Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Rare-earth-catalyzed regio- and enantioselective hydrosilylation of aryl-substituted terminal and internal alkenes

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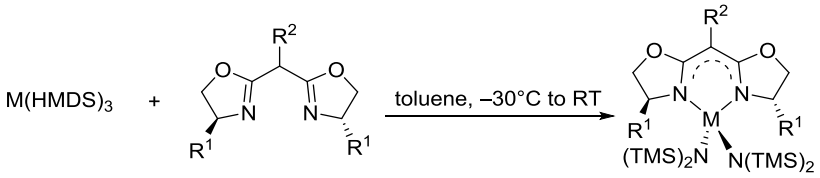
1. General remarks

^{1}HNMR spectra were recorded on Bruker ASCENDTM 400M (400 MHz) and ASCENDTM 600M (600 MHz). Chemical shifts were reported in ppm from tetramethylsilane with the solvent resonance as the internal standard ($CDCl_3$, δ = 7.26). Spectra were reported as follows: chemical shift (δ ppm), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, dd = doublet of doublets, dt = doublet of triplets), coupling constants (Hz), integration and assignment. $^{13}C\{^{1}H\}$ NMR spectra were collected on ASCENDTM 400M (101 MHz) and ASCENDTM 600M (153 MHz) with complete proton decoupling. Chemical shifts are reported in ppm from the tetramethylsilane with the solvent resonance as internal standard ($CDCl_3$, δ = 77.0). GC-MS analysis was performed on Shimadzu GCMS-2020 NX gas chromatograph with a SH-I-5MS column. Enantiomeric ratio (er) were determined by HPLC analysis using the corresponding commercial chiral column as stated in the experimental procedures at 23 ℃ with UV detector at 254 nm. Optical rotations were measured on Rudolph Research Analytic Automatic Polarimeter and reported as follows: $[\alpha]_D^T$ (*c* g/100 mL, in CH_2Cl_2). Infrared spectra (IR) were recorded on Bruker Tensor II spectrometer with Plantium ATR accessory and the peaks were reported as absorption maxima (v, cm^{-1}). Melting point ranges were determined on OptiMelt. X-ray crystallographic data were collected by a Bruker D8 Venture Photon II. All manipulations were carried out using standard Schlenk, high-vacuum and glovebox techniques unless otherwise noted. The solvents (THF, toluene, *n*-pentane and *n*-hexane) were freshly distilled from sodium prior to use. Alkenes were prepared according to Wittig reaction or the previously reported procedures.[1] Phenylsilanes were prepared according to the previously reported procedures.[2] Alkenes and phenylsilanes were vacuum-distilled over CaH_2 prior to use. Other chemicals were of analytical grade and were used as received. $La(HMDS)_3$, $Y(HMDS)_3$, $Cd(HMDS)_3$ were purchased from Sigma-Aldrich. $Ce(HMDS)_3$, $Nd(HMDS)_3$ was prepared according to known procedures.[3]

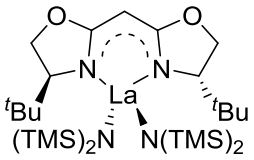
2. Preparation of catalysts

2.1 General procedure for the synthesis of rare-earth/bis(oxazoline) complexes.

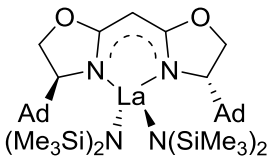


Bis(oxazoline) were synthesized according to the reported procedure[4].

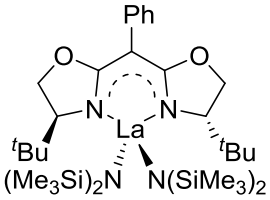
General Procedure (GP): In a glovebox, a dry Schlenk bottle was charged with rare earth metal amide and toluene (0.2 mol/L). Then, a solution of bis(oxazoline) in toluene (1 equiv.) was slowly added to the stirred solution at –30 °C and the resulting reaction mixture was warmed up and stirred at room temperature for more than 12 h. The volatiles were removed under vacuum. The remaining residue was extracted by *n*-hexane and the filtrate was removed under vacuum to afford the desired chiral catalyst.



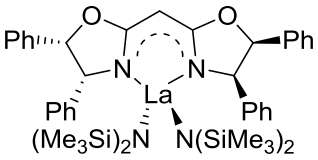
La-BOX-^{t}Bu ($C_{27}H_{61}LaN_4O_2Si_4$) Prepared according to the general procedure to yield 620.0 mg (85%) of yellow solid. **^{1}H NMR** (400 MHz, Benzene-d_6) δ 4.68 (s, 1H), 3.74 – 3.65 (m, 6H), 0.81 (s, 18H), 0.38 (s, 36H). **$^{13}C\{^{1}H\}$ NMR** (101 MHz, Benzene-d_6) δ 172.7, 74.8, 68.0, 57.5, 34.6, 26.9, 4.7.



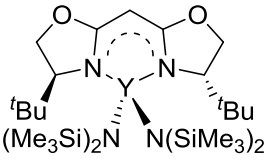
La-BOX-Ad ($C_{39}H_{73}LaN_4O_2Si_4$) Prepared according to the general procedure to yield 47.0 mg (53%) of pale brown solid. **^{1}H NMR** (400 MHz, Benzene-d_6) δ 4.65 (s, 1H), 3.94 (dd, J = 8.3, 3.1 Hz, 2H), 3.85 (dd, J = 8.8, 3.1 Hz, 2H), 3.77 (t, J = 8.5 Hz, 2H), 1.61 (s, 15H), 1.36 (s, 15H), 0.39 (s, 36H). **$^{13}C\{^{1}H\}$ NMR** (101 MHz, Benzene-d_6) δ 173.6, 74.7, 66.5, 57.7, 38.9, 38.6, 37.1, 36.9, 31.7, 30.2, 28.4, 23.1, 5.0.



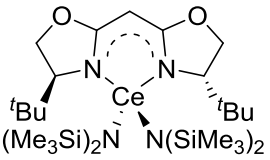
La-^{Ph}BOX-^{t}Bu ($C_{33}H_{65}LaN_4O_2Si_4$) Prepared according to the general procedure to yield 53 mg (66%) of yellow solid. **^{1}H NMR** (400 MHz, Benzene-d_6) δ 7.62 – 7.52 (m, 2H), 7.32 (t, *J* = 7.6 Hz, 2H), 7.13 (t, *J* = 7.4 Hz, 1H), 3.89 (dd, *J* = 8.5, 2.9 Hz, 2H), 3.68 (dd, *J* = 9.0, 2.9 Hz, 2H), 3.61 (t, *J* = 8.7 Hz, 2H), 0.85 (s, 18H), 0.37 (s, 36H). **$^{13}C\{^{1}H\}$ NMR** (101 MHz, Benzene-d_6) δ 172.5, 138.9, 133.2, 125.5, 75.4, 73.7, 67.9, 35.2, 26.4, 4.9.



La-BOX-DPh ($C_{43}H_{61}LaN_4O_2Si_4$) Prepared according to the general procedure to yield 68.0 mg (74%) of yellow solid. **^{1}H NMR** (400 MHz, Benzene-d_6) δ 7.03 – 6.98 (m, 4H), 6.97 – 6.90 (m, 9H), 6.90 – 6.85 (m, 5H), 6.84 (s, 2H), 5.68 (d, J = 8.2 Hz, 2H), 5.56 (d, J = 8.2 Hz, 2H), 5.25 (s, 1H), 0.21 (s, 36H). **^{13}C{^{1}H} NMR** (101 MHz, Benzene-d_6) δ 174.4, 139.0, 136.3, 128.7, 128.5, 126.6, 84.8, 72.3, 58.6, 4.0.



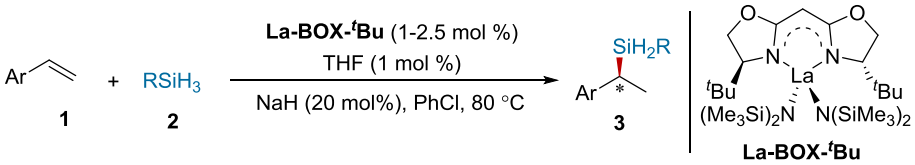
Y-BOX-^{t}Bu ($C_{27}H_{61}YN_4O_2Si_4$) Prepared according to the general procedure to yield 30.0 mg (41%) of pale brown solid. **^{1}H NMR (400 MHz, Benzene-d_6)** δ 4.66 (s, 1H), 4.01 (dd, J = 8.5, 3.1 Hz, 2H), 3.83 – 3.73 (m, 4H), 0.84 (s, 18H), 0.38 (s, 36H). **^{13}C{^{1}H} NMR** (101 MHz, Benzene-d_6) δ 174.4, 174.4, 74.2, 68.4, 58.5, 34.9, 26.3, 6.1



Ce-BOX-^{t}Bu ($C_{27}H_{61}CeN_4O_2Si_4$) Prepared according to the general procedure to yield 30.0 mg (41%) of pale brown solid. Complexes **Ce-BOX-^{t}Bu** are paramagnetic and display broad NMR signals. The structure was confirmed by X-ray single-crystal analysis.

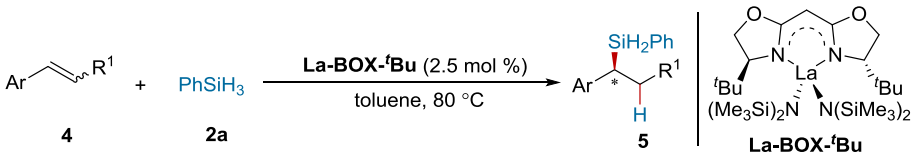
3. Typical procedure for the catalytic asymmetric reaction

3.1 General procedure for the synthesis of chiral hydrosilylation of aryl-substituted terminal alkenes



In a glovebox, a dry reaction tube was charged with **La-BOX-^{t}Bu** (1 mol %, 3.6 mg), olefins **1** (0.50 mmol) and phenylsilanes **2** (0.50 mmol). Then, chlorobenzene (0.50 mL), THF (1 mol %, 0.4 μL) and NaH (20 mol %, 2.4 mg) was added under argon atmosphere and the mixture was stirred at corresponding temperature for the indicated time. The residue was subjected to flash chromatography on silica gel (Eluent: petroleum) to afford the desired chiral product **3**.

3.2 General procedure for the chiral hydrosilylation of aryl-substituted internal alkenes

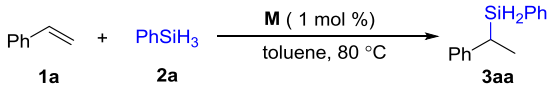


In a glovebox, a dry reaction tube was charged with **La-BOX-^{t}Bu** (2.5 mol %, 9.1 mg), phenylsilane **2a** (0.50 mmol) and aryl-substituted internal alkenes **4** (0.50 mmol). Then, toluene (0.50 mL) was added under argon atmosphere and the mixture was stirred at corresponding temperature for the indicated time. The residue was purified by flash chromatography on silica gel (Eluent: petroleum) to afford the desired chiral product **5**.

4. Optimization of the reaction conditions

4.1. Hydrosilylation of terminal alkenes.

(a) Screening of different rare-earth metal salts.[a]



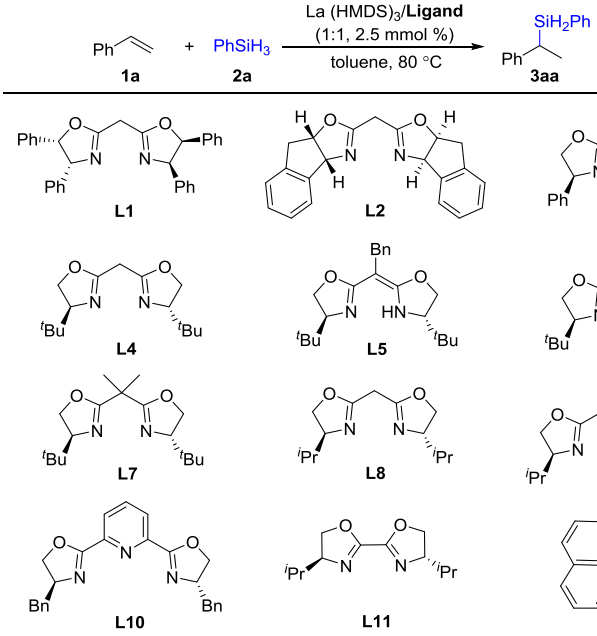
1a **2a** **3aa**

Entry[a]	**M**	Radius (Å)	Yield (%)[b]	b:l
1	La(HMDS)$_3$	1.032	71	19:1
2	Ce(HMDS)$_3$	1.01	68	11:1
3	Nd(HMDS)$_3$	0.983	50	9:1
4	Gd(HMDS)$_3$	0.938	36	5.5:1
5	Y(HMDS)$_3$	0.900	7	6:1
6	Er(HMDS)$_3$	0.890	NR	-

[a] All reactions were carried out with rare-earth metal salts (2.5 mol %), ethenylbenzene **1a** (0.50 mmol) and phenylsilane **2a** (0.50 mmol) in toluene (0.5 mL) at 80 °C for 22 h.
[b] Yield was determined by ^{1}H NMR.

Note: The above results indicated that the radius of rare-earth ions had a significant effect on the reactivity and regioselectivity. La(HMDS)$_3$ with large ionic radius (1.032 Å) provided the desired product in high yield and regioselectivity. Therefore, La(HMDS)$_3$ was selected the central metal for further investigation.

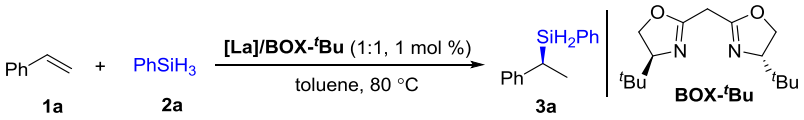
(b) Screening of chiral ligands.[a]



Entry[a]	Ligand	Yield (%)[b]	b:l	er (%)[c]
1	**L1**	76	15:1	51:49
2	**L2**	67	10:1	58.5:41.5
3	**L3**	74	13:1	racemic
4	**L4**	70	>19:1	76.5:23.5
5	**L5**	32	>19:1	58:42
6	**L6**	51	14:1	56:44
7	**L7**	86	>19:1	racemic
8	**L8**	67	>19:1	54.5:45.5
9	**L9**	12	17:1	56.5:43.5
10	**L10**	32	>19:1	52.5:47.5
11	**L11**	77	>19:1	racemic
12	**L12**	83	>19:1	51:49
13[d]	**L4**	81	>19:1	88:12
14[d],[e]	**L4**	79	>19:1	89:11

[a] Unless otherwise noted, all reactions were carried out with in-situ generated catalyst. La(HMDS)$_3$/**Ligand** (1:1, 2.5 mol %) in toluene (0.5 mL) was stirred at room temperature for 12 h. Then, ethenylbenzene **1a** (0.50 mmol) and phenylsilane **2a** (0.50 mmol) was added, the resulting mixture was stirred at 80 °C for 22 h. [b] Yield was determined by ^{1}H NMR. [c] Determined by HPLC analysis on a chiral stationary phase. [d] The catalyst **La-BOX-^{t}Bu** was prepared in advance. [e] **La-BOX-^{t}Bu** (1 mol %)

(b) Screening of different rare-earth metal salts.[a]

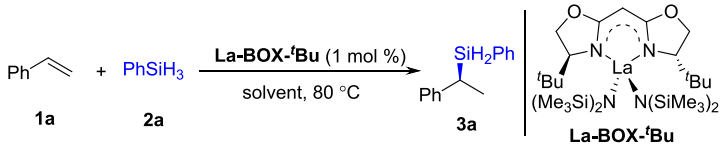


Entry[a]	[La]	Yield (%)[b]	b:l	er (%)[c]
1	**La(HMDS)$_3$**	80	>19:1	81.5:18.5
2	**La(CH$_2$C$_6$H$_4$NMe$_2$-o)$_3$**	20	>19:1	70:30
3	**La(2,6-^{t}Bu$_2$-C$_6$H$_4$O)$_3$**	NR	-	-
4	**La(CH$_2$TMS)$_3$**	trace	-	-
5[d]	**La-BOX-^{t}Bu**	79	>19:1	89:11
6[d],[e]	**La-BOX-^{t}Bu**	76	>19:1	76.5:23.5

[a] Unless otherwise noted, all reactions were carried out with in-situ generated catalyst. La^{III}/**Box-^{t}Bu** (1:1, 1 mol %) in toluene (0.5 mL) was stirred at room temperature for 12 h. Then, ethenylbenzene **1a** (0.50 mmol) and phenylsilane **2a** (0.50 mmol) was added and the resulting mixture was stirred at 80 °C for 22 h. [b] Yield was determined by ^{1}H NMR. [c] Determined by HPLC analysis on a chiral stationary phase. [d] The catalyst **La-BOX-^{t}Bu** was prepared in advance. [e] 1,1,1,3,3,3-hexamethyldisilazane (1 mol %) was added.

Note: The above outcomes suggested that the basic ligand had a significant effect on the reactivity and enantioselectivity. Moreover, 1,1,1,3,3,3-hexamethyldisilazane generated in the process of catalyst preparation exhibited an adverse influence on the enantioselectivity.

