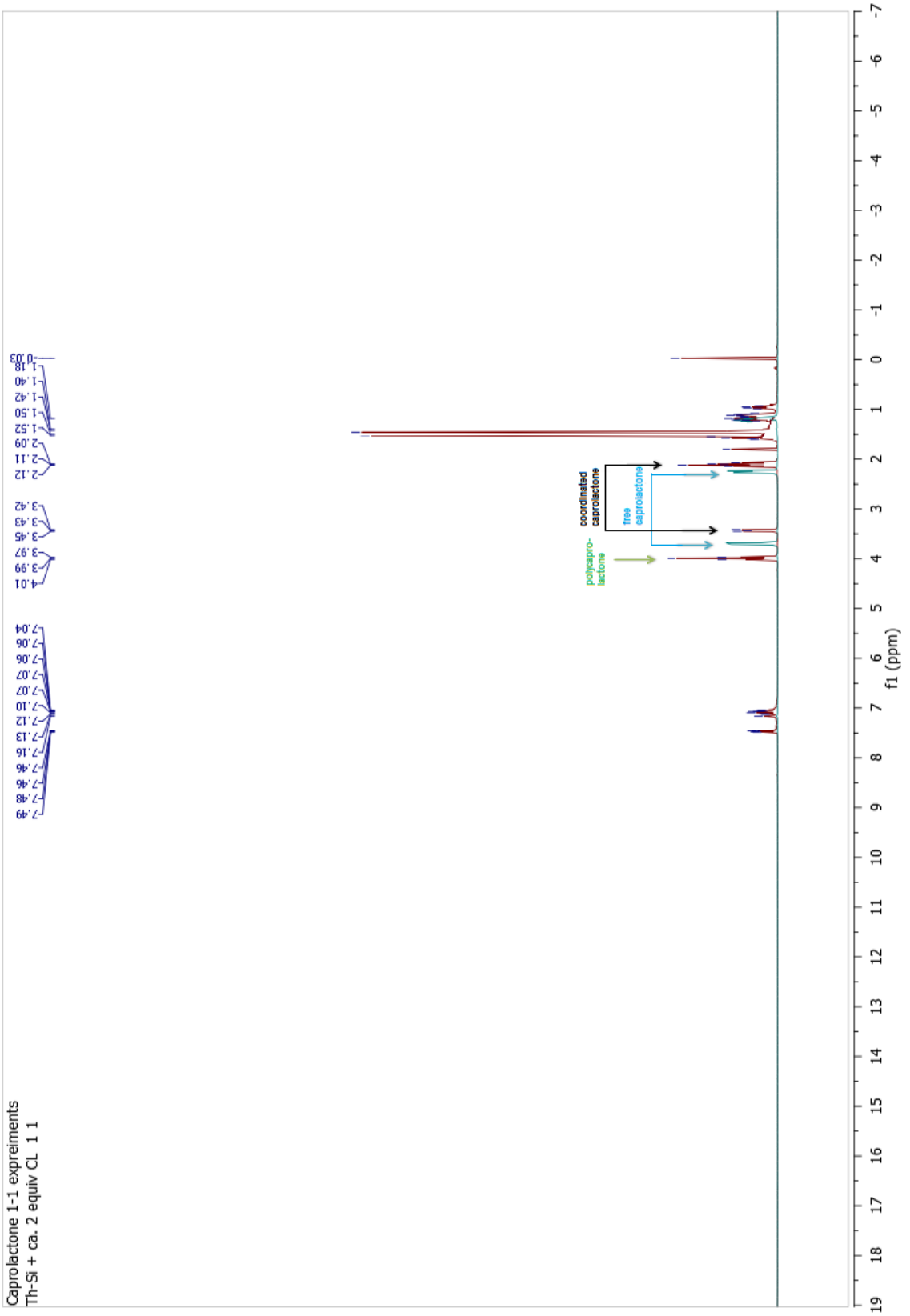
5.1. ^{1}H-NMR Spectrum of ε-Caprolactone



5.2. ^{1}H-NMR Spectrum of Stoichiometric Addition of ε-Caprolactone to Complex **2**, after 10 minutes.



5.3. Overlay of ^{1}H-NMR Spectra of ε-Caprolactone and ε-Caprolactone in Stoichiometric Amount with Complex **2**



6. Crystallographic data for complex **2**

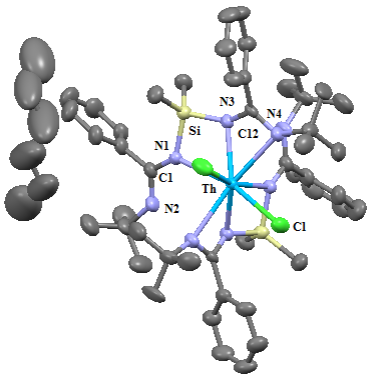


Figure 1: Molecular Molecular structure of complex 2. Color code: Th, blue, Cl, green, Si, yellow, N, purple, C, grey. Hydrogen atoms are omitted for clarity.

Table 1: Crystal data and structure refinement for complex **2**.

Complex	
Empirical Formula	$C_{52}H_{84}Si_2Cl_2Th$
Formula weight/g·mol^{-1}	1068.34
T/K	250(2)
λ/Å	0.71073
Crystal system	Orthorhombic
Space group	Pccn
a/Å	15.7880(5)
b/Å	18.7850(6)
c/Å	20.1863(7)
α/°	90
β/°	90
γ/°	90
V/Å^3	5986.8(3)
Z	4
ρ/g·cm^{-3}	1.336
μ(Mo-K$_\alpha$)/mm^{-1}	2.660
F(000)	2464
Θ range for data collection/°	1.68 to 25.68
Limiting indices	-19≤h≤19 -22≤k≤22 -24≤l≤15
Reflections collected/unique (R_{int})	23969/5626 (0.0195)
Completeness to Θ	98.8%
GOF on F^2	1.005
R_1, wR_2 [I>2σ(I)]	0.0305, 0.0884
R_1, wR_2 (all data)	0.0499, 0.0989
Largest diff. peak and hole (eÅ^{-3})	1.188 and -0.765

Table 2: U(eq) is defined as one third of the trace of the orthogonalized Uij tensor for complex **2.**

	x	y	z	U(eq)
Th(1)	2500	2500	1017(1)	25(1)
N(1)	1299(2)	2444(1)	1904(2)	29(1)
N(2)	1219(2)	3550(2)	2350(2)	48(1)
N(3)	2117(2)	1387(2)	1485(2)	32(1)
N(4)	3133(2)	1244(2)	743(2)	35(1)
Si(1)	1177(1)	1507(1)	1892(1)	33(1)
Cl(1)	3614(1)	2887(1)	72(1)	51(1)
C(1)	936(2)	2890(2)	2310(2)	35(1)
C(2)	869(3)	4199(2)	2688(3)	53(1)
C(3)	-45(4)	4308(3)	2517(3)	79(2)
C(4)	1010(4)	4163(3)	3431(3)	78(2)
C(5)	1386(4)	4812(3)	2411(3)	85(2)
C(6)	219(3)	2645(2)	2736(2)	42(1)
C(7)	333(4)	2514(2)	3406(2)	44(1)
C(8)	-340(4)	2240(3)	3778(3)	65(2)
C(9)	-1091(4)	2096(4)	3491(3)	76(2)
C(10)	-1212(3)	2218(3)	2822(3)	70(2)
C(11)	-556(3)	2494(2)	2449(3)	50(1)
C(12)	2458(2)	964(2)	1006(2)	28(1)
C(13)	1986(3)	299(2)	809(2)	36(1)
C(14)	1557(3)	261(2)	220(2)	48(1)
C(15)	1099(3)	-346(3)	59(2)	57(1)
C(16)	1085(3)	-921(2)	475(3)	60(1)
C(17)	1515(3)	-886(3)	1063(3)	59(1)
C(18)	1954(3)	-283(2)	1241(2)	47(1)
C(19)	3708(3)	904(2)	260(2)	47(1)
C(20)	3442(3)	1066(3)	-448(2)	64(2)
C(21)	4577(3)	1229(3)	410(3)	64(2)
C(22)	3785(4)	88(2)	343(3)	76(2)
C(23)	227(3)	1197(3)	1430(2)	50(1)
C(24)	1228(3)	1084(2)	2726(2)	49(1)
C(25)	7168(12)	1060(12)	1263(10)	258(11)
C(26)	6987(9)	1565(9)	763(10)	244(11)
C(27)	7566(9)	2132(3)	745(13)	305(15)

Table 3: Bond lengths [A] and angles [deg] for shelxl for complex **2**.

Th(1)-N(3)#1	2.374(3)
Th(1)-N(3)	2.374(3)
Th(1)-N(1)	2.611(3)
Th(1)-N(1)#1	2.611(3)
Th(1)-N(4)#1	2.621(3)
Th(1)-N(4)	2.621(3)
Th(1)-Cl(1)#1	2.6939(11)
Th(1)-Cl(1)	2.6939(11)
Th(1)-C(12)#1	2.885(4)
Th(1)-C(12)	2.886(4)
Th(1)-Si(1)#1	3.3119(11)
Th(1)-Si(1)	3.3119(11)
N(1)-C(1)	1.303(5)
N(1)-Si(1)	1.772(3)
N(2)-C(1)	1.320(5)
N(2)-C(2)	1.502(5)
N(3)-C(12)	1.362(5)
N(3)-Si(1)	1.711(4)
N(4)-C(12)	1.300(5)
N(4)-C(19)	1.477(5)
Si(1)-C(23)	1.859(5)
Si(1)-C(24)	1.862(4)
C(1)-C(6)	1.494(6)
C(2)-C(3)	1.498(7)
C(2)-C(4)	1.518(7)
C(2)-C(5)	1.518(7)
C(6)-C(11)	1.383(7)
C(6)-C(7)	1.386(7)
C(7)-C(8)	1.400(8)
C(8)-C(9)	1.348(9)
C(9)-C(10)	1.384(8)
C(10)-C(11)	1.381(7)
C(12)-C(13)	1.509(6)
C(13)-C(14)	1.370(6)
C(13)-C(18)	1.399(6)
C(14)-C(15)	1.389(6)
C(15)-C(16)	1.370(7)
C(16)-C(17)	1.369(7)
C(17)-C(18)	1.377(6)
C(19)-C(20)	1.520(7)
C(19)-C(21)	1.533(6)
C(19)-C(22)	1.547(6)
C(25)-C(26)	1.413(12)
C(26)-C(27)	1.405(11)
C(27)-C(27)#2	1.397(12)
N(3)#1-Th(1)-N(3)	133.02(14)
N(3)#1-Th(1)-N(1)	86.94(10)
N(3)-Th(1)-N(1)	60.41(10)
N(3)#1-Th(1)-N(1)#1	60.41(10)
N(3)-Th(1)-N(1)#1	86.95(10)

