Supporting Information

for

Highly selective synthesis of substituted (*E*)-alkenylsilatranes via catalytic trans-silylation and mechanistic implications

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1. General considerations

1.1. Analytical methods

^{1}H and $^{13}C\{^{1}H\}$ NMR spectra were recorded on a Bruker Ultrashield 300 MHz operating at 300 and 75 MHz, respectively. $^{29}Si\{^{1}H\}$ NMR and $^{31}P\{^{1}H\}$ spectra were recorded on a Bruker Ascend 400 MHz Nanobay operating at 79 and 162 MHz, respectively. Elemental analyses were carried out with a Vario EL III instrument (Elementar GmbH). Mass spectrometry analyses were performed using QTOF mass spectrometer (Impact HD, Bruker) equipped with the Electrospray ion source and quadrupole-Time-of-flight mass analyser. Dichloromethane-methanol and chloroform-methanol mixtures were used as solvents. The measurements was performed in the positive ion mode with the desolvation gas flow 4.0 L/h and capillary voltage set to 4500 V. The elemental compositions prediction for all the sodated ions confirmed their molecular formula and the isotopic profile.

1.2. Reagents and solvents

The chemicals were purchased from the following sources: trimethoxyvinylsilane, triethanolamine, styrene, 4-methylstyrene, 4-fluorostyrene, 4-chlorostyrene, 4-bromostyrene, 4-methoxystyrene, 4-vinylbiphenyl, 2-vinylnaphtalene, 9-vinylcarbazole, 9-vinylanthracene, 4-vinylpyridine, *tert*-butyl vinyl ether, calcium hydride, tricyclohexylphosphine, triphenylphosphine, 2-methoxyethanol, cycloocta-1,5-diene, toluene, formaldehyde, benzene-d_6, toluene-d_8 chloroform-d_1, molecular sieves (4A, 5A) and silica gel 60 from Aldrich; dichloromethane, *n*-hexane, methanol from Avantor Performance Materials Poland S.A.; ruthenium(III) chloride hydrate from ABCR.

1-Vinylsilatrane,[1] $RuHCl(CO)(PCy_3)_2$,[2] $RuHCl(CO)(PPh_3)_3$[3] were prepared according to the literature procedures.

Liquid olefins were dried with CaH_2 (24 h) and distilled. Solid olefins were used as received. Toluene and hexane were dried and purified with MB SPS 800 Solvent Drying System. Dichloromethane, ethanol and deuterated solvents were dried over CaH_2, distilled and stored under argon atmosphere in Rotaflo Schlenk flasks.

1.3. Reaction setup for the catalytic synthesis of alkenylsilatranes

Unless mentioned otherwise, all operations were performed by using standard Schlenk techniques. Catalytic reactions were carried out in a custom built glass reactors connected to a Davies condenser and argon inlet equipped with bubbler (Figure 1).

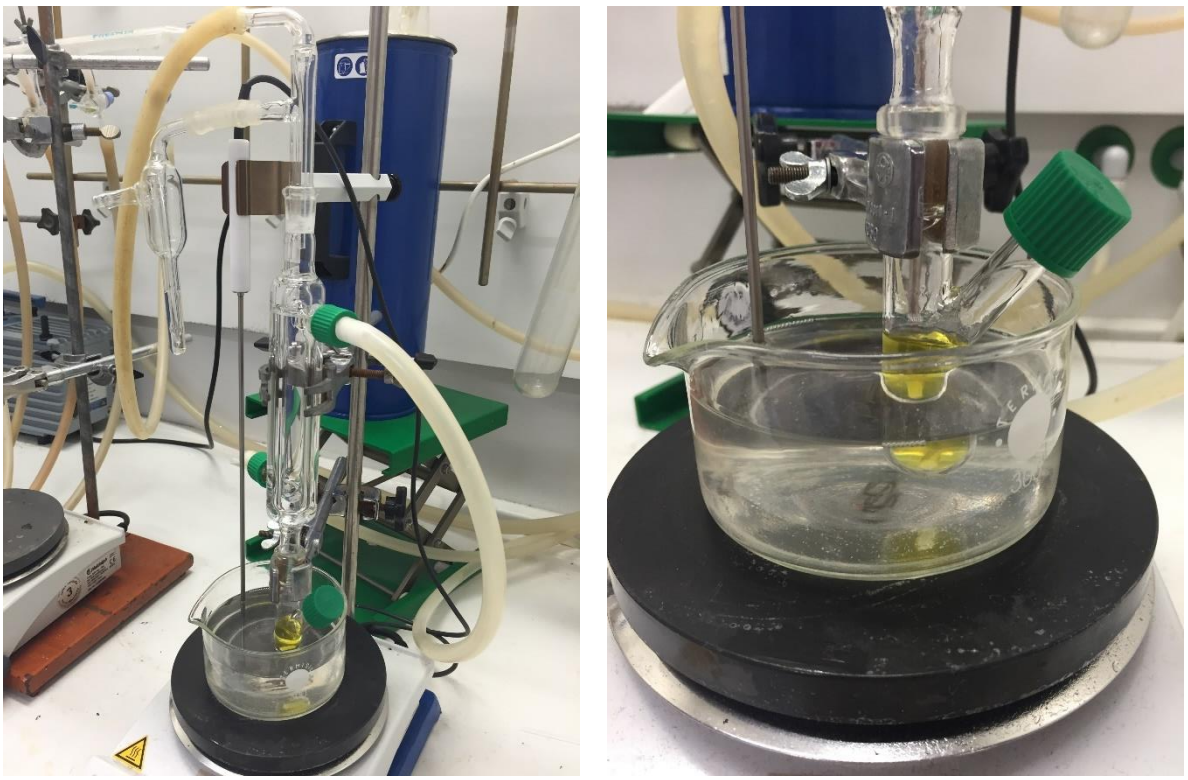


Figure 1. Reaction setup for the catalytic synthesis of alkenylsilatranes.

References

1 J. D. Nies, J. M. Bellama, N. Ben-Zvi, *J. Organomet. Chem.* 1985, **296**, 315

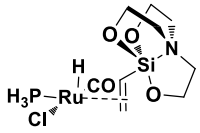
2 C. S. Yi; D. W. Lee, Y. Chen, *Organometallics,* 1999, **18**, 2043

3 J. Levison, S.D. Robinson, *J. Chem. Soc.,* 1970, *A*, 2947

2. DFT Calculations

All the optimizations, DFT calculations for molecules, geometries of potential energy minima and saddle points were performed using B3LYP (hybrid Becke's three parameter functional and Lee-Young-Parr exchange correlation potential) in connection with SDD bases. Frequency calculations at the same level of theory were also performed. Thermal corrections to Gibbs free energies calculated at 298 K were included. All computations were carried out with Gaussian09.

2.1. Geometries and Cartesian coordinates for all the structures calculated in this study using B3LYP/SDD



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C	0.89520000	-0.04150000	-1.55740000
H	0.06780000	-0.62780000	-1.95560000
C	0.19480000	1.78570000	2.21370000
H	1.23410000	2.07080000	2.43140000
H	-0.18910000	1.20600000	3.06050000
C	-1.53290000	3.95570000	-0.22620000
H	-1.15480000	4.57300000	-1.04880000
H	-2.27090000	4.55170000	0.33520000
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C	1.54080000	-2.92920000	-1.30630000
O	1.15580000	-3.86800000	-1.93280000
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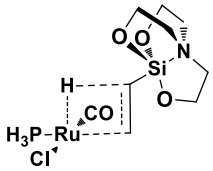
Si	0.35190000	1.48340000	-0.57990000



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H	-5.25270000	3.37750000	0.13920000
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O	-1.90940000	3.65570000	-2.11340000
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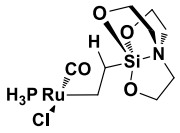

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C	-2.67750000	1.96010000	-1.57170000
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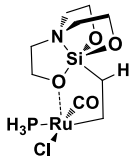

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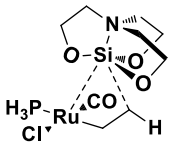

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H	3.14320000	2.81050000	1.77960000
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Ru	2.15730000	-1.06200000	-0.22810000
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P	4.51600000	-1.80960000	0.48460000
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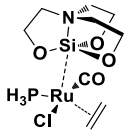

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C	1.00090000	-3.05310000	-0.05690000
H	0.94330000	-3.44750000	0.96490000
H	1.65350000	-3.73340000	-0.63490000
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H	1.42500000	0.68420000	-2.46160000
C	-3.12410000	2.81140000	0.45580000
H	-3.80480000	3.18340000	-0.30600000
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O	-3.21940000	0.10390000	3.09390000
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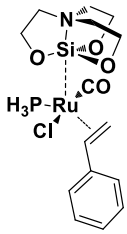

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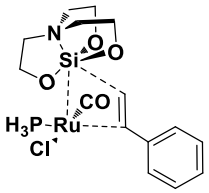
C	4.27360000	-0.88200000	0.08770000
H	4.36230000	-0.78890000	-1.00470000
H	4.78850000	-1.79660000	0.40720000
C	4.89320000	0.35300000	0.78080000
H	4.92080000	0.17170000	1.86240000
H	5.94030000	0.45810000	0.44080000
C	2.36500000	1.57900000	2.31310000
H	2.70740000	0.67110000	2.83190000
H	1.86230000	2.22710000	3.04080000
C	3.56440000	2.31250000	1.66920000
H	3.22460000	3.28950000	1.30430000
H	4.32700000	2.50180000	2.44700000
C	4.12940000	2.17910000	-0.79320000
H	4.77010000	1.57300000	-1.44540000
H	4.55700000	3.19840000	-0.77110000
C	2.71470000	2.24540000	-1.41530000
H	2.09500000	2.97330000	-0.86970000
H	2.77200000	2.55020000	-2.46700000
Si	1.60390000	0.08200000	0.02770000
Ru	-0.34930000	-1.19660000	-0.33790000
P	0.94820000	-3.22190000	-0.11160000
H	0.20210000	-4.41940000	-0.33620000
H	2.00130000	-3.40270000	-1.04140000
H	1.59210000	-3.55150000	1.11110000
C	-0.61680000	-1.07830000	1.48000000
O	-0.80630000	-1.08230000	2.65390000
Cl	-0.33210000	-1.78560000	-2.71060000
C	-1.05790000	0.95040000	-0.79920000
H	-0.50530000	1.18970000	-1.70270000
H	-0.89660000	1.60830000	0.05000000
C	-2.17990000	0.11840000	-0.88810000
H	-2.38620000	-0.32300000	-1.86220000
C	-3.28360000	-0.01070000	0.09160000
C	-4.31890000	-0.94010000	-0.18150000
H	-4.26670000	-1.54090000	-1.08800000
C	-5.40550000	-1.08950000	0.69630000
H	-6.19050000	-1.80690000	0.47020000
C	-5.47810000	-0.30790000	1.86570000
H	-6.31770000	-0.41970000	2.54750000
C	-4.45630000	0.62340000	2.14670000
H	-4.50810000	1.22970000	3.04770000
C	-3.37130000	0.77210000	1.27020000
H	-2.59380000	1.49520000	1.50240000



A5A6

E = - -2205.61153509 a. u.

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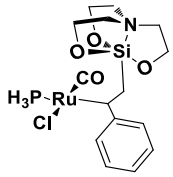
N	4.75150000	0.17310000	-0.04470000
O	2.50020000	-0.67770000	1.09300000
O	2.71120000	2.01520000	0.04570000
C	3.59750000	-1.61940000	1.21070000
H	3.51730000	-2.38990000	0.43180000
H	3.53520000	-2.09940000	2.19290000
C	3.88660000	2.31380000	0.84740000
H	3.71200000	1.99730000	1.88590000
H	4.02990000	3.39870000	0.82730000
C	5.16290000	-0.32550000	-1.38190000
H	5.09070000	-1.41850000	-1.37360000
H	6.19920000	-0.04810000	-1.63170000

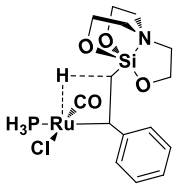
C	5.11460000	1.58620000	0.25030000
H	5.38830000	2.07310000	-0.69180000
H	5.97880000	1.65360000	0.92900000
C	4.89620000	-0.78590000	1.08390000
H	5.03570000	-0.21180000	2.00640000
H	5.77220000	-1.43930000	0.95470000
C	4.17010000	0.22590000	-2.43050000
H	4.34450000	1.29580000	-2.61780000
H	4.26280000	-0.31570000	-3.37710000
Ru	0.21460000	-0.46520000	0.26390000
P	0.32740000	-1.89120000	2.35100000
H	0.67330000	-1.36770000	3.63760000
H	-0.89060000	-2.53680000	2.72240000
H	1.17990000	-3.03310000	2.32530000
C	-0.06270000	1.01370000	1.32990000
O	-0.21690000	1.92530000	2.07830000
Cl	0.66840000	-2.57560000	-0.98160000
C	-1.44280000	-0.06300000	-1.09420000
C	-0.23500000	0.52210000	-1.61550000
H	-1.69030000	-1.05160000	-1.48170000
H	-0.11050000	1.60300000	-1.63550000
H	0.30350000	-0.00430000	-2.39760000
C	-2.63450000	0.69710000	-0.62350000
C	-3.86210000	0.00620000	-0.46910000
C	-2.61680000	2.08760000	-0.35170000
C	-5.02720000	0.67380000	-0.05260000
H	-3.90370000	-1.05800000	-0.69820000
C	-3.77690000	2.75780000	0.06830000
H	-1.69390000	2.65110000	-0.46150000
C	-4.99060000	2.05480000	0.21910000
H	-5.95880000	0.12170000	0.05230000
H	-3.74770000	3.81460000	0.29980000
H	-5.88920000	2.57590000	0.54110000
Si	2.31420000	0.37620000	-0.34500000



A6

E = --2205.61586229 a. u.

O	2.25000700	-2.04306400	-1.23825000
N	4.07359700	-0.86328300	0.39925800
O	1.58105300	-1.12717000	1.44030400
O	2.23609600	0.81591400	-0.68780700
C	2.66023500	-1.65752700	2.24312000
H	2.73868600	-2.74181500	2.07577200
H	2.40484200	-1.49040800	3.29477700
C	3.43342400	1.44029200	-0.16714700
H	3.23138800	1.82252300	0.84414200
H	3.67058300	2.28936400	-0.81612800
C	4.50881100	-2.10102000	-0.29281600
H	4.33877600	-2.94696100	0.38206800
H	5.57952700	-2.08190500	-0.55135900
C	4.58849200	0.41295100	-0.15520600
H	4.91422500	0.23160400	-1.18538300
H	5.45153200	0.79730000	0.41140000
C	3.98106100	-0.94219300	1.87675400
H	3.95313100	0.07943300	2.27165000
H	4.84520400	-1.45757800	2.32574300
C	3.63806300	-2.28606300	-1.55776900
H	3.95572900	-1.59747600	-2.35525800
H	3.71651100	-3.31044200	-1.93667400
Ru	-2.40872300	-1.11365100	-0.09605200
P	-4.55688200	-0.19354400	0.12701400
H	-4.80242400	0.94525800	-0.69109300
H	-5.68542700	-0.99118700	-0.23226800
H	-5.00271700	0.30538200	1.38626600
C	-2.13351200	-1.13759600	1.72315800
O	-2.04154400	-1.23865400	2.90928500
Cl	-3.00497400	-1.52108100	-2.42916000
C	-1.10040600	0.45973900	-0.52205900
C	-0.14645400	-0.71222000	-0.79330800
H	-1.47434000	0.86178500	-1.46865400
H	-0.14047200	-0.91243200	-1.86977600
H	-0.54186300	-1.70323300	-0.34835600
C	-0.88275700	1.58519800	0.43841300
C	-1.36613100	2.86551600	0.06476100
C	-0.25966900	1.45596000	1.70507100
C	-1.24202500	3.97490500	0.91956700
H	-1.83292000	2.99076400	-0.91119700
C	-0.13229800	2.56365400	2.55815500
H	0.11914500	0.49110700	2.02616100
C	-0.62223000	3.82962600	2.17573300
H	-1.62257700	4.94490800	0.60657100
H	0.34021700	2.43782400	3.53033800
H	-0.52518400	4.68252400	2.84381200
Si	1.67549500	-0.75316500	-0.24301500

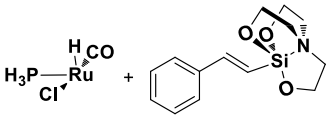


A6A7

E = -2205.59127177 a. u.

O	-2.20100000	-1.65920000	-0.62030000
N	-3.81620000	0.49570000	-1.06980000
O	-1.16610000	0.89930000	-1.55140000
O	-2.22320000	0.64510000	1.15010000
C	-2.06540000	1.19010000	-2.64540000
H	-2.10000000	0.32700000	-3.32620000
H	-1.65290000	2.04360000	-3.19290000
C	-3.34470000	1.55780000	1.09850000
H	-2.99840000	2.53880000	0.74090000
H	-3.71980000	1.67760000	2.12040000
C	-4.29090000	-0.81050000	-1.58150000
H	-3.98620000	-0.89700000	-2.63060000
H	-5.38810000	-0.90610000	-1.53830000
C	-4.44740000	0.98770000	0.17590000
H	-4.92300000	0.13800000	0.67780000
H	-5.22360000	1.74630000	-0.01700000
C	-3.47090000	1.51300000	-2.08800000
H	-3.44330000	2.49340000	-1.59910000
H	-4.21140000	1.56240000	-2.90310000
C	-3.61300000	-1.93610000	-0.76650000
H	-4.06960000	-2.02740000	0.22980000
H	-3.70780000	-2.89820000	-1.28090000
Ru	2.04280000	-1.06060000	-0.58720000
P	4.51410000	-0.77670000	-0.47160000
H	5.02010000	-0.64780000	0.85220000
H	5.31710000	-1.86790000	-0.91450000
H	5.21770000	0.29710000	-1.09690000
C	1.84100000	0.23580000	-1.88380000
O	1.79830000	0.99390000	-2.80150000
Cl	2.46940000	-3.05950000	0.76370000
C	1.25450000	0.06510000	1.05650000

C	0.14920000	-0.70730000	0.47500000
H	1.70660000	-0.43620000	1.91630000
H	-0.03750000	-1.62330000	1.04300000
H	0.55700000	-1.62530000	-0.86640000
C	1.45020000	1.53910000	1.15030000
C	2.26300000	2.01320000	2.21280000
C	0.89100000	2.49280000	0.26270000
C	2.51140000	3.38520000	2.38910000
H	2.69320000	1.29640000	2.91090000
C	1.13880000	3.86320000	0.44010000
H	0.27650000	2.16660000	-0.57000000
C	1.94810000	4.32080000	1.50020000
H	3.13460000	3.72180000	3.21460000
H	0.70540000	4.57850000	-0.25600000
H	2.13660000	5.38430000	1.62900000
Si	-1.51410000	-0.13060000	-0.21720000