(c) Screening of the solvents.[a]

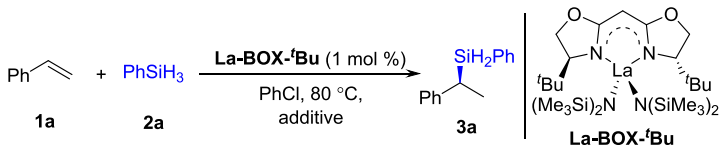


Entry[a]	Solvent	Yield (%)[b]	b:l	er (%)[c]
1	toluene	79	>19:1	89:11
2	benene	18	>19:1	82:18
3	THF	40	>19:1	73:27
4	MTBE	55	>19:1	74:26
5	Et_2O	79	>19:1	87.5:12.5
6	cyclohexane	75	>19:1	86:14
7	toluene[d]	79	>19:1	89:11
8	toluene[e]	75	>19:1	88:12
9	chlorobenzene	79	>19:1	90:10
10	benzotrifluoride	trace	>19:1	-
11	*o*-xylene	9	>19:1	73:27
12	*m*-xylene	48	>19:1	85.5:14.5
13	*p*-xylene	66	>19:1	85:15
14	mesitylene	55	>19:1	77.5:22.5
15[f]	chlorobenzene	76	>19:1	90.5:9.5

[a] Unless otherwise noted, all reactions were carried out with **La-BOX-^{t}Bu** (1 mol %, 3.6 mg), phenylsilanes (0.50 mmol), ethenylbenzene (0.50 mmol) and chlorobenzene (0.50 mL) at 80 °C for 22 h. [b] Yield was determined by ^{1}H NMR. [c] Determined by HPLC analysis on a chiral stationary phase. [d] 0.3 mL. [e] 1 mL. [f] THF (0.4 μL) was added. THF: tetrahedrofuran, MTBE: methyl *t*-butyl ether.

According to previous work[5] by Teuben, we envisioned that the addition of THF was benefit to the stereoselectivity through coordination with presume rare-earth hydride species.

(d) Screening of the additive.[a]

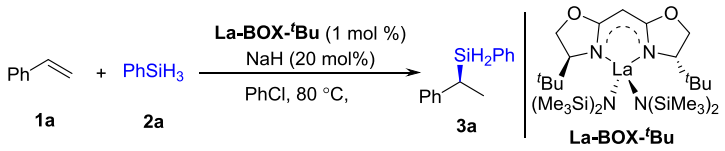


Entry[a]	Additive	Yield (%)[b]	b:l	er (%)[c]
1	no additive	76	>19:1	90.5:9.5
2	NaH (50 mol %)	99	>19:1	91:9
3	NaH (20 mol %)	99	>19:1	92.5:7.5
4	NaH (10 mol %)	96	>19:1	90.5:9.5
5	NaH (10 mol %)	93	>19:1	90:10
6	CaH_2 (20 mol %)	88	>19:1	88.5:11.5
7	CaH_2 (10 mol %)	92	>19:1	89:11
8	$NaBH_4$ (20 mol %)	92	>19:1	89.5:10.5
9	$NaBH_4$ (10 mol %)	86	>19:1	89:11

10	$LiAlH_4$ (20 mol %)	90	>19:1	racemic
11	$LiAlH_4$ (10 mol %)	88	>19:1	racemic
12	KH (20 mol %)	94	>19:1	81.5:18.5
13	KH (10 mol %)	96	>19:1	89:11

[a] Unless otherwise noted, all reactions were carried out with **La-BOX-^{t}Bu** (1 mol %, 3.6 mg), phenylsilanes (0.50 mmol), ethenylbenzene (0.50 mmol), chlorobenzene (0.50 mL), THF (0.4 μL) and additive (20 mol%) at 80 °C for 22 h. [b] Yield was determined by ^{1}H NMR. [c] Determined by HPLC analysis on a chiral stationary phase.

(e) Screening of reaction temperature.[a]

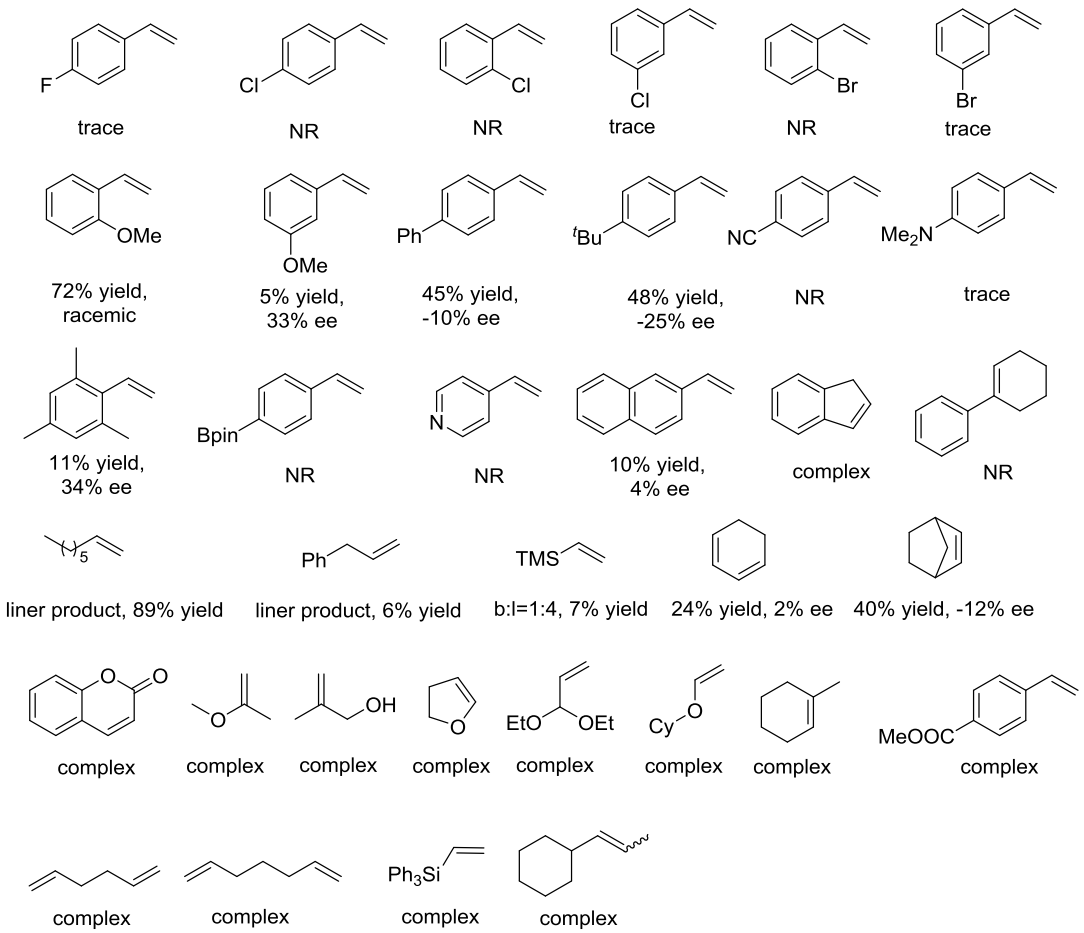


Entry[a]	T (°C)	Yield (%)[b]	b:l	er (%)[c]
1	80	99	>19:1	92.5:7.5
2	100	92	>19:1	88:12
3	60	63	>19:1	89.5:10.5
4	40	trace	>19:1	75:25

[a] Unless otherwise noted, all reactions were carried out with **La-BOX-^{t}Bu** (1 mol %, 3.6 mg), phenylsilanes (0.50 mmol), olefins (0.50 mmol), chlorobenzene (0.50 mL), THF (0.4 μL) and NaH (20 mol %, 2.4 mg) at 80 °C for 22 h. [b] Yield was determined by ^{1}H NMR. [c] Determined by HPLC analysis on a chiral stationary phase.

(f) Scope limitation

olefins

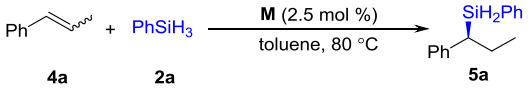


silanes

Ph_2SiH_2	$PhMeSiH_2$	*n*-$hexSiH_3$
trace	trace	79% yield, 29% ee

4.2 Hydrosilylation of internal alkenes.

(a) Screening of different rare-earth metal salts.[a]



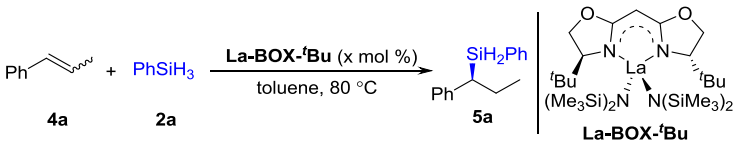
4a **2a** **5a**

Entry[a]	**M**	Radius (Å)	Yield (%)[b]
1	**La(HMDS)$_3$**	1.032	94
2	**Ce(HMDS)$_3$**	1.01	99
3	**Gd(HMDS)$_3$**	0.938	78
4	**Y(HMDS)$_3$**	0.900	trace

[a] Unless otherwise noted, all reactions were carried out with **M** (2.5 mol %), phenylsilanes (0.50 mmol), olefins (0.50 mmol) in toluene (0.5 mL) at 80 °C for 24 h. [b] Yield was determined by NMR.

Note: The above results indicated that the radius of rare-earth ions had a significant effect on the reactivity and regioselectivity. **La(HMDS)$_3$** and **Ce(HMDS)$_3$** with large ionic radius provided the desired product in high yield. Therefore, **La(HMDS)$_3$** was selected the central metal for further investigation because it was commercially available.

(b) Optimization of the reaction conditions.[a]



4a **2a** **5a** **La-BOX-^{t}Bu**

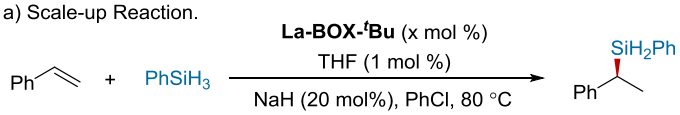
Entry[a]	solvent	x (mol%)	Yield (%)[b]	b:l	er (%)[c]
1	toluene	1	57	>19:1	86.5:13.5
2	toluene	2.5	67	>19:1	83.5:16.5
3	chlorobenzene	2.5	57	>19:1	86.5:13.5
4	*m*-xylene	2.5	50	>19:1	82:18
5	*p*-xylene	2.5	46	>19:1	82.5:17.5
6[d]	toluene	2.5	82	>19:1	88.5:11.5
7[d],[e]	toluene	2.5	trace	-	-
8[d],[f]	toluene	2.5	78	>19:1	88.5:11.5
9[d],[g]	toluene	2.5	trace	-	-

[a] Unless otherwise noted, all reactions were carried out with **La-BOX-^{t}Bu** (x mol %), phenylsilanes (0.10 mmol), olefins (0.10 mmol) in toluene (0.1 mL) at 80 °C for 24 h. [b] Yield was determined by NMR. [c] Determined by HPLC analysis on a chiral stationary phase. [d] 0.50 mmol scale. [e] **Y-BOX-^{t}Bu** (2.5 mol %) was used. [f] NaH (20 mol %, 2.4 mg) was added. [g] **Ce-BOX-^{t}Bu** (2.5 mol %) was used.

***Note*:** During the process of optimization, we found that 0.5 mmol scale reaction could assure reproducibility probably due to the small amount of solvent and volatility of product.

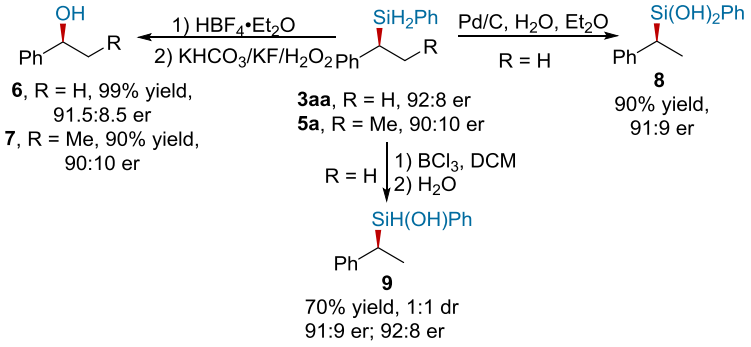
5. Experimental procedure for the scale-up reaction and transformation of the product

a) Scale-up Reaction.



5.0 mmol	1 equiv	x = 1	1.05 g, 99% yield, 92:8 er
1.0 mmol	1 equiv	x = 0.5	0.21 g, >99% yield, 92:8 er
5.0 mmol	1 equiv	x = 0.1	0.85 g, 81% yield, 86:14 er

b) Further Transformations of the Chiral Products.



i) A Schlenk bottle was charged with **La-BOX-^{t}Bu** (1 mol%, 36.4 mg), phenylsilanes (5.0 mmol) and olefins (5.0 mmol). Then, chlorobenzene (5 mL), THF (4 μL) and NaH (20 mol %, 24.0 mg) was added under argon atmosphere and the mixture was stirred at 80 °C for 22 h. The residue was subjected to flash chromatography on silica gel (Eluent: petroleum) to afford the desired chiral product **3aa** (1.05 g, 99% yield, 92:8 er).

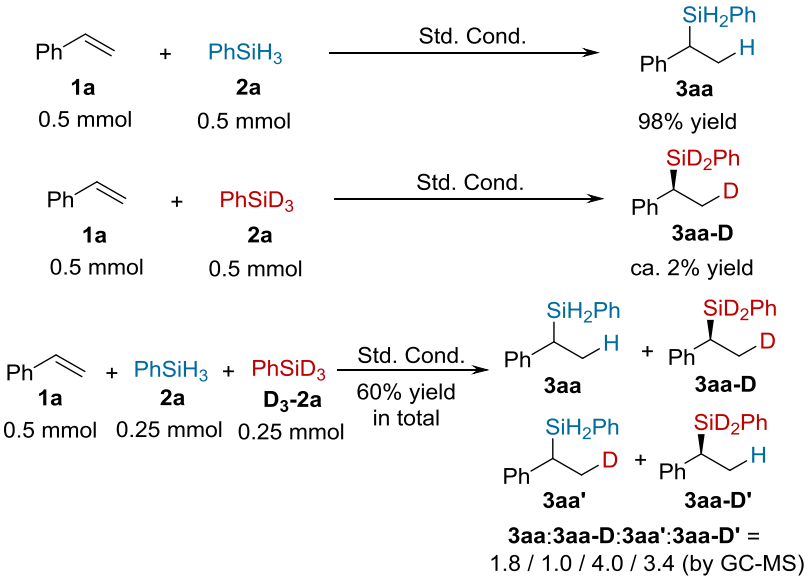
ii) Preparation of (*S*)-1-Phenylethan-1-ol (6). Prepared according to a previous reported method[8a]. To a 50 mL vial, **3aa** (0.106 g, 0.5 mmol) and 25 mL of DCM were added. The solution was stirred at 0 °C. Then HBF_4•Et_2O (0.426 g, 2.6 mmol, 50% Wt) was added. After stirred for 3 h at ambient temperature, the solvent was removed under reduced pressure. To the residue, 3.0 mL of THF, 3.0 mL of MeOH, KF (0.116 g, 2 mmol), $KHCO_3$ (0.50 g, 5.0 mmol) and H_2O_2 (2.5 mL, 30% Wt) were added in sequence. After stirred at room temperature for 15 h, the mixture was diluted with H_2O, extracted with Et_2O for three times. The combined organic layers were washed with brine, dried over Na_2SO_4 and concentrated in vacuo. The crude mixture was subjected to flash column chromatography silica gel and eluted with PE/EtOAc (4/1, v/v) to give 60.4 mg (0.495 mmol, 99% yield, 91.5:8.5 er) of the title compound **6** as a colorless oil.

iii) Preparation of (*S*)-1-Phenylpropan-1-ol (**7**). Prepared according to a previous reported method[8a]. To a 50 mL vial, **5a** (0.027 g, 0.12 mmol) and 5 mL of DCM were added. The solution was stirred at 0 °C. Then HBF_4•Et_2O (0.102 g, 0.6 mmol, 50% Wt) was added. After stirred for 3 h at ambient temperature, the solvent was removed under reduced pressure. To the residue, 0.8 mL of THF, 0.8 mL of MeOH, KF (0.028 g, 0.48 mmol), $KHCO_3$ (0.12 g, 1.2 mmol) and H_2O_2 (0.6 mL, 30% Wt) were added in sequence. After stirred at room temperature for 15 h, the mixture was diluted with H_2O, extracted with Et_2O for three times. The combined organic layers were washed with brine, dried over Na_2SO_4 and concentrated in vacuo. The crude mixture was subjected to flash column chromatography silica gel and eluted with PE/EtOAc (4/1, v/v) to give 15 mg (0.11 mmol, 92% yield,90:10 er) of the title compound **7** as a colorless oil.

iv) Preparation of (*S*)-Phenyl(1-phenylethyl)silanediol (8). Prepared according to a previous reported method[6] using **3aa** (0.13 g, 0.62 mmol), Pd/C (0.062 g, 0.059 mmol, 10% Wt), H_2O (0.2 mL) and Et_2O (2.0 mL). After stirred overnight, the mixture was then filtered through Celite, dried over Na_2SO_4 and concentrated in vacuo. The crude mixture was subjected to flash column chromatography on silica gel and eluted with PE/EtOAc (4/1, v/v) to give 0.134g (0.55 mmol, 90% yield, 91: 9 er) of the title compound **8** as a white solid.

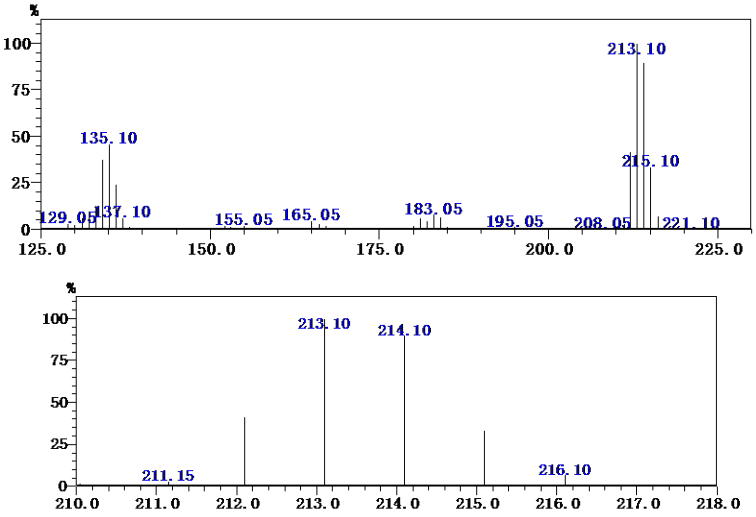
v) Preparation of (*S*)-Phenyl((S)-1-phenylethyl)silanol (9). Prepared according to a previously reported method[6] using **3aa** (0.106 g, 0.5 mmol), BCl_3 (0.5 mmol, 0.5 mL, 1.0 M in DCM), H_2O (1.2 mL) and DCM (2.0 mL). After stirred overnight, the mixture was then diluted with H_2O and extracted with DCM for three times. The combined organic layers were washed with brine, dried over Na_2SO_4 and concentrated in vacuo. The crude mixture was subjected to flash column chromatography on silica gel and eluted with PE/EtOAc (10/1, v/v) to give 79.0 mg (0.35mmol, 70% yield) of the title compound **9** as a colorless oil with 1:1 *dr*.