N(1)-Th(1)-N(1)#1	93.34(15)
N(3)#1-Th(1)-N(4)#1	52.24(11)
N(3)-Th(1)-N(4)#1	141.27(11)
N(1)-Th(1)-N(4)#1	84.48(10)
N(1)#1-Th(1)-N(4)#1	112.65(9)
N(3)#1-Th(1)-N(4)	141.27(11)
N(3)-Th(1)-N(4)	52.24(11)
N(1)-Th(1)-N(4)	112.65(9)
N(1)#1-Th(1)-N(4)	84.48(10)
N(4)#1-Th(1)-N(4)	155.69(15)
N(3)#1-Th(1)-Cl(1)#1	133.33(8)
N(3)-Th(1)-Cl(1)#1	82.99(8)
N(1)-Th(1)-Cl(1)#1	90.04(8)
N(1)#1-Th(1)-Cl(1)#1	166.08(6)
N(4)#1-Th(1)-Cl(1)#1	81.10(8)
N(4)-Th(1)-Cl(1)#1	81.76(8)
N(3)#1-Th(1)-Cl(1)	82.99(8)
N(3)-Th(1)-Cl(1)	133.33(8)
N(1)-Th(1)-Cl(1)	166.08(6)
N(1)#1-Th(1)-Cl(1)	90.04(8)
N(4)#1-Th(1)-Cl(1)	81.76(8)
N(4)-Th(1)-Cl(1)	81.10(8)
Cl(1)#1-Th(1)-Cl(1)	89.90(5)
N(3)#1-Th(1)-C(12)#1	27.91(10)
N(3)-Th(1)-C(12)#1	152.82(10)
N(1)-Th(1)-C(12)#1	93.54(9)
N(1)#1-Th(1)-C(12)#1	87.05(9)
N(4)#1-Th(1)-C(12)#1	26.76(9)
N(4)-Th(1)-C(12)#1	152.84(9)
Cl(1)#1-Th(1)-C(12)#1	106.24(7)
Cl(1)-Th(1)-C(12)#1	73.14(7)
N(3)#1-Th(1)-C(12)	152.82(10)
N(3)-Th(1)-C(12)	27.91(10)
N(1)-Th(1)-C(12)	87.05(9)
N(1)#1-Th(1)-C(12)	93.54(9)
N(4)#1-Th(1)-C(12)	152.84(9)
N(4)-Th(1)-C(12)	26.76(9)
Cl(1)#1-Th(1)-C(12)	73.14(7)
Cl(1)-Th(1)-C(12)	106.23(7)
C(12)#1-Th(1)-C(12)	179.15(14)
N(3)#1-Th(1)-Si(1)#1	29.57(8)
N(3)-Th(1)-Si(1)#1	116.38(8)
N(1)-Th(1)-Si(1)#1	96.57(7)
N(1)#1-Th(1)-Si(1)#1	32.13(6)
N(4)#1-Th(1)-Si(1)#1	81.11(8)
N(4)-Th(1)-Si(1)#1	112.29(8)
Cl(1)#1-Th(1)-Si(1)#1	160.32(3)
Cl(1)-Th(1)-Si(1)#1	79.27(3)
C(12)#1-Th(1)-Si(1)#1	54.99(7)
C(12)-Th(1)-Si(1)#1	125.57(7)
N(3)#1-Th(1)-Si(1)	116.38(8)
N(3)-Th(1)-Si(1)	29.57(8)
N(1)-Th(1)-Si(1)	32.13(6)
N(1)#1-Th(1)-Si(1)	96.57(7)
N(4)#1-Th(1)-Si(1)	112.29(8)
N(4)-Th(1)-Si(1)	81.11(7)

Cl(1)#1-Th(1)-Si(1)	79.27(3)
Cl(1)-Th(1)-Si(1)	160.31(3)
C(12)#1-Th(1)-Si(1)	125.57(7)
C(12)-Th(1)-Si(1)	54.99(7)
Si(1)#1-Th(1)-Si(1)	115.49(4)
C(1)-N(1)-Si(1)	126.8(3)
C(1)-N(1)-Th(1)	136.4(3)
Si(1)-N(1)-Th(1)	96.27(13)
C(1)-N(2)-C(2)	131.8(4)
C(12)-N(3)-Si(1)	139.5(3)
C(12)-N(3)-Th(1)	97.4(2)
Si(1)-N(3)-Th(1)	107.22(15)
C(12)-N(4)-C(19)	126.7(3)
C(12)-N(4)-Th(1)	88.0(2)
C(19)-N(4)-Th(1)	139.7(3)
N(3)-Si(1)-N(1)	92.50(16)
N(3)-Si(1)-C(23)	114.68(19)
N(1)-Si(1)-C(23)	113.9(2)
N(3)-Si(1)-C(24)	109.88(19)
N(1)-Si(1)-C(24)	113.99(19)
C(23)-Si(1)-C(24)	110.8(2)
N(3)-Si(1)-Th(1)	43.21(11)
N(1)-Si(1)-Th(1)	51.60(11)
C(23)-Si(1)-Th(1)	114.67(15)
C(24)-Si(1)-Th(1)	134.04(17)
N(1)-C(1)-N(2)	119.6(4)
N(1)-C(1)-C(6)	119.8(4)
N(2)-C(1)-C(6)	120.6(4)
C(3)-C(2)-N(2)	111.1(4)
C(3)-C(2)-C(4)	112.0(5)
N(2)-C(2)-C(4)	111.0(4)
C(3)-C(2)-C(5)	109.2(5)
N(2)-C(2)-C(5)	104.6(4)
C(4)-C(2)-C(5)	108.7(5)
C(11)-C(6)-C(7)	119.2(5)
C(11)-C(6)-C(1)	119.5(4)
C(7)-C(6)-C(1)	121.2(5)
C(6)-C(7)-C(8)	119.4(6)
C(9)-C(8)-C(7)	120.7(6)
C(8)-C(9)-C(10)	120.5(5)
C(11)-C(10)-C(9)	119.4(6)
C(10)-C(11)-C(6)	120.8(5)
N(4)-C(12)-N(3)	112.2(4)
N(4)-C(12)-C(13)	129.2(3)
N(3)-C(12)-C(13)	118.3(3)
N(4)-C(12)-Th(1)	65.2(2)
N(3)-C(12)-Th(1)	54.7(2)
C(13)-C(12)-Th(1)	147.3(3)
C(14)-C(13)-C(18)	118.8(4)
C(14)-C(13)-C(12)	121.1(4)
C(18)-C(13)-C(12)	120.0(4)
C(13)-C(14)-C(15)	120.2(4)
C(16)-C(15)-C(14)	120.8(5)
C(15)-C(16)-C(17)	119.1(4)
C(18)-C(17)-C(16)	121.0(5)
C(17)-C(18)-C(13)	119.9(5)

N(4)-C(19)-C(20)	111.4(4)
N(4)-C(19)-C(21)	104.4(4)
C(20)-C(19)-C(21)	110.7(4)
N(4)-C(19)-C(22)	114.0(4)
C(20)-C(19)-C(22)	108.7(4)
C(21)-C(19)-C(22)	107.6(4)
C(27)-C(26)-C(25)	113(2)
C(27)#2-C(27)-C(26)	130.7(19)

Table 4: Anisotropic displacement parameters (A^2 x 10^3) for complex 2. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Th(1)	29(1)	22(1)	25(1)	0	0	3(1)
N(1)	29(2)	27(2)	31(2)	1(1)	2(1)	2(1)
N(2)	40(2)	36(2)	68(3)	-10(2)	17(2)	6(2)
N(3)	29(2)	29(2)	36(2)	-3(1)	3(1)	2(2)
N(4)	34(2)	30(2)	43(2)	-3(2)	8(2)	5(2)
Si(1)	36(1)	30(1)	34(1)	-2(1)	4(1)	2(1)
Cl(1)	65(1)	39(1)	49(1)	5(1)	23(1)	5(1)
C(1)	35(2)	35(2)	35(2)	-2(2)	3(2)	8(2)
C(2)	60(3)	34(2)	63(3)	-11(2)	19(3)	9(2)
C(3)	76(4)	56(3)	104(5)	-13(3)	11(4)	23(3)
C(4)	98(5)	66(4)	69(4)	-29(3)	9(3)	4(3)
C(5)	112(5)	42(3)	103(5)	-14(3)	48(4)	1(3)
C(6)	39(3)	45(2)	41(2)	-2(2)	8(2)	10(2)
C(7)	44(3)	50(3)	37(2)	3(2)	8(2)	8(2)
C(8)	77(4)	67(3)	52(3)	8(3)	31(3)	12(3)
C(9)	65(4)	78(5)	85(5)	3(3)	39(3)	5(4)
C(10)	40(3)	77(4)	92(5)	-11(4)	15(3)	7(3)
C(11)	36(2)	60(3)	53(3)	-3(2)	1(2)	7(2)
C(12)	35(2)	20(2)	28(2)	-3(1)	-5(2)	9(2)
C(13)	36(2)	32(2)	41(2)	-6(2)	7(2)	1(2)
C(14)	64(3)	38(2)	44(3)	-8(2)	4(2)	5(2)
C(15)	68(3)	52(3)	51(3)	-10(2)	-6(3)	14(3)
C(16)	71(3)	42(3)	66(3)	-10(2)	10(3)	21(3)
C(17)	70(4)	40(3)	67(4)	4(2)	15(3)	14(3)
C(18)	55(3)	40(2)	45(2)	1(2)	3(2)	3(2)
C(19)	53(3)	30(2)	59(3)	-8(2)	22(2)	1(2)
C(20)	74(4)	62(3)	56(3)	-18(3)	25(3)	6(3)
C(21)	46(3)	52(3)	93(4)	-4(3)	22(3)	6(2)
C(22)	72(4)	32(2)	124(5)	-15(3)	46(4)	12(3)
C(23)	39(3)	53(3)	58(3)	-6(2)	0(2)	6(2)
C(24)	60(3)	44(2)	44(3)	9(2)	12(2)	7(2)
C(25)	214(17)	240(30)	320(30)	-140(20)	-17(18)	37(18)
C(26)	114(10)	187(16)	430(30)	-167(18)	-3(15)	15(11)
C(27)	144(13)	210(20)	560(40)	-190(30)	11(18)	22(16)