A7

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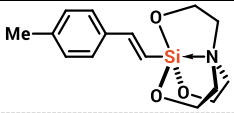
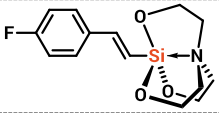
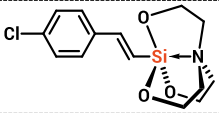
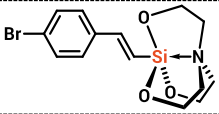
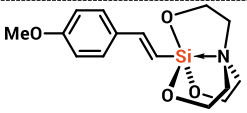
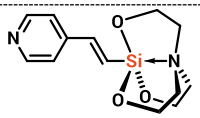
O	4.17077000	0.88284100	0.30827900
N	5.06814400	-1.66101900	-0.22124000
O	2.54300100	-1.07960000	-1.11129400
O	3.15567200	-1.41972100	1.72646700
C	3.47810300	-1.57112000	-2.09498600
H	3.91308700	-0.72158400	-2.64346500
H	2.91718900	-2.18826400	-2.80515000
C	3.90102200	-2.65671900	1.70352200
H	3.31841000	-3.42695000	1.17508300
H	4.03488600	-2.97999500	2.74154300
C	6.00922500	-0.54683900	-0.46507500
H	5.93217000	-0.25588400	-1.51879800
H	7.05744700	-0.82796600	-0.26882600
C	5.27127500	-2.44243400	1.01737300
H	5.91575700	-1.86182600	1.68679600
H	5.76603600	-3.40966500	0.82885300
C	4.58705600	-2.40113600	-1.40679100
H	4.15918800	-3.35084700	-1.06632400
H	5.39615900	-2.63175200	-2.11980200
C	5.59558800	0.65363300	0.41604400
H	5.85652800	0.47065800	1.46921300
H	6.10057600	1.56845800	0.08758500
Ru	-3.77156600	-0.30366000	-0.08877700
P	-4.98467600	-2.31744700	-0.02579400
H	-6.36816900	-2.27048500	-0.37057600
H	-4.54427900	-3.32594300	-0.92633900
H	-5.06381600	-3.07270400	1.18223900
C	-3.63770600	-0.18548100	1.73753000
O	-3.58167200	-0.13965200	2.92715600
Cl	-4.28196600	-0.39089800	-2.49685800
C	0.31210400	0.68051100	0.03182300
C	1.40834700	0.61425000	0.82794200
H	0.33220700	0.13260100	-0.91073900
H	1.41832700	1.13683700	1.78538200
H	-2.51420700	-1.21394000	0.01143700
C	-0.93927900	1.42015200	0.29960300
C	-1.99891500	1.32469300	-0.66450900
C	-1.13504400	2.23910600	1.42695000
C	-3.20585100	2.05706200	-0.48888500
H	-1.80329000	0.83678800	-1.61493900
C	-2.33758900	2.96132400	1.60727200
H	-0.34701400	2.33471400	2.16829600
C	-3.36782500	2.88164900	0.66235800
H	-3.91483400	2.12138800	-1.31009300
H	-2.45539100	3.59168300	2.48503200
H	-4.27861300	3.46166500	0.78634000
Si	2.95121700	-0.34181600	0.39388100

3. Synthetic procedures

3.1. General protocol for the synthesis of alkenylsilatranes using liquid olefins

A dried, argon filled glass reactor was charged with vinylsilatrane (100 mg, 0.5 mmol) and $RuHCl(CO)(PCy_3)_2$ (7.2 mg, 0.01 mmol, 2 mol%). The reactor was evacuated under reduced pressure on the Schlenk line for 15 min and filled again with argon. Then, the reactor was equipped with Davies condenser and argon inlet with bubbler and the solids were added 1 mL of toluene under intense stirring. After dissolution of the solids, an olefin (1 mmol, two-fold excess in relation to vinylsilatrane) and 2 mL of toluene were added to the reaction mixture and the reactor was heated at 120°C for 24 h in an oil bath. Then, the volatiles were removed under reduced pressure and the residue was dissolved in dichloromethane and preliminary purified on a short silica column. The resulting solution was concentrated, then pentane was added in order to precipitate the product. The solvent was decanted and the product was washed two times with pentane. The obtained powder or fluffy needles were kept under reduced pressure for 3 h in order to remove traces of solvents. Products **2c-g**, and **2j** were obtained in the above described manner.

Product		Isolated yield
	**2c**	80
	**2d**	80
	**2e**	83
	**2f**	81
	**2g**	86
	**2j**	60

Products **2c-g** were isolated as white or greyish-white powders or needles. Product **2j** was isolated as orange powder. The color may be due to formation of traces of unspecified impurities in the 4-vinylpyridine itself. After the distillation of 4-vinylpyridine the compound is colorless. However, after ca. 48 h in the refrigerator the color changes to deep orange.

3.1.1. Synthesis of (E)-1-styryl-2,8,9-trioxa-5-aza-1-silabicyclo[3.3.3]undecane (2a)

Compound **2a** was prepared in the same manner as described in section 3.1., but was isolated in a different way, because styryl derivative has low solubility in toluene (Figure 2). Solvent was decanted from the reaction mixture and the remaining solid was washed three times with small portions of cold toluene. After the volatiles were removed under reduced pressure, the pure product was isolated in 85% yield as a white, crystalline solid.

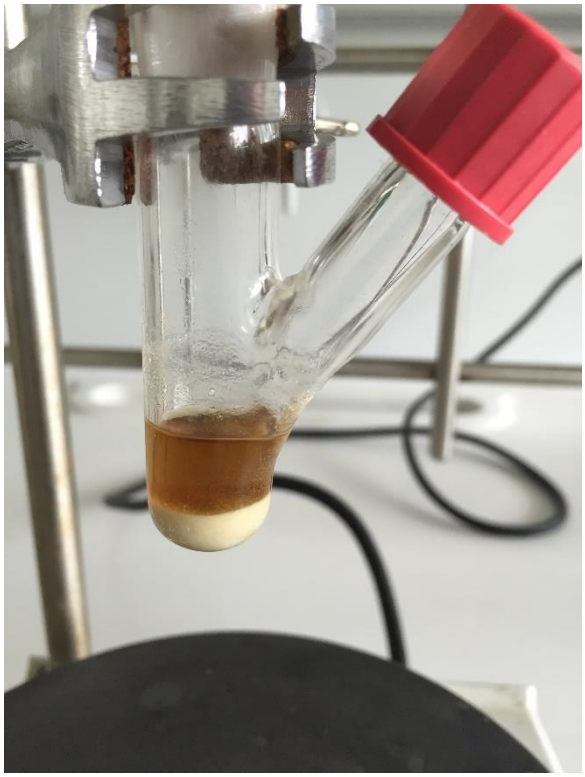
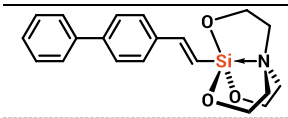
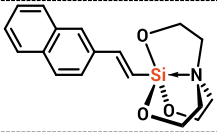
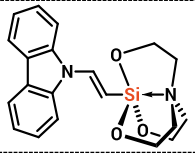


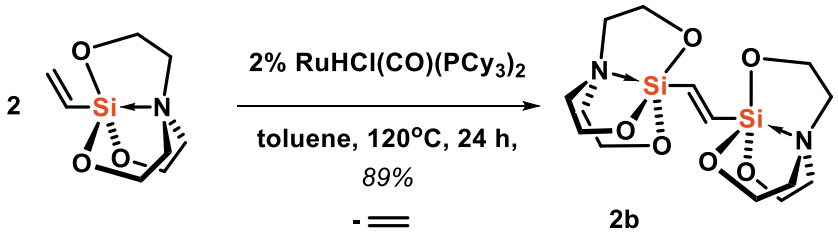
Figure 2. Product **2a** precipitated from the reaction mixture.

3.2. General protocol for the synthesis of alkenylsilatranes using solid olefins

A dried, argon filled glass reactor was charged with vinylsilatrane (100 mg, 0.5 mmol), a solid olefin (0.5 mmol, equimolar amount in relation to vinylsilatrane) and $RuHCl(CO)(PCy_3)_2$ (7.2 mg, 0.01 mmol, 2 mol%). The reactor was evacuated under reduced pressure on the Schlenk line for 15 min and filled again with argon. Then, the reactor was equipped with Davies condenser and argon inlet with bubbler and the solids were added 3 mL of toluene under intense stirring. After dissolution of the solids, the reactor was heated at 120°C for 24 h on an oil bath. Then, the volatiles were removed under reduced pressure and residue was dissolved in dichloromethane and preliminary purified on the short silica column. The resulting solution was concentrated and added pentane in order to precipitate the product. The solvent was decanted and the product was washed two times with pentane. The obtained powders were kept under reduced pressure for 3 h in order to remove traces of solvents. Products **2h, 2i** and **2k** were prepared in the above described manner.

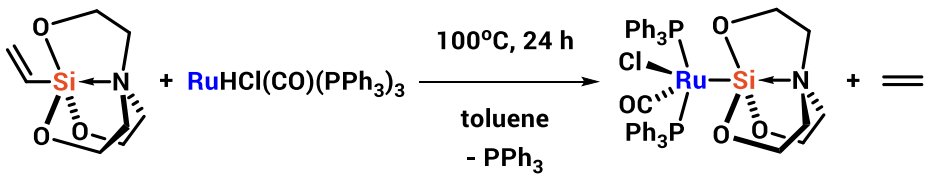
Product		Isolated yield
	**2h**	89
	**2i**	86
	**2k**	81

3.3. Homocoupling reaction of 1-vinylsilatrane



A dried, argon filled glass reactor was charged with vinylsilatrane (200 mg, 1 mmol) and $RuHCl(CO)(PCy_3)_2$ (7.2 mg, 0.01 mmol, 2 mol%). The reactor was evacuated under reduced pressure on the Schlenk line for 15 min and filled again with argon. Then, the reactor was equipped with Davies condenser and argon inlet with bubbler and the solids were added 3 mL of toluene under intense stirring. After dissolution of the solids, the reactor was heated at 120°C on an oil bath. After ca. 20 min, white crystalline solid started to precipitate from the solution. After 24 h, the suspension was cooled down to room temperature and volatiles were removed under reduced pressure. The remaining residue was washed with ethyl acetate and hexane. (*E*)-1,2-bis(silatranyl)ethene was obtained as colourless, crystalline solid in 89% yield.

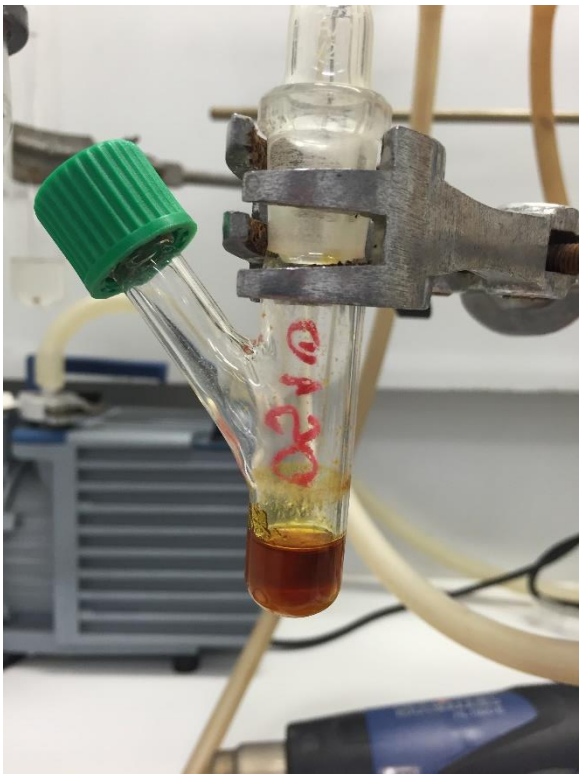
3.4. Synthesis of the ruthenium silatranyl complex 3.



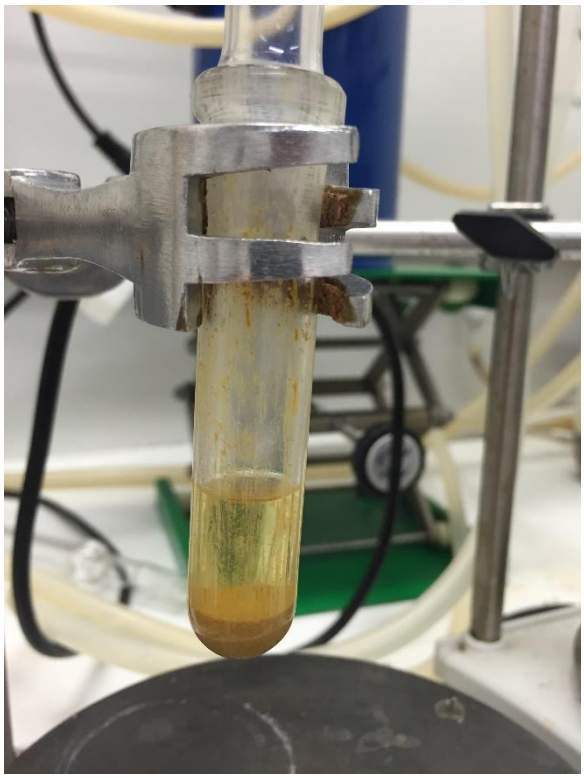
A dried, argon filled glass reactor was charged with vinylsilatrane (50 mg, 0.25 mmol) and $RuHCl(CO)(PPh_3)_3$ (238 mg, 0.25 mmol). The reactor was evacuated under reduced pressure on the Schlenk line for 15 min and filled again with argon. Then, the reactor was equipped with Davies condenser and argon inlet with bubbler and the solids were added 3 mL of toluene upon intense stirring. Then, the reactor was heated at 100°C for 24 h on an oil bath. The initial suspension gradually

turned into clear, deep orange-brown solution (Figure 3a). After 24 h, the solution was cooled down to room temperature and toluene was removed under reduced pressure. The remaining solid was washed three times with ethanol (Figure 3b). Isolated complex was kept under reduced pressure for 5 h to remove traces of the solvents. Complex **3** was isolated as a pale yellow powder in 99% yield.

Figure 3. Synthesis of ruthenium silatranyl complex **3**.



3a) Reaction mixture after 24 h.



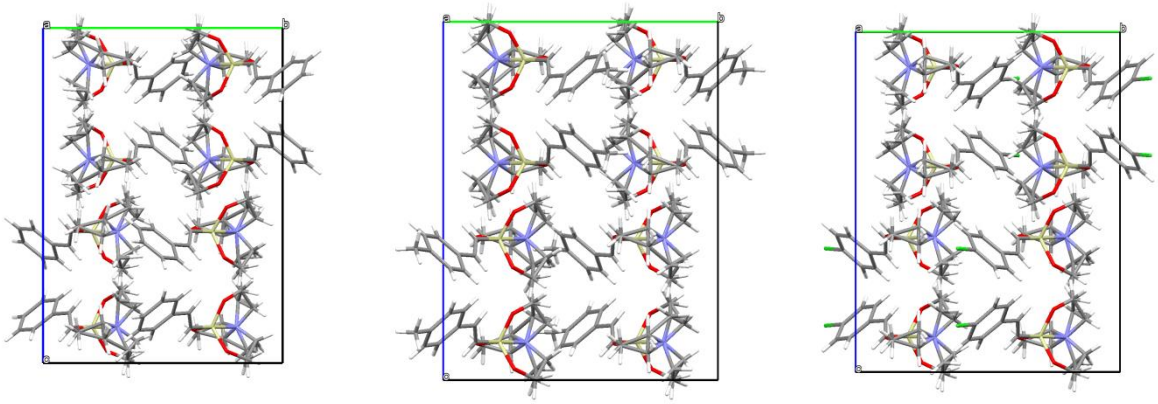
3b) Washing of **3** with ethanol.

4. Crystallographic data

4.1. Analytical methods

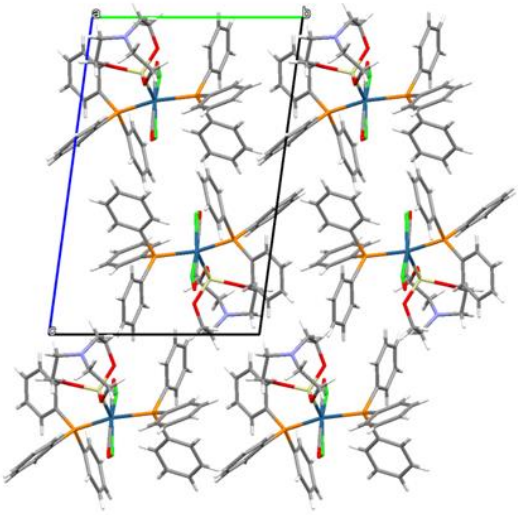
The diffraction data were collected at room temperature with an Oxford Diffraction NewXcalibur diffractometer Mo Kα radiation (λ=0.71073 Å). Data collectionand reduction were performed with the CrysAlis Pro software.[1] The structures of **2a**, **2b** and **2c** were solved by VLD procedure with the program Sir2014[2] and the structure of **2d** was solved by charge flipping implemented in SUPERFLIP.[3] The structure of **3** was solved by direct method with the SHELXS-2014.[4] All structures were refined by the full-matrix least-squares method on F^2 with SHELXL-2014.[4] The positions of C bound hydrogen atoms were placed in idealized positions and refined using the riding model and their isotropic displacement parameters were set equal to $1.2U_{eq}$(C). Additional details concerning crystal data and structure refinement are given in Table 1. Molecular graphics were generated with Mercury 3.8 software.[5]

4.2. Crystal packing of 2a, 2b, 2c (viewed along a-axis)



2a **2b** **2c**

4.4. Crystal packing of 3



4.5. Crystallographic data

Table 1. Crystallographic data and refinement details for compounds **2b, 2c, 2e, 3**.

	2b*	**2c**	**2e**	**3**
empirical formula	$C_{14}H_{26}N_2O_6Si_8$	$C_{15}H_{21}NO_3Si$	$C_{14}H_{18}ClNO_3Si$	$C_{43}H_{42}ClNO_4P_2RuSi$
CCDC no.	-	CCDC 1524197	CCDC 1524196	CCDC 1524198
formula weight	372.54	291.42	311.83	863.32
crystal system	Orthorhombic	Orthorhombic	Orthorhombic	Triclinic
space group	*P*bca	*P*bca	*P*bca	$P\bar{1}$
a (Å)	11.649 (9)	11.4618(3)	11.5758(6)	9.6141(3)
b (Å)	11.796 (8)	14.1740(4)	14.1553(7)	12.1035(4)
c (Å)	12.183 (7)	18.5112(5)	18.2251(9)	18.1419(5)
α(°)	90	90	90	94.833(2)
β(°)	90	90	90	100.853(2)
γ(°)	90	90	90	104.855(2)
volume (Å^3)	1674.1 (19)	3007.32(14)	2986.3(3)	1984.39(17)
Z	8	8	8	2
temperature (K)	298 (2)	298 (2)	298 (2)	293(2)
radiation type	Mo *K*	Mo *K*	Mo *K*	Mo *K*
D_c		1.287	1.387	1.445
No. of measured, independent and observed [$I > 2\ (I)$] reflections		22931, 2641, 2015	20303, 2629,2031	56101, 6989, 6043
R_{int}		0.046	0.060	0.063
$R[F^2 > 2\ (F^2)]$, $wR(F^2)$,		0.042, 0.109	0.044, 0.095	0.045, 0.095
S		1.04	1.06	1.09
No. of reflections		2641	2629	6989
No. of parameters		210	209	476
No. of restraints		0	0	0
H-atom treatment		H-atom parameters constrained	H-atom parameters constrained	H-atom parameters constrained
$_{max}$, $_{min}$ (e Å^{-3})		0.17, −0.18	0.22, −0.25	0.86, −0.49

*Due to poor quality of the obtained crystals, structure **2b** was not deposited in CDDC base.

In silatranes the distance between the Si and N atoms falls in a range 2.05 – 2.20 Å and this value is shorter than the sum of van der Waals radii (3.5 Å). The Si-N distance found in the crystal structures of **2b**, **2c** and **2e** are typical and showed in Table 2. The Si-N distance can be correlated to nature of styryl group. Only in the compound **3** the distance increases (2.944(2) Å) and is slightly shorter than observed in analogous osmium complex (Si – N 3.000(7) Å).