6. Control experiments



Prepared according to the general procedure using 0.5 mmol of D_3-**2a** or 0.5 mmol phenylsilanes (**2a**/D_3-2a =1:1, v/v) instead of phenylsilanes. After 22 hours, the crude mixture was subjected to flash column chromatography on silica gel and eluted with PE to give the title compound as a colorless oil.

GC-MS Spectra



Mass Table
Line#:1 R.Time:27.405(Scan#:4982)
MassPeaks:5
RawMode:Averaged 27.400-27.410(4981-4983) BasePeak:213(152868)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan

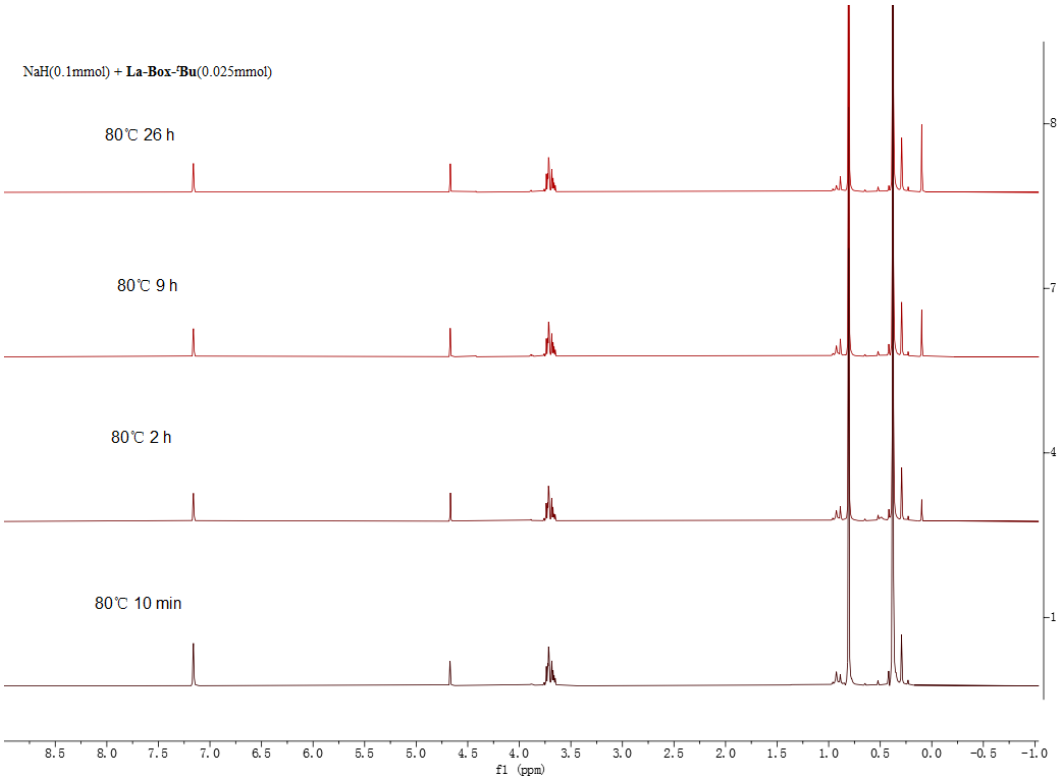
#	m/z	Abs. Int.	Rel. Int.
1	212.10	63303	41.41
2	213.10	152868	100.00
3	214.10	137167	89.73
4	215.10	50776	33.22
5	216.10	10288	6.73

The ratio of these four products was ca. 1.8/1.0/4.0/3.4 based on the relative strength of their signals..

The La hydride formation

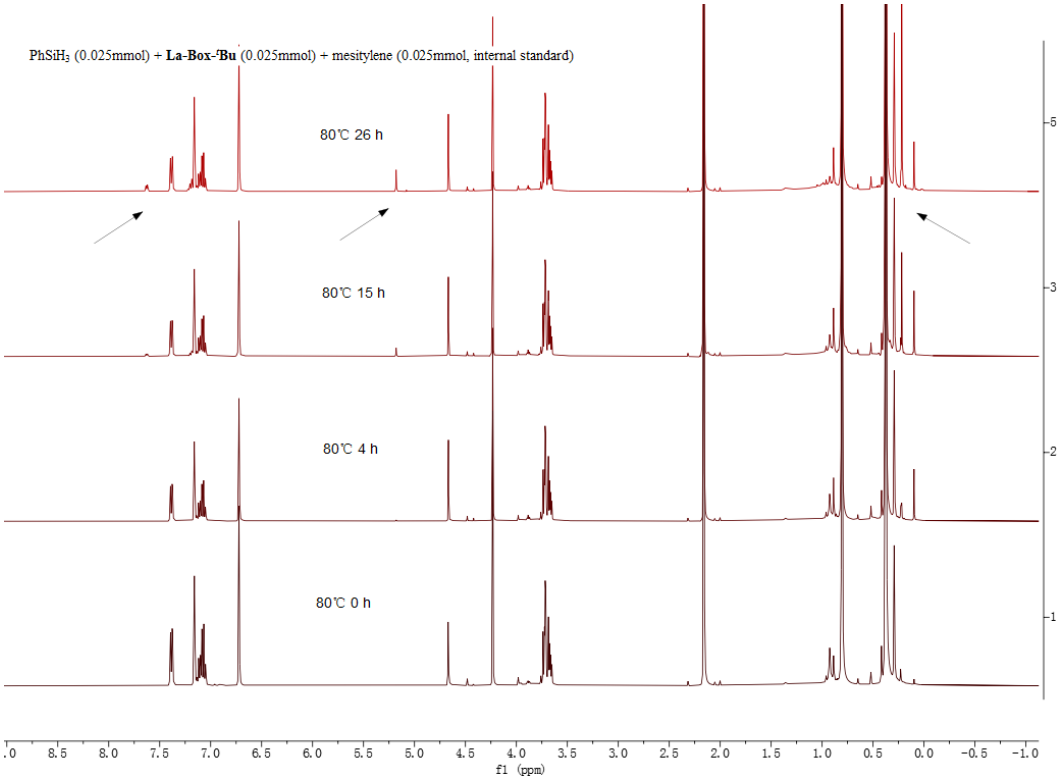
We believe that the La hydride may be formed by the reaction of **La-Box-^{t}Bu** with $PhSiH_3$, and the addition of sodium hydride can accelerate this process. To prove this hypothesis, we conducted the following experiments.

NaH (0.1mmol) + **La-Box-^{t}Bu** (0.025mmol)



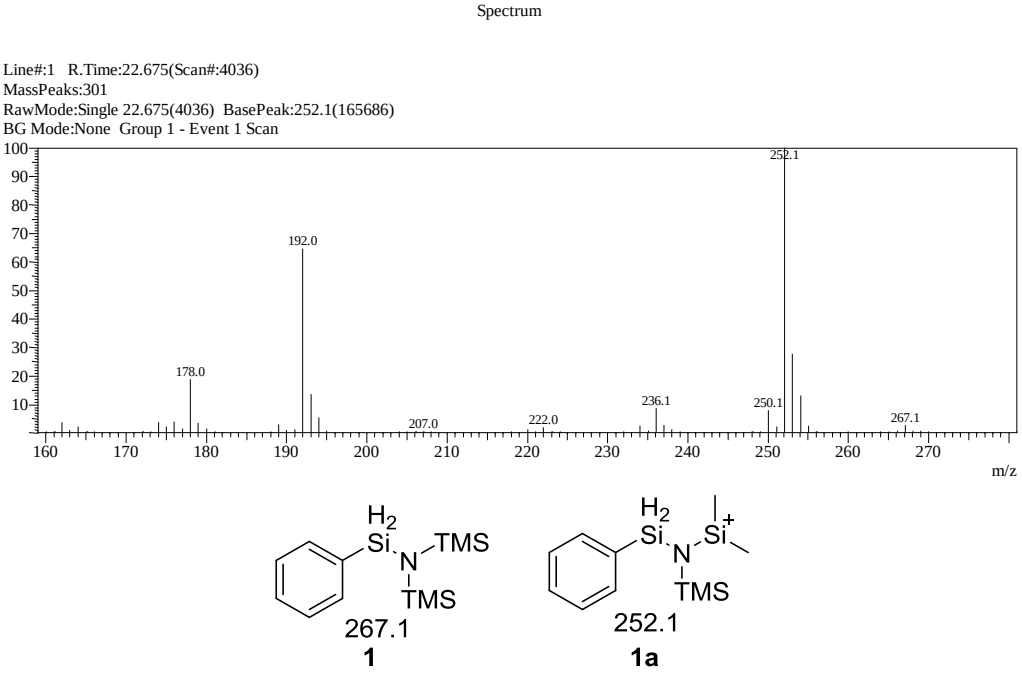
Note: Heating the mixture of **La-Box-^{t}Bu** and NaH in toluene led to no change at 80 °C after 26 h, which suggested that the form of ate complex with La amide was not feasible in current system.

$PhSiH_3$ (0.025mmol) + **La-Box-^{t}Bu** (0.025mmol) + mesitylene (0.025mmol, internal standard)

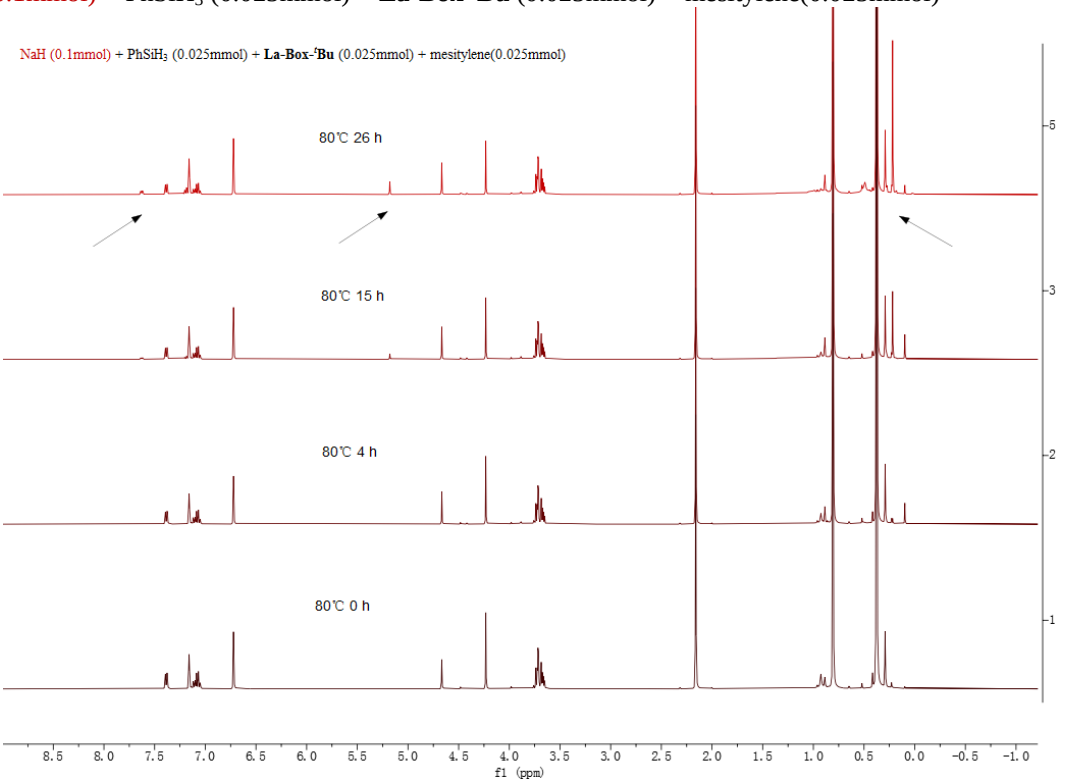


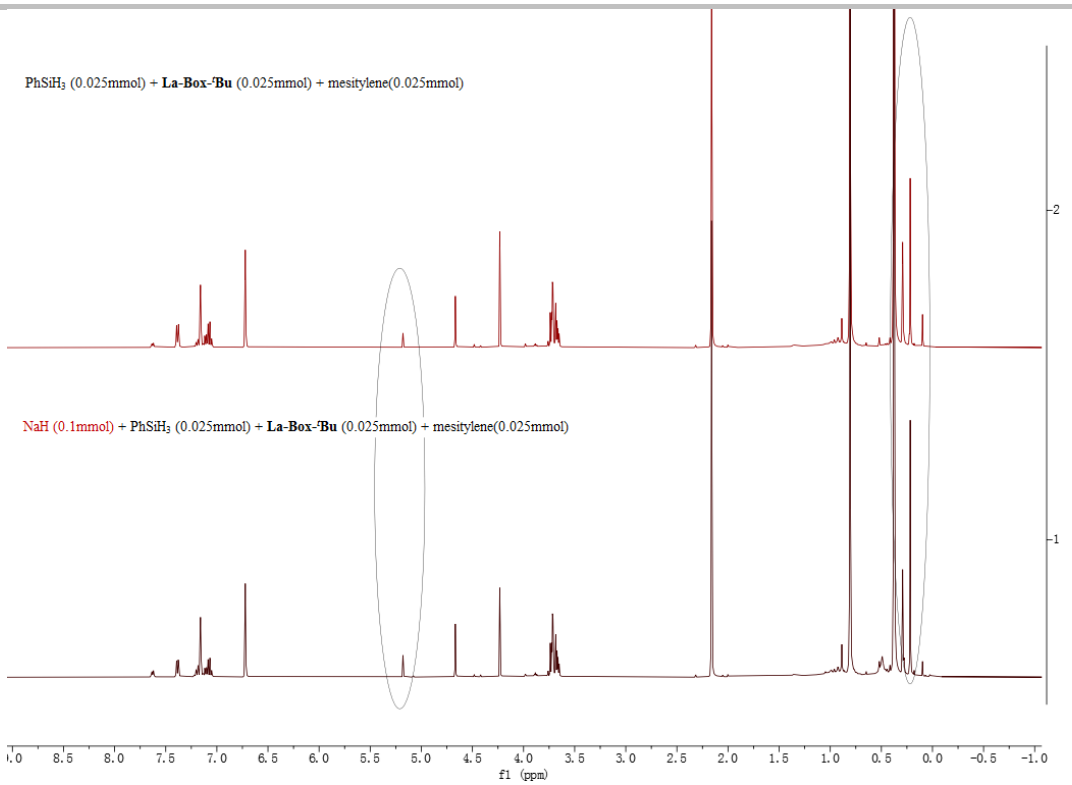
Note: According to the of ^{1}H NMR spectra, the reaction of $PhSiH_3$ (0.025mmol) with **La-Box-^{t}Bu** occurred slowly at 80 °C. The product was isolated and characterized. The ^{1}H NMR spectrum and GC-MS analysis suggested this new compound was TMS_2SiH_2Ph. The above results indicated that LaH may be formed. However, we could not isolate this very active species at current stage.

The characterized data were in according with those in the literature[8e].



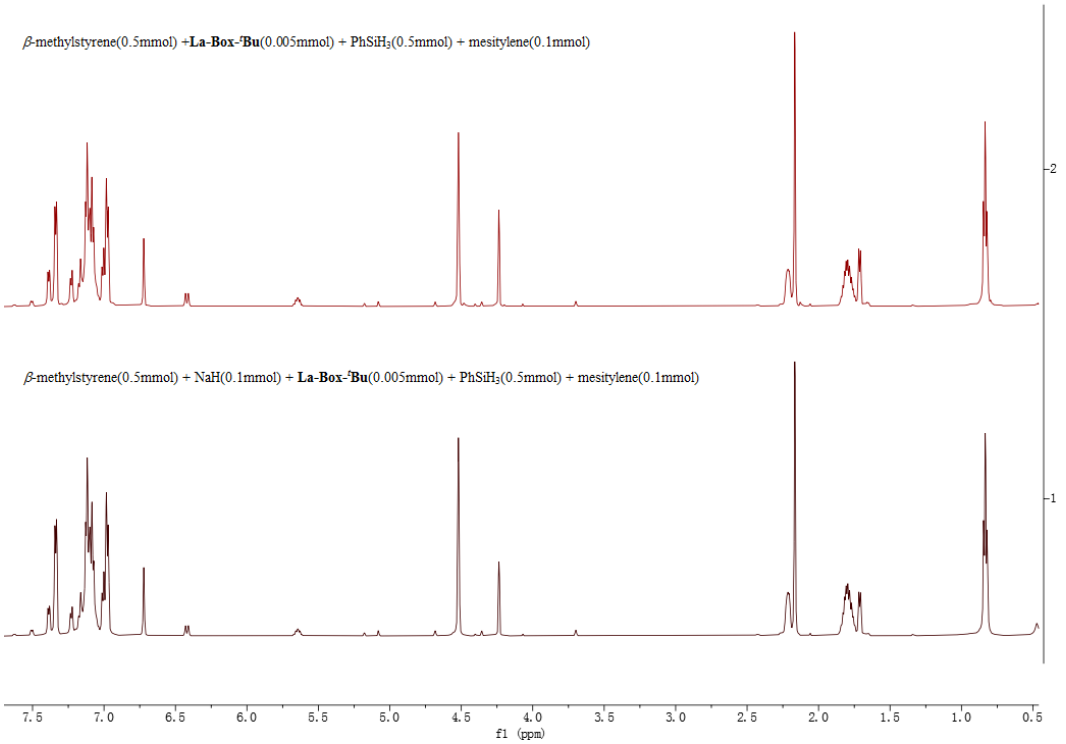
(3) NaH (0.1mmol) + $PhSiH_3$ (0.025mmol) + **La-Box-^{t}Bu** (0.025mmol) + mesitylene(0.025mmol)





Note: According to the NMR analysis, the amount of TMS_2SiH_2Ph increased slightly with the addition of NaH (from 8.25% to 8.7%).