Table 5: Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for complex **2.**

	x	y	z	U(eq)

H(2)	1694	3622	2144	58
H(3A)	-256	4728	2743	118
H(3B)	-370	3896	2655	118
H(3C)	-101	4371	2042	118
H(4A)	784	4589	3638	116
H(4B)	1611	4128	3523	116
H(4C)	723	3748	3609	116
H(5A)	1201	5255	2612	128
H(5B)	1306	4838	1935	128
H(5C)	1981	4736	2508	128
H(7)	857	2609	3608	53
H(8)	-267	2156	4234	79
H(9)	-1536	1910	3747	91
H(10)	-1736	2115	2623	83
H(11)	-637	2579	1994	60
H(14)	1574	646	-77	58
H(15)	794	-362	-341	68
H(16)	785	-1335	359	71
H(17)	1510	-1280	1351	71
H(18)	2233	-261	1652	56
H(20A)	2893	854	-534	96
H(20B)	3856	869	-752	96
H(20C)	3408	1577	-509	96
H(21A)	4735	1122	863	96
H(21B)	4551	1741	351	96
H(21C)	4995	1031	110	96
H(22A)	3953	-22	794	114
H(22B)	4209	-93	38	114
H(22C)	3243	-133	248	114
H(23A)	-125	910	1720	75
H(23B)	404	913	1053	75
H(23C)	-93	1605	1276	75
H(24A)	704	832	2812	74
H(24B)	1309	1449	3060	74
H(24C)	1698	752	2740	74
H(25A)	6757	677	1242	387
H(25B)	7138	1288	1693	387
H(25C)	7732	870	1195	387
H(26A)	6988	1325	332	293
H(26B)	6417	1756	836	293
H(27A)	7943	2048	1123	366
H(27B)	7910	2043	350	366

7. Crystallographic data for complex **3**

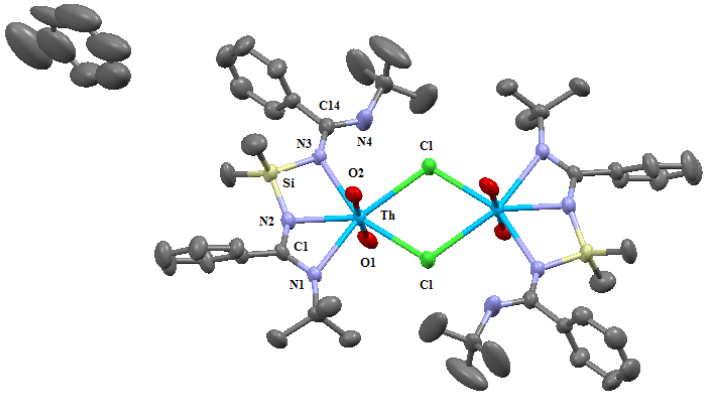


Figure 2: Molecular structure of complex 3. Color code: Th, blue, Cl, green, Si, yellow, N, purple, O, red, C, grey. Hydrogen atoms are omitted for clarity.

Table 6: Crystallographic data and structure refinement for complex **3**

Complex	**3**
Empirical Formula	$C_{56}H_{82}N_8Si_2Cl_2O_4Th_2$
Formula weight/g·mol^{-1}	1522.45
T/K	250(2)
λ/Å	0.71073
Crystal system	Triclinic
Space group	P-1
a/Å	10.9649(6)
b/Å	12.6366(7)
c/Å	12.9693(7)
α/°	97.368
β/°	97.368
γ/°	98.750
V/Å^3	1696.07(16)
Z	1
ρ/g·cm^{-3}	1.563
μ(Mo-K$_\alpha$)/mm^{-1}	4.542
F(000)	786
Θ range for data collection/°	1.64 to 25.02
Limiting indices	-13≤h≤13 -15≤k≤15 -15≤l≤15
Reflections collected/unique (R_{int})	62495/5981(0.0392)
Completeness to Θ	99.7%
GOF on F^2	1.060
R_1, wR_2 [I>2σ(I)]	0.354, 0.1074
R_1, wR_2 (all data)	0.0384, 0.1092
Largest diff. peak and hole (eÅ^{-3})	3.228 and -0.960

Table 7: Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for complex **3**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Th(1)	4056(1)	10129(1)	1402(1)	30(1)
Cl(1)	5479(2)	8855(1)	347(1)	40(1)
Si(1)	2792(2)	8992(2)	3134(2)	37(1)
O(1)	5480(5)	10883(4)	2273(4)	44(1)
O(2)	2690(5)	9350(4)	479(4)	37(1)
N(1)	2741(5)	11536(4)	1757(5)	33(1)
N(2)	2945(6)	10213(5)	2717(5)	36(1)
N(3)	4071(5)	8641(4)	2638(5)	33(1)
N(4)	5780(7)	7823(6)	2593(7)	59(2)
C(1)	2242(6)	10949(5)	2361(5)	32(1)
C(2)	2306(7)	12499(6)	1348(6)	40(2)
C(3)	3512(8)	13236(6)	1284(7)	51(2)
C(4)	1365(9)	12143(8)	231(7)	60(2)
C(5)	1708(10)	13145(7)	2107(9)	65(3)
C(6)	996(7)	10937(6)	2647(6)	36(2)
C(7)	989(8)	11157(7)	3720(6)	51(2)
C(8)	-170(9)	11071(10)	3994(7)	67(3)
C(9)	-1311(9)	10773(9)	3208(8)	63(2)
C(10)	-1305(7)	10522(8)	2152(7)	52(2)
C(11)	-164(7)	10607(6)	1868(6)	41(2)
C(12)	1249(9)	8063(8)	2412(10)	72(3)
C(13)	2997(10)	9156(8)	4616(7)	62(3)
C(14)	4766(6)	7936(6)	2955(6)	35(1)
C(15)	4481(7)	7289(5)	3788(6)	35(1)
C(16)	3538(8)	6363(7)	3505(7)	49(2)
C(17)	3283(11)	5802(8)	4314(9)	69(3)
C(18)	3942(12)	6198(9)	5373(8)	71(3)
C(19)	4852(10)	7124(8)	5656(7)	61(2)
C(20)	5138(8)	7670(6)	4866(6)	45(2)
C(21)	6571(8)	6947(7)	2595(7)	49(2)
C(22)	7027(16)	6626(14)	3676(11)	126(7)
C(23)	7711(14)	7417(13)	2276(18)	151(9)
C(24)	5829(15)	6004(13)	1815(17)	158(9)
C(25)	1753(13)	5975(12)	8931(14)	183(11)
C(26)	2318(11)	6751(8)	8436(18)	138(8)
C(27)	1937(16)	6667(12)	7319(19)	199(14)
C(28)	990(17)	5806(16)	6699(14)	208(15)
C(29)	424(10)	5030(10)	7194(17)	197(15)
C(30)	806(12)	5114(8)	8311(17)	155(11)
C(31)	2120(30)	6100(30)	10067(17)	234(17)

Table 8: Bond lengths [A] and angles [deg] for complex 3.

Th(1)-O(2)	1.737(5)
Th(1)-O(1)	1.741(5)
Th(1)-N(2)	2.327(5)
Th(1)-N(1)	2.520(5)
Th(1)-N(3)	2.623(5)
Th(1)-C(1)	2.844(6)
Th(1)-Cl(1)	2.8536(16)
Th(1)-Cl(1)#1	2.8572(16)
Th(1)-Si(1)	3.2831(18)
Cl(1)-Th(1)#1	2.8572(16)
Si(1)-N(2)	1.697(6)
Si(1)-N(3)	1.771(5)
Si(1)-C(12)	1.858(10)
Si(1)-C(13)	1.860(8)
N(1)-C(1)	1.304(9)
N(1)-C(2)	1.486(8)
N(2)-C(1)	1.351(8)
N(3)-C(14)	1.300(9)
N(4)-C(14)	1.328(9)
N(4)-C(21)	1.506(9)
C(1)-C(6)	1.498(9)
C(2)-C(3)	1.523(11)
C(2)-C(4)	1.524(11)
C(2)-C(5)	1.530(11)
C(6)-C(7)	1.385(10)
C(6)-C(11)	1.384(10)
C(7)-C(8)	1.394(12)
C(8)-C(9)	1.371(13)
C(9)-C(10)	1.368(13)
C(10)-C(11)	1.381(11)
C(14)-C(15)	1.500(9)
C(15)-C(16)	1.381(11)
C(15)-C(20)	1.390(10)
C(16)-C(17)	1.399(12)
C(17)-C(18)	1.373(16)
C(18)-C(19)	1.362(15)
C(19)-C(20)	1.377(12)
C(21)-C(24)	1.449(17)
C(21)-C(23)	1.476(14)
C(21)-C(22)	1.497(15)
C(25)-C(26)	1.3900
C(25)-C(30)	1.3900
C(25)-C(31)	1.410(16)
C(26)-C(27)	1.3900
C(27)-C(28)	1.3900
C(28)-C(29)	1.3900
C(29)-C(30)	1.3900
O(2)-Th(1)-O(1)	176.4(2)
O(2)-Th(1)-N(2)	89.7(2)
O(1)-Th(1)-N(2)	93.7(2)
O(2)-Th(1)-N(1)	88.4(2)