Table 2. Selected geometrical parameters (Å, °)

	2b	**2c**	**2e**	**3**
Si – N	2.194(2)	2.162(2)	2.151(2)	2.944(2)

References

1 Agilent (2014). *CrysAlis PRO*. Agilent Technologies Ltd, Yarnton, Oxfordshire, England.

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3 L. Palatinus, G. Chapuis *J. Appl. Cryst.* 2007, **40**, 786

4 G. M. Sheldrick, *Acta Cryst. C* 2015, **71**, 3

5 C. F. Macrae, P. R. Edgington, P. McCabe, E. Pidcock, G. P. Shields, R. Taylor, M. Towler, J. van de Streek, *J. Appl. Cryst.* 2006, **39**, 453

5. Analytical data

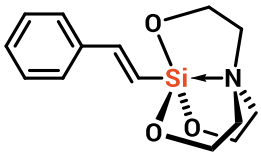
5.1. 1-vinylsilatrane (vinylsilatrane)

^{1}H NMR (DCCl$_3$, 300 MHz): δ 2.85 (t, *J* = 5.9 Hz, 6H, C*H*$_2$-N), 3.82 (t, *J* = 5.9 Hz, 6H, C*H*$_2$-O), 5.79 (m, 2H, *H*$_2$C=), 5.99 (dd, *J* = 20.7, 13.4 Hz, 1H, =C*H*-Si); **^{13}C NMR (DCCl$_3$, 75 MHz):** δ 51.13 (*C*-N), 57.63 (*C*-O), 129.72 (=*C*-Si), 139.53 (*C*=C-Si); **^{29}Si NMR (DCCl$_3$, 79 MHz):** δ -81.32

^{1}H NMR of vinylsilatrane in C$_6$D$_6$CD$_3$

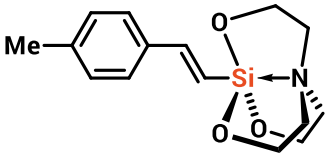
^{1}H NMR (C$_6$D$_5$CD$_3$, 300 MHz): δ 1.93 (t, *J* = 5.8 Hz, 6H, C*H*$_2$-N), 3.36 (t, *J* = 5.8 Hz, 6H, C*H*$_2$-O), 6.00 (dd, *J* = 14.2, 5.5 Hz, 1H, *H*$_2$C=), 6.24 (dd, *J* = 20.1, 5.4 Hz, 1H, *H*$_2$C=), 6.47 (dd, *J* = 20.1, 14.2 Hz, 1H, =C*H*-Si)

5.2. (*E*)-1-styryl-2,8,9-trioxa-5-aza-1-silabicyclo[3.3.3]undecane (2a)



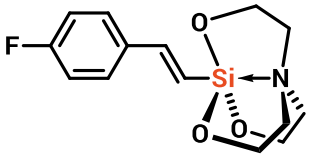
^{1}H NMR (DCCl$_3$, 300 MHz): δ 2.85 (t, *J* = 5.8 Hz, 6H, C*H*$_2$-N), 3.84 (t, *J* = 5.8 Hz, 6H, C*H*$_2$-O), 6.31 (d, *J* = 18.9 Hz, 1H, =C*H*-Si), 7.09 (d, *J* = 19.0 Hz, 1H, -C*H*=CH-Si), 7.06–7.46 (m, 5H, Ph); **^{13}C NMR (DCCl$_3$, 75 MHz):** δ 51.14, 57.78, 126.66, 127.03, 128.14, 128.99, 139.48, 142.79; **^{29}Si NMR (DCCl$_3$, 79 MHz):** δ -80.06; **MS (ESI):** *m/z* 300 (M+Na, 100%), 192 (19), 174 (15); Found: C, 60.60; H, 6.91. Calc. for $C_{14}H_{19}NO_3Si$: C, 60.62; H, 6.90%.

5.3. (*E*)-1-(4-methylstyryl)-2,8,9-trioxa-5-aza-1-silabicyclo[3.3.3]undecane (2c)



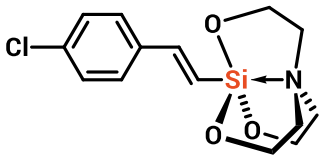
^{1}H NMR (DCCl$_3$, 300 MHz): δ 2.29 (s, 1H, Me), 2.87 (t, *J* = 5.9 Hz, 6H, C*H*$_2$-N), 3.86 (t, *J* = 5.9 Hz, 6H, C*H*$_2$-O), 6.27 (d, *J* = 18.8 Hz, 1H, =C*H*-Si), 6.99-7.12 (m, 3H, phenyl fing doublet overlapping with -C*H*=CH-Si), 7.33 (d, *J* = 8.0 Hz, 2H, =CH-C$_6$*H*$_4$-Me); **^{13}C NMR (DCCl$_3$, 75 MHz):** δ 21.51, 51.35, 58.02, 126.78, 127.76, 129.08, 136.94, 137.04, 142.94; **^{29}Si NMR (DCCl$_3$, 79 MHz):** δ -79.62; **MS (ESI):** *m/z* 330 (M+K, 100%), 314 (M+Na, 49%), 292 (M+H, 19%), 192 (46), 174 (51); Found: C, 61.77; H, 7.20. Calc. for $C_{15}H_{21}NO_3Si$: C, 61.82; H, 7.26%.

5.4. (*E*)-1-(4-fluorostyryl)-2,8,9-trioxa-5-aza-1-silabicyclo[3.3.3]undecane (2d)



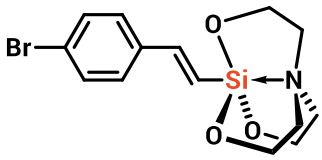
^{1}H NMR (DCCl$_3$, 300 MHz): δ 2.87 (t, *J* = 5.9 Hz, 6H, C*H*$_2$-N), 3.86 (t, *J* = 5.9 Hz, 6H, C*H*$_2$-O), 6.24 (d, *J* = 18.8 Hz, 1H, =C*H*-Si), 6.92 (t, *J* = 8.7 Hz, 2H, =CH-C$_6$*H*$_4$-F), 7.06 (d, *J* = 18.9 Hz, 1H, -C*H*=CH-Si); 7.39 (dd, *J* = 8.5, 5.7 Hz, 2H, =CH-C$_6$*H*$_4$-F); **^{13}C NMR (DCCl$_3$, 75 MHz):** δ 51.13, 57.75, 114.96 (d, $^{2}J_{C\text{-}F}$ = 21.4 Hz), 128.01 (d, $^{3}J_{C\text{-}F}$ = 8 Hz), 128.88, 135.78, 141.42, 162.22 (d, $^{1}J_{C\text{-}F}$ = 245.2 Hz); **^{29}Si NMR (DCCl$_3$, 79 MHz):** δ -80.43; **MS (ESI):** *m/z* 334 (M+K, 30%), 318 (M+Na, 100%), 192 (16), 174 (22), 150 (; Found: C, 56.89; H, 6.10. Calc. for $C_{14}H_{18}FNO_3Si$: C, 56.93; H, 6.14%.

5.5. (*E*)-1-(4-chlorostyryl)-2,8,9-trioxa-5-aza-1-silabicyclo[3.3.3]undecane (2e)



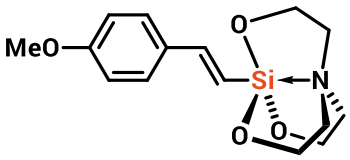
^{1}H NMR (DCCl$_3$, 300 MHz): δ 2.87 (t, *J* = 5.9 Hz, 6H, C*H*$_2$-N), 3.86 (t, *J* = 5.9 Hz, 6H, C*H*$_2$-O), 6.31 (d, *J* = 18.8 Hz, 1H, =C*H*-Si), 7.05 (d, *J* = 18.8 Hz, 1H, -C*H*=CH-Si), 7.20 (d, *J* = 8.5 Hz, 2H, =CH-C$_6$*H*$_4$-Cl), 7.35 (d, *J* = 8.4 Hz, 2H, =CH-C$_6$*H*$_4$-Cl); **^{13}C NMR (DCCl$_3$, 75 MHz):** δ 51.12, 57.71, 127.80, 128.31, 130.19, 132.55, 138.08, 141.24; **^{29}Si NMR (DCCl$_3$, 79 MHz):** δ -80.89; **MS (ESI):** *m/z* 350 (M+K, 42%), 334 (M+Na, 100%), 242 (8), 192 (29), 174 (21); Found: C, 53.90; H, 5.79. Calc. for $C_{14}H_{18}ClNO_3Si$: C, 53.92; H, 5.82%.

5.6. (*E*)-1-(4-bromostyryl)-2,8,9-trioxa-5-aza-1-silabicyclo[3.3.3]undecane (2f)



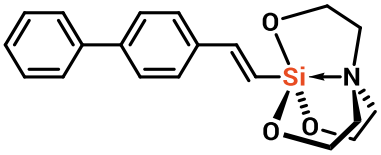
^{1}H NMR (DCCl$_3$, 300 MHz): δ 2.88 (t, *J* = 5.8 Hz, 6H, C*H*$_2$-N), 3.86 (t, *J* = 5.8 Hz, 6H, C*H*$_2$-O), 6.33 (d, *J* = 18.8 Hz, 1H, =C*H*-Si), 7.03 (d, *J* = 18.8 Hz, 1H, -C*H*=CH-Si), 7.29 (d, *J* = 8.5 Hz, 2H, =CH-C$_6$*H*$_4$-Br), 7.36 (d, *J* = 8.4 Hz, 2H, =CH-C$_6$*H*$_4$-Br); **^{13}C NMR (DCCl$_3$, 75 MHz):** δ 51.11, 57.71, 120.82, 128.17, 130.38, 131.26, 138.51, 141.30; **^{29}Si NMR (DCCl$_3$, 79 MHz):** δ -80.89; **MS (ESI):** *m/z* 395 (M+K, 100%), 380 (M+Na, 49%), 353 (13), 192 (36), 174 (30); Found: C, 47.21; H, 5.11. Calc. for $C_{14}H_{18}BrNO_3Si$: C, 47.20; H, 5.09%.

5.7. (*E*)-1-(4-methoxystyryl)-2,8,9-trioxa-5-aza-1-silabicyclo[3.3.3]undecane (2g)



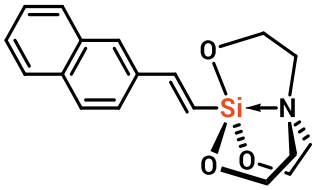
^{1}H NMR (DCCl$_3$, 300 MHz): δ 2.86 (t, *J* = 5.8 Hz, 6H, C*H*$_2$-N), 3.77 (s, 3H, OMe), 3.85 (t, *J* = 5.8 Hz, 6H, C*H*$_2$-O), 6.17 (d, *J* = 18.8 Hz, 1H, =C*H*-Si), 6.78 (d, *J* = 8.5 Hz, 2H, =CH-C$_6$*H*$_4$-OMe), 7.06 (d, *J* = 18.9 Hz, 1H, -C*H*=CH-Si), 7.37 (d, *J* = 8.5 Hz, 2H, =CH-C$_6$*H*$_4$-OMe); **^{13}C NMR (DCCl$_3$, 75 MHz):** δ 51.16, 55.29, 57.83, 113.54, 126.16, 127.79, 132.57, 142.3, 158.95; **^{29}Si NMR (DCCl$_3$, 79 MHz):** δ -79.39; **MS (ESI):** *m/z* 346 (M+K, 14%), 330 (M+Na, 100%), 308 (M+H, 57%), 192 (26), 174 (34); Found: C, 58.59; H, 6.90. Calc. for $C_{15}H_{21}NO_4Si$: C, 58.61; H, 6.89%.

5.8. *(E)*-1-(2-([1,1'-biphenyl]-4-yl)vinyl)-2,8,9-trioxa-5-aza-1-silabicyclo[3.3.3]undecane (2h)



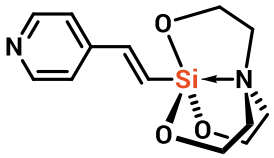
^{1}H NMR (DCCl$_3$, 300 MHz): δ 2.82 (t, *J* = 5.8 Hz, 6H, C*H*$_2$-N), 3.81 (t, *J* = 5.8 Hz, 6H, C*H*$_2$-O), 6.33 (d, *J* = 18.9 Hz, 1H, =C*H*-Si), 7.09 (d, *J* = 18.8 Hz, 1H, -C*H*=CH-Si), 7.18-7.59 (m, 9H, Ph-C$_6$H$_4$-); **^{13}C NMR (DCCl$_3$, 75 MHz):** δ 51.16, 57.80, 126.85, 126.99, 127.08, 128.77, 129.30, 138.69, 139.66, 141.16, 142.25; **^{29}Si NMR (DCCl$_3$, 79 MHz):** δ -80.07; **MS (ESI):** *m/z* 392 (M+K, 7%), 376 (M+Na, 100%), 354 (M+H, 18%), 192 (70), 174 (56); Found: C, 67.93; H, 6.55. Calc. for C$_{20}$H$_{23}$NO$_3$Si: C, 67.96; H, 6.56%.

5.9. (*E*)-1-(2-(naphthalen-2-yl)vinyl)-2,8,9-trioxa-5-aza-1-silabicyclo[3.3.3]undecane (2i)



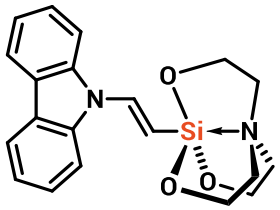
^{1}H NMR (DCCl$_3$, 300 MHz): δ 2.89 (t, *J* = 5.8 Hz, 6H, C*H*$_2$-N), 3.89 (t, *J* = 5.7 Hz, 6H, C*H*$_2$-O), 6.48 (d, *J* = 18.8 Hz, 1H, =C*H*-Si), 7.24-7.84 (m, 8H, naphtalene ring and -C*H*=CH-Si which is overlapped by chloroform signal); **^{13}C NMR (DCCl$_3$, 75 MHz):** δ 51.13, 57.77, 124.17, 125.42, 125.80, 126.54, 142.75, 127.60, 127.67, 128.24, 129.70, 133.11, 133.76, 137.11, 142.75; **^{29}Si NMR (DCCl$_3$, 79 MHz):** δ -80.32; **MS (ESI):** *m/z* 350 (M+Na, 100%), 192 (28), 174 (17); Found: C, 66.06; H, 6.43. Calc. for C$_{18}$H$_{21}$NO$_3$Si: C, 66.02; H, 6.46%.

5.10. (*E*)-1-(2-(pyridin-4-yl)vinyl)-2,8,9-trioxa-5-aza-1-silabicyclo[3.3.3]undecane (2j)



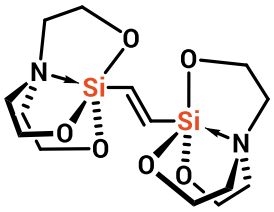
^{1}H NMR (DCCl$_3$, 300 MHz): δ 2.83 (t, *J* = 5.9 Hz, 6H, C*H*$_2$-N), 3.80 (t, *J* = 5.7 Hz, 6H, C*H*$_2$-O), 6.54 (d, *J* = 18.8 Hz, 1H, =C*H*-Si), 6.96 (d, *J* = 18.8 Hz, 1H, -C*H*=CH-Si), 7.12 (d, *J* = 5.6 Hz, 2H, =CH-C$_5$*H*$_4$N), 8.39 (d, *J* = 5.5 Hz, 2H, =CH-C$_5$*H*$_4$N) ; **^{13}C NMR (DCCl$_3$, 75 MHz):** δ 51.08, 57.59, 121.11, 135.74, 139.84, 146.66, 149.83; **^{29}Si NMR (DCCl$_3$, 79 MHz):** δ -82.44; **MS (ESI):** *m/z* 301 (M+Na, 22%), 279 (M+H, 100%); Found: C, 56.06; H, 6.47. Calc. for C$_{13}$H$_{18}$N$_2$O$_3$Si: C, 56.09; H, 6.52%.

5.11. (*E*)-1-(2-(9H-carbazol-9-yl)vinyl)-2,8,9-trioxa-5-aza-1-silabicyclo[3.3.3]undecane (2k)



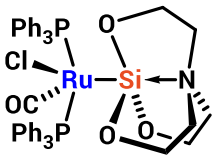
^{1}H NMR (DCCl$_3$, 300 MHz): δ 2.82 (t, *J* = 5.8 Hz, 6H, C*H*$_2$-N), 3.85 (t, *J* = 5.7 Hz, 6H, C*H*$_2$-O), 5.92 (d, *J* = 16.8 Hz, 1H, =C*H*-Si), 7.22 (*pseudo* t, 2H, Ar), 7.41 (*pseudo* t, 2H, Ar), 7.64 (d, *J* = 16.8 Hz, 1H, -C*H*=CH-Si), 7.81 (d, *J* = 8.2 Hz, 2H, Ar), 8.02 (d, *J* = 7.6 Hz, 1H, Ar); **^{13}C NMR (DCCl$_3$, 75 MHz):** δ 51.04, 57.70, 111.48, 113.93, 119.87, 120.05, 123.88, 125.87, 133.39, 139.69; **^{29}Si NMR (DCCl$_3$, 79 MHz):** δ -79.68; **MS (ESI):** *m/z* 405 (M+K, 13%), 389 (M+Na, 19%), 367 (M+H, 88%), 192 (99), 174 (100); Found: C, 65.54; H, 6.03. Calc. for $C_{20}H_{22}N_2O_3Si$: C, 65.55; H, 6.05%.

5.12. (*E*)-1,2-bis(2,8,9-trioxa-5-aza-1-silabicyclo[3.3.3]undecan-1-yl)ethene (2b)



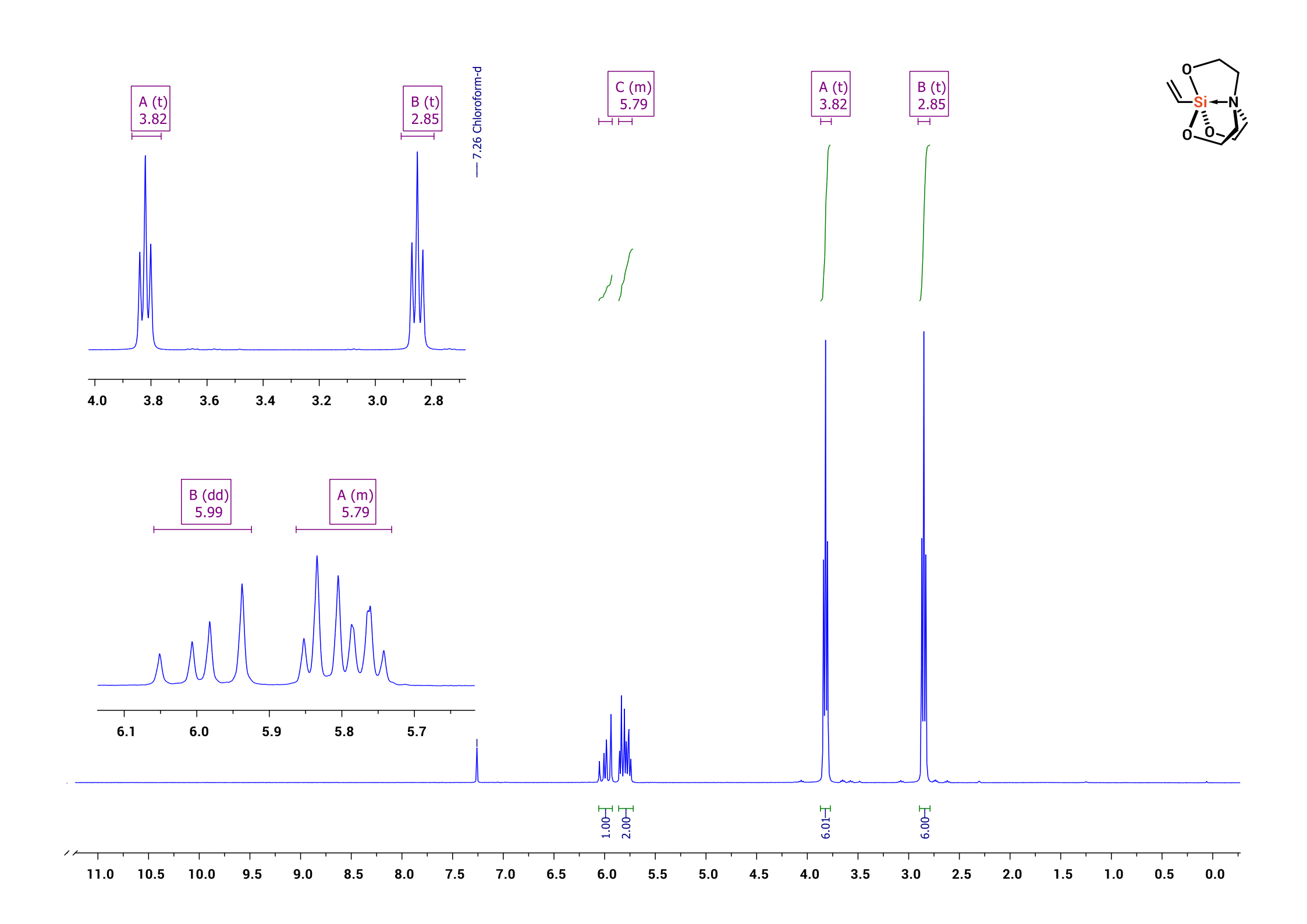
^{1}H NMR (DCCl$_3$, 300 MHz): δ 2.67–2.92 (m, 6H, C*H*$_2$-N), 3.67-3.92 (m, 6H, C*H*$_2$-O), 6.58 (s, 2H, =C*H*-Si); Found: C, 44.87; H, 6.98. Calc. for $C_{14}H_{26}N_2O_6Si_2$: C, 44.90; H, 7.00%.