(4) β-methylstyrene (0.5mmol) + NaH (0.1mmol) + **La-Box-^{t}Bu** (0.005mmol) + $PhSiH_3$ (0.5mmol) + mesitylene(0.1mmol)
(5) β-methylstyrene (0.5mmol) + **La-Box-^{t}Bu** (0.005mmol) + $PhSiH_3$ (0.5mmol) + mesitylene (0.1mmol)



Note: To probe the role of NaH, we carried out the in-situ NMR studies. The results indicated that the yield of desired product increased from 82% to 90% with the addition of NaH. DFT calculation were performed to elucidate the role of NaH, However, no clear-cut explanation was obtained at the current stage.

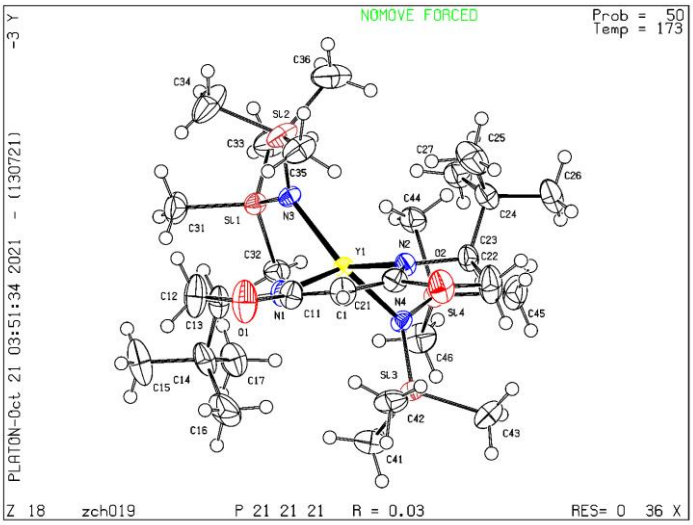
7. X-ray crystallography data

Determination of the structure of rare earth metals by X-ray crystallography

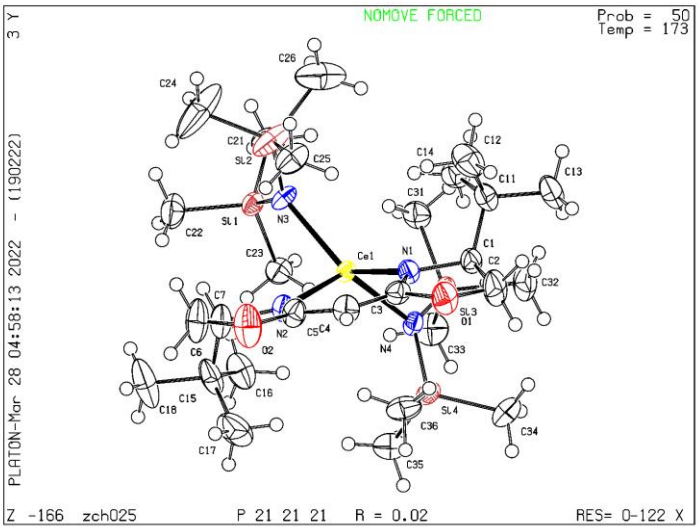
Crystals of **Y-Box-^{t}Bu** for the X-ray crystal structure analysis were obtained from a concentrated solution of **Y-Box-^{t}Bu** in pentane at –35 °C. The colorless crystal in flake-shape, with approximate dimensions of 0.109 × 0.187 × 0.392 mm^3, was selected and mounted for the single-crystal X-ray diffraction. The data set was collected by Bruker D8 Venture Photon II diffractometer at 170(2)K equipped with micro-focus Cu radiation source (K_α = 1.54178Å) Mo radiation source (K_α = 0.71073Å). Applied with face-indexed numerical absorption correction, the structure solution was solved and refinement was processed by SHELXTL (version 6.14) and OLEX 2.3 program package[7a-d] The value observed herein is indicative of racemic twinning and was accommodated during the refinement (using the SHELXL TWIN instruction). In this case, the relatively large standard uncertainty indicates that the structural data alone should not be used to confirm absolute stereochemistry, but should be used in conjunction with the established stereochemistry of the precursor compound. The Flack parameter is provided for informational purposes only. The structure was analyzed by ADDSYM routine implemented in PLATON suite and no higher symmetry was suggested[7e]. The absolute stereochemistry of chiral complex was assigned by the corresponding chiral ligand **Box-^{t}Bu**. **CCDC: 2202534** contains the supplementary crystallographic data which can be obtained free of charge from The Cambridge Crystallographic Data Centere via www.ccdc.cam.ac.uk/data_request/cif.

Crystals of **Ce-Box-^{t}Bu** for the X-ray crystal structure analysis were obtained from a concentrated solution of **Ce-Box-^{t}Bu** in pentane at –35 °C. The yellow crystal in block-shape, with approximate dimensions of 0.356 × 0.437 × 0.610 mm^3, was selected and mounted for the single-crystal X-ray diffraction. The data set was collected by Bruker D8 Venture Photon II diffractometer at 170(2)K equipped with micro-focus Mo radiation source (K_α = 0.71073Å). Applied with face-indexed numerical absorption correction, the structure solution was solved and refinement was processed by SHELXTL (version 6.14) and OLEX 2.3 program package[7a-d]. The structure was analyzed by ADDSYM routine implemented in PLATON suite and no higher symmetry was suggested[7e]. The absolute stereochemistry of chiral complex was assigned by the corresponding chiral ligand **Box-^{t}Bu**. **CCDC: 2202535** contains the supplementary crystallographic data which can be obtained free of charge from The Cambridge Crystallographic Data Centere via www.ccdc.cam.ac.uk/data_request/cif.

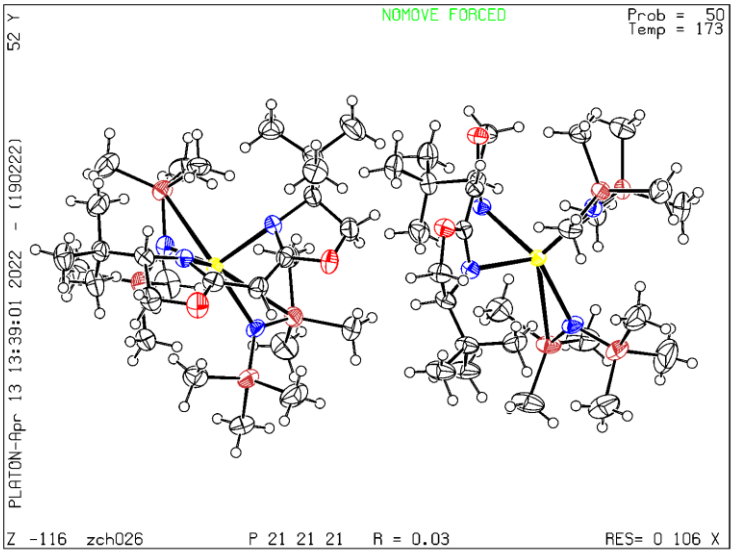
La-Box-^{t}Bu for the X-ray crystal structure analysis were obtained from a concentrated solution of **La-Box-^{t}Bu** in pentane at –35 °C. The colorless crystal in flake-shape, with approximate dimensions of 0.102 × 0.256 × 0.538 mm^3, was selected and mounted for the single-crystal X-ray diffraction. The data set was collected by Bruker D8 Venture Photon II diffractometer at 173(2)K equipped with micro-focus Cu radiation source (K_α = 1.54178Å). Applied with face-indexed numerical absorption correction, the structure solution was solved and refinement was processed by SHELXTL (version 6.14) and OLEX 2.3 program package[7a-d]. The structure was analyzed by ADDSYM routine implemented in PLATON suite and no higher symmetry was suggested[7e]. The absolute stereochemistry of chiral complex was assigned by the corresponding chiral ligand **Box-^{t}Bu**. **CCDC: 2202536** contains the supplementary crystallographic data which can be obtained free of charge from The Cambridge Crystallographic Data Centere via www.ccdc.cam.ac.uk/data_request/cif.



Y-Box-^{t}Bu



Ce-Box-^{t}Bu



La-Box-^{t}Bu

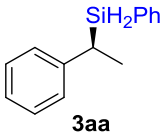
Crystallographic data for catalysts

Formula	$C_{27}H_{61}N_4O_2Si_4Y$	$C_{27}H_{61}CeN_4O_2Si_4$	$C_{54}H_{122}La_2N_8O_4Si_8$
Formula mass (amu)	675.06	726.27	1450.13
Space group	P 21 21 21	P 21 21 21	P 21 21 21
a (Å)	11.9697(3)	12.0950(5)	10.9205(2)
b (Å)	17.8874(5)	17.8554(7)	17.7934(4)
c (Å)	17.8874(5)	18.0760(7)	40.2620(8)
α (deg)	90	90	90
β (deg)	90	90	90
γ (deg)	90	90	90
V (Å^3)	3829.81(18)	3903.7(3)	7823.4(3)
Z	4	4	4
λ (Å)	1.54178	0.71073	1.54178
T (K)	173 K	173 K	173 K
ρ_{calcd} (g cm^{-3})	1.171	1.236	1.231
μ (mm^{-1})	3.546	1.315	9.811
Transmission factors	0.449,0.807	0.482,0.613	0.031,0.341
θ_{max} (deg)	68.421	27.513	68.313
No. of unique data, including $F_o^2 < 0$	6849	8757	12899
No. of unique data, with $F_o^2 > 2\sigma(F_o^2)$	6686	8279	12713
No. of variables	362	361	722
$R(F)$ for $F_o^2 > 2\sigma(F_o^2)$ [a]	0.0267	0.0244	0.0339
$R_w(F_o^2)$ [b]	0.0687	0.0598	0.0821
Goodness of fit	1.080	1.059	1.065

[a] $R(F) = \sum||F_o| - |F_c|| / \sum|F_o|$.

[b] $R_w(F_o^2) = [\sum[w(F_o^2 - F_c^2)^2] / \sum wF_o^4]^{1/2}$; $w^{-1} = [\sigma^2(F_o^2) + (Ap)^2 + Bp]$, where $p = [\max(F_o^2,0) + 2F_c^2] / 3$.

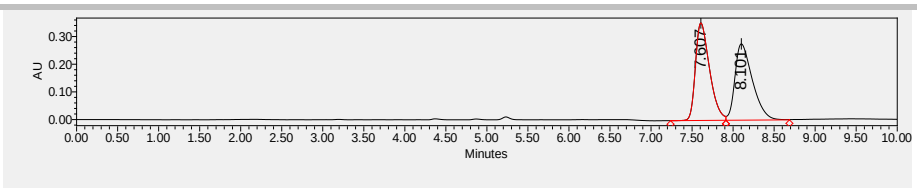
8. The analytical and spectral characterization data of products



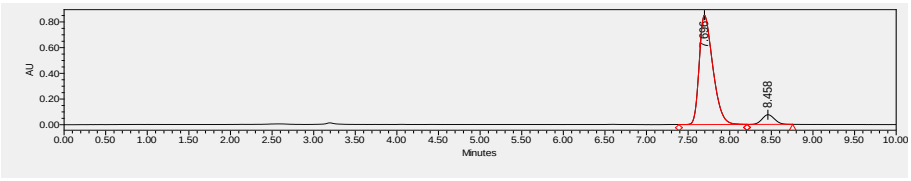
3aa

(*S*)-Phenyl(1-phenylethyl)silane (3aa)

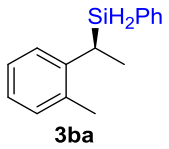
($C_{14}H_{16}Si$) colorless oil; 104.1 mg, 98% yield, 92.5:7.5 er, $[\alpha]_D^{28}$ = –17.8 (c = 0.60, in CH_2Cl_2), dissolved in hexane for HPLC; **HPLC** (Daicel chiralcel **OJH**, hexane/^{i}PrOH = 99.7/0.3, flow rate 1.0 mL/min) retention time: t_{major} = 7.70 min, t_{minor} = 8.46 min. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.38 – 7.28 (m, 2H), 7.28 – 7.23 (m, 1H), 7.23 – 7.17 (m, 2H), 7.17 – 7.10 (m, 2H), 7.05 – 6.95 (m, 3H), 4.24 (d, J = 3.2 Hz, 2H), 2.68 – 2.28 (m, 1H), 1.36 (d, J = 7.5 Hz, 3H). **^{13}C{^{1}H} NMR** (101 MHz, Chloroform-*d*) δ 144.6, 135.7, 131.4, 129.8, 128.4, 127.9, 127.2, 125.1, 25.4, 16.4. **IR** (film, cm^{-1}): 2955, 2924, 2135, 1600, 1492, 1116, 929, 839, 697. These spectroscopic data was correspond to the previously reported data.[8a].



	Retention Time	% Area
1	7.607	50.69
2	8.101	49.31



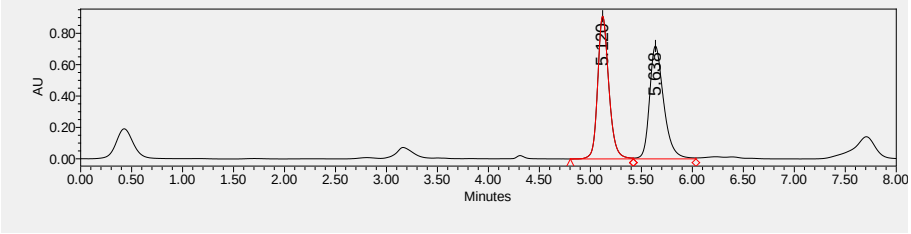
	Retention Time	% Area
1	7.696	92.46
2	8.458	7.54



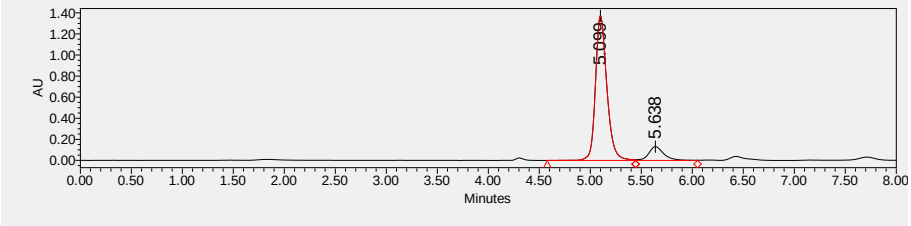
3ba

(*S*)-Phenyl(1-(o-tolyl)ethyl)silane (3ba)

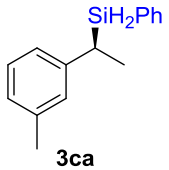
($C_{15}H_{18}Si$) colorless oil; 95 mg, 84% yield, 88.5:11.5 er, $[\alpha]_D^{28}$ = 17.2 (*c* = 2.12, in CH_2Cl_2), dissolved in hexane for HPLC; **HPLC** (Daicel chiralcel **OJH**, hexane/^{i}PrOH = 99.5/0.5, flow rate 1.0 mL/min) retention time: t_{major} = 5.10 min, t_{minor} = 5.64 min. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.43 – 7.33 (m, 3H), 7.32 – 7.25 (m, 2H), 7.19 – 7.12 (m, 1H), 7.12 – 7.06 (m, 2H), 7.06 – 7.00 (m, 1H), 4.61 – 3.94 (m, 2H), 2.85 – 2.65 (m, 1H), 2.19 (s, 3H), 1.44 (d, *J* = 7.4 Hz, 3H). **^{13}C{^{1}H} NMR** (101 MHz, Chloroform-*d*) δ 142.9, 135.7, 134.9, 131.7, 130.2, 129.9, 128.0, 126.3, 126.1, 124.9, 20.9, 20.1, 20.1, 16.7. **IR** (film, cm^{-1}) : 2956, 2134, 1486, 1459, 1429, 1116, 929, 840, 734, 699. These spectroscopic data correspond to the previously reported data.[8a]



	Retention Time	% Area
1	5.120	49.88
2	5.638	50.12



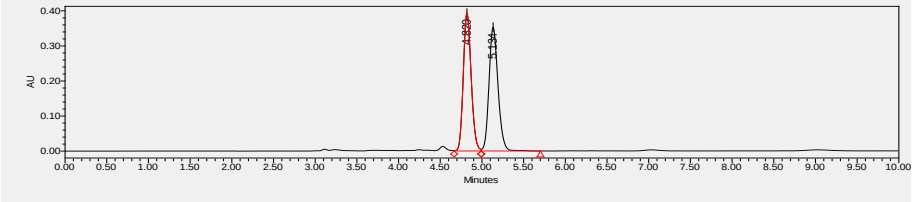
	Retention Time	% Area
1	5.099	88.66
2	5.638	11.34



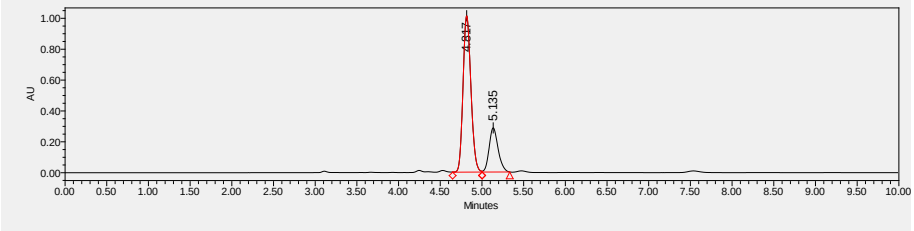
3ca

(*S*)-Phenyl(1-(m-tolyl)ethyl)silane (3ca)