O(1)-Th(1)-N(1)	94.5(2)
N(2)-Th(1)-N(1)	54.22(19)
O(2)-Th(1)-N(3)	90.2(2)
O(1)-Th(1)-N(3)	90.6(2)
N(2)-Th(1)-N(3)	60.26(18)
N(1)-Th(1)-N(3)	114.46(17)
O(2)-Th(1)-C(1)	83.0(2)
O(1)-Th(1)-C(1)	100.5(2)
N(2)-Th(1)-C(1)	28.08(19)
N(1)-Th(1)-C(1)	27.29(18)
N(3)-Th(1)-C(1)	87.65(17)
O(2)-Th(1)-Cl(1)	86.68(15)
O(1)-Th(1)-Cl(1)	89.94(16)
N(2)-Th(1)-Cl(1)	144.68(14)
N(1)-Th(1)-Cl(1)	160.31(13)
N(3)-Th(1)-Cl(1)	84.60(12)
C(1)-Th(1)-Cl(1)	167.10(15)
O(2)-Th(1)-Cl(1)#1	86.70(17)
O(1)-Th(1)-Cl(1)#1	91.23(19)
N(2)-Th(1)-Cl(1)#1	142.33(14)
N(1)-Th(1)-Cl(1)#1	88.18(13)
N(3)-Th(1)-Cl(1)#1	157.06(12)
C(1)-Th(1)-Cl(1)#1	114.44(13)
Cl(1)-Th(1)-Cl(1)#1	72.53(5)
O(2)-Th(1)-Si(1)	82.47(17)
O(1)-Th(1)-Si(1)	100.02(18)
N(2)-Th(1)-Si(1)	29.39(14)
N(1)-Th(1)-Si(1)	82.63(13)
N(3)-Th(1)-Si(1)	32.52(12)
C(1)-Th(1)-Si(1)	55.44(14)
Cl(1)-Th(1)-Si(1)	115.50(5)
Cl(1)#1-Th(1)-Si(1)	165.96(5)
Th(1)-Cl(1)-Th(1)#1	107.47(5)
N(2)-Si(1)-N(3)	92.1(3)
N(2)-Si(1)-C(12)	113.2(4)
N(3)-Si(1)-C(12)	111.5(4)
N(2)-Si(1)-C(13)	111.5(4)
N(3)-Si(1)-C(13)	117.9(4)
C(12)-Si(1)-C(13)	109.7(5)
N(2)-Si(1)-Th(1)	42.30(19)
N(3)-Si(1)-Th(1)	52.76(18)
C(12)-Si(1)-Th(1)	110.1(4)
C(13)-Si(1)-Th(1)	139.2(4)
C(1)-N(1)-C(2)	126.9(6)
C(1)-N(1)-Th(1)	90.3(4)
C(2)-N(1)-Th(1)	141.2(4)
C(1)-N(2)-Si(1)	141.1(5)
C(1)-N(2)-Th(1)	97.7(4)
Si(1)-N(2)-Th(1)	108.3(3)
C(14)-N(3)-Si(1)	126.5(5)
C(14)-N(3)-Th(1)	138.4(4)
Si(1)-N(3)-Th(1)	94.7(2)
C(14)-N(4)-C(21)	132.9(7)
N(1)-C(1)-N(2)	113.1(6)
N(1)-C(1)-C(6)	129.4(6)
N(2)-C(1)-C(6)	117.4(6)

N(1)-C(1)-Th(1)	62.4(3)
N(2)-C(1)-Th(1)	54.2(3)
C(6)-C(1)-Th(1)	157.0(5)
N(1)-C(2)-C(3)	105.6(6)
N(1)-C(2)-C(4)	109.7(6)
C(3)-C(2)-C(4)	110.4(7)
N(1)-C(2)-C(5)	113.2(6)
C(3)-C(2)-C(5)	107.5(7)
C(4)-C(2)-C(5)	110.3(7)
C(7)-C(6)-C(11)	118.6(7)
C(7)-C(6)-C(1)	119.9(6)
C(11)-C(6)-C(1)	121.2(6)
C(6)-C(7)-C(8)	120.1(8)
C(9)-C(8)-C(7)	120.5(8)
C(8)-C(9)-C(10)	119.5(8)
C(9)-C(10)-C(11)	120.7(8)
C(10)-C(11)-C(6)	120.7(7)
N(3)-C(14)-N(4)	120.6(6)
N(3)-C(14)-C(15)	120.3(6)
N(4)-C(14)-C(15)	119.0(6)
C(16)-C(15)-C(20)	120.2(7)
C(16)-C(15)-C(14)	121.0(7)
C(20)-C(15)-C(14)	118.6(7)
C(15)-C(16)-C(17)	119.0(8)
C(18)-C(17)-C(16)	119.6(9)
C(19)-C(18)-C(17)	121.4(8)
C(18)-C(19)-C(20)	119.6(9)
C(19)-C(20)-C(15)	120.1(8)
C(24)-C(21)-C(23)	110.9(13)
C(24)-C(21)-C(22)	109.9(13)
C(23)-C(21)-C(22)	107.7(12)
C(24)-C(21)-N(4)	108.8(9)
C(23)-C(21)-N(4)	105.3(7)
C(22)-C(21)-N(4)	114.2(8)
C(26)-C(25)-C(30)	120.0
C(26)-C(25)-C(31)	119.1(19)
C(30)-C(25)-C(31)	120.8(19)
C(27)-C(26)-C(25)	120.0
C(26)-C(27)-C(28)	120.0
C(29)-C(28)-C(27)	120.0
C(28)-C(29)-C(30)	120.0
C(29)-C(30)-C(25)	120.0

Table 9: Anisotropic displacement parameters (A^2 x 10^3) for complex **3**. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Th(1)	26(1)	33(1)	36(1)	10(1)	14(1)	10(1)
Cl(1)	46(1)	40(1)	48(1)	19(1)	28(1)	21(1)
Si(1)	32(1)	43(1)	46(1)	19(1)	21(1)	14(1)
O(1)	50(3)	44(3)	44(3)	5(2)	12(2)	28(2)
O(2)	34(3)	34(2)	46(3)	9(2)	14(2)	16(2)
N(1)	32(3)	35(3)	40(3)	11(2)	18(2)	13(2)
N(2)	38(3)	41(3)	37(3)	13(2)	19(2)	17(3)
N(3)	32(3)	37(3)	40(3)	16(2)	18(2)	15(2)
N(4)	60(4)	66(5)	87(5)	50(4)	49(4)	43(4)
C(1)	35(3)	37(3)	27(3)	6(3)	10(3)	18(3)
C(2)	49(4)	32(3)	49(4)	13(3)	19(3)	20(3)
C(3)	54(5)	37(4)	68(5)	17(4)	21(4)	11(4)
C(4)	60(5)	58(5)	60(5)	25(4)	3(4)	14(4)
C(5)	85(7)	49(5)	86(7)	21(5)	48(6)	40(5)
C(6)	33(4)	40(4)	43(4)	10(3)	17(3)	15(3)
C(7)	38(4)	76(6)	41(4)	3(4)	14(3)	23(4)
C(8)	61(6)	113(8)	38(4)	12(5)	22(4)	35(6)
C(9)	47(5)	94(7)	61(5)	24(5)	26(4)	30(5)
C(10)	30(4)	71(6)	55(5)	16(4)	11(3)	7(4)
C(11)	33(4)	50(4)	43(4)	11(3)	15(3)	7(3)
C(12)	45(5)	58(6)	114(9)	22(6)	22(5)	11(4)
C(13)	82(7)	83(6)	54(5)	34(5)	45(5)	51(6)
C(14)	31(3)	40(4)	39(4)	11(3)	14(3)	10(3)
C(15)	39(4)	32(3)	41(4)	14(3)	16(3)	13(3)
C(16)	54(5)	46(4)	49(4)	9(3)	18(4)	3(4)
C(17)	85(7)	50(5)	82(7)	23(5)	44(6)	1(5)
C(18)	105(8)	70(6)	64(6)	40(5)	44(6)	32(6)
C(19)	84(7)	67(6)	42(4)	20(4)	17(4)	33(5)
C(20)	49(4)	45(4)	42(4)	10(3)	8(3)	16(3)
C(21)	50(5)	49(4)	70(5)	29(4)	33(4)	32(4)
C(22)	154(14)	180(16)	101(10)	63(10)	55(10)	140(13)
C(23)	108(11)	136(13)	310(30)	152(16)	146(15)	96(10)
C(24)	88(10)	114(12)	230(20)	-76(14)	14(12)	38(9)
C(25)	150(20)	160(20)	280(30)	30(20)	90(20)	111(19)
C(26)	112(13)	75(10)	250(30)	35(13)	89(16)	20(9)
C(27)	200(30)	109(17)	360(50)	80(20)	180(30)	77(18)
C(28)	123(18)	100(14)	420(50)	20(20)	110(20)	45(13)
C(29)	83(13)	92(14)	410(50)	0(20)	70(20)	34(11)
C(30)	55(8)	51(7)	330(30)	-36(12)	43(13)	17(6)
C(31)	280(40)	290(40)	160(20)	20(20)	30(20)	210(30)

Table 10: Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for complex **3.**

	x	y	z	U(eq)
H(3A)	4090	13473	2002	77
H(3B)	3282	13864	981	77
H(3C)	3931	12839	827	77
H(4A)	1751	11726	-239	90
H(4B)	1155	12779	-66	90
H(4C)	591	11696	289	90
H(5A)	880	12733	2091	98
H(5B)	1599	13833	1874	98
H(5C)	2266	13281	2836	98
H(7)	1768	11364	4263	61
H(8)	-169	11219	4724	81
H(9)	-2091	10742	3394	75
H(10)	-2085	10288	1614	62
H(11)	-176	10438	1138	50
H(12A)	546	8371	2575	107
H(12B)	1244	7363	2645	107
H(12C)	1153	7970	1641	107
H(13A)	3850	9562	4992	94
H(13B)	2887	8446	4826	94
H(13C)	2363	9546	4802	94
H(16)	3074	6114	2780	59
H(17)	2664	5158	4135	82
H(18)	3762	5821	5915	85
H(19)	5282	7390	6386	74
H(20)	5778	8301	5055	54
H(22A)	6389	6049	3765	189
H(22B)	7159	7249	4240	189
H(22C)	7828	6373	3723	189
H(23A)	8248	6879	2232	226
H(23B)	8191	8047	2808	226
H(23C)	7443	7634	1577	226
H(24A)	6381	5688	1433	237
H(24B)	5146	6220	1304	237
H(24C)	5463	5471	2186	237
H(26)	2959	7334	8855	165
H(27)	2319	7192	6984	238
H(28)	731	5749	5944	250
H(29)	-217	4447	6775	236
H(30)	423	4589	8646	185
H(31A)	1641	5498	10290	351
H(31B)	1933	6778	10374	351
H(31C)	3028	6103	10318	351

8. Crystallographic Data for complex **4**.

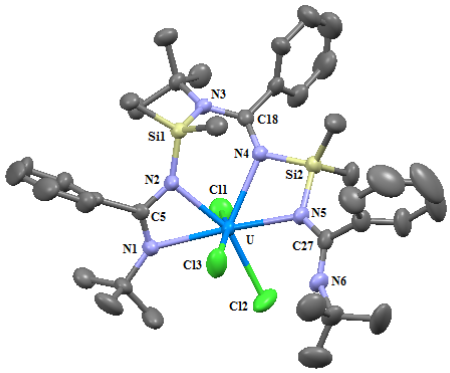


Figure 3: Molecular structure of complex 4. Color code: U, blue, Cl, green, Si, yellow, N, purple, C, grey. Hydrogen atoms are omitted for clarity.