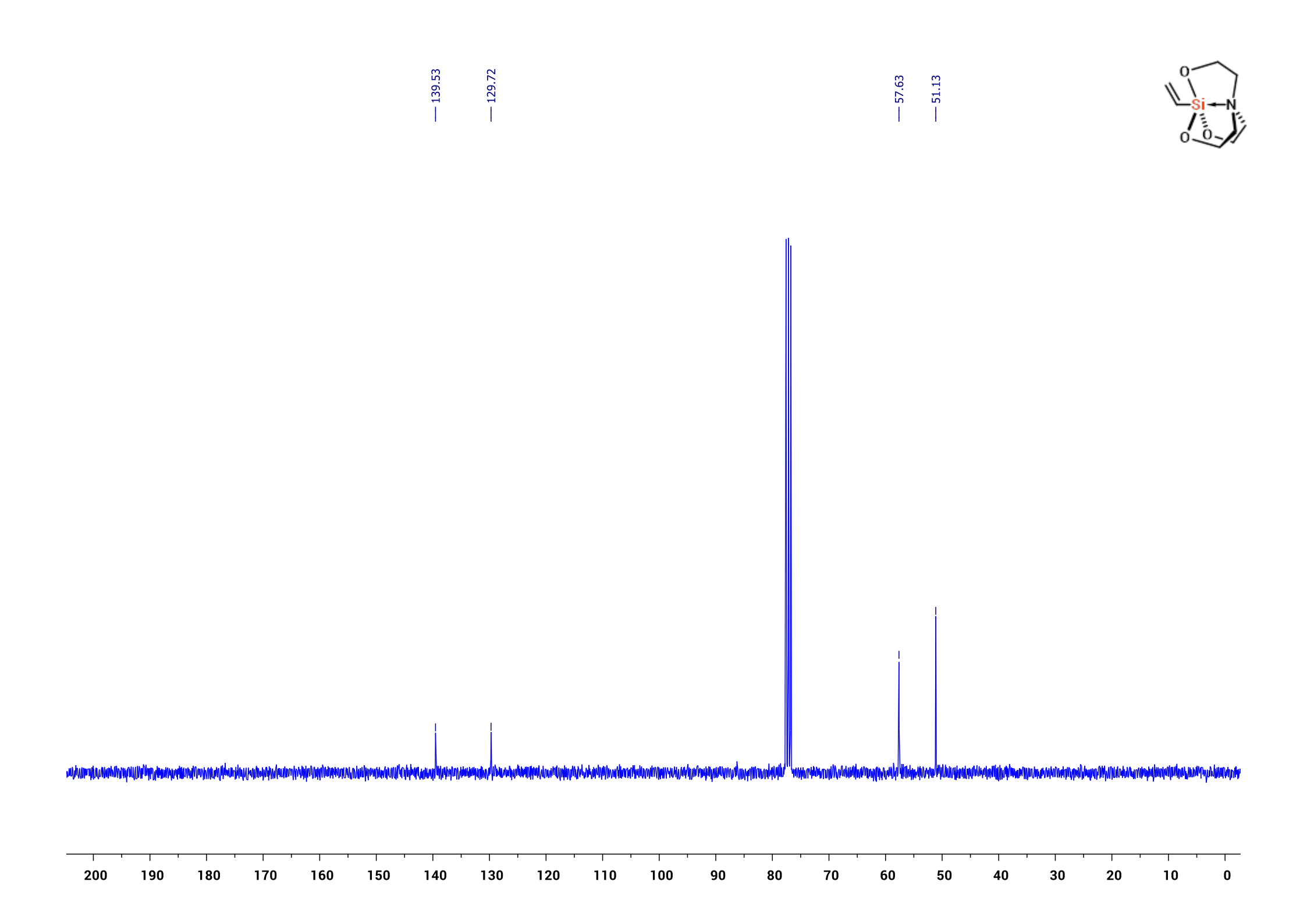
5.13. Ruthenium silatranyl complex (3)

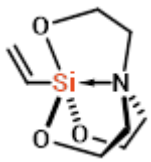


^{1}H NMR (DCCl$_3$, 300 MHz): δ 2.54 (bs, 6H), 3.25 (bs, 6H), 7.74 – 7.10 (m, 30H); **^{13}C NMR (DCCl$_3$, 75 MHz):** δ 128.01 (t, *J* = 4.9 Hz), 129.74, 134.90 (t, *J* = 5.7 Hz); **^{31}P NMR (DCCl$_3$, 162 MHz):** δ 37.35; **IR:** ν(CO): 1922 cm^{-1}**; MS (ESI):** *m/z* 828 (M-Cl, 100%), 655 (15), 579 (6); Found: C, 44.87; H, 6.98. Calc. for $C_{14}H_{26}N_2O_6Si_2$: C, 44.90; H, 7.00%.

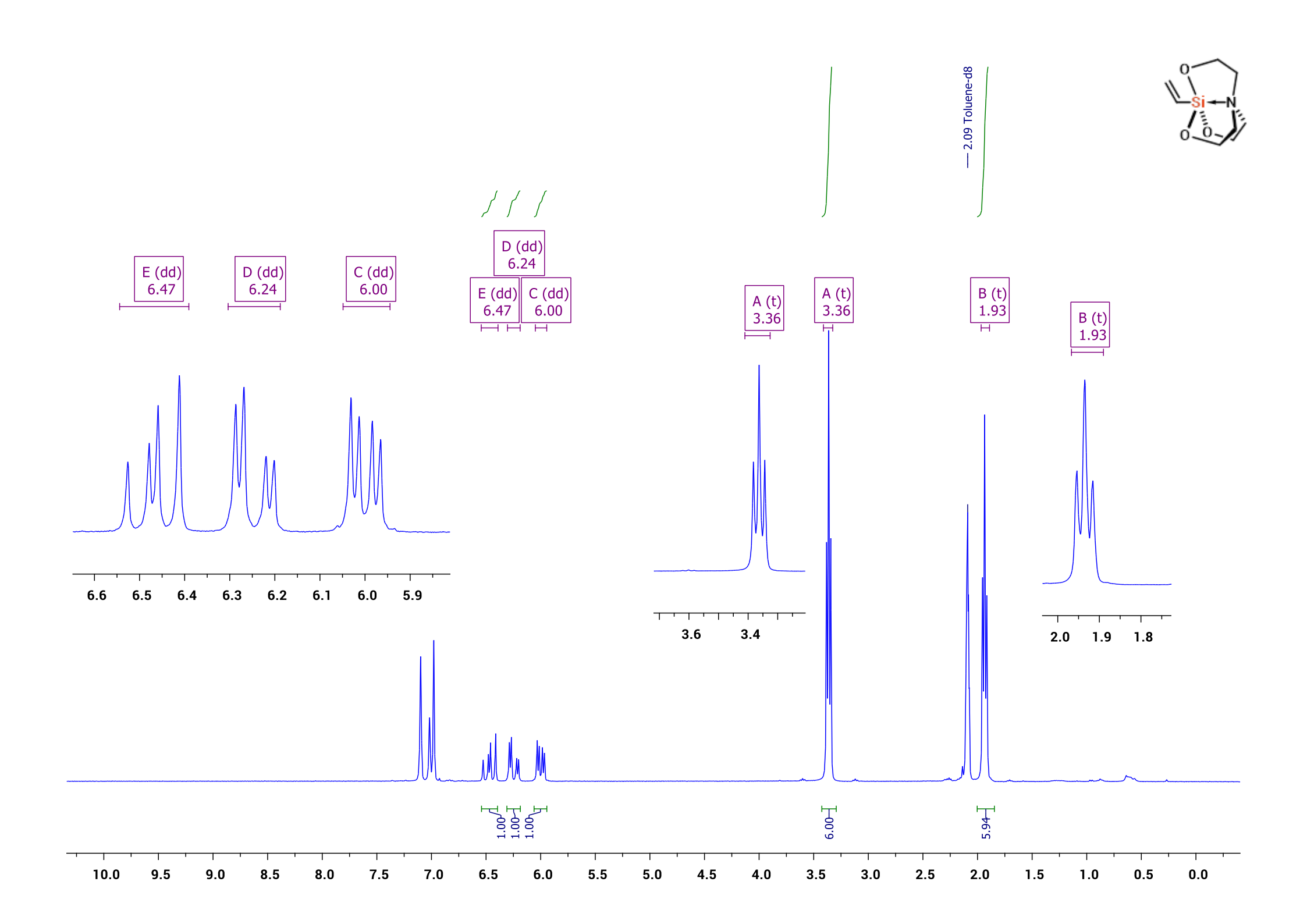
6. NMR Spectra

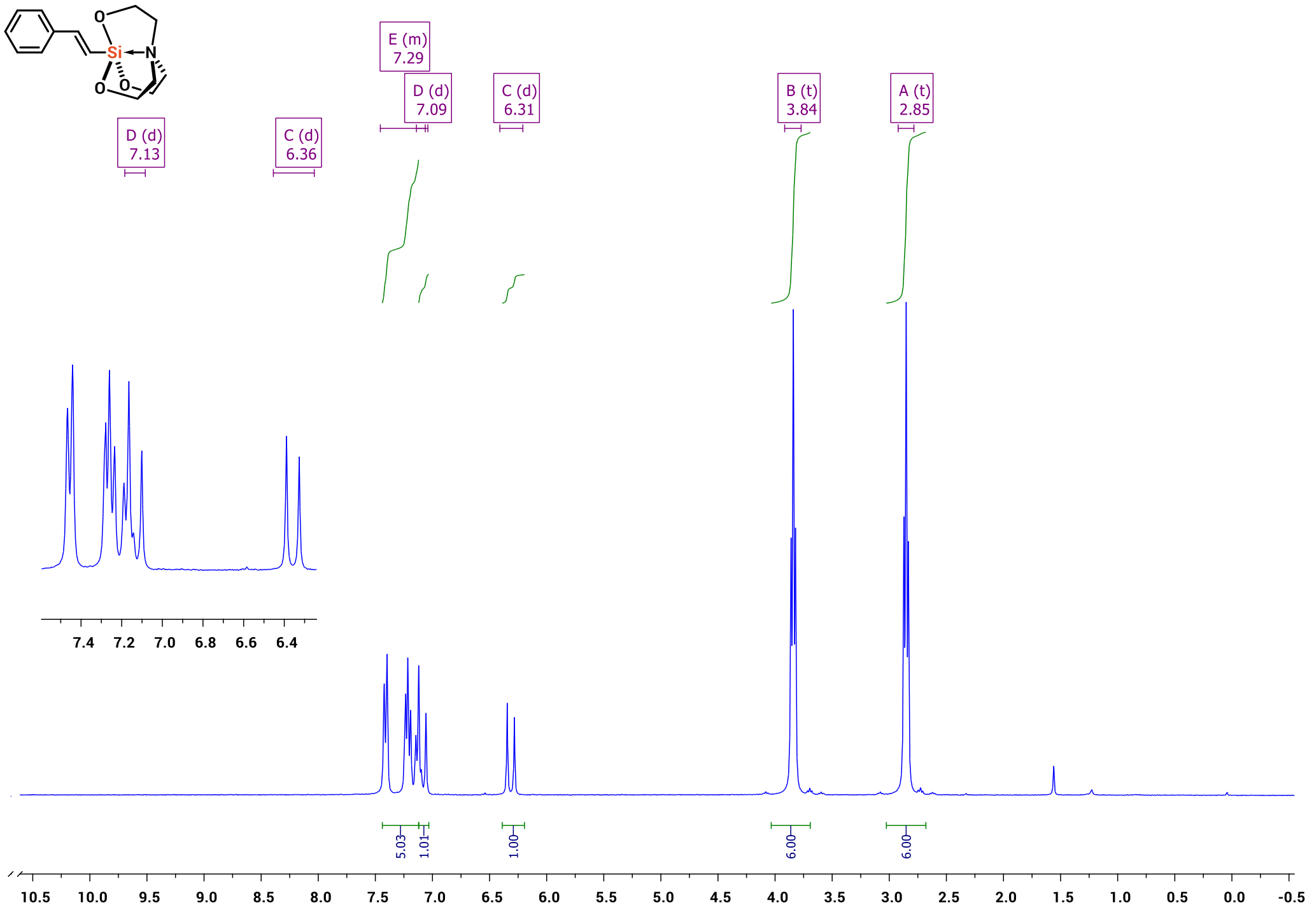

A (t)
3.82
B (t)
2.85
C (m)
5.79
A (t)
3.82
B (t)
2.85
7.26 Chloroform-d
B (dd)
5.99
A (m)
5.79
Si
N
O
O
O
4.0
3.8
3.6
3.4
3.2
3.0
2.8
6.1
6.0
5.9
5.8
5.7
1.00
2.00
6.01
6.00
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

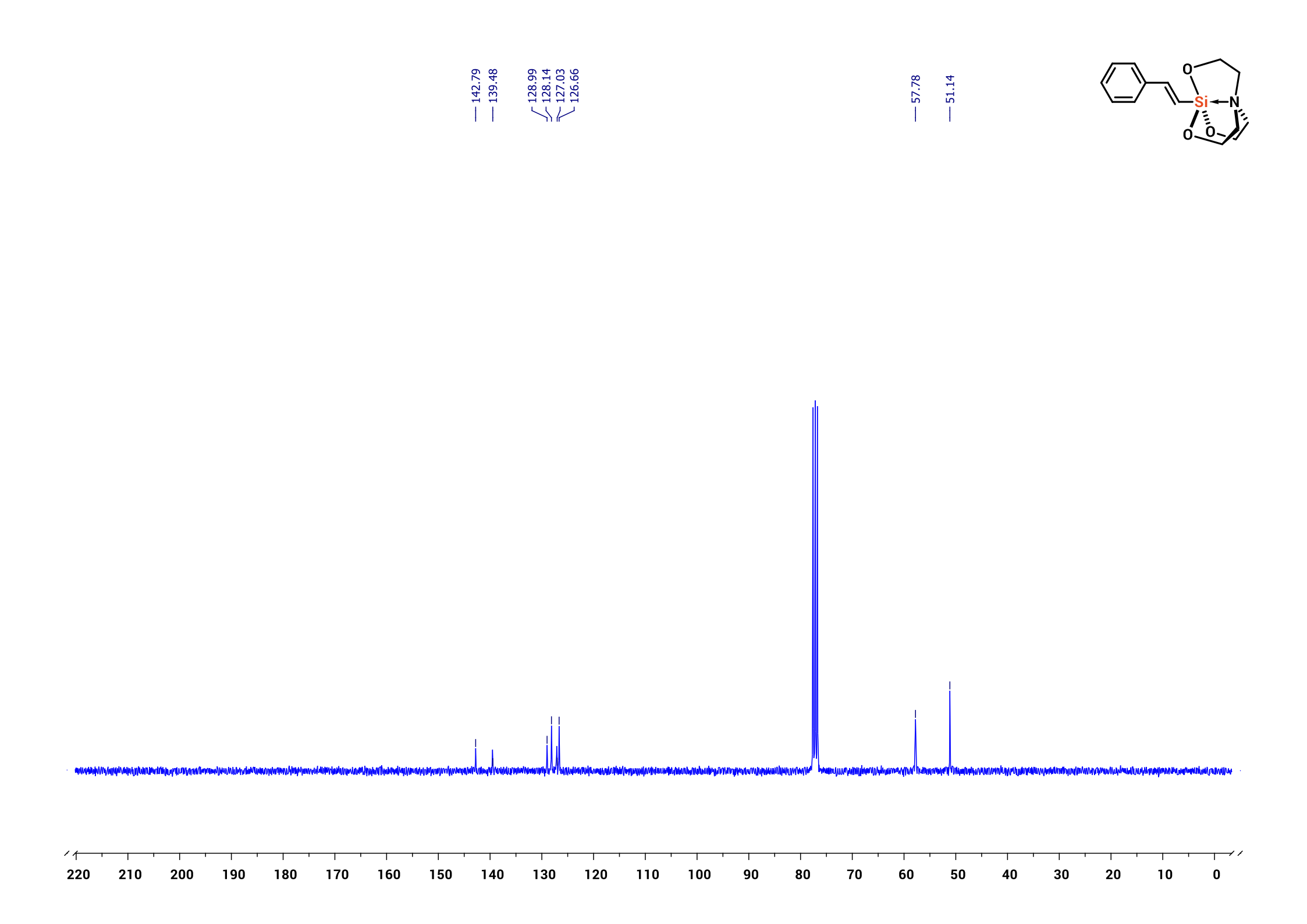

139.53
129.72
57.63
51.13
O
Si
N
O
O
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

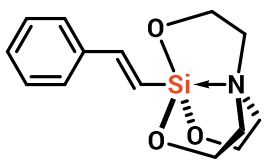

O
Si
N
O
O

-81.32
100
80
60
40
20
0
-20
-40
-60
-80
-100
-130
-160
-190
-220
-250
-280

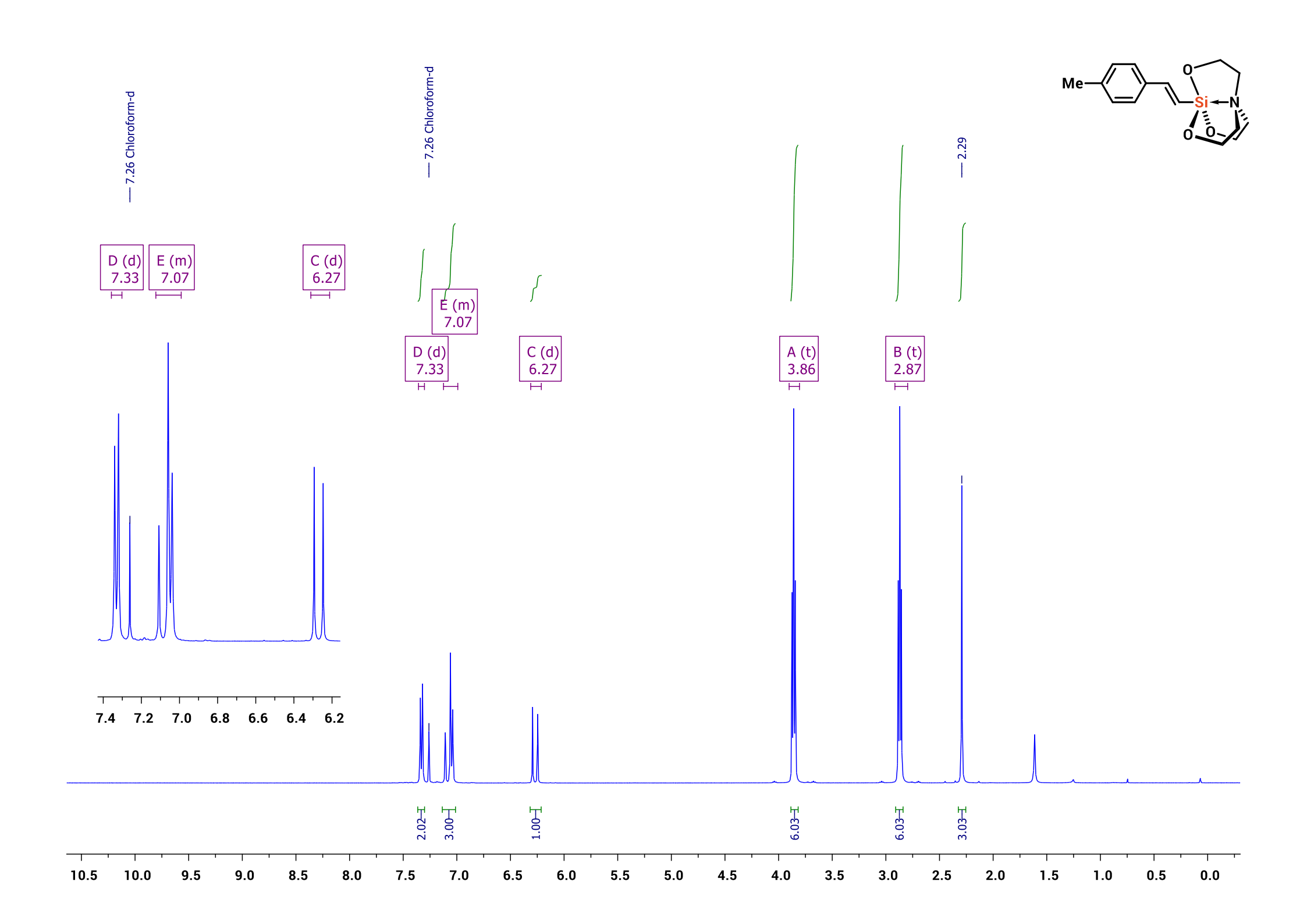

E (dd)
6.47
D (dd)
6.24
C (dd)
6.00
D (dd)
6.24
E (dd)
6.47
C (dd)
6.00
A (t)
3.36
A (t)
3.36
B (t)
1.93
B (t)
1.93
2.09 Toluene-d8
1.00
1.00
1.00
6.00
5.94
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