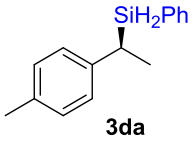
($C_{15}H_{18}Si$) colorless oil; 103.0 mg, 91% yield, 75.5:24.5 er $[\alpha]_D^{28}$ = –14.7 (*c* = 1.83, in CH_2Cl_2), dissolved in hexane for HPLC; **HPLC** (Daicel chiralcel **OJH**, hexane/^{i}PrOH = 95/5, flow rate 1.0 mL/min) retention time: t_{major} = 5.10 min, t_{minor} = 5.64 min. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.75 – 7.68 (m, 2H), 7.67 – 7.60 (m, 1H), 7.60 – 7.54 (m, 2H), 7.46 – 7.39 (m, 1H), 7.26 – 7.17 (m, 3H), 4.97 – 4.33 (m, 2H), 2.96 – 2.78 (m, 1H), 2.58 (s, 3H), 1.75 (d, *J* = 7.5 Hz, 3H). **^{13}C{^{1}H} NMR** (101 MHz, Chloroform-*d*) δ 144.5, 137.8, 135.7, 131.5, 129.7, 128.3, 128.0, 127.8, 125.9, 124.2, 25.3, 21.5, 16.5. **IR** (film, cm^{-1}) 2954, 2134, 1603, 1429, 1116, 929, 838, 785, 734, 699. These spectroscopic data correspond to the previously reported data.[8a]



	Retention Time	% Area
1	4.820	49.29
2	5.134	50.71



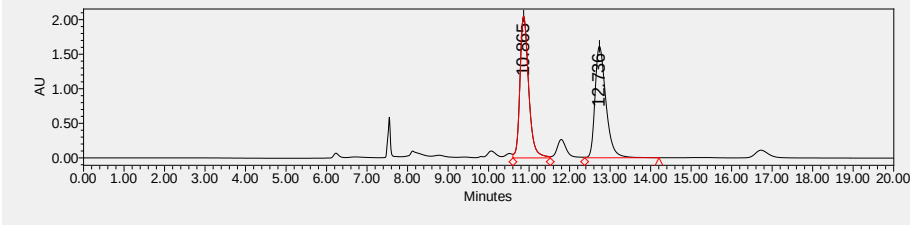
	Retention Time	% Area
1	4.817	75.65
2	5.135	24.35



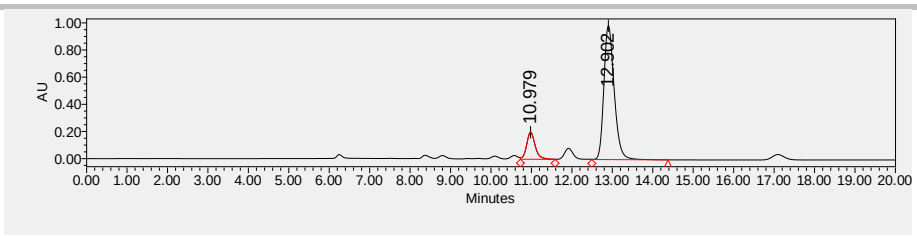
3da

(*S*)-Phenyl(1-(*p*-tolyl)ethyl)silane (3da)

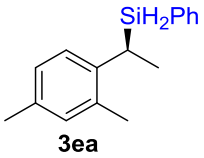
($C_{15}H_{18}Si$) colorless oil; 107.5 mg, 95% yield, 84.5:15.5 er, $[\alpha]_D^{28}$ = –18.9 (*c* = 0.42, in CH_2Cl_2), dissolved in hexane for HPLC; **HPLC** (Daicel chiralcel **OJH**, hexane/^{i}PrOH = 99/1, flow rate 0.5 mL/min) retention time: t_{major} =12.90 min, t_{minor} = 10.98 min. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.50 – 7.44 (m, 2H), 7.45 – 7.40 (m, 1H), 7.38 – 7.32 (m, 2H), 7.16 – 7.07 (m, 2H), 7.07 – 6.99 (m, 2H), 4.76 – 3.95 (m, 2H), 2.68 – 2.55 (m, 1H), 2.35 (s, 3H), 1.48 (d, *J* = 7.5 Hz, 3H). **^{13}C{^{1}H} NMR** (101 MHz, Chloroform-*d*) δ 141.5, 135.7, 134.5, 131.6, 129.8, 129.2, 127.9, 127.1, 24.9, 21.0, 16.6. **IR** (film, cm^{-1}): 2954, 2360, 2135, 1510, 1428, 1116, 929, 842. These spectroscopic data correspond to the previously reported data. [8a]



	Retention Time	% Area
1	10.865	50.38
2	12.736	49.62



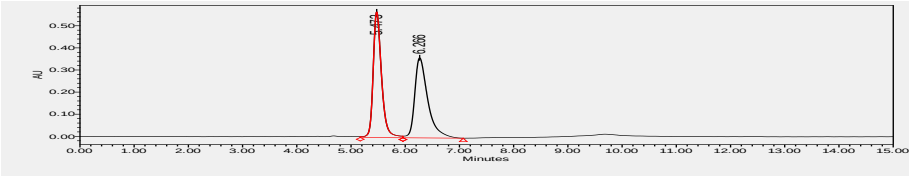
	Retention Time	% Area
1	10.979	15.30
2	12.902	84.70



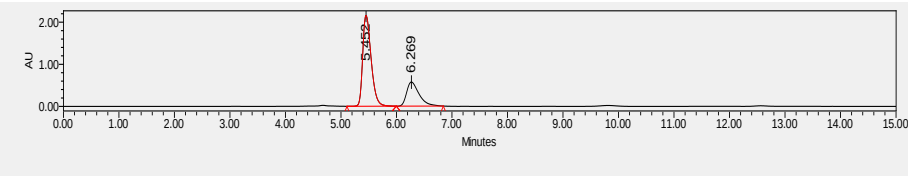
3ea

(*S*)-(1-(2,4-Dimethylphenyl)ethyl)(phenyl)silane (3ea)

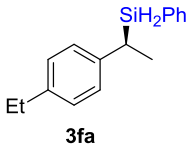
($C_{16}H_{20}Si$) colorless oil; 81.8 mg, 68% yield, 72:28 er, $[\alpha]_D^{28}$ = –8.4 (*c* = 0.75, in CH_2Cl_2), dissolved in hexane for HPLC; **HPLC** (Daicel chiralcel **OJH**, hexane/^{i}PrOH = 99.7/0.3, flow rate 1.0 mL/min) retention time: t_{major} = 5.45 min, t_{minor} = 6.27 min. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.51 – 7.45 (m, 2H), 7.44 – 7.39 (m, 1H), 7.35 (t, *J* = 7.4 Hz, 2H), 7.08 – 6.94 (m, 3H), 4.53 – 4.09 (m, 2H), 2.76 (tt, *J* = 7.6, 4.2 Hz, 1H), 2.32 (s, 3H), 2.22 (s, 3H), 1.46 (d, *J* = 7.4 Hz, 3H). **^{13}C{^{1}H} NMR** (101 MHz, Chloroform-*d*) δ 139.8, 135.6, 134.7, 134.2, 131.8, 131.1, 129.8, 127.9, 127.0, 126.0, 20.9, 20.3, 20.0, 16.7. **IR** (film, cm^{-1}) 2954, 2133, 1500, 1429, 1116, 929, 841, 733, 699, 550. These spectroscopic data correspond to the previously reported data.[8b]



	Retention Time	% Area
1	5.473	50.00
2	6.266	50.00



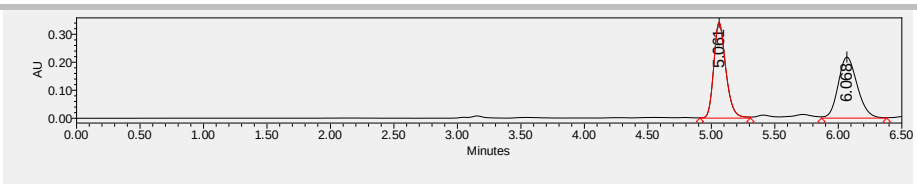
	Retention Time	% Area
1	5.452	71.82
2	6.269	28.18



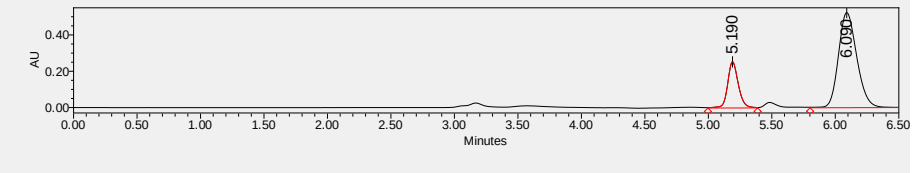
3fa

(*S*)-(1-(4-Ethylphenyl)ethyl)(phenyl)silane (3fa)

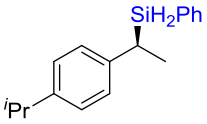
($C_{16}H_{20}Si$) colorless oil; 96.2 mg, 80% yield, 81:19 er, $[\alpha]_D^{28}$ = –15.9 (*c* = 0.86, in CH_2Cl_2), dissolved in hexane for HPLC; **HPLC** (Daicel chiralcel **OJH**, hexane/^{i}PrOH = 99/1, flow rate 1.0 mL/min) retention time: t_{major} = 6.09 min, t_{minor} = 5.19 min. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.55 – 7.48 (m, 2H), 7.48 – 7.42 (m, 1H), 7.43 – 7.35 (m, 2H), 7.23 – 7.14 (m, 2H), 7.15 – 7.08 (m, 2H), 4.70 – 4.07 (m, 2H), 2.78 – 2.55 (m, 3H), 1.53 (d, *J* = 7.5 Hz, 3H), 1.31 (t, *J* = 7.6 Hz, 3H). **^{13}C{^{1}H} NMR** (101 MHz, Chloroform-*d*) δ 141.7, 140.9, 135.7, 131.7, 129.8, 128.0, 127.9, 127.1, 28.5, 24.9, 16.6, 15.7. **GC-MS** (EI): Calcd for $C_{16}H_{20}Si$: 240.1, found: 240.1. **IR** (film, cm^{-1}) 2962, 2134, 1510, 1428, 1117, 929, 843, 734, 699, 583.



	Retention Time	% Area
1	5.061	49.80
2	6.068	50.20



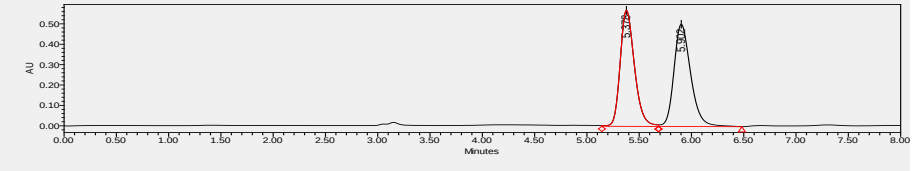
	Retention Time	% Area
1	5.190	19.11
2	6.090	80.89



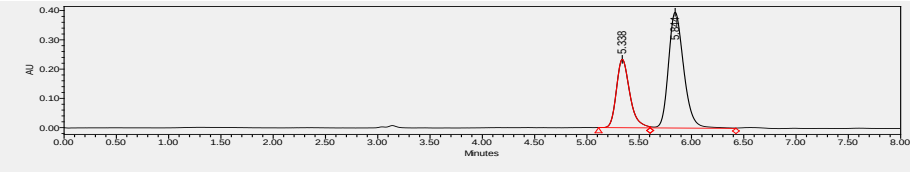
3ga

(*S*)-(1-(4-Isopropylphenyl)ethyl)(phenyl)silane (3ga)

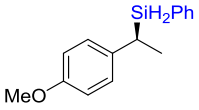
($C_{17}H_{22}Si$) colorless oil; 86.5 mg, 68% yield, 66:34 er, $[\alpha]_D^{28}$ = –7.7 (*c* = 1.36, in CH_2Cl_2), dissolved in hexane for HPLC; **HPLC** (Daicel chiralcel **OJH**, hexane/^{i}PrOH = 99.7/0.3, flow rate 1.0 mL/min) retention time: t_{major} = 5.84 min, t_{minor} = 5.34 min. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.35 – 7.29 (m, 2H), 7.27 – 7.24 (m, 1H), 7.24 – 7.15 (m, 2H), 7.05 – 6.98 (m, 2H), 6.98 – 6.88 (m, 2H), 4.53 – 3.91 (m, 2H), 2.82 – 2.71 (m, 1H), 2.56 – 2.39 (m, 1H), 1.34 (d, *J* = 7.5 Hz, 3H), 1.14 (d, *J* = 7.0 Hz, 6H). **^{13}C{^{1}H} NMR** (101 MHz, Chloroform-*d*) δ 145.5, 141.8, 135.7, 131.7, 129.7, 127.9, 127.0, 126.4, 33.6, 24.8, 24.1, 16.5. **GC-MS** (EI): Calcd for $C_{17}H_{22}Si$: 254.1, found: 254.1. **IR** (film, cm^{-1}) 2959, 2134, 1511, 1458, 1427, 1116, 929, 843, 733, 699, 557.



	Retention Time	% Area
1	5.378	49.52
2	5.902	50.48



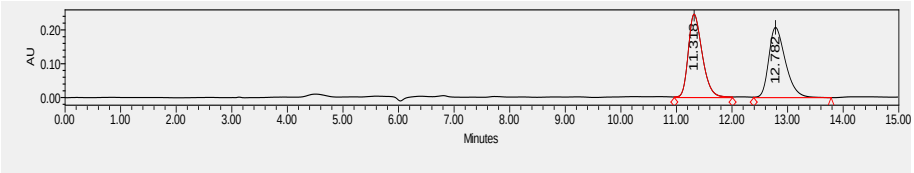
	Retention Time	% Area
1	5.338	34.14
2	5.844	65.86



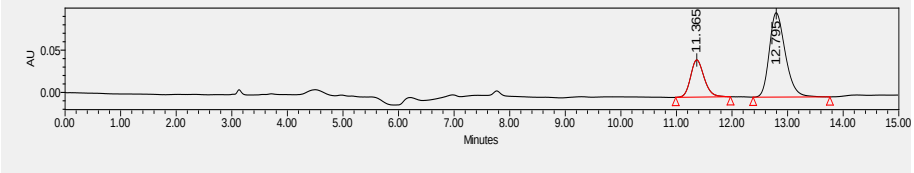
3ha

(*S*)- (1-(4-Methoxyphenyl)ethyl)(phenyl)silane (3ha)

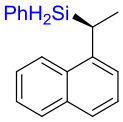
($C_{15}H_{18}OSi$) colorless oil; 64.2 mg, 53% yield, 73:27 er, $[\alpha]_D^{28}$ = –11.5 (*c* = 0.40, in CH_2Cl_2), dissolved in hexane for HPLC; **HPLC** (Daicel chiralcel **OJH**, hexane/^{i}PrOH = 99.5/0.5, flow rate 1.0 mL/min) retention time: t_{major} = 12.80 min, t_{minor} = 11.37 min. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.36 – 7.31 (m, 2H), 7.30 – 7.26 (m, 1H), 7.25 – 7.19 (m, 2H), 6.97 – 6.88 (m, 2H), 6.78 – 6.65 (m, 2H), 4.34 – 4.08 (m, 2H), 3.69 (s, 3H), 2.54 – 2.41 (m, 1H), 1.34 (d, *J* = 7.6 Hz, 3H). **^{13}C{^{1}H} NMR** (101 MHz, Chloroform-*d*) δ 156.1, 135.5, 134.6, 130.5, 128.7, 126.9, 126.8, 112.8, 54.2, 23.2, 15.7. **IR** (film, cm^{-1}): 2953, 2133, 1610, 1509, 1246, 1116, 1038, 929, 841. These spectroscopic data correspond to the previously reported data.[8a]



	Retention Time	% Area
1	11.318	49.97
2	12.782	50.03



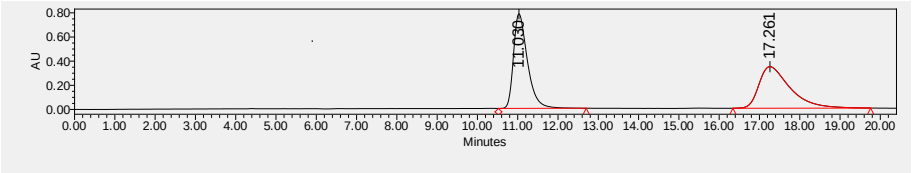
	Retention Time	% Area
1	11.365	27.22
2	12.795	72.78



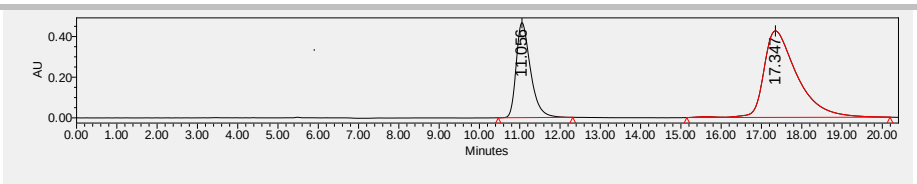
3ia

(*S*)-(1-(Naphthalen-1-yl)ethyl)(phenyl)silane (3ia)

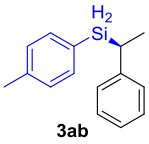
($C_{18}H_{18}Si$) colorless oil; 72.2 mg, 55% yield, 68:32 er, $[\alpha]_D^{28}$ = 52.7 (*c* = 1.12, in CH_2Cl_2), dissolved in hexane for HPLC; **HPLC** (Daicel chiralcel **OJH**, hexane/^{i}PrOH = 99.7/0.3, flow rate 1.0 mL/min) retention time: t_{major} = 17.35 min, t_{minor} = 11.06 min. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.08 – 8.00 (m, 1H), 7.89 – 7.79 (m, 1H), 7.68 – 7.61 (m, 1H), 7.47 – 7.42 (m, 2H), 7.42 – 7.37 (m, 3H),7.37 – 7.33 (m, 1H), 7.30 – 7.26 (m, 2H), 7.25 – 7.21 (m, 1H), 4.67 – 4.16 (m, 2H), 3.54 – 3.35 (m, 1H), 1.58 (d, *J* = 7.3 Hz, 3H). **^{13}C{^{1}H} NMR** (101 MHz, Chloroform-*d*) δ 141.0, 135.8, 134.0, 131.5, 131.2, 129.9, 129.0, 128.0, 125.7, 125.7, 125.6, 125.5, 123.5, 123.3, 20.1, 16.9. **IR** (film, cm^{-1}) 3049, 2137, 1428, 1394, 1116, 928, 837, 776, 733, 699. These spectroscopic data correspond to the previously reported data.[8a]