Table 11: Crystallographic data for complexes **4**

Complex	4
Empirical Formula	$C_{37}H_{55}Cl_3N_6Si_2U$
Formula weight/g·mol^{-1}	984.43
T/K	240(2)
λ/Å	0.71073
Crystal system	Monoclinic
Space group	P21/C
a/Å	19.5150(4)
b/Å	10.5640(2)
c/Å	22.4540(4)
α/°	90
β/°	109.1960(9)
γ/°	90
V/Å^3	4371.66(14)
Z	4
ρ/g·cm^{-3}	1.496
μ(Mo-K$_\alpha$)/mm^{-1}	3.983
F(000)	1960
Θ range for data collection/°	1.10 to 25.05
Limiting indices	0≤h≤23 0≤k≤12 -26≤1≤25
Reflections collected/unique (R_{int})	7747/7747 (0.0000)
Completeness to Θ	99.9%
GOF on F^2	1.028
R_1, wR_2 [I>2σ(I)]	0.0317, 0.0692
R_1, wR_2 (all data)	0.0538, 0.0759
Largest diff. peak and hole (eÅ^{-3})	0.604, -0.788

Table 12: Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for shelxl. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
U(1)	2648(1)	2430(1)	3546(1)	28(1)
Si(1)	1977(1)	5171(1)	4095(1)	31(1)
Si(2)	3258(1)	4729(1)	2834(1)	36(1)
Cl(1)	1469(1)	2102(1)	2573(1)	56(1)
Cl(2)	3111(1)	389(1)	3097(1)	67(1)
Cl(3)	3681(1)	2137(2)	4642(1)	61(1)
N(1)	1956(2)	1477(3)	4186(2)	33(1)
N(2)	2061(2)	3576(3)	4133(2)	34(1)
N(3)	1496(2)	5519(3)	3275(2)	31(1)
N(4)	2477(2)	4621(3)	3061(2)	30(1)
N(5)	3696(2)	3469(3)	3313(2)	34(1)
N(6)	4606(2)	1995(4)	3662(2)	41(1)
C(1)	1844(3)	218(4)	4426(2)	42(1)
C(2)	2060(4)	-705(5)	4008(3)	78(2)
C(3)	2337(3)	53(5)	5107(3)	70(2)
C(4)	1061(3)	-33(5)	4380(3)	54(1)
C(5)	1863(2)	2577(4)	4396(2)	28(1)
C(6)	1521(3)	2826(4)	4915(2)	36(1)
C(7)	1981(3)	3101(5)	5516(2)	53(2)
C(8)	1693(5)	3384(6)	5985(3)	76(2)
C(9)	962(5)	3408(6)	5861(3)	84(2)
C(10)	504(4)	3166(6)	5267(3)	76(2)
C(11)	775(3)	2862(5)	4790(3)	50(1)
C(12)	1541(3)	5883(4)	4646(2)	42(1)
C(13)	2888(3)	5920(5)	4334(2)	45(1)
C(14)	682(2)	5750(4)	3022(2)	36(1)
C(15)	511(3)	7071(5)	3210(2)	49(1)
C(16)	332(3)	4715(5)	3304(2)	46(1)
C(17)	338(3)	5617(5)	2307(2)	52(1)
C(18)	1922(2)	5379(4)	2900(2)	30(1)
C(19)	1775(3)	6212(5)	2329(2)	38(1)
C(20)	1598(3)	5719(6)	1727(2)	55(2)
C(21)	1461(4)	6542(8)	1217(3)	79(2)
C(22)	1514(4)	7823(8)	1316(3)	87(2)
C(23)	1708(4)	8315(6)	1906(3)	70(2)
C(24)	1824(3)	7519(4)	2417(2)	46(1)
C(25)	3667(3)	6327(5)	2993(3)	59(2)
C(26)	3130(3)	4240(5)	2011(2)	54(2)
C(27)	4392(3)	3170(5)	3479(2)	34(1)
C(28)	4949(3)	4124(5)	3451(2)	45(1)
C(29)	5179(3)	4152(6)	2936(3)	63(2)
C(30)	5672(4)	5068(9)	2899(4)	101(3)
C(31)	5921(5)	5915(10)	3369(5)	125(4)
C(32)	5696(5)	5908(8)	3884(4)	106(3)
C(33)	5196(3)	4998(6)	3927(3)	67(2)
C(34)	5336(3)	1443(5)	4020(2)	51(1)

C(35)	5893(4)	1657(8)	3697(3)	95(3)
C(36)	5184(4)	43(6)	4042(3)	87(2)
C(37)	5596(3)	1971(7)	4682(3)	79(2)

Table 13: Bond lengths [A] and angles [deg] for shelxl for complex **4**.

U(1)-N(2)	2.349(4)
U(1)-N(1)	2.486(4)
U(1)-N(5)	2.523(4)
U(1)-N(4)	2.533(3)
U(1)-Cl(1)	2.6233(12)
U(1)-Cl(3)	2.6372(12)
U(1)-Cl(2)	2.6608(13)
U(1)-C(5)	2.817(4)
U(1)-Si(2)	3.3345(13)
Si(1)-N(2)	1.691(4)
Si(1)-N(3)	1.808(4)
Si(1)-C(13)	1.857(5)
Si(1)-C(12)	1.874(5)
Si(2)-N(5)	1.747(4)
Si(2)-N(4)	1.762(4)
Si(2)-C(25)	1.852(5)
Si(2)-C(26)	1.856(5)
N(1)-C(5)	1.289(5)
N(1)-C(1)	1.478(6)
N(2)-C(5)	1.327(5)
N(3)-C(18)	1.370(6)
N(3)-C(14)	1.520(6)
N(4)-C(18)	1.300(5)
N(5)-C(27)	1.322(6)
N(6)-C(27)	1.331(6)
N(6)-C(34)	1.505(6)
N(6)-H(6)	0.9599
C(1)-C(2)	1.507(7)
C(1)-C(4)	1.521(7)
C(1)-C(3)	1.524(7)
C(2)-H(2A)	0.9600
C(2)-H(2B)	0.9600
C(2)-H(2C)	0.9601
C(3)-H(3A)	0.9601
C(3)-H(3B)	0.9601
C(3)-H(3C)	0.9600
C(4)-H(4A)	0.9600
C(4)-H(4B)	0.9600
C(4)-H(4C)	0.9599
C(5)-C(6)	1.545(6)
C(6)-C(7)	1.384(7)
C(6)-C(11)	1.389(7)
C(7)-C(8)	1.380(8)
C(7)-H(7)	0.9599
C(8)-C(9)	1.360(10)
C(8)-H(8)	0.9600
C(9)-C(10)	1.364(10)
C(9)-H(9)	0.9599
C(10)-C(11)	1.379(8)
C(10)-H(10)	0.9601
C(11)-H(11)	0.9600

C(12)-H(12A)	0.9602
C(12)-H(12B)	0.9599
C(12)-H(12C)	0.9601
C(13)-H(13A)	0.9599
C(13)-H(13B)	0.9600
C(13)-H(13C)	0.9600
C(14)-C(15)	1.526(6)
C(14)-C(17)	1.528(6)
C(14)-C(16)	1.534(6)
C(15)-H(15A)	0.9600
C(15)-H(15B)	0.9601
C(15)-H(15C)	0.9600
C(16)-H(16A)	0.9600
C(16)-H(16B)	0.9599
C(16)-H(16C)	0.9600
C(17)-H(17A)	0.9601
C(17)-H(17B)	0.9599
C(17)-H(17C)	0.9600
C(18)-C(19)	1.503(6)
C(19)-C(20)	1.383(7)
C(19)-C(24)	1.394(6)
C(20)-C(21)	1.391(8)
C(20)-H(20)	0.9600
C(21)-C(22)	1.370(10)
C(21)-H(21)	0.9600
C(22)-C(23)	1.356(9)
C(22)-H(22)	0.9600
C(23)-C(24)	1.379(7)
C(23)-H(23)	0.9600
C(24)-H(24)	0.9600
C(25)-H(25A)	0.9599
C(25)-H(25B)	0.9601
C(25)-H(25C)	0.9600
C(26)-H(26A)	0.9598
C(26)-H(26B)	0.9601
C(26)-H(26C)	0.9600
C(27)-C(28)	1.499(7)
C(28)-C(29)	1.373(7)
C(28)-C(33)	1.374(7)
C(29)-C(30)	1.386(9)
C(29)-H(29)	0.9601
C(30)-C(31)	1.348(12)
C(30)-H(30)	0.9599
C(31)-C(32)	1.365(12)
C(31)-H(31)	0.9600
C(32)-C(33)	1.395(9)
C(32)-H(32)	0.9600
C(33)-H(33)	0.9599
C(34)-C(35)	1.508(8)
C(34)-C(37)	1.511(8)
C(34)-C(36)	1.513(8)
C(35)-H(35A)	0.9600
C(35)-H(35B)	0.9601
C(35)-H(35C)	0.9601
C(36)-H(36A)	0.9600
C(36)-H(36B)	0.9601