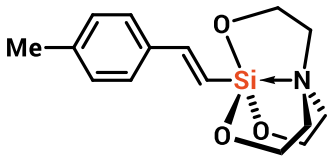

O
Si
N
O
O
E (m)
7.29
D (d)
7.09
C (d)
6.31
B (t)
3.84
A (t)
2.85
D (d)
7.13
C (d)
6.36
7.4
7.2
7.0
6.8
6.6
6.4
5.03
1.01
1.00
6.00
6.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5


142.79
139.48
128.99
128.14
127.03
126.66
57.78
51.14
O
Si
N
O
O
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0


O
Si
N
O
O

-80.06
-80.06
-50
-60
-70
-80
-90
-100
-110
100
80
60
40
20
0
-20
-40
-60
-80
-100
-130
-160
-190
-220
-250
-280


— 7.26 Chloroform-d
D (d) 7.33
E (m) 7.07
C (d) 6.27
— 7.26 Chloroform-d
E (m) 7.07
D (d) 7.33
C (d) 6.27
A (t) 3.86
B (t) 2.87
— 2.29
Me
O
Si
N
O
O
7.4 7.2 7.0 6.8 6.6 6.4 6.2
2.02
3.00
1.00
6.03
6.03
3.03
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

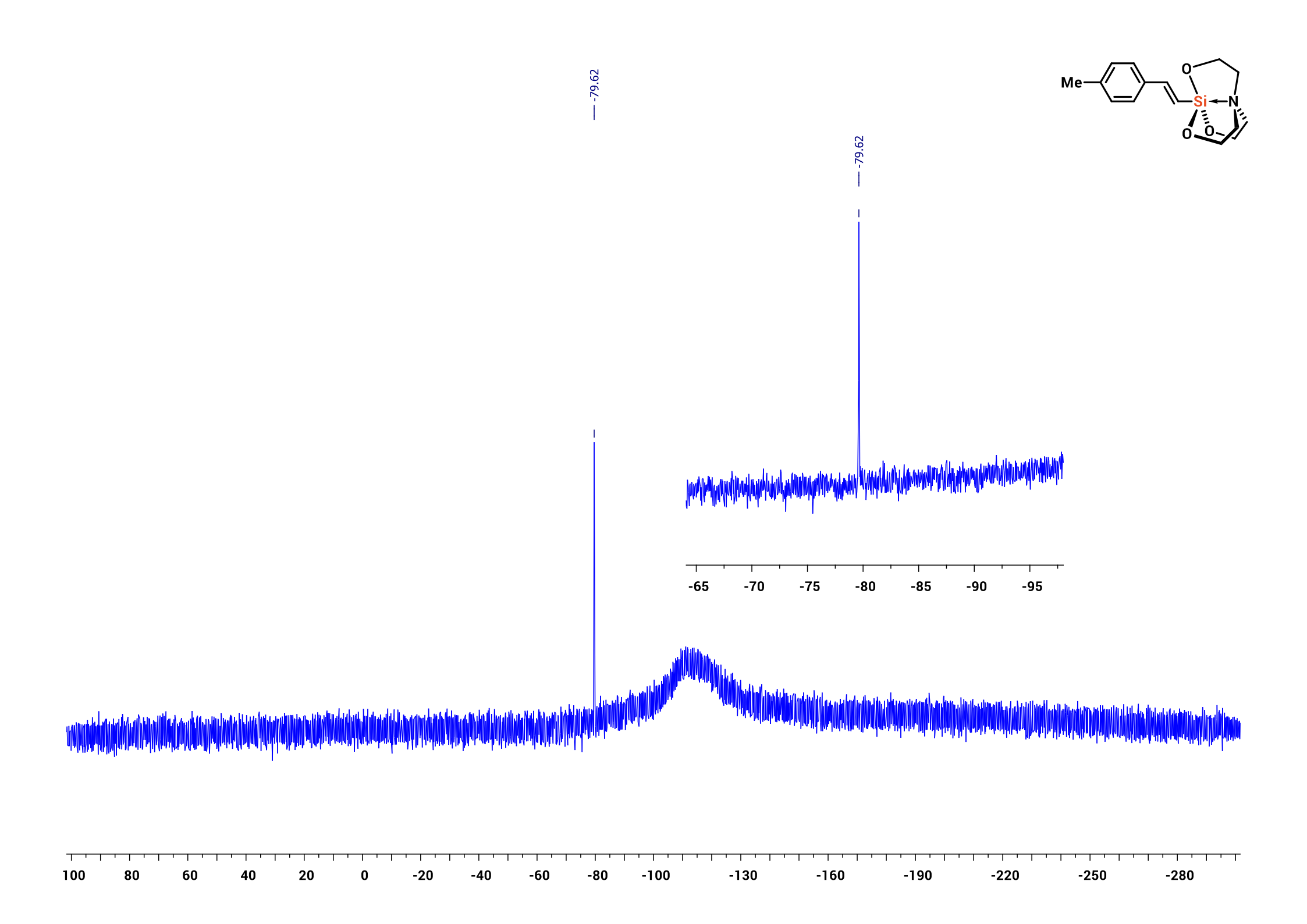


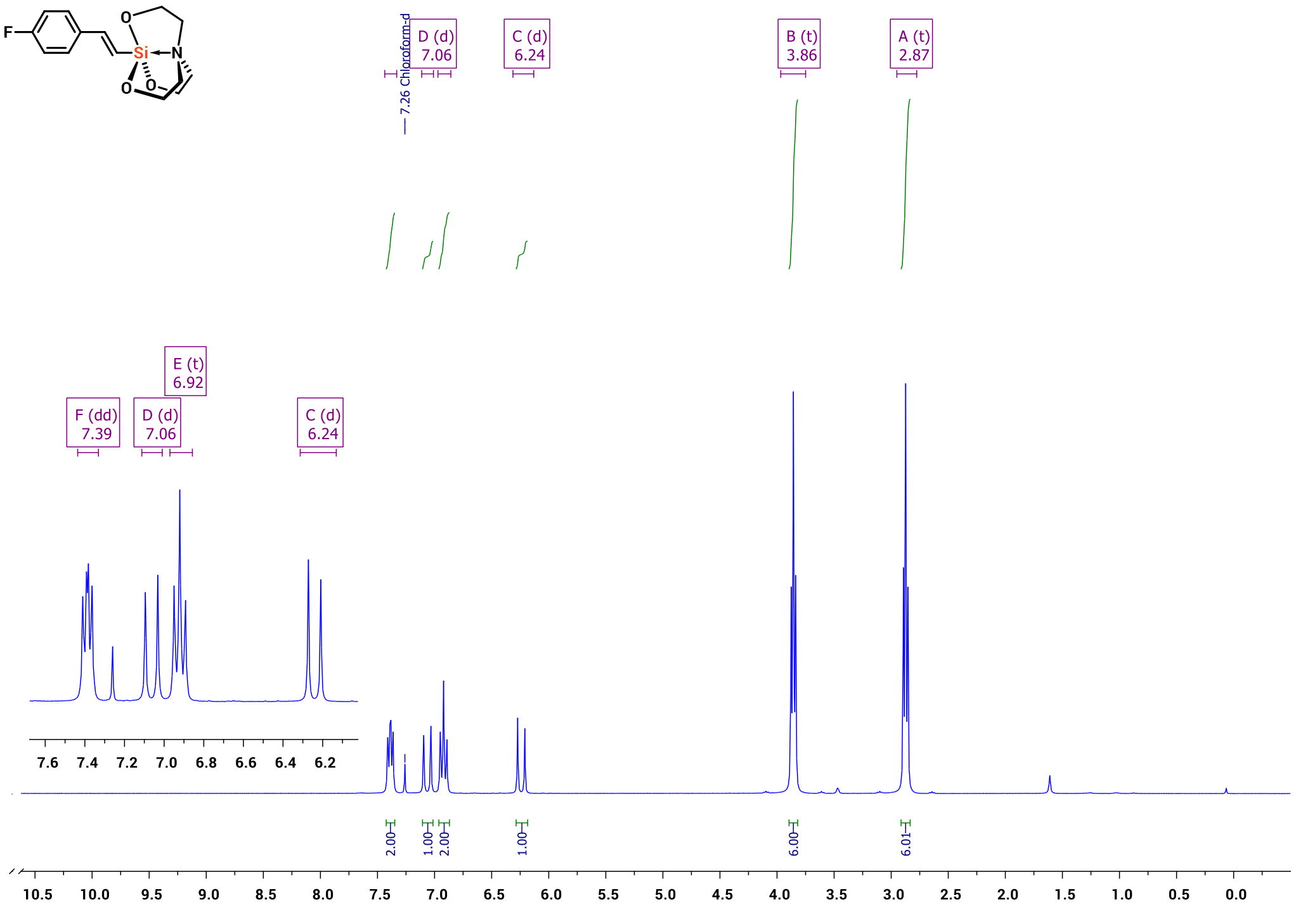
142.94
137.04
136.94
129.08
127.76
126.78
77.16 Chloroform-d
58.02
51.35
21.51

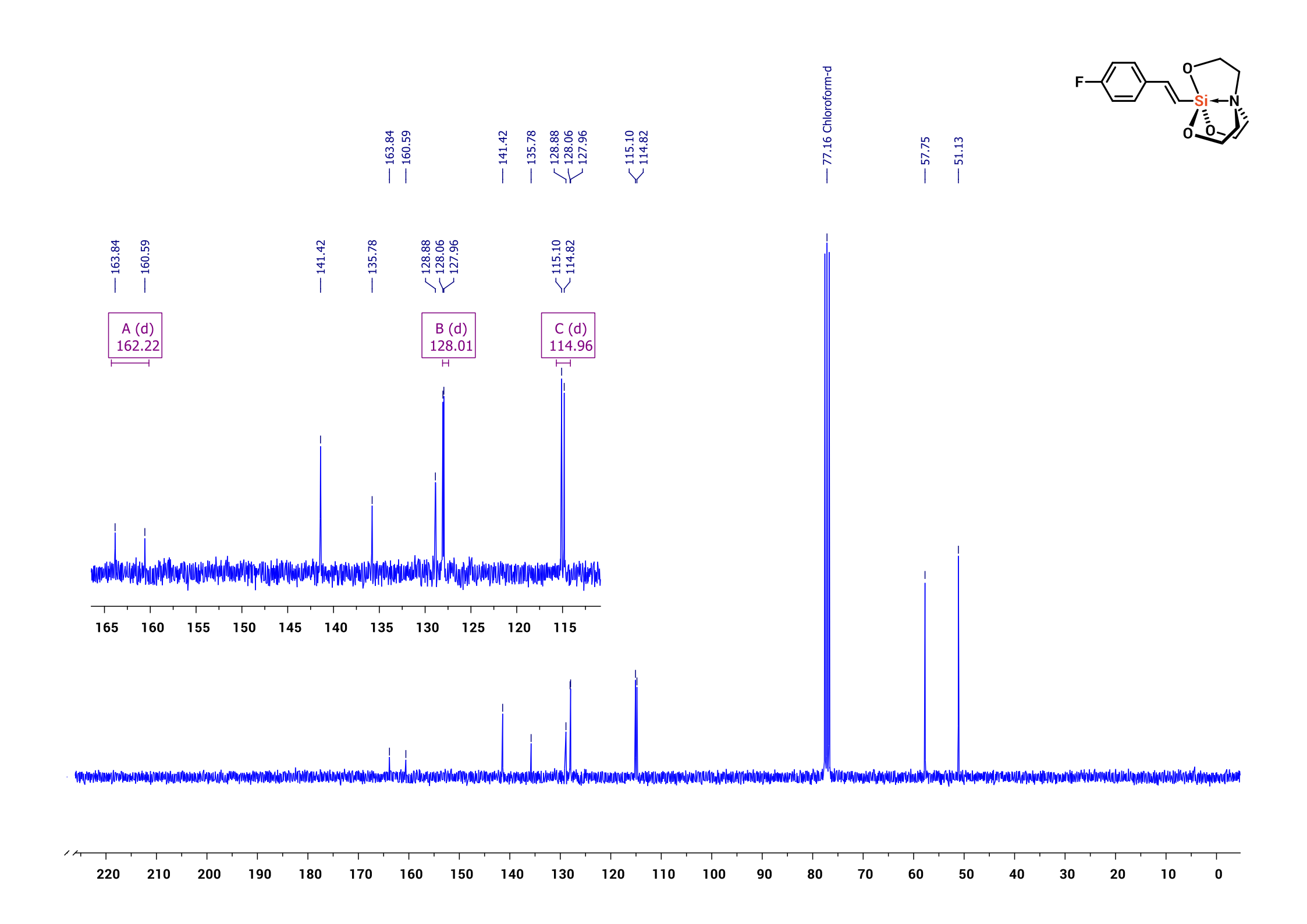
142.73
136.84
136.74
128.87
127.55
126.57

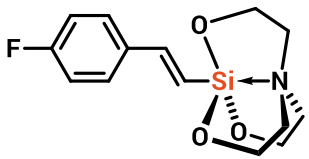
140
135
130
125

200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0


-79.62
-79.62
Me
O
Si
N
O
O
-65
-70
-75
-80
-85
-90
-95
100
80
60
40
20
0
-20
-40
-60
-80
-100
-130
-160
-190
-220
-250
-280


F
O
Si
N
O
O
7.26 Chloroform-d
D (d)
7.06
C (d)
6.24
B (t)
3.86
A (t)
2.87
E (t)
6.92
F (dd)
7.39
D (d)
7.06
C (d)
6.24
7.6
7.4
7.2
7.0
6.8
6.6
6.4
6.2
2.00
1.00
2.00
1.00
6.00
6.01
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0


F
O
Si
N
O
O
163.84
160.59
141.42
135.78
128.88
128.06
127.96
115.10
114.82
77.16 Chloroform-d
57.75
51.13
A (d)
162.22
B (d)
128.01
C (d)
114.96
165 160 155 150 145 140 135 130 125 120 115
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0


F
O
Si
N
O
O

-80.43
-80.43
-75
-80
-85
-90
-95
100
80
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20
0
-20
-40
-60
-80
-100
-130
-160
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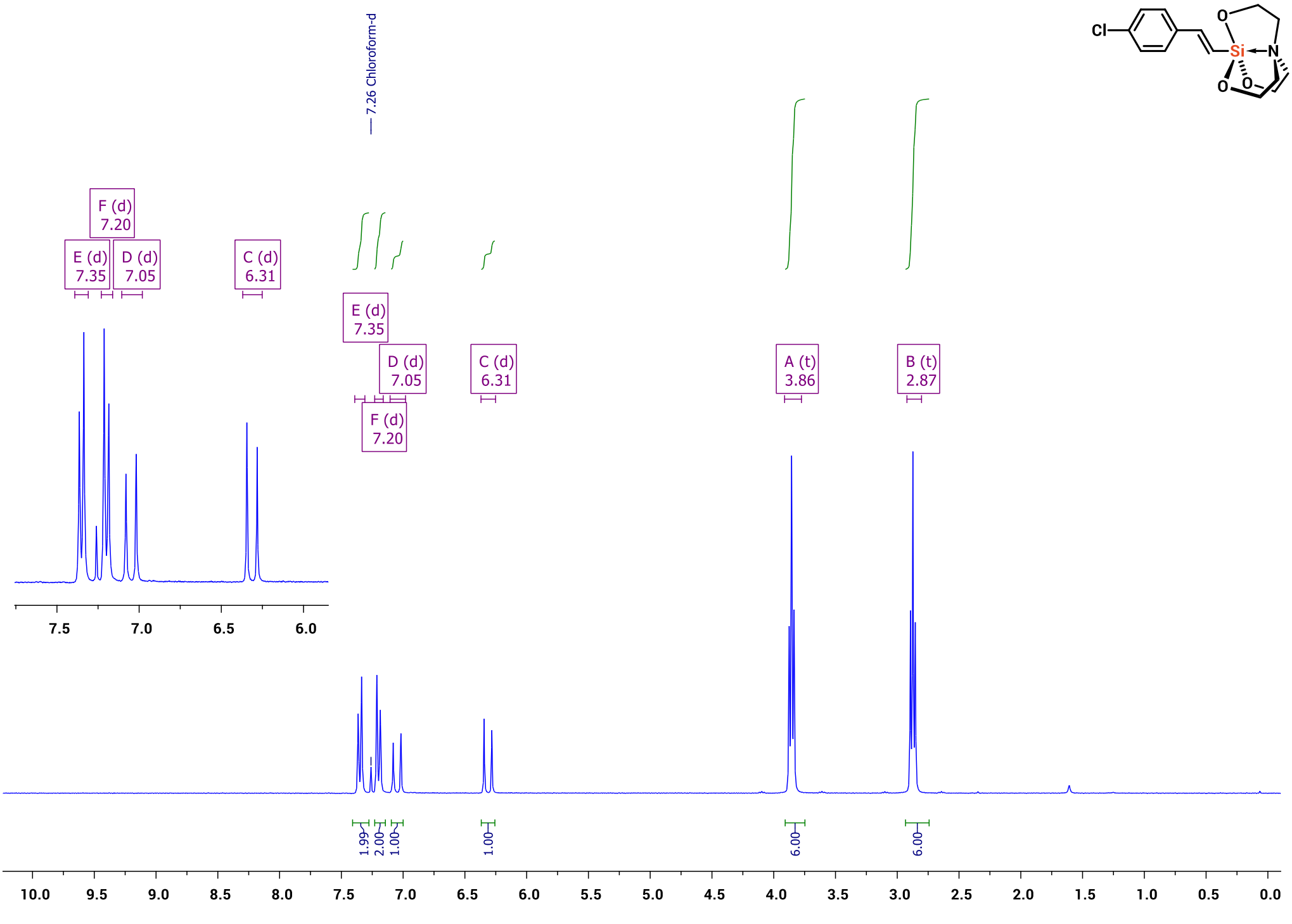
-220
-250
-280


— 7.26 Chloroform-d
F (d)
7.20
E (d)
7.35
D (d)
7.05
C (d)
6.31
A (t)
3.86
B (t)
2.87
1.99
2.00
1.00
1.00
6.00
6.00
Cl
O
Si
N
O
O
7.5
7.0
6.5
6.0
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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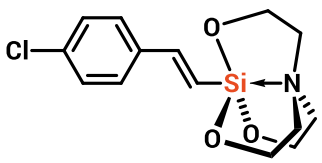
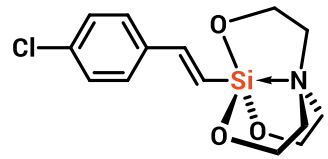