	Retention Time	% Area
1	11.030	50.49
2	17.261	49.51



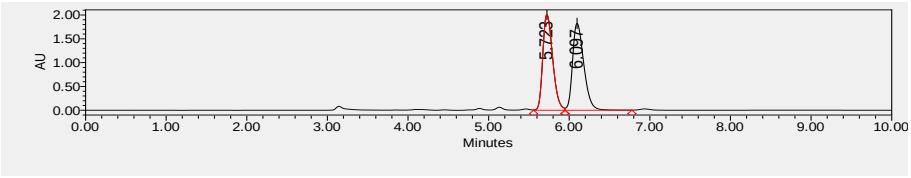
	Retention Time	% Area
1	11.056	31.97
2	17.347	68.03



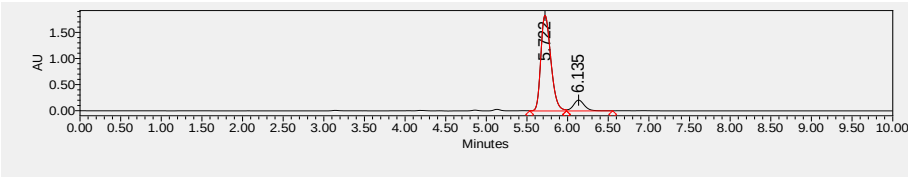
3ab

(*S*)-(1-Phenylethyl)(p-tolyl)silane (3ab)

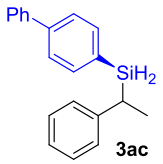
($C_{15}H_{18}Si$) colorless oil; 95.1 mg, 84% yield, 89:11 er, $[\alpha]_D^{28}$ = 11.6 (*c* = 1.88, in CH_2Cl_2), dissolved in hexane for HPLC; **HPLC** (Daicel chiralcel **OJH**, hexane/^{i}PrOH = 99/1, flow rate 1.0 mL/min) retention time: t_{major} = 5.72 min, t_{minor} = 6.13 min. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.24 – 7.18 (m, 2H), 7.18 – 7.12 (m, 2H), 7.06 – 6.93 (m, 5H), 4.54 – 3.91 (m, 2H), 2.59 – 2.40 (m, 1H), 2.24 (s, 3H), 1.35 (d, *J* = 7.5 Hz, 3H). **^{13}C{1H} NMR** (101 MHz, Chloroform-*d*) δ 144.8, 139.8, 135.8, 128.8, 128.4, 127.7, 127.2, 125.0, 25.6, 21.6, 21.6, 16.5. **GC-MS** (EI): Calcd for $C_{15}H_{18}Si$: 226.1, found: 226.1 **IR** (film, cm^{-1}) 2955, 2132, 1601, 1486, 1458, 1110, 929, 844, 796, 766.



	Retention Time	% Area
1	5.720	48.53
2	6.097	51.47



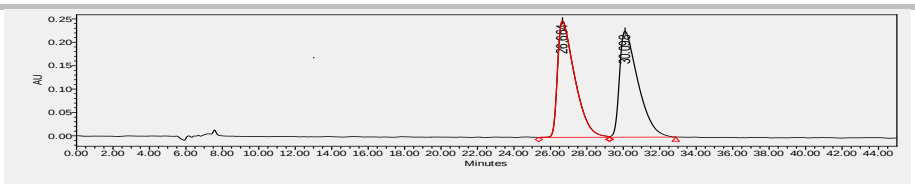
	Retention Time	% Area
1	5.722	88.86
2	6.135	11.14



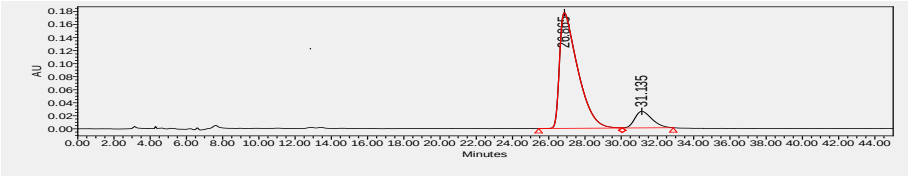
3ac

(*S*)-[1,1'-Biphenyl]-4-yl(1-phenylethyl)silane (3ac)

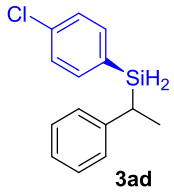
($C_{20}H_{20}Si$) white solid; M.p. 64 – 67 °C, 99.5 mg, 69% yield, 88:12 er $[\alpha]_D^{28}$ = –24.3 (*c* = 2.27, in CH_2Cl_2), dissolved in hexane for HPLC; **HPLC** (Daicel chiralcel **OJH**, hexane/^{i}PrOH = 99.7/0.3, flow rate 1.0 mL/min) retention time: t_{major} = 26.86 min, t_{minor} = 31.14 min. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.61 – 7.56 (m, 2H), 7.56 – 7.51 (m, 2H), 7.49 – 7.39 (m, 4H), 7.37 – 7.31 (m, 1H), 7.29 – 7.21 (m, 2H), 7.17 – 7.07 (m, 3H), 4.71 – 3.98 (m, 2H), 2.74 – 2.56 (m, 1H), 1.48 (d, *J* = 7.4 Hz, 3H). **^{13}C{^{1}H} NMR** (101 MHz, Chloroform-*d*) δ 144.6, 142.5, 140.8, 136.2, 130.1, 128.9, 128.5, 127.6, 127.2, 127.2, 126.6, 125.1, 25.5, 16.5. **GC-MS** (EI): Calcd for $C_{20}H_{20}Si$: 288.1, found: 288.1.**IR** (film, cm^{-1}) 3024, 2955, 2134, 1597, 1486, 1450, 1384, 1117, 1007, 919, 844, 823, 757, 696, 597.



	Retention Time	% Area
1	26.664	50.41
2	30.098	49.59



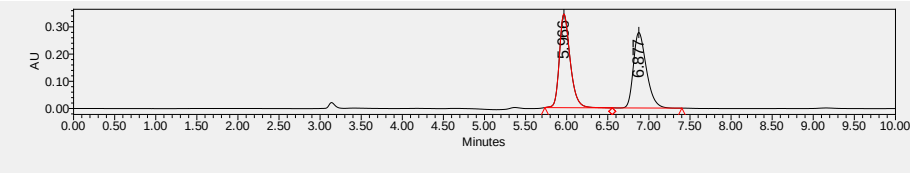
	Retention Time	% Area
1	26.864	88.11
2	31.139	11.89



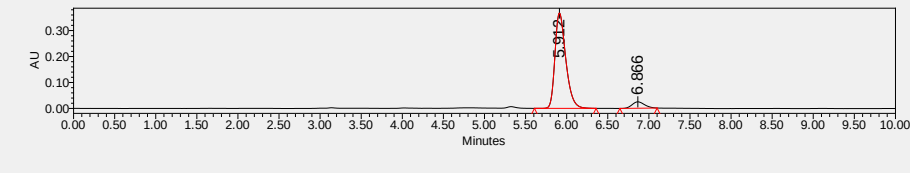
3ad

(*S*)-(4-Chlorophenyl)(1-phenylethyl)silane (3ad)

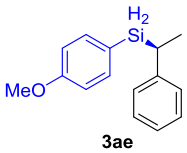
($C_{14}H_{15}ClSi$) colorless oil; 101.2 mg, 82% yield, 93:7 er, $[\alpha]_D^{28}$ = –21.1 (*c* = 2.02, in CH_2Cl_2), dissolved in hexane for HPLC; **HPLC** (Daicel chiralcel **OJH**, hexane/^{i}PrOH = 99/1, flow rate 1.0 mL/min) retention time: t_{major} = 5.91 min, t_{minor} = 6.87 min. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.23 – 7.10 (m, 6H), 7.06 – 7.00 (m, 1H), 6.99 – 6.90 (m, 2H), 4.22 (d, *J* = 3.2 Hz, 2H), 2.60 – 2.37 (m, 1H), 1.34 (d, *J* = 7.5 Hz, 3H). **^{13}C{^{1}H} NMR** (101 MHz, Chloroform-*d*) δ 144.2, 137.1, 136.4, 129.7, 128.5, 128.2, 127.2, 125.3, 25.4, 16.3. **IR** (film, cm^{-1}) 2955, 2137, 1578, 1484, 1451, 1380, 1088, 1013, 928, 841, 809, 763, 738, 698, 595. These spectroscopic data correspond to the previously reported data. [8a]



	Retention Time	% Area
1	5.966	50.84
2	6.877	49.16



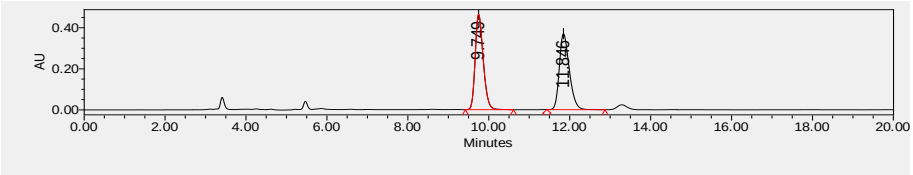
	Retention Time	% Area
1	5.912	92.90
2	6.866	7.10



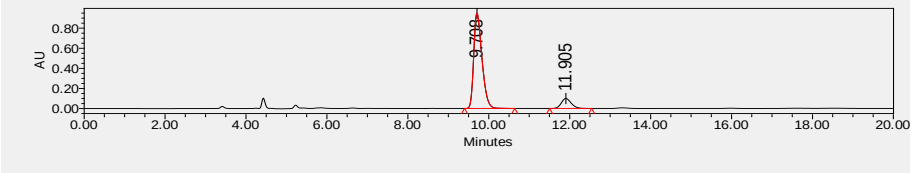
3ae

(*S*)-(4-Methoxyphenyl)(1-phenylethyl)silane (3ae)

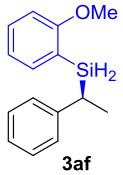
($C_{15}H_{18}OSi$) colorless oil; 94.5 mg, 78% yield, 89:11 er, $[\alpha]_D^{28}$ = –21.5 (*c* = 1.45, in CH_2Cl_2), dissolved in hexane for HPLC; **HPLC** (Daicel chiralcel **OJH**, hexane/^{i}PrOH = 99/1, flow rate 1.0 mL/min) retention time: t_{major} = 9.71 min, t_{minor} = 11.91 min. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.25 – 7.20 (m, 2H), 7.20 – 7.12 (m, 2H), 7.06 – 6.96 (m, 3H), 6.82 – 6.73 (m, 2H), 4.29 – 4.11 (m, 2H), 3.70 (s, 3H), 2.57 – 2.41 (m, 1H), 1.36 (d, *J* = 7.5 Hz, 3H). **^{13}C{^{1}H} NMR** (101 MHz, Chloroform-*d*) δ 161.1, 144.8, 137.3, 128.4, 127.2, 125.0, 122.0, 113.7, 55.1, 25.7, 16.4. **IR** (film, cm^{-1}) 2955, 2131, 1594, 1501, 1454, 1280, 1248, 1182, 1115, 1032, 929, 845, 824, 699. These spectroscopic data correspond to the previously reported data.[8a]



	Retention Time	% Area
1	9.749	50.12
2	11.846	49.88



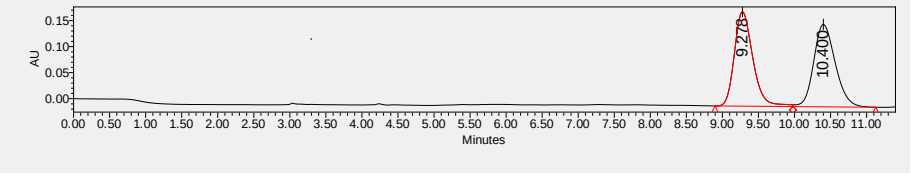
	Retention Time	% Area
1	9.708	88.79
2	11.905	11.21



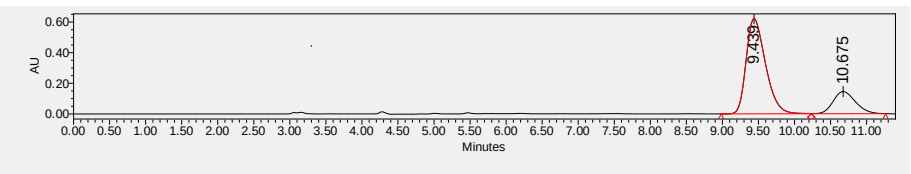
3af

(*S*)-(2-Methoxyphenyl)(1-phenylethyl)silane (3af)

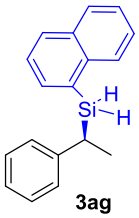
($C_{15}H_{18}OSi$) colorless oil; 24.2 mg, 20% yield, 79:21 er $[\alpha]_D^{28}$ = –53.6 (*c* = 0.06, in CH_2Cl_2), dissolved in hexane for HPLC; **HPLC** (Daicel chiralcel **OJH**, hexane/^{i}PrOH = 99/1, flow rate 1.0 mL/min) retention time: t_{major} = 9.44 min, t_{minor} = 10.67 min. **^{1}HNMR** (400 MHz, Chloroform-*d*) δ 7.45 – 7.31 (m, 2H), 7.26 – 7.19 (m, 2H), 7.18 – 7.04 (m, 3H), 6.95 – 6.85 (m, 1H), 6.86 – 6.77 (m, 1H), 4.52 – 3.97 (m, 2H), 3.76 (s, 3H), 2.81 – 2.66 (m, 1H), 1.42 (d, *J* = 7.5 Hz, 3H). **^{13}C{^{1}H} NMR** (101 MHz, Chloroform-*d*) δ 164.2, 145.6, 137.8, 132.0, 128.3, 127.0, 124.8, 120.7, 120.4, 109.4, 55.3, 24.9, 16.7. **GC-MS** (EI): Calcd for $C_{15}H_{18}OSi$: 242.1, found: 242.1 **IR** (film, cm^{-1}) 2955, 2360, 2134, 1588, 1460, 1429, 1272, 1240, 1085, 1023, 935, 840, 758, 698.



	Retention Time	% Area
1	9.278	49.55
2	10.400	50.45



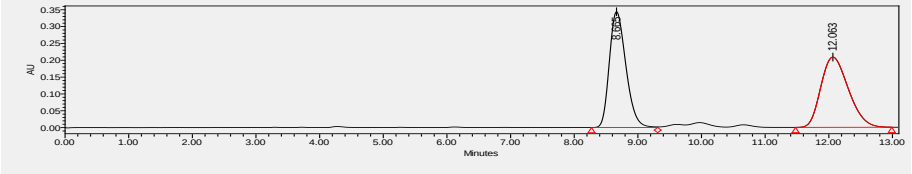
	Retention Time	% Area
1	9.439	78.73
2	10.675	21.27



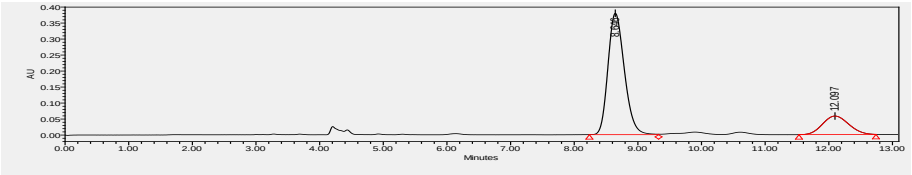
3ag

(*S*)-Naphthalen-1-yl(1-phenylethyl)silane (3ag)

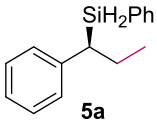
($C_{18}H_{18}Si$) colorless oil; 68.2 mg, 52% yield, 80.5:19.5 er, $[\alpha]_D^{28}$ = –63.9 (*c* = 0.58, in CH_2Cl_2), dissolved in hexane for HPLC; **HPLC** (Daicel chiralcel **OJH**, hexane/^{i}PrOH = 98/2, flow rate 1.0 mL/min) retention time: t_{major} =8.65 min, t_{minor} = 12.10 min. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.91 – 7.78 (m, 3H), 7.69 – 7.64 (m, 1H), 7.50 – 7.27 (m, 3H), 7.24 – 7.13 (m, 2H), 7.13 – 7.03 (m, 3H), 5.00 – 4.27 (m, 2H), 2.90 – 2.64 (m, 1H), 1.44 (d, *J* = 7.5 Hz, 3H). **^{13}C{^{1}H} NMR** (101 MHz, Chloroform-*d*) δ 144.9, 137.3, 136.7, 133.2, 130.8, 130.4, 128.9, 128.5, 128.0, 127.1, 126.2, 125.8, 125.2, 125.1, 25.7, 16.7. **GC-MS** (EI): Calcd for $C_{18}H_{18}Si$: 262.1, found: 262.1. **IR** (film, cm^{-1}) 3055, 2136, 1502, 1452, 1444, 985, 937, 840, 795, 777, 698, 511.