C(36)-H(36C)	0.9600
C(37)-H(37A)	0.9602
C(37)-H(37B)	0.9602
C(37)-H(37C)	0.9600
N(2)-U(1)-N(1)	54.95(13)
N(2)-U(1)-N(5)	118.10(13)
N(1)-U(1)-N(5)	158.11(12)
N(2)-U(1)-N(4)	75.53(12)
N(1)-U(1)-N(4)	126.75(12)
N(5)-U(1)-N(4)	60.96(11)
N(2)-U(1)-Cl(1)	94.51(10)
N(1)-U(1)-Cl(1)	86.15(9)
N(5)-U(1)-Cl(1)	115.70(9)
N(4)-U(1)-Cl(1)	78.89(8)
N(2)-U(1)-Cl(3)	84.30(9)
N(1)-U(1)-Cl(3)	78.86(9)
N(5)-U(1)-Cl(3)	79.75(9)
N(4)-U(1)-Cl(3)	117.41(9)
Cl(1)-U(1)-Cl(3)	162.50(5)
N(2)-U(1)-Cl(2)	156.94(10)
N(1)-U(1)-Cl(2)	102.00(9)
N(5)-U(1)-Cl(2)	82.77(9)
N(4)-U(1)-Cl(2)	126.21(9)
Cl(1)-U(1)-Cl(2)	83.79(5)
Cl(3)-U(1)-Cl(2)	90.49(5)
N(2)-U(1)-C(5)	27.93(12)
N(1)-U(1)-C(5)	27.22(11)
N(5)-U(1)-C(5)	140.84(12)
N(4)-U(1)-C(5)	102.49(11)
Cl(1)-U(1)-C(5)	92.70(9)
Cl(3)-U(1)-C(5)	78.08(9)
Cl(2)-U(1)-C(5)	129.02(9)
N(2)-U(1)-Si(2)	102.15(9)
N(1)-U(1)-Si(2)	156.82(9)
N(5)-U(1)-Si(2)	30.94(8)
N(4)-U(1)-Si(2)	31.33(9)
Cl(1)-U(1)-Si(2)	92.91(4)
Cl(3)-U(1)-Si(2)	104.43(4)
Cl(2)-U(1)-Si(2)	100.91(4)
C(5)-U(1)-Si(2)	130.07(9)
N(2)-Si(1)-N(3)	105.33(17)
N(2)-Si(1)-C(13)	110.0(2)
N(3)-Si(1)-C(13)	109.5(2)
N(2)-Si(1)-C(12)	115.0(2)
N(3)-Si(1)-C(12)	113.3(2)
C(13)-Si(1)-C(12)	103.7(2)
N(5)-Si(2)-N(4)	93.90(17)
N(5)-Si(2)-C(25)	118.9(2)
N(4)-Si(2)-C(25)	111.2(2)
N(5)-Si(2)-C(26)	106.2(2)
N(4)-Si(2)-C(26)	115.1(2)
C(25)-Si(2)-C(26)	110.7(3)
N(5)-Si(2)-U(1)	47.95(13)
N(4)-Si(2)-U(1)	48.35(11)
C(25)-Si(2)-U(1)	140.43(19)

C(26)-Si(2)-U(1)	108.82(18)
C(5)-N(1)-C(1)	128.5(4)
C(5)-N(1)-U(1)	90.8(3)
C(1)-N(1)-U(1)	138.5(3)
C(5)-N(2)-Si(1)	141.1(3)
C(5)-N(2)-U(1)	96.1(3)
Si(1)-N(2)-U(1)	122.79(19)
C(18)-N(3)-C(14)	123.9(3)
C(18)-N(3)-Si(1)	112.8(3)
C(14)-N(3)-Si(1)	122.8(3)
C(18)-N(4)-Si(2)	126.9(3)
C(18)-N(4)-U(1)	131.5(3)
Si(2)-N(4)-U(1)	100.32(16)
C(27)-N(5)-Si(2)	127.3(3)
C(27)-N(5)-U(1)	131.6(3)
Si(2)-N(5)-U(1)	101.11(17)
C(27)-N(6)-C(34)	132.3(4)
C(27)-N(6)-H(6)	119.2
C(34)-N(6)-H(6)	108.5
N(1)-C(1)-C(2)	104.5(4)
N(1)-C(1)-C(4)	113.4(4)
C(2)-C(1)-C(4)	108.9(5)
N(1)-C(1)-C(3)	110.5(4)
C(2)-C(1)-C(3)	109.7(5)
C(4)-C(1)-C(3)	109.7(4)
C(1)-C(2)-H(2A)	110.3
C(1)-C(2)-H(2B)	110.1
H(2A)-C(2)-H(2B)	109.5
C(1)-C(2)-H(2C)	108.0
H(2A)-C(2)-H(2C)	109.5
H(2B)-C(2)-H(2C)	109.5
C(1)-C(3)-H(3A)	110.4
C(1)-C(3)-H(3B)	109.2
H(3A)-C(3)-H(3B)	109.5
C(1)-C(3)-H(3C)	108.8
H(3A)-C(3)-H(3C)	109.5
H(3B)-C(3)-H(3C)	109.5
C(1)-C(4)-H(4A)	109.9
C(1)-C(4)-H(4B)	110.1
H(4A)-C(4)-H(4B)	109.5
C(1)-C(4)-H(4C)	108.4
H(4A)-C(4)-H(4C)	109.5
H(4B)-C(4)-H(4C)	109.5
N(1)-C(5)-N(2)	117.3(4)
N(1)-C(5)-C(6)	125.2(4)
N(2)-C(5)-C(6)	117.4(4)
N(1)-C(5)-U(1)	61.9(2)
N(2)-C(5)-U(1)	56.0(2)
C(6)-C(5)-U(1)	170.7(3)
C(7)-C(6)-C(11)	119.5(5)
C(7)-C(6)-C(5)	118.0(5)
C(11)-C(6)-C(5)	122.4(4)
C(8)-C(7)-C(6)	119.5(6)
C(8)-C(7)-H(7)	122.3
C(6)-C(7)-H(7)	118.2
C(9)-C(8)-C(7)	120.8(6)

C(9)-C(8)-H(8)	118.4
C(7)-C(8)-H(8)	120.8
C(8)-C(9)-C(10)	120.1(6)
C(8)-C(9)-H(9)	120.3
C(10)-C(9)-H(9)	119.5
C(9)-C(10)-C(11)	120.5(7)
C(9)-C(10)-H(10)	120.0
C(11)-C(10)-H(10)	119.5
C(10)-C(11)-C(6)	119.6(6)
C(10)-C(11)-H(11)	121.4
C(6)-C(11)-H(11)	119.0
Si(1)-C(12)-H(12A)	109.5
Si(1)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
Si(1)-C(12)-H(12C)	109.4
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
Si(1)-C(13)-H(13A)	109.3
Si(1)-C(13)-H(13B)	109.6
H(13A)-C(13)-H(13B)	109.5
Si(1)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
N(3)-C(14)-C(15)	109.9(4)
N(3)-C(14)-C(17)	115.0(4)
C(15)-C(14)-C(17)	108.3(4)
N(3)-C(14)-C(16)	106.5(4)
C(15)-C(14)-C(16)	111.7(4)
C(17)-C(14)-C(16)	105.4(4)
C(14)-C(15)-H(15A)	109.6
C(14)-C(15)-H(15B)	109.9
H(15A)-C(15)-H(15B)	109.5
C(14)-C(15)-H(15C)	108.9
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(14)-C(16)-H(16A)	109.7
C(14)-C(16)-H(16B)	109.0
H(16A)-C(16)-H(16B)	109.5
C(14)-C(16)-H(16C)	109.7
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(14)-C(17)-H(17A)	110.4
C(14)-C(17)-H(17B)	109.3
H(17A)-C(17)-H(17B)	109.5
C(14)-C(17)-H(17C)	108.7
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
N(4)-C(18)-N(3)	120.9(4)
N(4)-C(18)-C(19)	120.4(4)
N(3)-C(18)-C(19)	118.4(4)
C(20)-C(19)-C(24)	119.7(5)
C(20)-C(19)-C(18)	122.1(5)
C(24)-C(19)-C(18)	118.3(4)
C(19)-C(20)-C(21)	119.2(6)
C(19)-C(20)-H(20)	118.6
C(21)-C(20)-H(20)	122.2

C(22)-C(21)-C(20)	120.0(6)
C(22)-C(21)-H(21)	118.1
C(20)-C(21)-H(21)	121.9
C(23)-C(22)-C(21)	121.2(6)
C(23)-C(22)-H(22)	119.8
C(21)-C(22)-H(22)	119.0
C(22)-C(23)-C(24)	119.8(6)
C(22)-C(23)-H(23)	121.4
C(24)-C(23)-H(23)	118.8
C(23)-C(24)-C(19)	120.0(5)
C(23)-C(24)-H(24)	120.8
C(19)-C(24)-H(24)	119.2
Si(2)-C(25)-H(25A)	108.8
Si(2)-C(25)-H(25B)	109.4
H(25A)-C(25)-H(25B)	109.5
Si(2)-C(25)-H(25C)	110.2
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
Si(2)-C(26)-H(26A)	109.4
Si(2)-C(26)-H(26B)	109.1
H(26A)-C(26)-H(26B)	109.5
Si(2)-C(26)-H(26C)	109.9
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
N(5)-C(27)-N(6)	119.9(4)
N(5)-C(27)-C(28)	121.2(4)
N(6)-C(27)-C(28)	118.8(4)
C(29)-C(28)-C(33)	120.8(6)
C(29)-C(28)-C(27)	119.6(5)
C(33)-C(28)-C(27)	119.6(5)
C(28)-C(29)-C(30)	119.5(7)
C(28)-C(29)-H(29)	119.2
C(30)-C(29)-H(29)	121.2
C(31)-C(30)-C(29)	119.7(8)
C(31)-C(30)-H(30)	120.0
C(29)-C(30)-H(30)	120.3
C(30)-C(31)-C(32)	121.7(8)
C(30)-C(31)-H(31)	121.3
C(32)-C(31)-H(31)	117.0
C(31)-C(32)-C(33)	119.3(8)
C(31)-C(32)-H(32)	121.4
C(33)-C(32)-H(32)	119.2
C(28)-C(33)-C(32)	119.0(7)
C(28)-C(33)-H(33)	119.8
C(32)-C(33)-H(33)	121.3
N(6)-C(34)-C(35)	113.0(4)
N(6)-C(34)-C(37)	109.5(4)
C(35)-C(34)-C(37)	110.9(6)
N(6)-C(34)-C(36)	103.6(5)
C(35)-C(34)-C(36)	110.0(6)
C(37)-C(34)-C(36)	109.6(5)
C(34)-C(35)-H(35A)	110.0
C(34)-C(35)-H(35B)	109.3
H(35A)-C(35)-H(35B)	109.5
C(34)-C(35)-H(35C)	109.1
H(35A)-C(35)-H(35C)	109.5