141.24
138.08
132.55
130.19
128.31
127.80
77.16 Chloroform-d
57.71
51.12

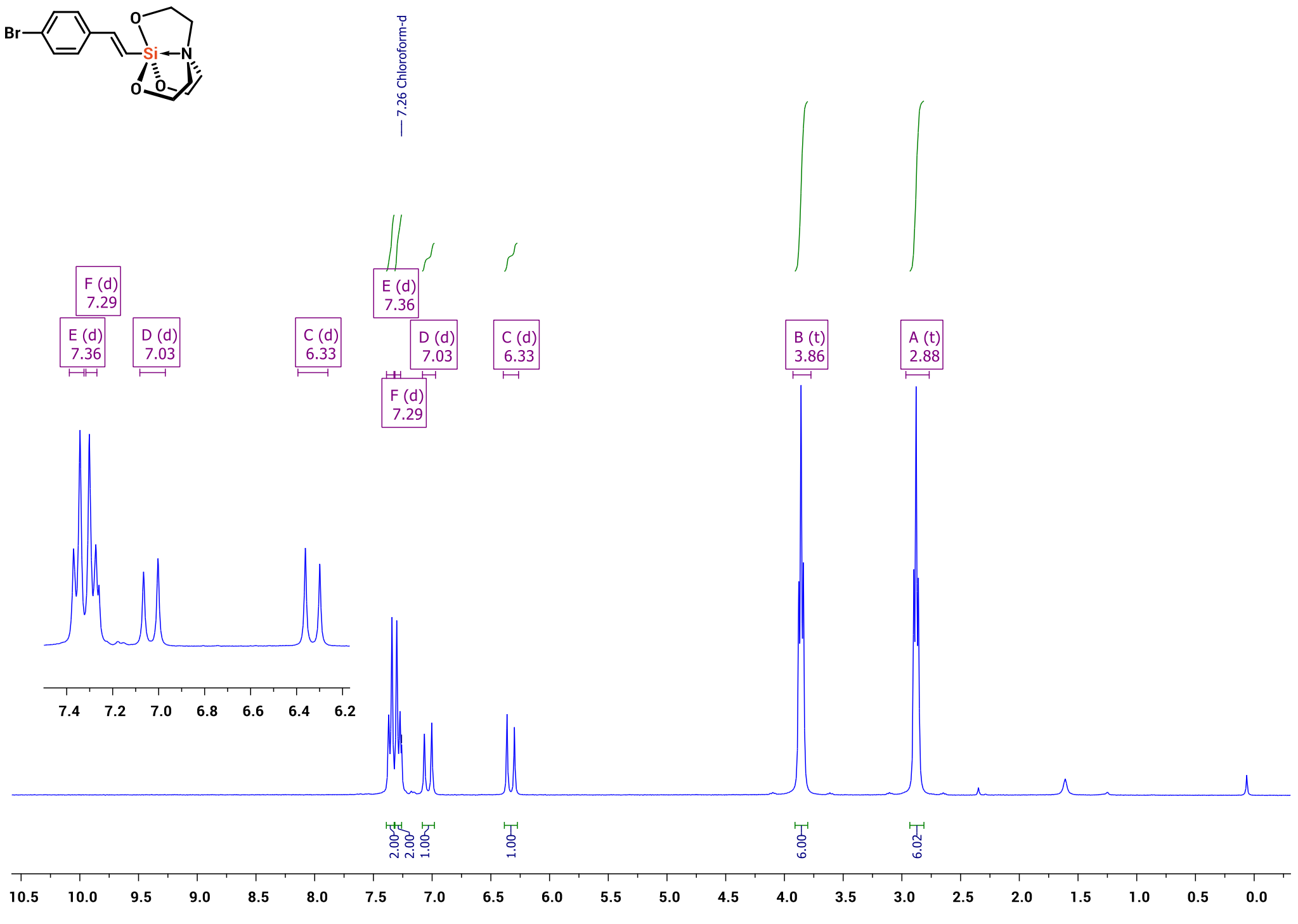


-80.89

-80.89

-60 -70 -80 -90 -100 -110

100 80 60 40 20 0 -20 -40 -60 -80 -100 -130 -160 -190 -220 -250 -280


Br
O
Si
N
O
O
7.26 Chloroform-d
F (d) 7.29
E (d) 7.36
D (d) 7.03
C (d) 6.33
E (d) 7.36
D (d) 7.03
C (d) 6.33
F (d) 7.29
B (t) 3.86
A (t) 2.88
7.4
7.2
7.0
6.8
6.6
6.4
6.2
2.00
2.00
1.00
1.00
6.00
6.02
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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2.0
1.5
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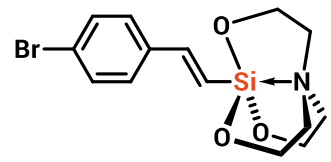
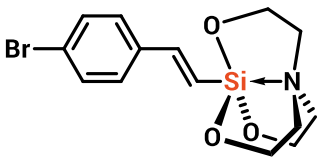


141.30
138.51
131.26
130.38
128.17
120.82
77.16 Chloroform-d
57.71
51.11

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0


Br
O
Si
N
O
O

-80.89
-80.89
-60
-65
-70
-75
-80
-85
-90
-95
-100
100
80
60
40
20
0
-20
-40
-60
-80
-100
-130
-160
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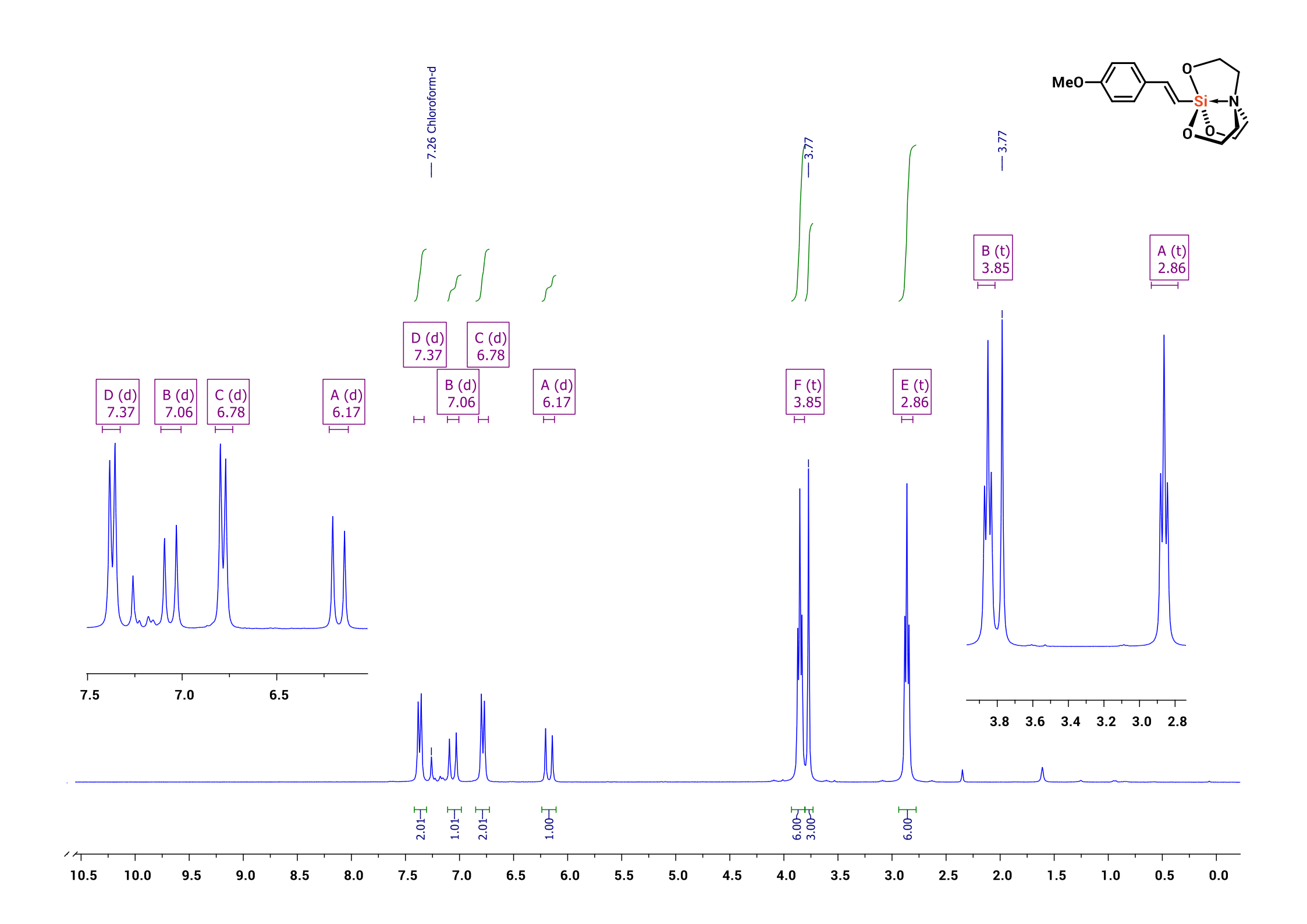
-220
-250
-280


MeO
O
Si
N
O
O
7.26 Chloroform-d
3.77
3.77
D (d) 7.37
C (d) 6.78
B (d) 7.06
A (d) 6.17
F (t) 3.85
E (t) 2.86
B (t) 3.85
A (t) 2.86
D (d) 7.37
B (d) 7.06
C (d) 6.78
A (d) 6.17
7.5
7.0
6.5
3.8
3.6
3.4
3.2
3.0
2.8
2.01
1.01
2.01
1.00
6.00
3.00
6.00
10.5
10.0
9.5
9.0
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8.0
7.5
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6.0
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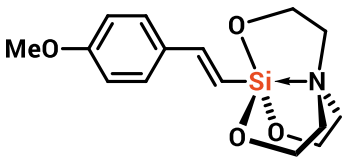
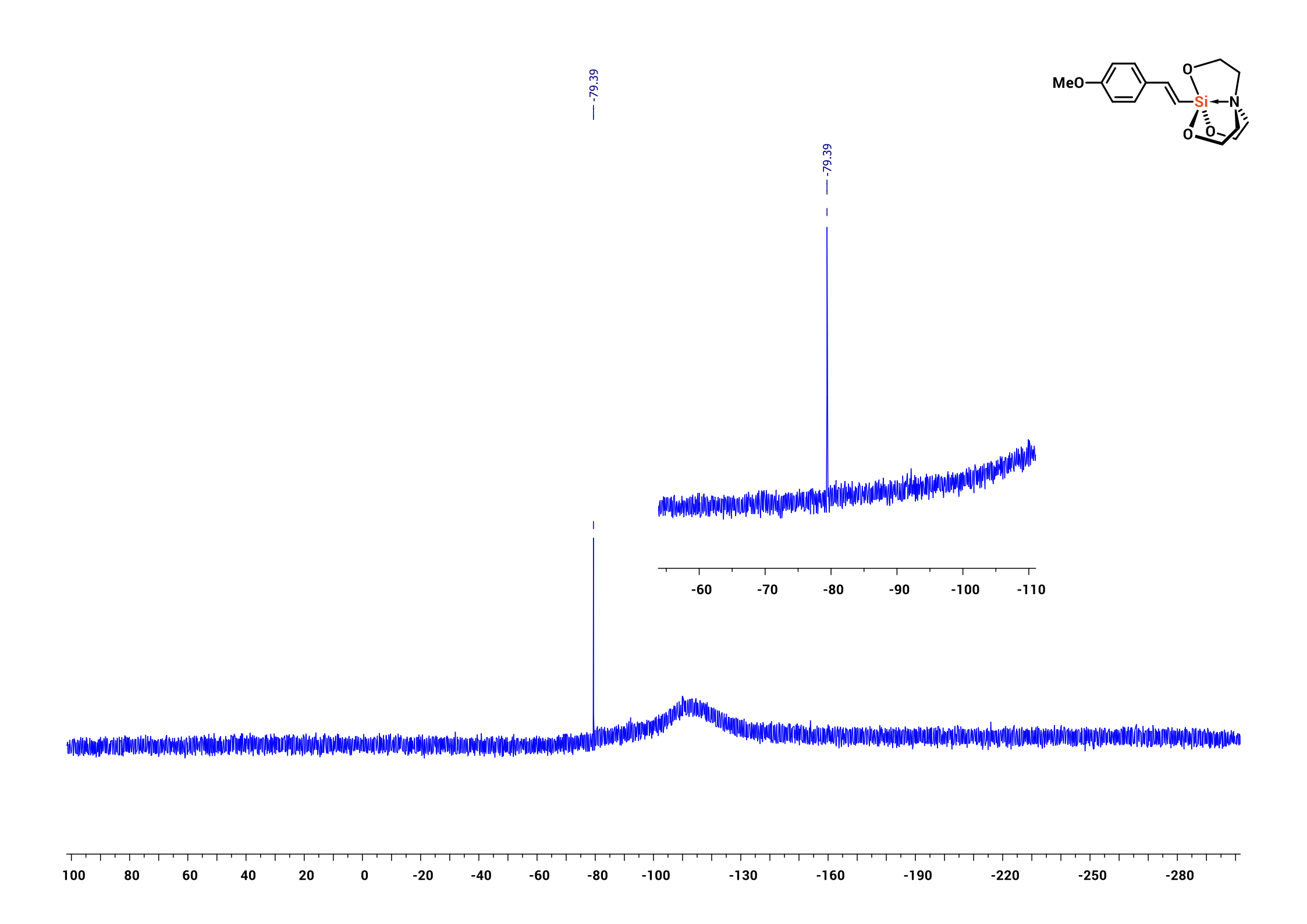


158.95
142.31
132.57
127.79
126.16
113.54
77.16 Chloroform-d
57.83
55.29
51.16

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0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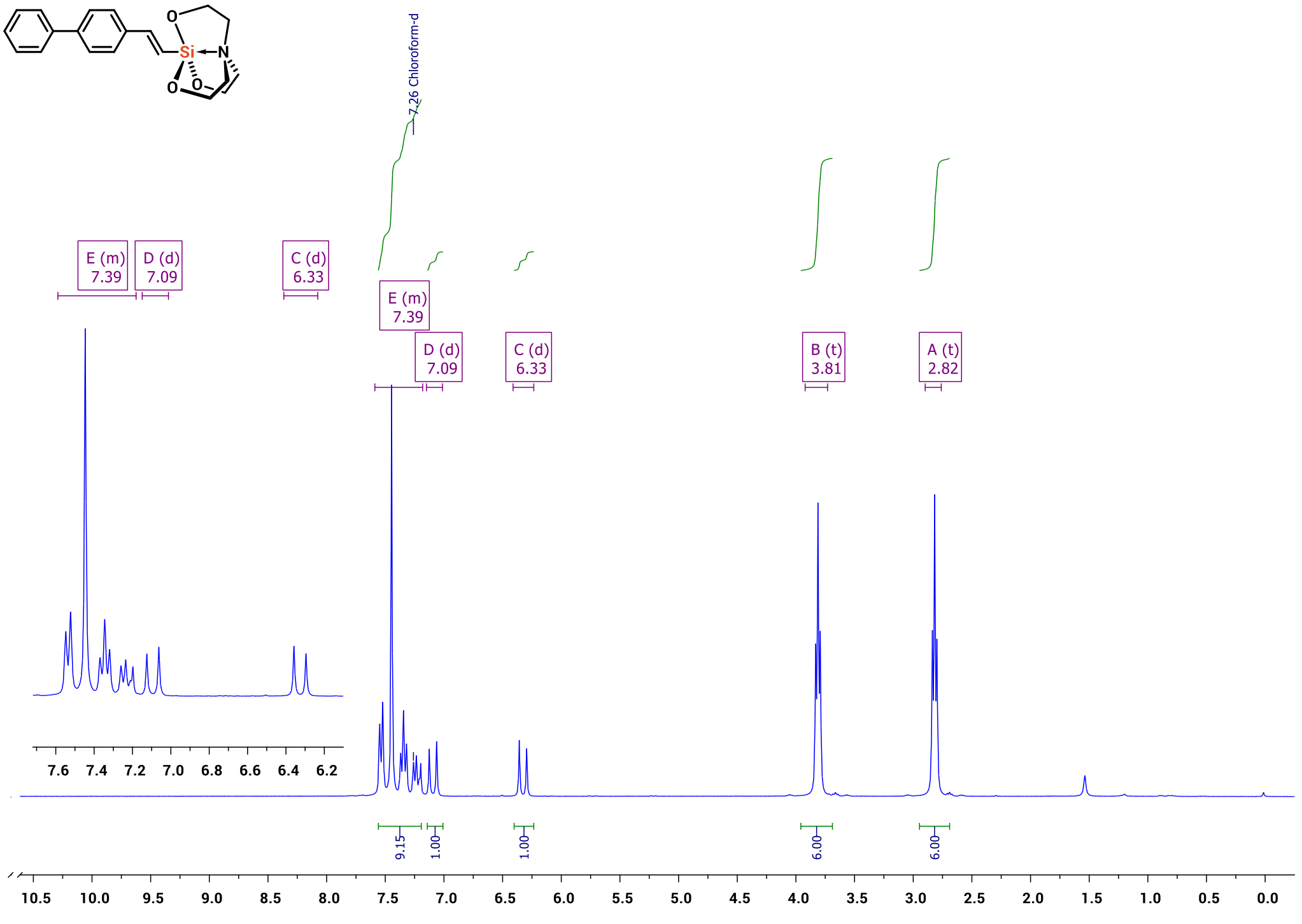
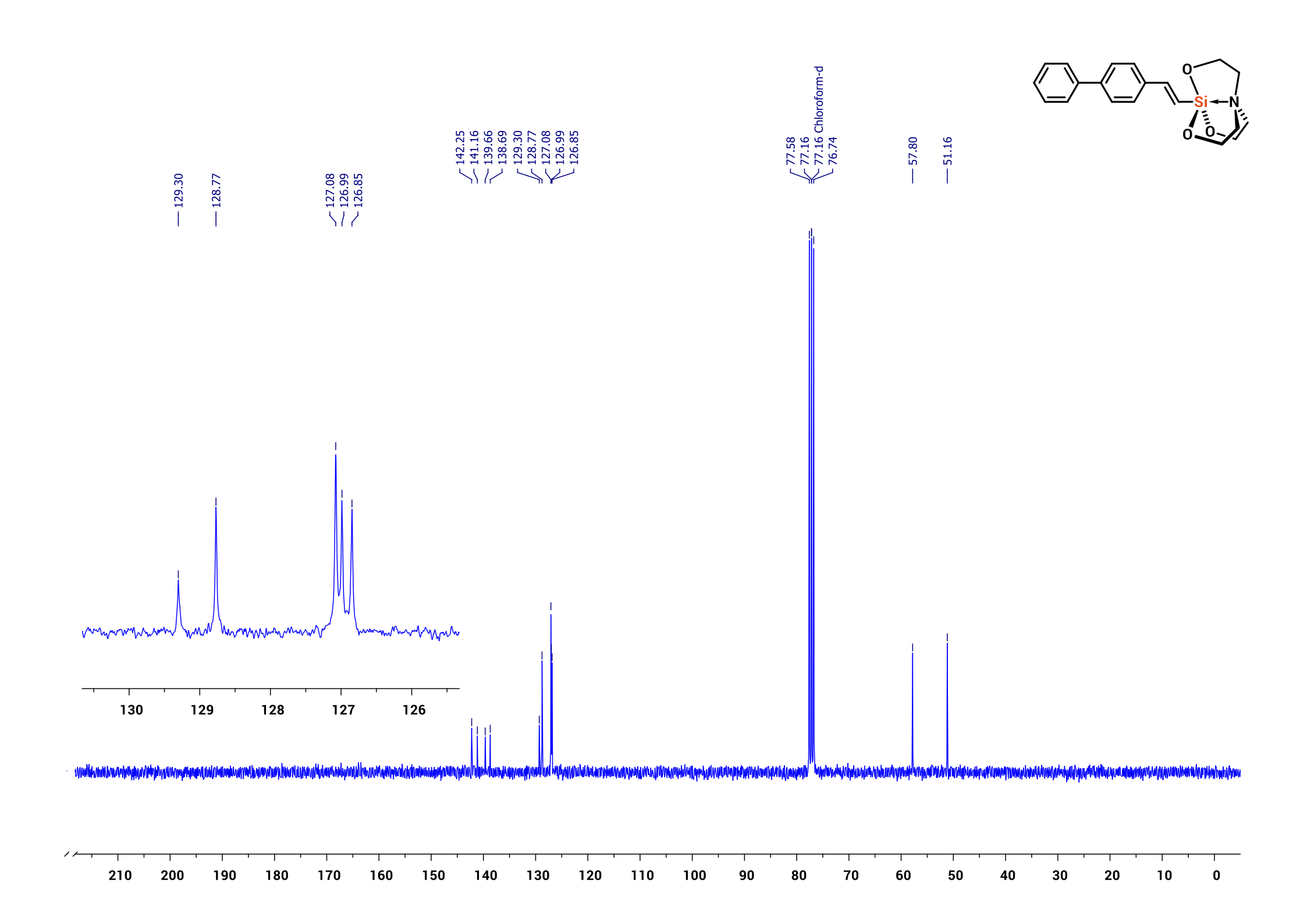
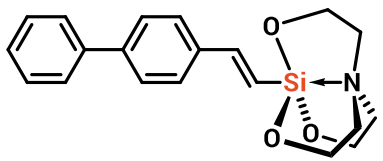
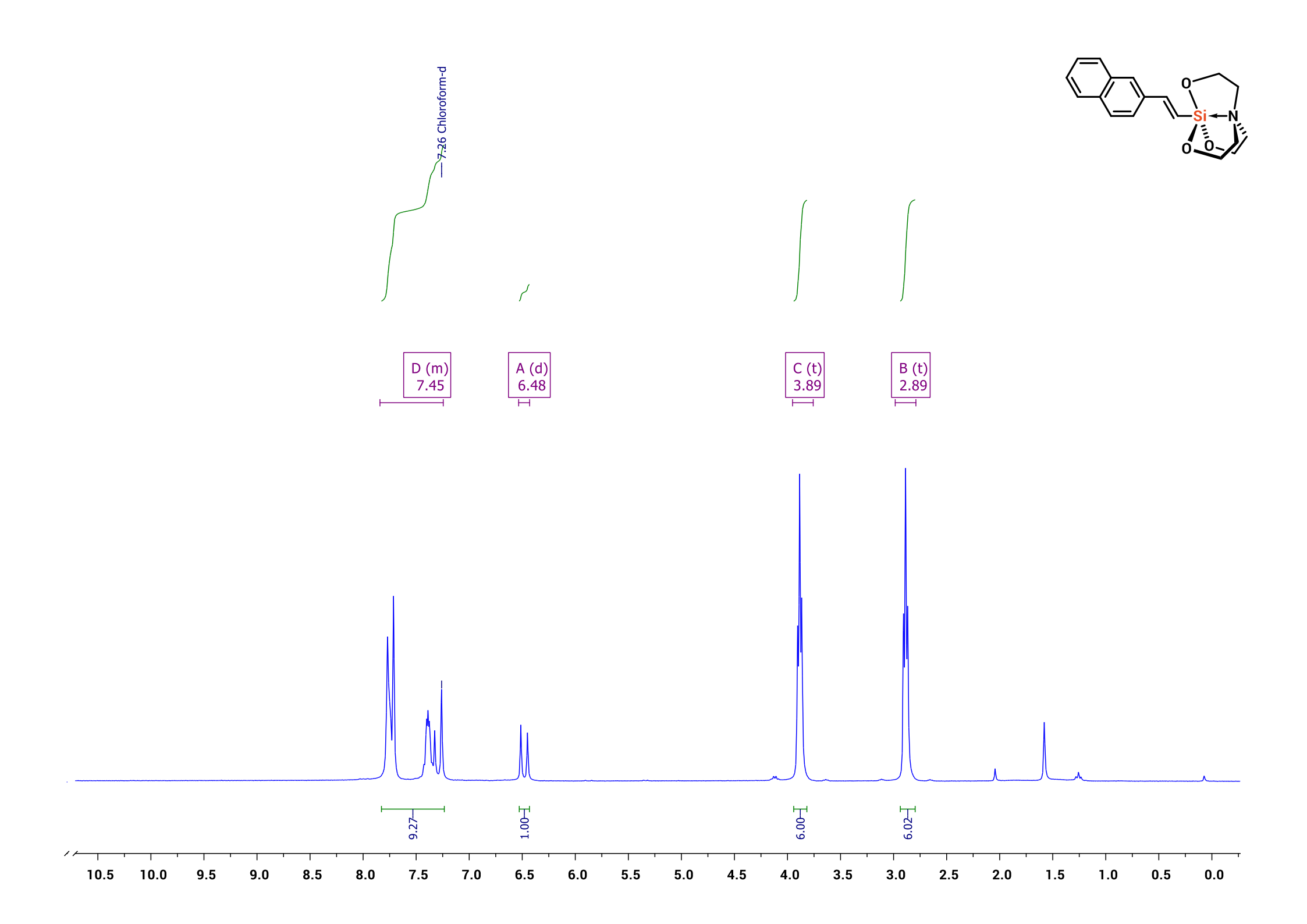
-79.39
MeO
O
Si
N
O
O
-60
-70
-80
-90
-100
-110
100
80
60
40
20
0
-20
-40
-60
-80
-100
-130
-160
-190
-220
-250
-280