	Retention Time	% Area
1	8.665	49.76
2	12.063	50.24



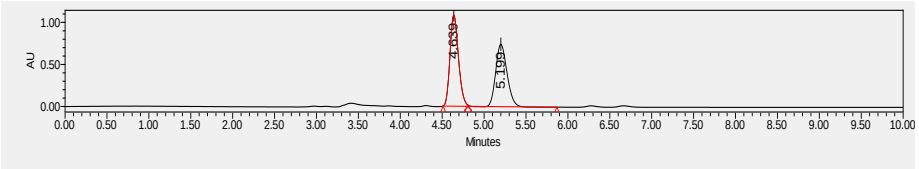
	Retention Time	% Area
1	8.646	80.50
2	12.097	19.50



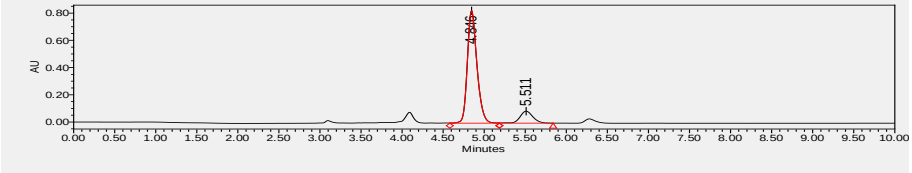
5a

(*S*)-Phenyl(1-phenylpropyl)silane (5a)

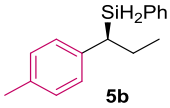
($C_{15}H_{18}Si$) colorless oil (*E* olefin); 92.8 mg, 82% yield, 88.5:11.5 er, ($C_{15}H_{18}Si$) colorless oil (*Z* olefin); 88.3 mg, 78% yield, 88.5:11.5 er ($C_{15}H_{18}Si$) colorless oil (olefin *E*:*Z* =1:1.3); 97.3 mg, 86% yield, 88.5:11.5 er $[\alpha]_D^{28}$ = –61 (*c* = 0.41, in CH_2Cl_2), dissolved in hexane for HPLC; **HPLC** (Daicel chiralcel **OJH**, hexane/^{i}PrOH = 95/5, flow rate 1 mL/min) retention time: t_{major} = 4.85 min, t_{minor} =5.51 min. **^{1}HNMR** (400 MHz, Chloroform-*d*) δ 7.21 – 7.12 (m, 3H), 7.12 – 6.99 (m, 4H), 6.94 – 6.88 (m, 1H), 6.88 – 6.81 (m, 2H), 4.44 – 3.86 (m, 2H), 2.28 – 2.02 (m, 1H), 1.92 – 1.49 (m, 2H), 0.71 (t, *J* = 7.3 Hz, 3H). **^{13}C{^{1}H} NMR** (101 MHz, Chloroform-*d*) δ142.9, 135.8, 131.6, 129.8, 128.4, 128.0, 127.9, 125.1, 34.5, 24.7, 14.0. **IR** (film, cm^{-1}) 3066, 2961, 2926, 2867, 2362, 2135, 1599, 1490, 1451, 1428, 1377, 1116, 1058, 930, 896, 850, 796, 735, 698,604, 509. These spectroscopic data correspond to the previously reported data.[7c]



	Retention Time	% Area
1	4.639	50.11
2	5.199	49.89



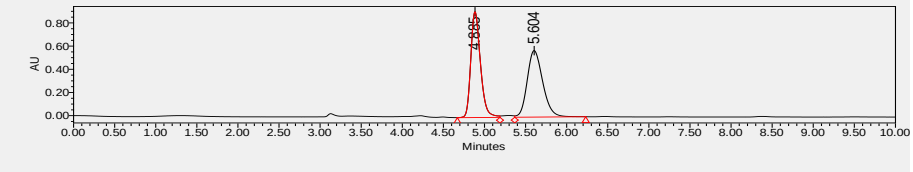
	Retention Time	% Area
1	4.846	88.50
2	5.511	11.50



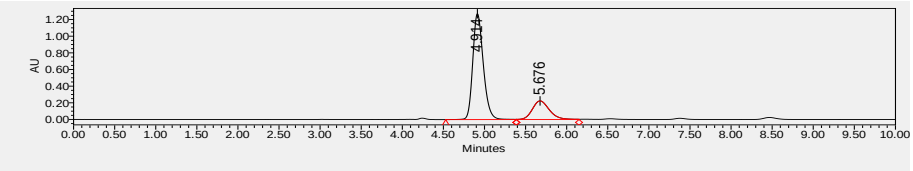
5b

(*S*)-Phenyl(1-(p-tolyl)propyl)silane (5b)

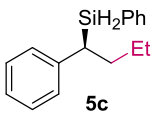
($C_{16}H_{20}Si$) (*E* olefin) colorless oil; 104.6 mg, 87% yield, 78.5:21.5 er, $[\alpha]_D^{28}$ = –36 (*c* = 0.30, in CH_2Cl_2), dissolved in hexane for HPLC; **HPLC** (Daicel chiralcel **OJH**, hexane/^{i}PrOH = 99/1, flow rate 1 mL/min) retention time: t_{major} = 4.91 min, t_{minor} = 5.68 min. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.42 – 7.37 (m, 2H), 7.37 – 7.31 (m, 1H), 7.30 – 7.23 (m, 2H), 7.07 – 6.99 (m, 2H), 6.97 – 6.89 (m, 2H), 4.67 – 3.97 (m, 2H), 2.47 – 2.10 (m, 4H), 1.96 – 1.71 (m, 2H), 0.88 (t, *J* = 7.3 Hz, 3H). **^{13}C{^{1}H} NMR** (101 MHz, Chloroform-*d*) δ 139.7, 135.8, 134.5, 131.8, 129.7, 129.2, 127.9, 33.9, 24.8, 21.1,14.0. **GC-MS** (EI): Calcd for $C_{16}H_{20}Si$: 240.1, found: 240.1. **IR** (film, cm^{-1}) 3049,3018, 2961, 2867, 2359, 2134, 1510, 1454, 1428, 1376, 1116, 1055, 930, 856, 837, 732, 699, 672, 575, 517.



	Retention Time	% Area
1	4.885	49.68
2	5.604	50.32



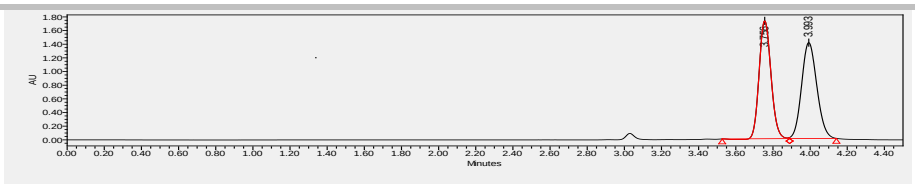
	Retention Time	% Area
1	4.914	78.49
2	5.676	21.51



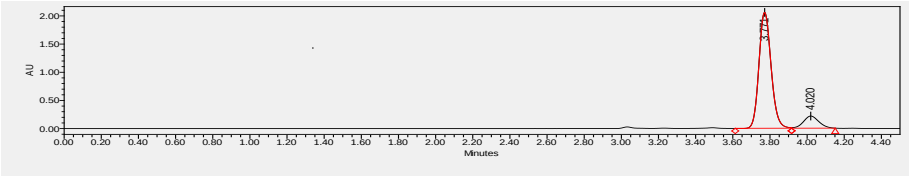
5c

(*S*)-phenyl(1-phenylbutyl)silane (5c)

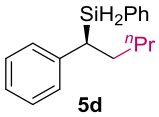
($C_{16}H_{20}Si$) colorless oil(olefin *E*:*Z* =1:4.8); 97.6 mg, 81% yield, 90.5:9.5 er, $[\alpha]_D^{26}$ = –26 (*c* = 1.95, in CH_2Cl_2), dissolved in hexane for HPLC; **HPLC** (Daicel chiralcel **OJH**, hexane/^{i}PrOH = 95/5, flow rate 1 mL/min) retention time: t_{major} = 3.77 min, t_{minor} =4.02 min. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.39 – 7.31 (m, 3H), 7.30 – 7.17 (m, 4H), 7.12 – 7.06 (m, 1H), 7.06 – 6.98 (m, 2H), 4.72 – 3.99 (m, 2H), 2.56 – 2.37 (m, 1H), 2.01 – 1.70 (m, 2H), 1.40 – 1.13 (m, 2H), 0.84 (t, J = 7.3 Hz, 3H). **^{13}C{^{1}H} NMR** (101 MHz, Chloroform-*d*) δ143.1, 135.8, 131.6, 129.8, 128.5, 128.0, 127.9, 125.1, 33.7, 32.1, 22.2, 14.0. **IR** (film, cm^{-1}) 3068,3022, 2956, 2926, 2870, 2360, 2133, 1599, 1491, 1451, 1429, 1378, 1116, 1074, 929, 886, 836, 733, 697, 606, 510. These spectroscopic data correspond to the previously reported data.[7c]



	Retention Time	% Area
1	3.756	49.16
2	3.993	50.84



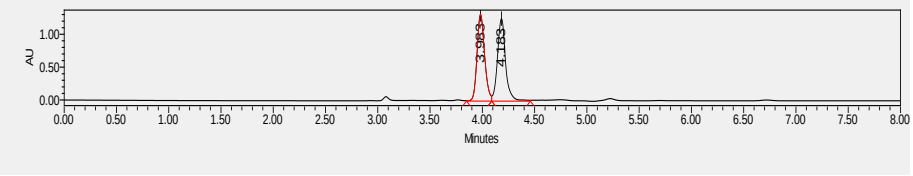
	Retention Time	% Area
1	3.771	90.46
2	4.020	9.54



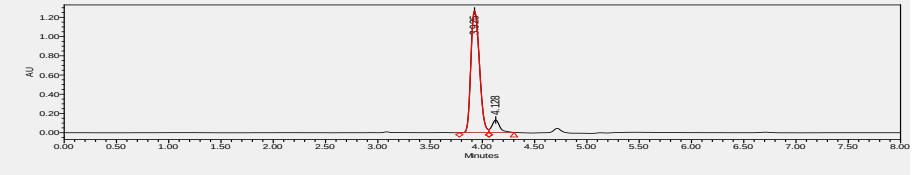
5d

(*S*)-phenyl(1-phenylpentyl)silane (5d)

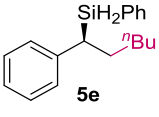
($C_{17}H_{22}Si$) colorless oil(olefin *E*:*Z* =1:4.3); 98.0 mg, 77% yield, 91.5:8.5 er, $[\alpha]_D^{25}$ = –27 (*c* = 1.48, in CH_2Cl_2), dissolved in hexane for HPLC; **HPLC** (Daicel chiralcel **IJ**, hexane/^{i}PrOH = 99/1, flow rate 1 mL/min) retention time: t_{major} = 3.93 min, t_{minor} =4.13 min. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ7.40 – 7.30 (m, 3H), 7.30 – 7.17 (m, 4H), 7.12 – 7.06 (m, 1H), 7.06 – 6.98 (m, 2H), 4.64 – 4.01 (m, 2H), 2.51 – 2.37 (m, 1H), 1.95 – 1.73 (m, 2H), 1.34 – 1.14 (m, 4H), 0.81 (t, J = 5.8 Hz, 3H). **^{13}C{^{1}H} NMR** (101 MHz, Chloroform-*d*) δ143.1, 135.8, 131.6, 129.8, 128.5, 128.0, 127.9, 125.1, 32.4, 31.4, 31.2, 22.6, 14.0. **IR** (film, cm^{-1}) 3066,3023, 2957, 2925, 2856, 2360, 2133, 1598, 1491, 1452, 1429, 1116, 1084, 929, 842, 734, 698, 603, 510. These spectroscopic data correspond to the previously reported data.[7c]



	Retention Time	% Area
1	3.983	49.46
2	4.183	50.54



	Retention Time	% Area
1	3.925	91.44
2	4.128	8.56

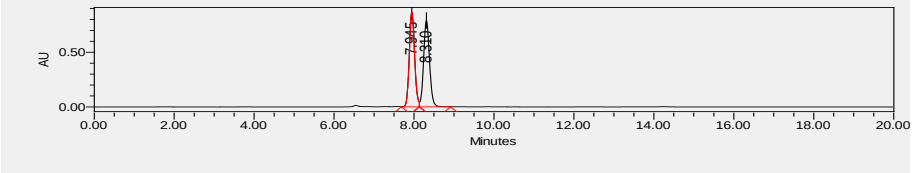


5e

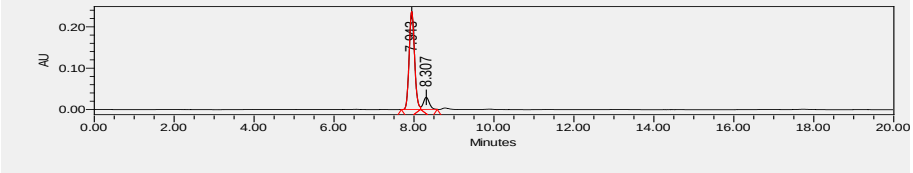
(*S*)-phenyl(1-phenylhexyl)silane (5e)

($C_{18}H_{24}Si$) colorless oil(olefin *E*:*Z* =1:5.8); 110.1 mg, 82% yield, 87.9:12.1 er, $[\alpha]_D^{25}$ = –17.5 (*c* = 0.45, in CH_2Cl_2), dissolved in hexane for HPLC; **HPLC** (Daicel chiralcel **OJH**, hexane/^{i}PrOH = 97/3, flow rate 0.5 mL/min) retention time: t_{major} = 7.94 min, t_{minor} = 8.30 min. **^{1}H NMR** (400 MHz, Chloroform-*d*)

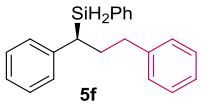
δ7.40 – 7.29 (m, 3H), 7.30 – 7.16 (m, 4H), 7.13 – 7.06 (m, 1H), 7.07 – 6.98 (m, 2H), 4.62 – 4.05 (m, 2H), 2.51 – 2.38 (m, 1H), 1.92 – 1.73 (m, 2H), 1.35 – 1.13 (m, 6H), 0.82 (t, 3H). **^{13}C{^{1}H} NMR** (101 MHz, Chloroform-*d*) δ143.2, 135.8, 131.6, 129.8, 128.5, 128.0, 127.9, 125.1, 32.4, 31.8, 31.4, 28.8, 22.6, 14.2. **IR** (film, cm^{-1}) 3023, 2956, 2925, 2855, 2134, 1492, 1453, 1429, 1116, 930, 838, 734, 698, 603, 511. These spectroscopic data correspond to the previously reported data.[7c]



	Retention Time	% Area
1	7.945	49.78
2	8.310	50.22



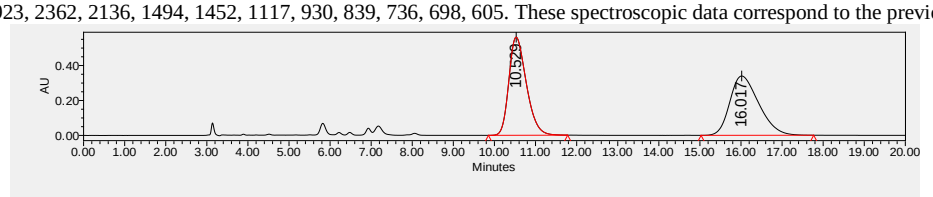
	Retention Time	% Area
1	7.943	87.91
2	8.307	12.09



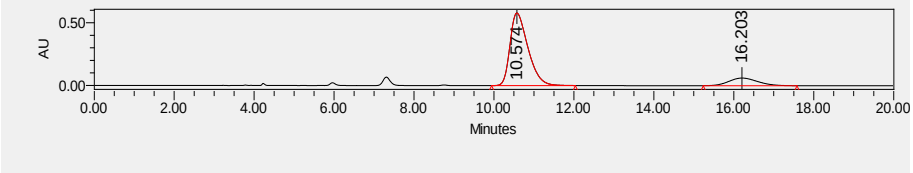
5f

(*S*)-(1,3-diphenylpropyl)(phenyl)silane (5f)

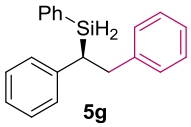
($C_{21}H_{22}Si$) colorless oil(olefin *E*:*Z*=1:1.6); 130.0 mg, 86% yield, 85.5:14.5 er $[\alpha]_D^{25}$ = –66.7 (*c* = 0.05, in CH_2Cl_2), dissolved in hexane for HPLC; **HPLC** (Daicel chiralcel **OJH**, hexane/^{i}PrOH = 95/5, flow rate 1 mL/min) retention time: t_{major} = 10.57 min, t_{minor} = 16.20 min. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ7.37 – 7.29 (m, 3H), 7.29 – 7.18 (m, 6H), 7.17 – 7.10 (m, 2H), 7.09 – 7.02 (m, 4H), 4.66 – 3.98 (m, 2H), 2.70 – 2.58 (m, 1H), 2.54 – 2.41 (m, 2H), 2.28 – 2.04 (m, 2H). **^{13}C{^{1}H} NMR** (101 MHz, Chloroform-*d*) δ142.5, 142.1, 135.8, 131.2, 129.9, 128.7, 128.6, 128.4, 128.1, 128.0, 125.9, 125.3, 35.1, 33.2, 31.8. **IR** (film, cm^{-1}) 3024, 2923, 2362, 2136, 1494, 1452, 1117, 930, 839, 736, 698, 605. These spectroscopic data correspond to the previously reported data.[7c]



	Retention Time	% Area
1	10.529	49.98
2	16.017	50.02



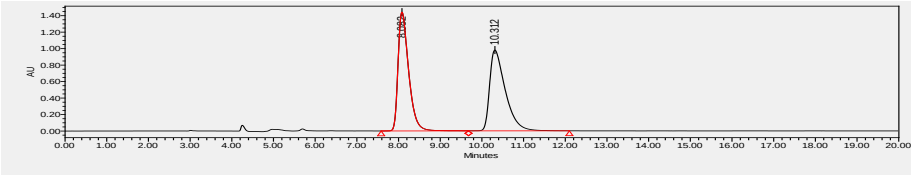
	Retention Time	% Area
1	10.574	85.50
2	16.203	14.50



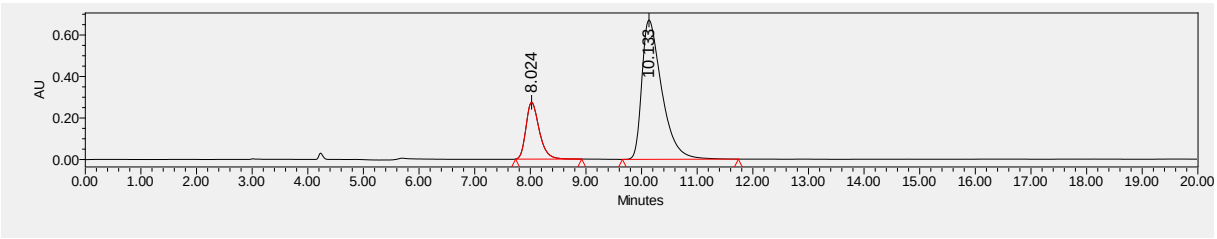
5g

(*S*)-Phenyl(1-(p-tolyl)propyl)silane (3ha)

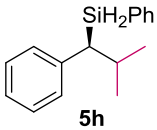
($C_{16}H_{20}Si$) colorless oil(*E* olefin); 102.4 mg, 71% yield, 78.5:21.5 er, $[\alpha]_D^{28}$ = 8.8 (*c* = 0.80, in CH_2Cl_2), dissolved in hexane for HPLC; **HPLC** (Daicel chiralcel **OJH**, hexane/^{i}PrOH = 99/1, flow rate 1 mL/min) retention time: t_{major} = 10.13 min, t_{minor} =8.02 min. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ7.38 – 7.30 (m, 3H), 7.30 – 7.23 (m, 2H), 7.22 – 7.12 (m, 4H), 7.12 – 7.01 (m, 6H), 4.76 – 3.95 (m, 2H), 3.15 (d, J = 7.9 Hz, 2H), 2.87 – 2.75 (m, 1H). **^{13}C{1H} NMR** (101 MHz, Chloroform-*d*) δ142.3, 141.2, 135.9, 131.1, 129.9, 128.8, 128.5, 128.3, 128.2, 128.0, 126.0, 125.4, 37.8, 34.3. **GC-MS** (EI): Calcd for $C_{16}H_{20}Si$: 288.1, found: 288.1. **IR** (film, cm^{-1}) 3024, 2138, 1599, 1493, 1451, 1429, 1117, 929, 832, 735, 698, 507.