H(35B)-C(35)-H(35C)	109.5
C(34)-C(36)-H(36A)	110.5
C(34)-C(36)-H(36B)	108.5
H(36A)-C(36)-H(36B)	109.5
C(34)-C(36)-H(36C)	109.4
H(36A)-C(36)-H(36C)	109.5
H(36B)-C(36)-H(36C)	109.5
C(34)-C(37)-H(37A)	110.0
C(34)-C(37)-H(37B)	110.6
H(37A)-C(37)-H(37B)	109.5
C(34)-C(37)-H(37C)	107.8
H(37A)-C(37)-H(37C)	109.5
H(37B)-C(37)-H(37C)	109.5

Table 14: Anisotropic displacement parameters (A^2 x 10^3) for shelxl. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
U(1)	27(1)	30(1)	29(1)	0(1)	13(1)	1(1)
Si(1)	34(1)	29(1)	30(1)	-2(1)	12(1)	1(1)
Si(2)	31(1)	37(1)	43(1)	7(1)	16(1)	2(1)
Cl(1)	43(1)	71(1)	43(1)	-5(1)	-1(1)	12(1)
Cl(2)	54(1)	49(1)	110(1)	-33(1)	45(1)	7(1)
Cl(3)	37(1)	106(1)	37(1)	15(1)	6(1)	(1)
N(1)	40(2)	29(2)	33(2)	3(2)	17(2)	3(2)
N(2)	41(2)	31(2)	35(2)	2(2)	22(2)	5(2)
N(3)	28(2)	30(2)	34(2)	1(2)	11(2)	5(2)
N(4)	26(2)	29(2)	34(2)	2(2)	11(2)	1(2)
N(5)	24(2)	35(2)	45(2)	2(2)	15(2)	2(2)
N(6)	25(2)	45(2)	54(3)	2(2)	14(2)	6(2)
C(1)	49(3)	29(2)	53(3)	10(2)	25(3)	1(2)
C(2)	123(6)	35(3)	107(5)	3(3)	80(5)	5(4)
C(3)	67(4)	53(4)	77(4)	33(3)	5(3)	5(3)
C(4)	53(4)	40(3)	67(4)	3(3)	20(3)	9(3)
C(5)	35(3)	30(2)	15(2)	1(2)	3(2)	3(2)
C(6)	50(3)	26(2)	37(3)	6(2)	24(2)	9(2)
C(7)	66(4)	59(3)	39(3)	9(3)	24(3)	16(3)
C(8)	124(7)	68(4)	45(3)	1(3)	42(4)	27(4)
C(9)	134(8)	79(5)	76(5)	13(4)	83(5)	38(5)
C(10)	78(5)	81(5)	99(5)	17(4)	71(5)	22(4)
C(11)	50(4)	49(3)	62(3)	9(3)	33(3)	8(3)
C(12)	54(3)	34(3)	41(3)	-3(2)	21(2)	7(2)
C(13)	47(3)	40(3)	44(3)	-6(2)	11(2)	1(2)
C(14)	26(3)	40(3)	41(3)	1(2)	13(2)	4(2)
C(15)	40(3)	48(3)	56(3)	2(2)	10(3)	16(2)
C(16)	31(3)	50(3)	59(3)	-3(3)	20(3)	5(2)
C(17)	29(3)	71(4)	49(3)	-3(3)	1(2)	1(3)
C(18)	29(3)	27(2)	33(2)	-3(2)	10(2)	5(2)
C(19)	31(3)	51(3)	35(3)	5(2)	15(2)	12(2)
C(20)	50(4)	75(4)	40(3)	6(3)	16(3)	23(3)
C(21)	88(5)	116(6)	38(3)	7(4)	30(3)	33(5)
C(22)	96(6)	108(6)	62(4)	44(4)	34(4)	35(5)
C(23)	75(5)	60(4)	82(5)	30(3)	35(4)	10(3)
C(24)	48(3)	43(3)	52(3)	18(2)	22(3)	12(3)
C(25)	50(4)	39(3)	94(4)	8(3)	34(3)	3(3)
C(26)	45(3)	77(4)	47(3)	12(3)	26(3)	10(3)
C(27)	29(3)	47(3)	29(2)	-5(2)	12(2)	2(2)
C(28)	26(3)	59(3)	47(3)	5(3)	9(2)	1(2)
C(29)	36(3)	95(5)	62(4)	16(3)	22(3)	5(3)
C(30)	42(4)	161(8)	101(6)	53(6)	27(4)	11(5)
C(31)	79(6)	146(9)	120(8)	51(7)	-9(6)	66(6)
C(32)	87(6)	88(6)	106(6)	-1(5)	-16(5)	38(5)
C(33)	61(4)	69(4)	61(4)	-4(3)	6(3)	20(3)

C(34)	35(3)	63(4)	52(3)	12(3)	10(3)	22(3)
C(35)	52(4)	150(7)	97(5)	47(5)	43(4)	51(5)
C(36)	75(5)	70(5)	97(5)	25(4)	3(4)	28(4)
C(37)	43(4)	101(5)	77(5)	4(4)	-1(3)	15(4)

Table 15: Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for shelxlfor complex **4.**

	x	y	z	U(eq)
H(6)	4255	1323	3558	49
H(2A)	2000	-1559	4129	93
H(2B)	2556	-570	4037	93
H(2C)	1751	-565	3582	93
H(3A)	2265	-766	5262	84
H(3B)	2228	697	5364	84
H(3C)	2832	135	5123	84
H(4A)	1019	-864	4538	64
H(4B)	751	29	3949	64
H(4C)	919	588	4629	64
H(7)	2495	3059	5594	64
H(8)	2003	3571	6405	91
H(9)	765	3595	6191	101
H(10)	-11	3211	5177	91
H(11)	459	2675	4372	60
H(12A)	1819	5669	5073	50
H(12B)	1057	5560	4549	50
H(12C)	1524	6787	4598	50
H(13A)	3152	5604	4072	53
H(13B)	3147	5721	4767	53
H(13C)	2835	6821	4285	53
H(15A)	-3	7212	3049	59
H(15B)	753	7697	3041	59
H(15C)	677	7131	3661	59
H(16A)	-186	4820	3157	55
H(16B)	512	4781	3755	55
H(16C)	451	3897	3179	55
H(17A)	-175	5773	2182	63
H(17B)	422	4777	2184	63
H(17C)	559	6220	2107	63
H(20)	1572	4816	1674	66
H(21)	1326	6241	791	95
H(22)	1407	8379	959	104
H(23)	1779	9208	1979	84
H(24)	1932	7855	2835	55
H(25A)	3750	6632	2620	71
H(25B)	4121	6278	3332	71
H(25C)	3348	6896	3108	71
H(26A)	3304	4897	1802	64
H(26B)	2623	4101	1794	64
H(26C)	3393	3473	2010	64
H(29)	4993	3539	2607	75
H(30)	5837	5098	2541	121
H(31)	6268	6551	3357	150
H(32)	5867	6525	4213	127
H(33)	5024	4974	4281	80
H(35A)	6351	1304	3945	114
H(35B)	5947	2550	3646	114

H(35C)	5731	1257	3290	114
H(36A)	5621	-407	4265	104
H(36B)	4996	-268	3617	104
H(36C)	4831	-84	4249	104
H(37A)	6065	1631	4912	94
H(37B)	5260	1768	4899	94
H(37C)	5630	2874	4652	94

9. Crystallographic data for complex **5**.

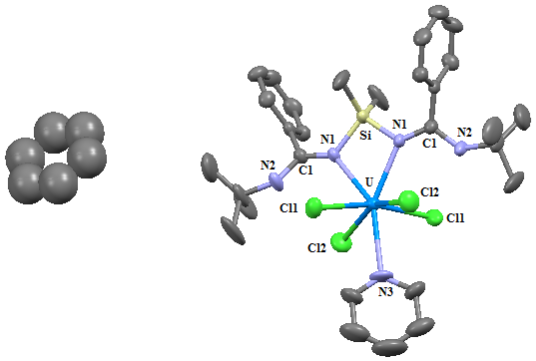


Figure 4: Molecular structure of complex 5. Color code: U, blue, Cl, green, Si, yellow, N, purple, C, grey. Hydrogen atoms are omitted for clarity.

Table 16: Crystallographic data for complexes **5.**

Complex	5
Empirical Formula	$C_{29}H_{41}N_5SiCl_4U$
Formula weight/g·mol^{-1}	867.60
T/K	250(2)
λ/Å	0.71073
Crystal system	Monoclinic
Space group	C 2/C
a/Å	12.2835(4)
b/Å	14.8751(5)
c/Å	23.0777(8)
α/°	90
β/°	93.3560(10)
γ/°	90
V/Å^3	4209.5(2)
Z	4
ρ/g·cm^{-3}	1.479
μ(Mo-K$_\alpha$)/mm^{-1}	4.166
F(000)	1832
Θ range for data collection/°	1.77 to 26.42
Limiting indices	-15≤h≤15 -18≤k≤18 -28≤l≤28
Reflections collected/unique (R_{int})	27898/4304 (0.0339)
Completeness to Θ	99.7%
GOF on F^2	1.163
R_1, wR_2 [I>2σ(I)]	0.0427, 0.1112
R_1, wR_2 (all data)	0.0466, 0.1128
Largest diff. peak and hole (eÅ^{-3})	1.482, -0.895