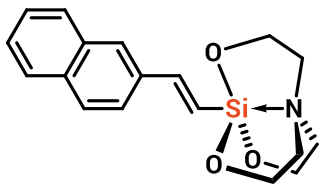

7.26 Chloroform-d
E (m) 7.39
D (d) 7.09
C (d) 6.33
B (t) 3.81
A (t) 2.82
9.15
1.00
1.00
6.00
6.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
7.6 7.4 7.2 7.0 6.8 6.6 6.4 6.2


129.30
128.77
127.08
126.99
126.85
142.25
141.16
139.66
138.69
129.30
128.77
127.08
126.99
126.85
77.58
77.16
77.16 Chloroform-d
76.74
57.80
51.16
O
Si
N
O
O
130
129
128
127
126
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

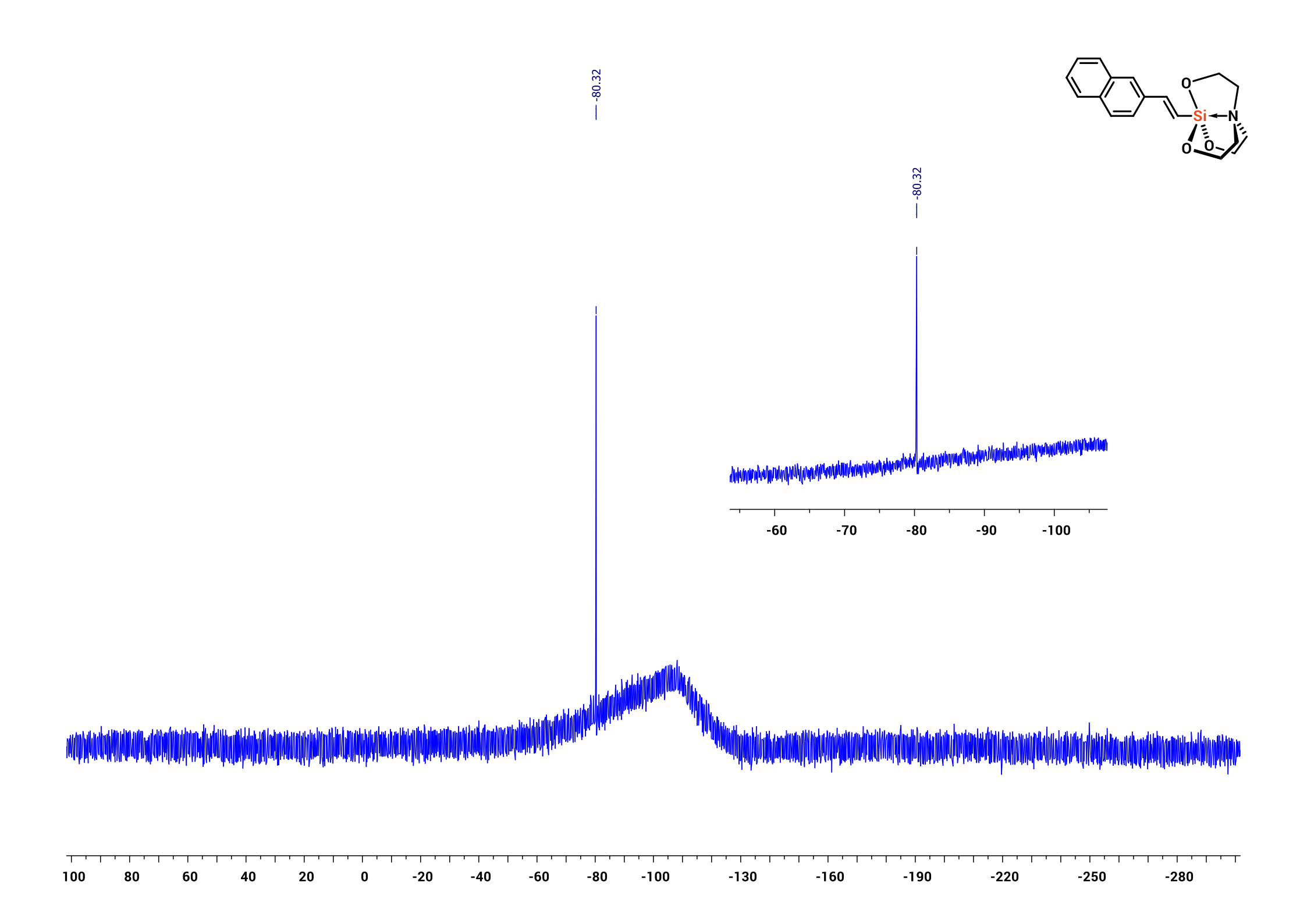

O
Si
N
O
O

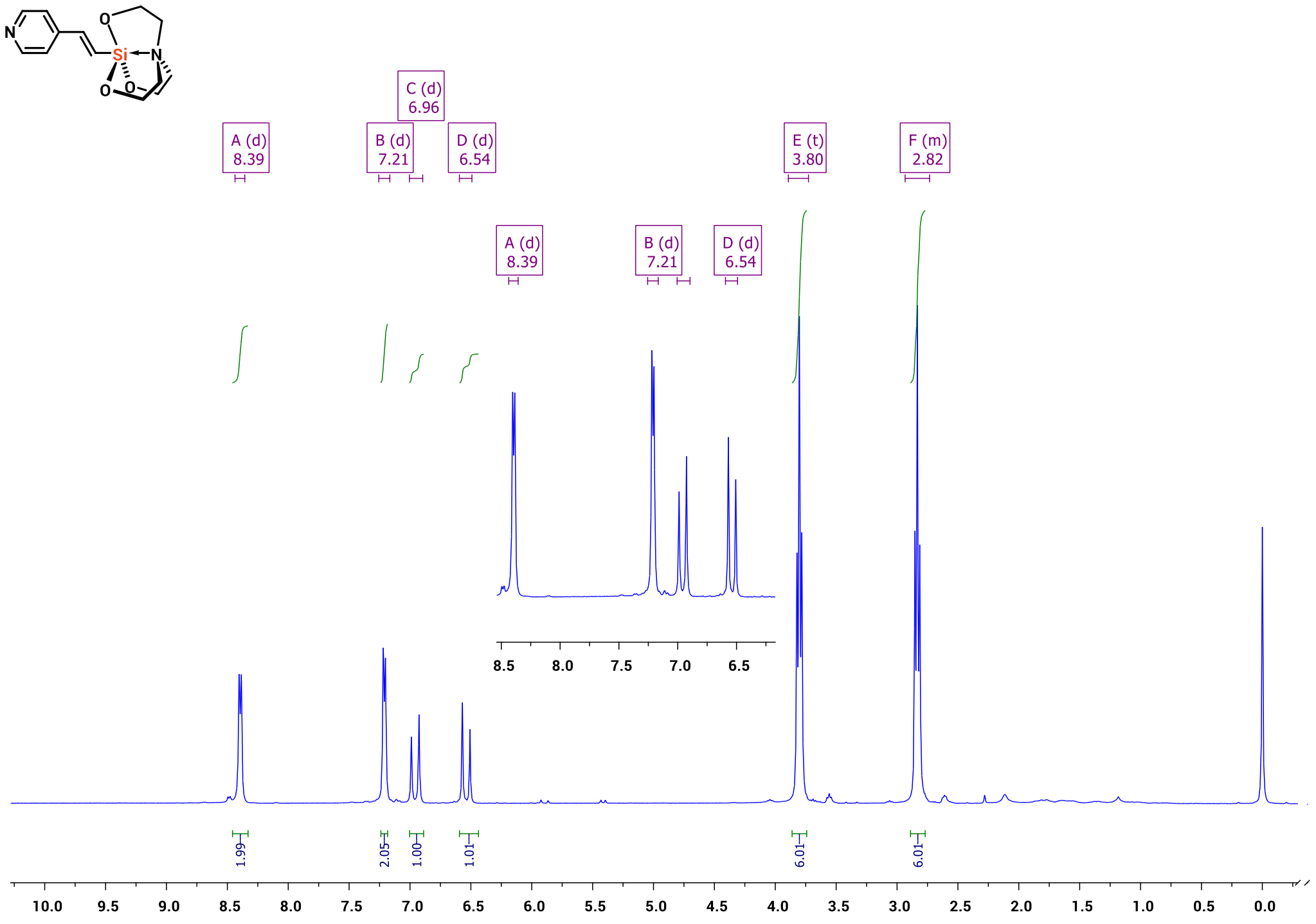
-80.07
-80.07
-70
-75
-80
-85
-90
-95
-100
100
80
60
40
20
0
-20
-40
-60
-80
-100
-130
-160
-190
-220
-250
-280

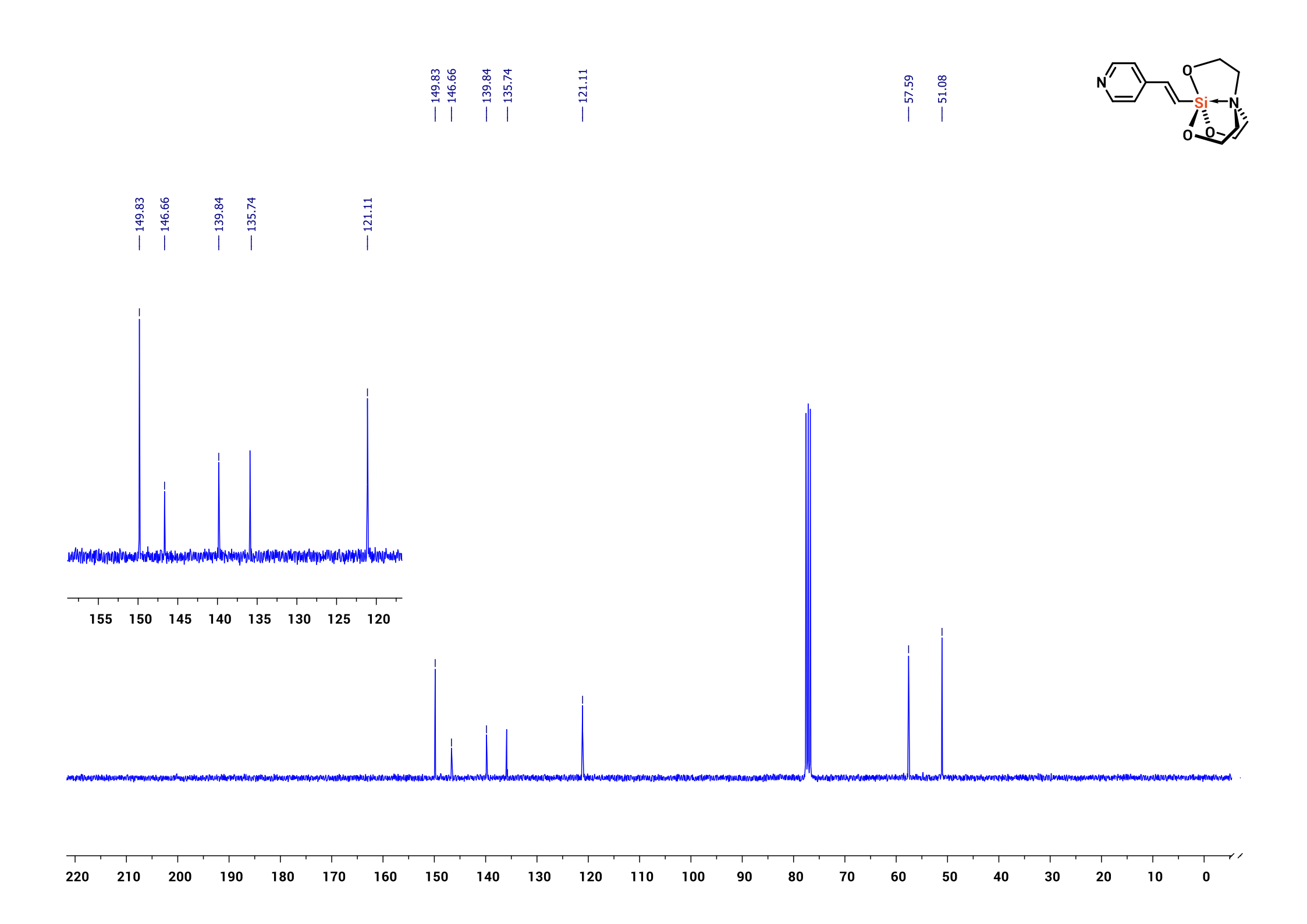

7.26 Chloroform-d
D (m)
7.45
A (d)
6.48
C (t)
3.89
B (t)
2.89
9.27
1.00
6.00
6.02
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
O
Si
N
O
O

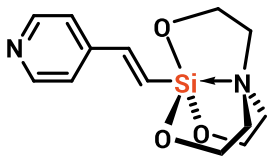


142.75
137.11
133.76
133.11
129.70
128.24
127.67
127.60
126.54
125.80
125.42
124.17
57.77
51.13