Table 16: Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for complex **5**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
U(1)	0	4610(1)	2500	31(1)
Cl(1)	2149(1)	4829(1)	2618(1)	49(1)
Si(1)	0	2385(2)	2500	32(1)
Cl(2)	93(2)	5064(2)	3602(1)	61(1)
N(3)	5000	1444(5)	2500	61(2)
C(1)	1208(4)	3022(4)	1628(2)	32(1)
N(1)	620(4)	3186(3)	2074(2)	31(1)
N(2)	1946(5)	3622(4)	1477(2)	45(1)
C(2)	1080(4)	2174(4)	1292(2)	29(1)
C(3)	1819(5)	1475(4)	1374(3)	41(1)
C(7)	194(5)	2066(4)	906(3)	38(1)
C(6)	45(6)	1270(5)	591(3)	48(2)
C(9)	3029(11)	4674(7)	995(5)	109(5)
C(5)	785(7)	582(5)	678(3)	51(2)
C(4)	1663(6)	686(5)	1069(3)	50(2)
C(8)	2551(7)	3730(5)	936(3)	64(2)
C(10)	1792(10)	3692(8)	398(4)	98(4)
C(11)	3454(9)	3043(8)	907(5)	102(4)
C(12)	-1060(8)	1688(6)	2110(4)	77(3)
C(13)	4172(7)	1874(5)	2709(4)	64(2)
C(14)	4136(10)	2801(6)	2703(5)	88(3)
C(15)	5000	3254(10)	2500	114(6)
C(161)	7855	3311(10)	280	217(6)
C(162)	7101	2758(10)	532	217(6)
C(163)	6746	1975(10)	251	217(6)
C(164)	7145	1745(10)	-280	217(6)
C(165)	7899	2297(10)	-532	217(6)
C(166)	8254	3080(10)	-251	217(6)

Table 17: Bond lengths [A] and angles [deg] for complex **5.**

U(1)-N(1)#1	2.474(5)
U(1)-N(1)	2.475(5)
U(1)-Cl(2)	2.6277(17)
U(1)-Cl(2)#1	2.6277(17)
U(1)-Cl(1)#1	2.6575(16)
U(1)-Cl(1)	2.6576(16)
U(1)-N(3)#2	2.727(7)
U(1)-Si(1)	3.311(2)
Si(1)-N(1)#1	1.747(5)
Si(1)-N(1)	1.747(5)
Si(1)-C(12)	1.855(8)
Si(1)-C(12)#1	1.855(8)
N(3)-C(13)#3	1.317(8)
N(3)-C(13)	1.317(8)
N(3)-U(1)#4	2.727(7)
C(1)-N(1)	1.315(7)
C(1)-N(2)	1.333(7)
C(1)-C(2)	1.484(7)
N(2)-C(8)	1.499(8)
C(2)-C(7)	1.374(8)
C(2)-C(3)	1.386(8)
C(3)-C(4)	1.376(9)
C(7)-C(6)	1.396(9)
C(6)-C(5)	1.376(10)
C(9)-C(8)	1.525(10)
C(5)-C(4)	1.373(11)
C(8)-C(10)	1.510(14)
C(8)-C(11)	1.512(14)
C(13)-C(14)	1.380(12)
C(14)-C(15)	1.363(13)
C(15)-C(14)#3	1.363(13)
C(161)-C(166)	1.3900
C(161)-C(162)	1.3900
C(162)-C(163)	1.3900
C(163)-C(164)	1.3900
C(164)-C(165)	1.3900
C(165)-C(166)	1.3900
N(1)#1-U(1)-N(1)	62.2(2)
N(1)#1-U(1)-Cl(2)	80.35(12)
N(1)-U(1)-Cl(2)	127.43(12)
N(1)#1-U(1)-Cl(2)#1	127.42(12)
N(1)-U(1)-Cl(2)#1	80.34(12)
Cl(2)-U(1)-Cl(2)#1	150.22(10)
N(1)#1-U(1)-Cl(1)#1	79.57(11)
N(1)-U(1)-Cl(1)#1	113.00(11)
Cl(2)-U(1)-Cl(1)#1	93.13(6)
Cl(2)#1-U(1)-Cl(1)#1	83.25(6)
N(1)#1-U(1)-Cl(1)	113.00(11)
N(1)-U(1)-Cl(1)	79.57(11)
Cl(2)-U(1)-Cl(1)	83.26(6)
Cl(2)#1-U(1)-Cl(1)	93.13(6)

Cl(1)#1-U(1)-Cl(1)	165.93(8)
N(1)#1-U(1)-N(3)#2	148.90(10)
N(1)-U(1)-N(3)#2	148.90(10)
Cl(2)-U(1)-N(3)#2	75.11(5)
Cl(2)#1-U(1)-N(3)#2	75.11(5)
Cl(1)#1-U(1)-N(3)#2	82.97(4)
Cl(1)-U(1)-N(3)#2	82.97(4)
N(1)#1-U(1)-Si(1)	31.10(10)
N(1)-U(1)-Si(1)	31.10(10)
Cl(2)-U(1)-Si(1)	104.89(5)
Cl(2)#1-U(1)-Si(1)	104.89(5)
Cl(1)#1-U(1)-Si(1)	97.03(4)
Cl(1)-U(1)-Si(1)	97.03(4)
N(3)#2-U(1)-Si(1)	180.0
N(1)#1-Si(1)-N(1)	94.0(3)
N(1)#1-Si(1)-C(12)	109.7(3)
N(1)-Si(1)-C(12)	115.1(3)
N(1)#1-Si(1)-C(12)#1	115.1(3)
N(1)-Si(1)-C(12)#1	109.7(3)
C(12)-Si(1)-C(12)#1	112.1(7)
N(1)#1-Si(1)-U(1)	47.00(16)
N(1)-Si(1)-U(1)	47.01(16)
C(12)-Si(1)-U(1)	124.0(4)
C(12)#1-Si(1)-U(1)	124.0(4)
C(13)#3-N(3)-C(13)	121.9(10)
C(13)#3-N(3)-U(1)#4	119.1(5)
C(13)-N(3)-U(1)#4	119.1(5)
N(1)-C(1)-N(2)	119.6(5)
N(1)-C(1)-C(2)	121.4(5)
N(2)-C(1)-C(2)	119.1(5)
C(1)-N(1)-Si(1)	126.3(4)
C(1)-N(1)-U(1)	131.8(4)
Si(1)-N(1)-U(1)	101.9(2)
C(1)-N(2)-C(8)	131.8(5)
C(7)-C(2)-C(3)	119.2(5)
C(7)-C(2)-C(1)	119.6(5)
C(3)-C(2)-C(1)	121.2(5)
C(4)-C(3)-C(2)	120.0(6)
C(2)-C(7)-C(6)	120.8(6)
C(5)-C(6)-C(7)	119.3(6)
C(4)-C(5)-C(6)	120.0(6)
C(5)-C(4)-C(3)	120.8(6)
N(2)-C(8)-C(10)	111.6(6)
N(2)-C(8)-C(11)	111.4(7)
C(10)-C(8)-C(11)	111.0(8)
N(2)-C(8)-C(9)	103.3(6)
C(10)-C(8)-C(9)	108.9(9)
C(11)-C(8)-C(9)	110.3(9)
N(3)-C(13)-C(14)	120.4(9)
C(15)-C(14)-C(13)	118.2(11)
C(14)#3-C(15)-C(14)	120.7(13)
C(166)-C(161)-C(162)	120.0
C(163)-C(162)-C(161)	120.0
C(162)-C(163)-C(164)	120.0
C(165)-C(164)-C(163)	120.0
C(164)-C(165)-C(166)	120.0

C(161)-C(166)-C(165) 120.0

Symmetry transformations used to generate equivalent atoms:
#1 -x,y,-z+1/2 #2 x-1/2,y+1/2,z #3 -x+1,y,-z+1/2
#4 x+1/2,y-1/2,z

Table 18: Anisotropic displacement parameters (A^2 x 10^3) for complex **5**. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
U(1)	37(1)	27(1)	31(1)	0	7(1)	0
Cl(1)	40(1)	50(1)	58(1)	-19(1)	5(1)	7(1)
Si(1)	37(1)	27(1)	35(1)	0	16(1)	0
Cl(2)	79(1)	66(1)	39(1)	-13(1)	9(1)	5(1)
N(3)	86(6)	15(3)	81(6)	0	8(5)	0
C(1)	34(3)	32(3)	29(3)	-2(2)	5(2)	7(2)
N(1)	32(2)	28(2)	33(2)	-2(2)	13(2)	6(2)
N(2)	54(3)	41(3)	44(3)	-14(2)	27(2)	21(2)
C(2)	32(3)	30(3)	25(2)	-3(2)	10(2)	6(2)
C(3)	46(3)	45(3)	31(3)	-2(3)	1(2)	6(3)
C(7)	40(3)	36(3)	39(3)	-1(2)	4(2)	3(2)
C(6)	54(4)	53(4)	37(3)	-6(3)	0(3)	18(3)
C(9)	149(11)	90(7)	96(8)	-26(6)	76(8)	84(7)
C(5)	83(5)	36(3)	37(3)	-10(3)	9(3)	7(3)
C(4)	71(5)	35(3)	45(4)	-3(3)	6(3)	14(3)
C(8)	79(5)	61(5)	57(4)	-19(4)	47(4)	36(4)
C(10)	125(9)	126(9)	47(5)	0(5)	43(5)	48(7)
C(11)	102(8)	109(8)	103(8)	-20(7)	73(7)	13(7)
C(12)	98(6)	77(6)	61(5)	-22(4)	44(5)	58(5)
C(13)	73(5)	40(4)	79(5)	-9(4)	14(4)	21(4)
C(14)	123(9)	49(5)	91(7)	-5(5)	-4(6)	32(6)
C(15)	190(20)	35(7)	119(14)	0	-1(14)	0

Table 19: Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for complex **5.**

	x	y	z	U(eq)
H(3)	2415	1537	1638	49
H(7)	-312	2528	855	46
H(6)	-549	1205	325	58
H(9A)	3439	4802	663	131
H(9B)	3497	4721	1342	131
H(9C)	2441	5097	1012	131
H(5)	693	46	474	62
H(4)	2163	220	1128	60
H(10A)	2203	3742	58	118
H(10B)	1267	4169	401	118
H(10C)	1422	3123	394	118
H(11A)	3811	3130	553	122
H(11B)	3169	2442	918	122
H(11C)	3969	3132	1232	122
H(12A)	-897	1062	2169	92
H(12B)	-1079	1823	1703	92
H(12C)	-1757	1821	2258	92
H(13)	3605	1522	2866	77
H(14)	3512	3110	2837	106
H(15)	5000	3900	2500	136