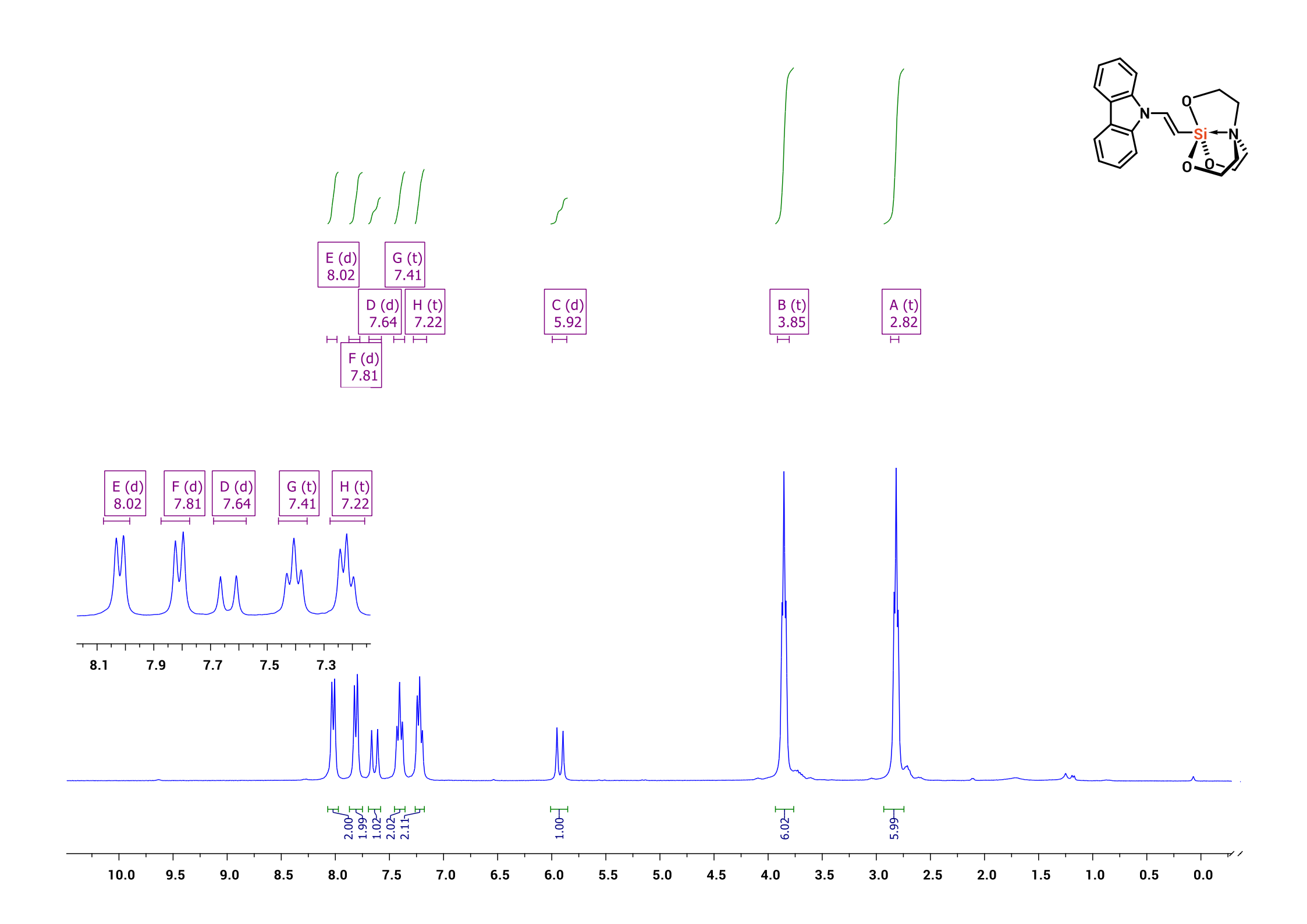

-80.32
-80.32
O
Si
N
O
O
-60
-70
-80
-90
-100
100
80
60
40
20
0
-20
-40
-60
-80
-100
-130
-160
-190
-220
-250
-280

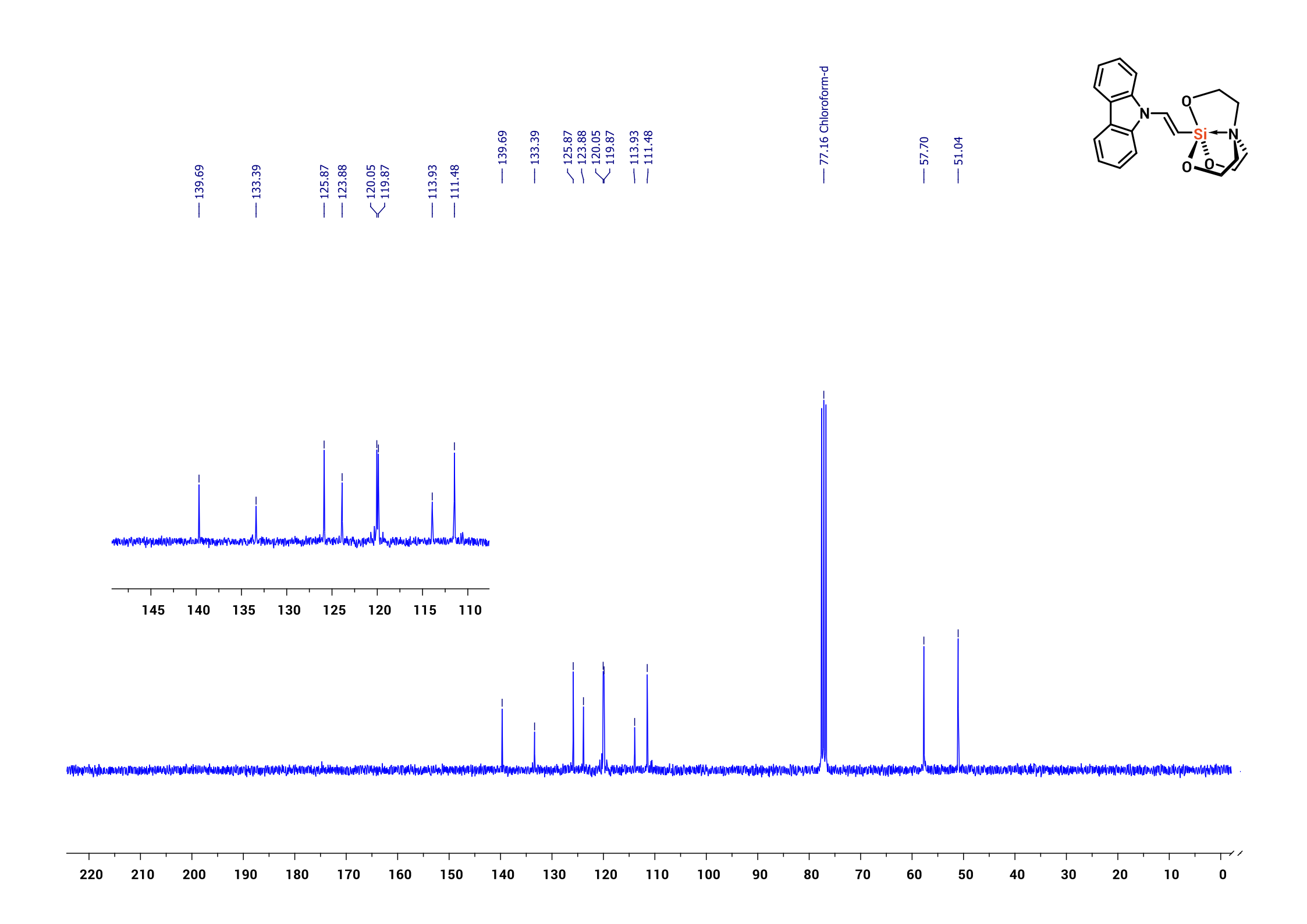

A (d)
8.39
B (d)
7.21
C (d)
6.96
D (d)
6.54
E (t)
3.80
F (m)
2.82
1.99
2.05
1.00
1.01
6.01
6.01
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

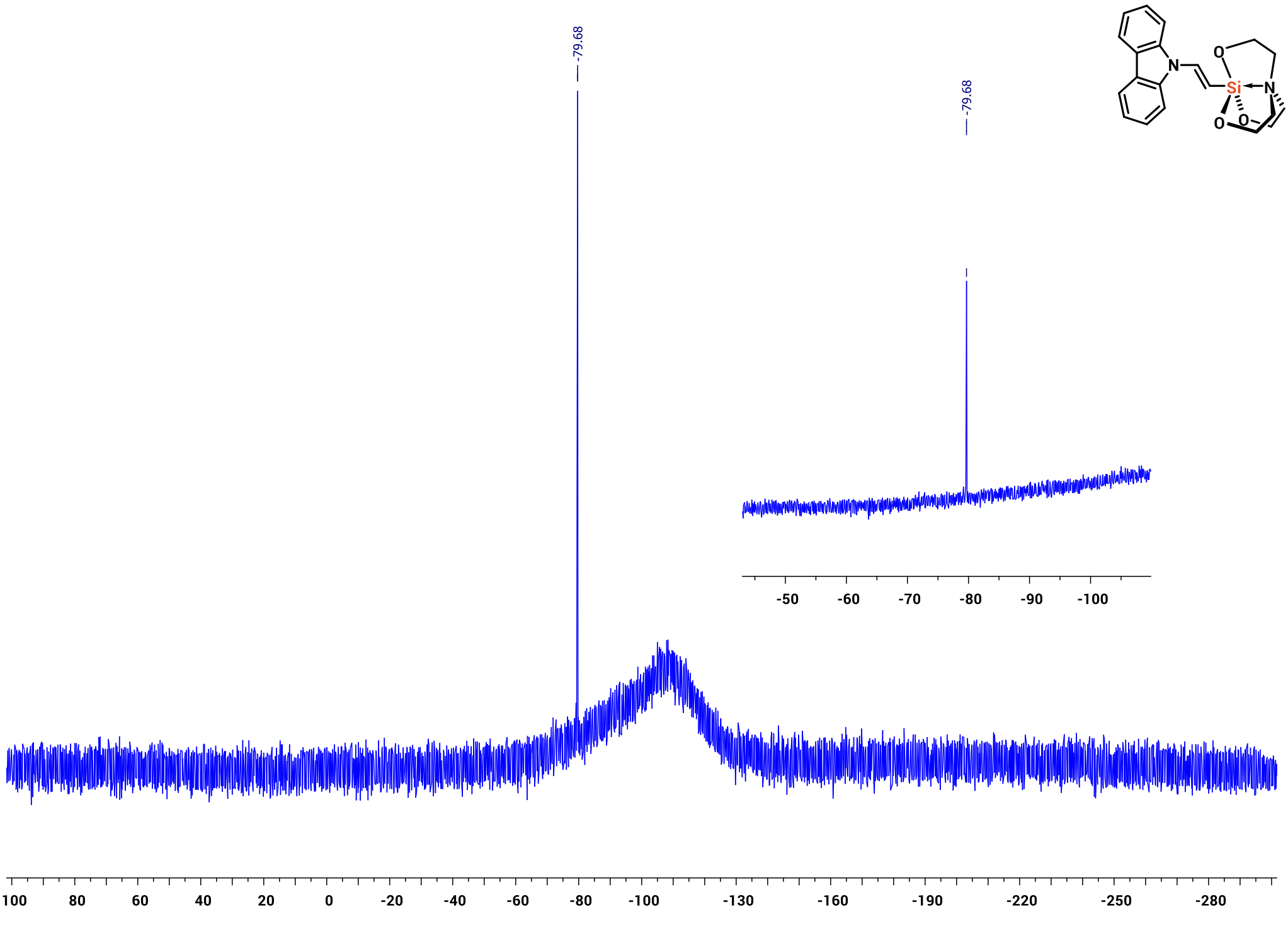

149.83
146.66
139.84
135.74
121.11
57.59
51.08
N
O
Si
N
O
O
155 150 145 140 135 130 125 120
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

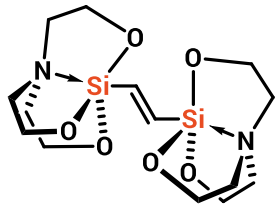

N
O
Si
N
O
O

-82.44
-82.44
-60
-65
-70
-75
-80
-85
-90
-95
100
80
60
40
20
0
-20
-40
-60
-80
-100
-130
-160
-190
-220
-250
-280

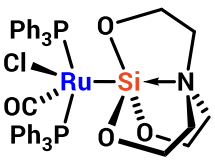

E (d) 8.02
G (t) 7.41
D (d) 7.64
H (t) 7.22
F (d) 7.81
C (d) 5.92
B (t) 3.85
A (t) 2.82
E (d) 8.02
F (d) 7.81
D (d) 7.64
G (t) 7.41
H (t) 7.22
8.1
7.9
7.7
7.5
7.3
2.00
1.99
1.02
2.02
2.11
1.00
6.02
5.99
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0


139.69
133.39
125.87
123.88
120.05
119.87
113.93
111.48
139.69
133.39
125.87
123.88
120.05
119.87
113.93
111.48
77.16 Chloroform-d
57.70
51.04
O
N
Si
N
O
O
145 140 135 130 125 120 115 110
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

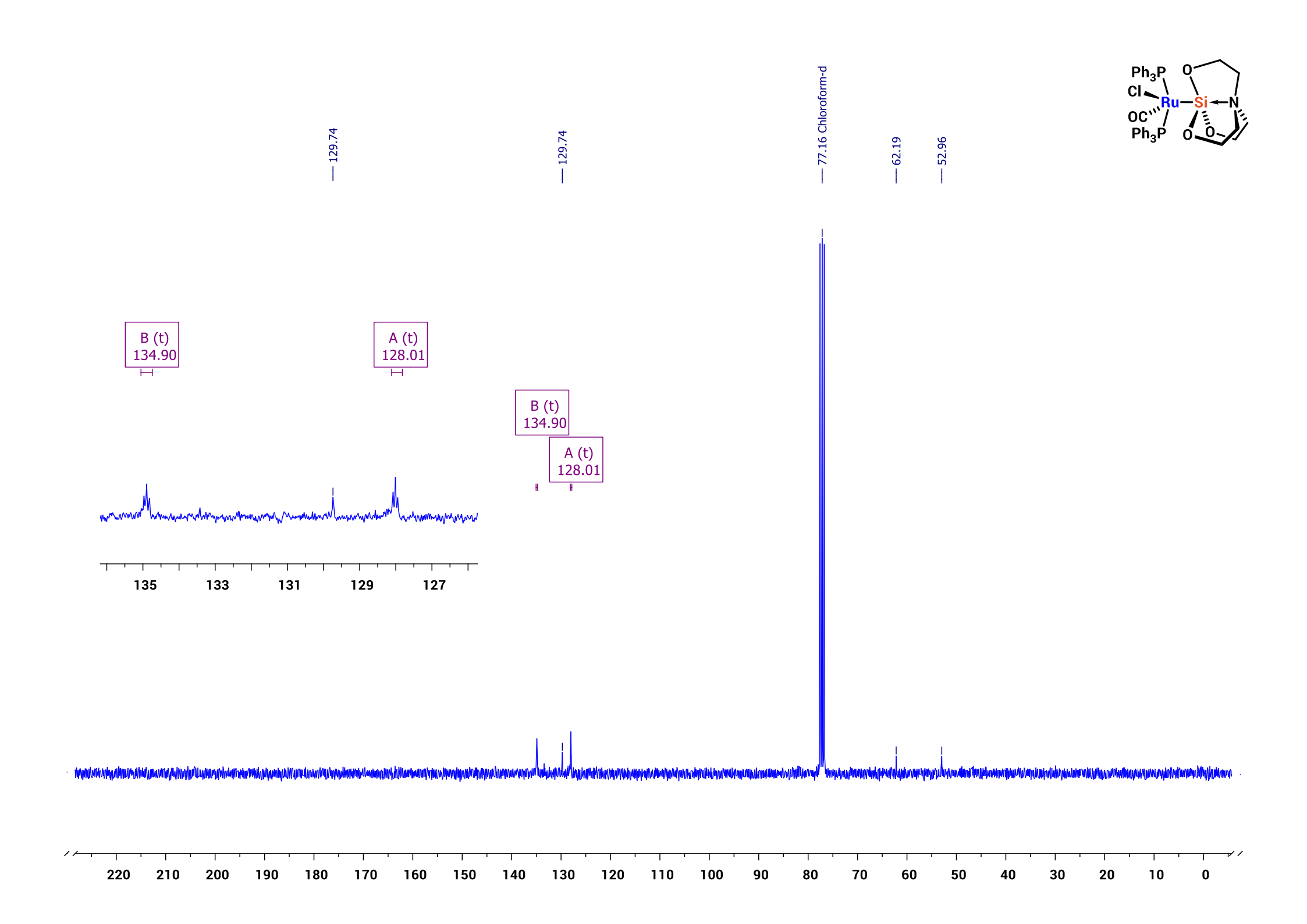

-79.68
-79.68
O
N
Si
N
O
O
-50
-60
-70
-80
-90
-100
100
80
60
40
20
0
-20
-40
-60
-80
-100
-130
-160
-190
-220
-250
-280

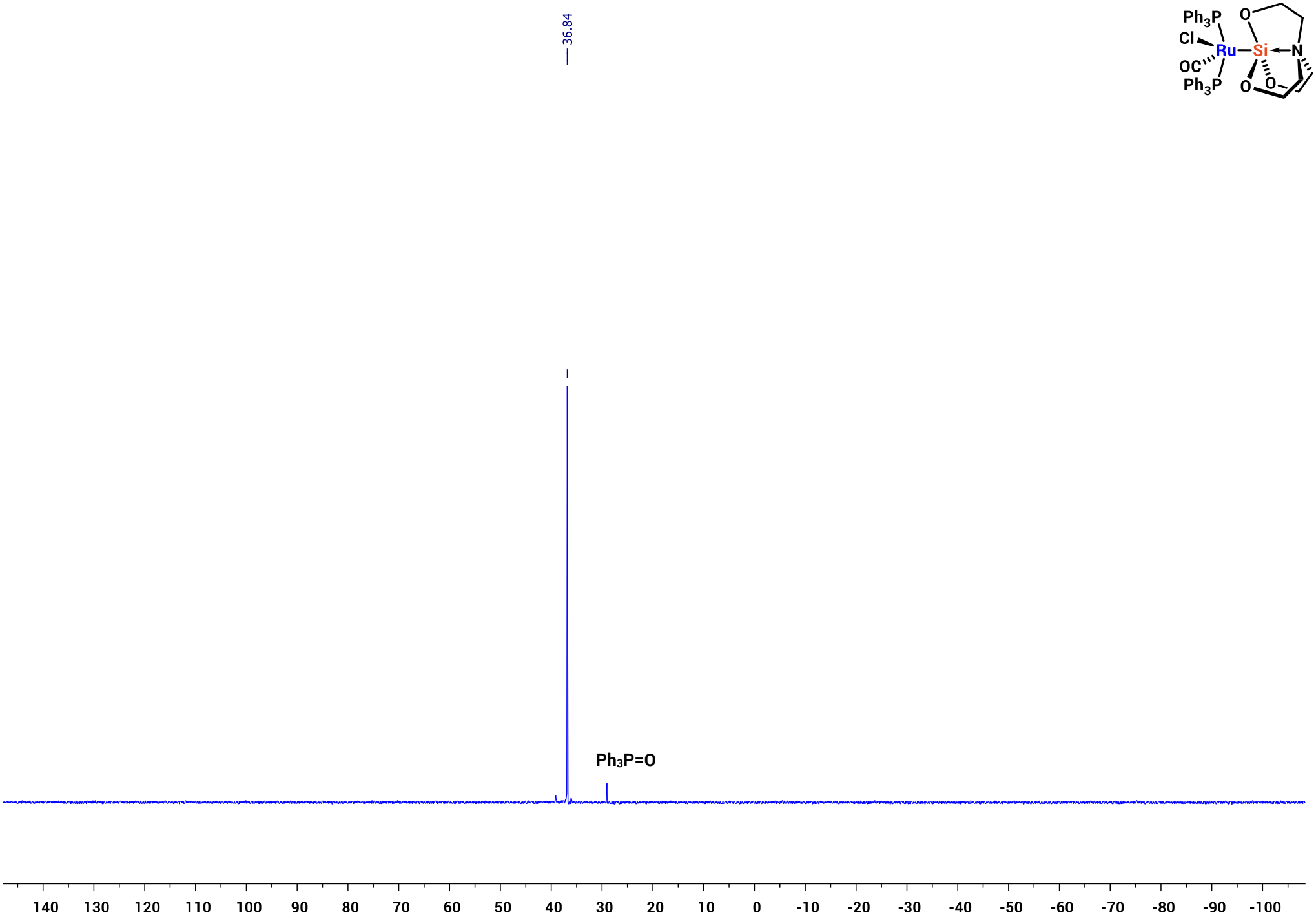

O
N
Si
O
O
Si
O
O
N
O

7.26 Chloroform-d
6.58
A (m)
3.78
B (m)
2.81
H2O
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0


Ph3P
Cl
Ru
Si
N
OC
Ph3P
O
O
O

7.26 Chloroform-d
A (m)
7.31
C (s)
3.25
B (s)
2.54
Silicone grease
6.39
1.00
1.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5


129.74
129.74
77.16 Chloroform-d
62.19
52.96
B (t)
134.90
A (t)
128.01
B (t)
134.90
A (t)
128.01
135
133
131
129
127
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0


36.84
Ph3P=O
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100