	Retention Time	% Area
1	8.082	49.89
2	10.312	50.11



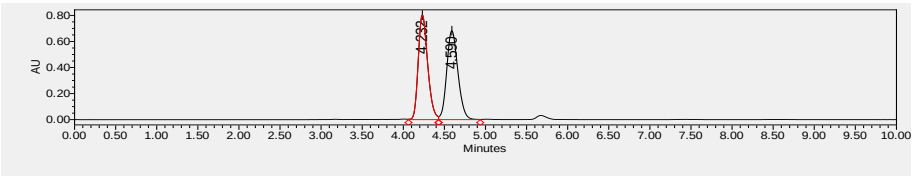
	Retention Time	% Area
1	8.024	21.31
2	10.133	78.69



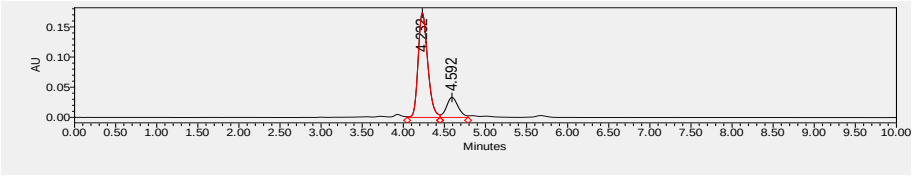
5h

(*S*)-(2-Methyl-1-phenylpropyl)(phenyl)silane (5h)

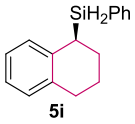
($C_{16}H_{20}Si$) colorless oil; 31.2 mg, 26% yield, 83:17 er, $[\alpha]_D^{28}$ = –13 (*c* = 1.80, in CH_2Cl_2), dissolved in hexane for HPLC; **HPLC** (Daicel chiralcel **OJH**, hexane/^{i}PrOH = 90/10, flow rate 1 mL/min) retention time: t_{major} = 4.23 min, t_{minor} =4.59 min. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.3 – 7.3 (m, 3H), 7.3 – 7.1 (m, 4H), 7.1 – 7.1 (m, 1H), 7.0 – 6.9 (m, 2H), 4.8 – 4.1 (m, 2H), 2.3 – 2.1 (m, 2H), 1.1 (d, *J* = 6.1 Hz, 3H), 0.8 (d, *J* = 6.0 Hz, 3H). **^{13}C{^{1}H} NMR** (101 MHz, Chloroform-*d*) δ 142.7, 135.8, 131.9, 129.6, 129.0, 128.3, 127.8, 125.2, 41.6, 31.0, 23.4, 22.8. **GC-MS** (EI): Calcd for $C_{16}H_{20}Si$: 240.1, found: 240.1. **IR** (film, cm^{-1}) 3067,3023, 2957, 2868, 2360, 2137, 1597, 1489, 1451, 1429, 1384, 1116, 1078, 936, 856, 824, 737, 699, 620, 510.



	Retention Time	% Area
1	4.232	49.70
2	4.590	50.30



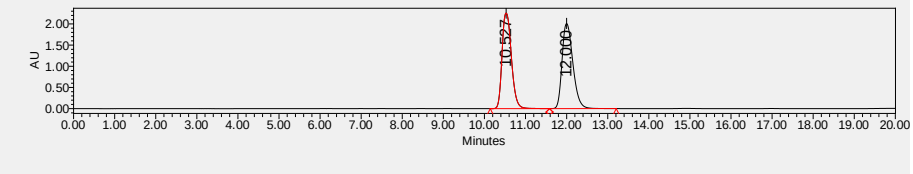
	Retention Time	% Area
1	4.231	82.75
2	4.592	17.25



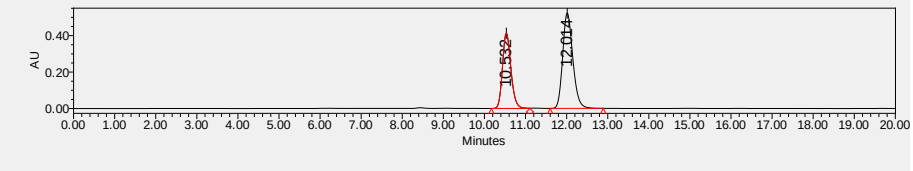
5i

(*S*)-Phenyl(1,2,3,4-tetrahydronaphthalen-1-yl)silane (5i)

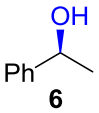
($C_{16}H_{18}Si$) colorless oil; 85.0 mg, 71% yield, 61.5:38.5 er, $[\alpha]_D^{28}$ = 4.5 (*c* = 0.33, in CH_2Cl_2), dissolved in hexane for HPLC; **HPLC** (Daicel chiralcel **OJH**, hexane/^{i}PrOH = 99/1, flow rate 0.5 mL/min) retention time: t_{major} = 12.01 min, t_{minor} =10.53 min. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.54 – 7.44 (m, 2H), 7.41 – 7.35 (m, 1H), 7.35 – 7.26 (m, 2H), 7.12 – 6.89 (m, 4H), 4.63 – 4.19 (m, 2H), 2.86 – 2.79 (m, 1H), 2.78 – 2.63 (m, 2H), 2.07 – 1.95 (m, 1H), 1.94 – 1.81 (m, 2H), 1.77 – 1.67 (m, 1H). **^{13}C{^{1}H} NMR** (101 MHz, Chloroform-*d*) δ 137.8, 136.5, 135.7, 132.0, 129.8, 129.5, 128.8, 128.0, 125.5, 124.7, 29.5, 25.3, 25.3, 21.5. **GC-MS** (EI): Calcd for $C_{16}H_{18}Si$: 238.1, found: 238.1. **IR** (film, cm^{-1}) 2929, 2136, 1489, 1116, 931, 867, 838, 741, 699.



	Retention Time	% Area
1	10.527	49.07
2	12.000	50.93



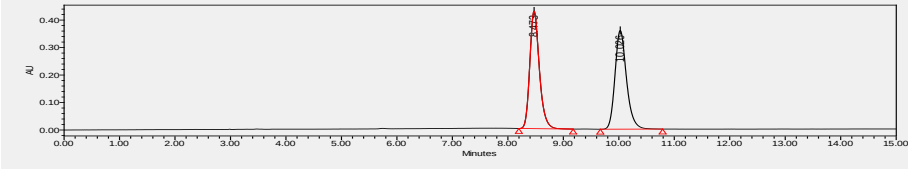
	Retention Time	% Area
1	10.532	38.35
2	12.014	61.65



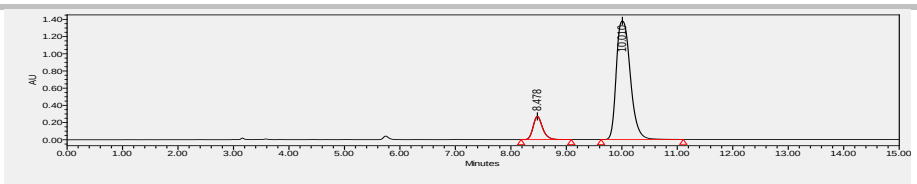
6

(*S*)-1-Phenylethan-1-ol (6)

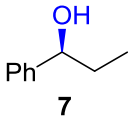
($C_8H_{10}O$) colorless oil; 61 mg, 99% yield, 91.5:8.5 er, $[\alpha]_D^{28}$ = –38 (*c* = 0.68, in CH_2Cl_2), dissolved in hexane for HPLC; **HPLC** (Daicel chiralcel **ODH**, hexane/^{i}PrOH = 95/5, flow rate 1 mL/min) retention time: t_{major} =10.01 min, t_{minor} =8.48 min. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.65 – 6.97 (m, 5H), 4.84 (q, *J* = 6.3 Hz, 1H), 2.22 (s, 1H), 1.46 (d, *J* = 6.5 Hz, 3H). **^{13}C{^{1}H} NMR** (101 MHz, Chloroform-*d*) δ 145.9, 128.5, 127.5, 125.4, 70.4, 25.2. **IR** (film, cm^{-1}) 3044, 3029, 2973, 2874, 1493, 1451, 1368, 1284, 1076, 1029, 1010, 760, 698, 606, 540. These spectroscopic data correspond to the previously reported data.[8a]



	Retention Time	% Area
1	8.473	49.73
2	10.026	50.27



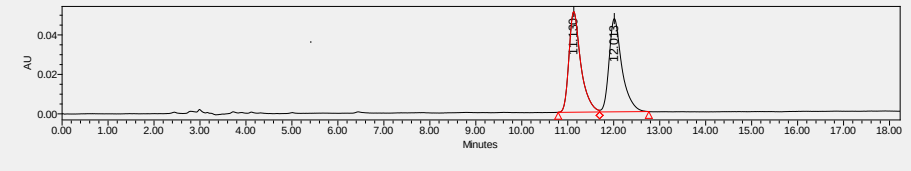
	Retention Time	% Area
1	8.478	8.47
2	10.010	91.53



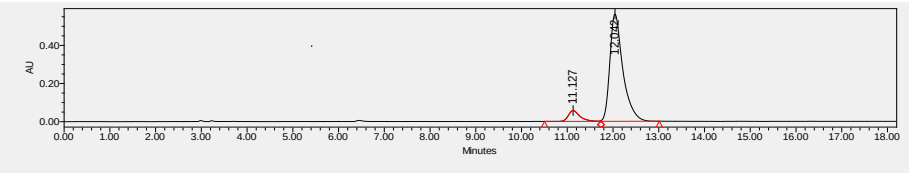
7

(*S*)-1-Phenylethan-1-ol (7)

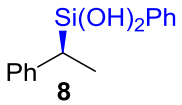
($C_9H_{12}O$) colorless oil; 15 mg, 92% yield, 90:10 er $[\alpha]_D^{28}$ = –29 (*c* = 0.28, in CH_2Cl_2), dissolved in hexane for HPLC; **HPLC** (Daicel chiralcel **OJH**, hexane/^{i}PrOH = 97/3, flow rate 1 mL/min) retention time: t_{major} =12.04 min, t_{minor} =11.13 min. **^{1}H NMR** (400 MHz, Chloroform-*d*) *δ*7.4 – 7.2 (m, 5H), 4.6 – 4.5 (m, 1H), 1.9 – 1.7 (m, 3H), 0.9 (t, J = 7.4 Hz, 3H). **^{13}C{^{1}H} NMR** (101 MHz, Chloroform-*d*) *δ* 144.7, 128.5, 127.6, 126.1, 76.2, 32.0, 10.3. **IR** (film, cm^{-1}) 3357, 3029, 2965, 2932, 2876, 1493, 1453, 1201, 1096, 1012, 974, 762, 699, 543. These spectroscopic data correspond to the previously reported data.[8d]



	Retention Time	% Area
1	11.130	49.90
2	12.013	50.10



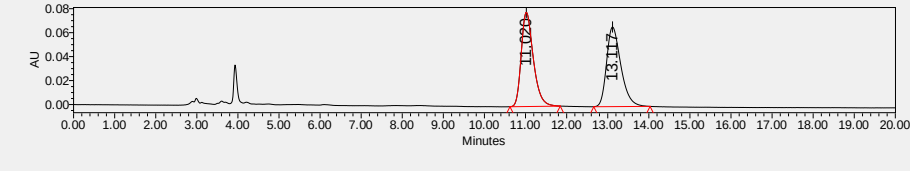
	Retention Time	% Area
1	11.127	10.13
2	12.042	89.87



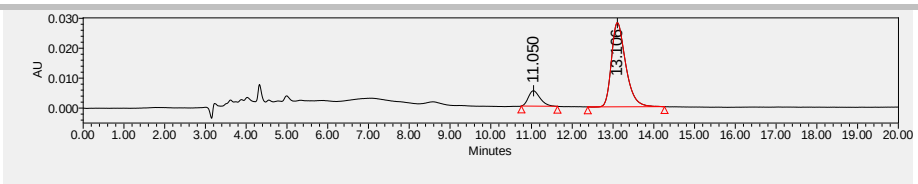
8

(*S*)-Phenyl(1-phenylethyl)silanediol (8)

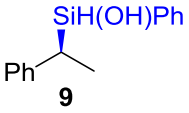
($C_{15}H_{18}Si$) white solid.M.p.120-122 °C. 110.0 mg, 90% yield, 91:9 er, $[\alpha]_D^{28}$ = –24 (*c* = 1.80, in CH_2Cl_2), dissolved in hexane for HPLC; **HPLC** (Daicel chiralcel **OJH**, hexane/^{i}PrOH = 90/10, flow rate 1 mL/min) retention time: t_{major} = 13.11 min, t_{minor} =11.05 min. **^{1}H NMR** (400 MHz, Chloroform-*d*) *δ* 7.60 – 7.49 (m, 2H), 7.45 – 7.39 (m, 1H), 7.37 – 7.30 (m, 2H), 7.27 – 7.21 (m, 2H), 7.15 – 7.06 (m, 3H), 2.85 (s, 2H), 2.48 (q, *J* = 7.6 Hz, 1H), 1.40 (d, *J* = 7.6 Hz, 3H). **^{13}C{^{1}H} NMR** (101 MHz, Chloroform-*d*) *δ* 143.4, 134.4, 133.5, 130.5, 128.5, 127.9, 127.7, 125.2, 29.0, 14.6. Found 646.0668. **IR** (film, cm^{-1}) 3319, 3072, 2963, 2874, 2361, 1598, 1491, 1453, 1429, 1122, 995, 841, 700, 522, 467. These spectroscopic data correspond to the previously reported data. [8a]



	Retention Time	% Area
1	11.020	49.99
2	13.117	50.01



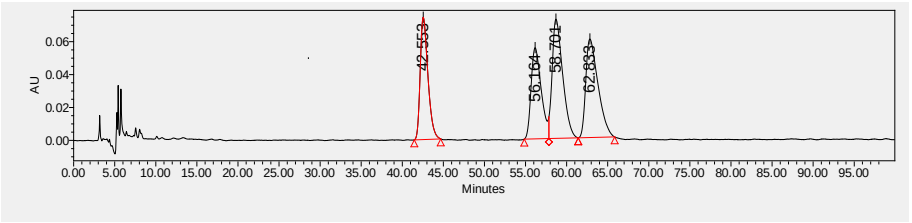
	Retention Time	% Area
1	11.050	8.99
2	13.106	91.01



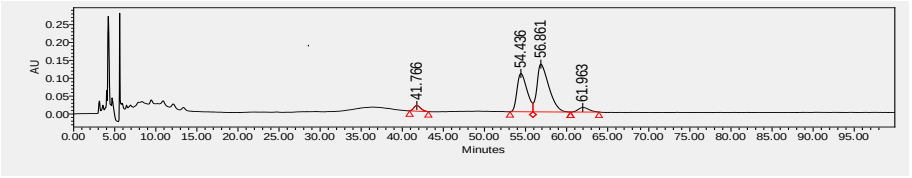
9

(S)-Phenyl(1-phenylethyl)silanol (9)

($C_{14}H_{16}OSi$) colorless oil; 79.9 mg, 70% yield, 1:1 dr, 91:9 er; 92:8 er, $[\alpha]_D^{28}$ = –2.5 (*c* = 1.58, in CH_2Cl_2), dissolved in hexane for HPLC; **HPLC** (Daicel chiralcel **OJH**, hexane/^{i}PrOH = 99/1, flow rate 1 mL/min) retention time: t_{major} = 54.44 min, 56.86 min, t_{minor} = 41.77 min, 61.96 min. **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.52 – 7.28 (m, 10H), 7.27 – 7.18 (m, 4H), 7.15 – 7.01 (m, 6H), 4.94 (d, J = 1.8 Hz, 1H), 4.91 (d, J = 2.6 Hz, 1H), 2.54 (q, J = 7.4 Hz, 2H), 2.14 (d, J = 17.8 Hz, 2H), 1.40 (dd, J = 13.2, 7.6 Hz, 6H). **^{13}C{^{1}H} NMR** (101 MHz, Chloroform-*d*) δ143.3, 143.2, 134.2, 134.2, 134.1, 130.5, 130.4, 128.6, 128.5, 128.0, 127.9, 127.6, 127.6, 125.3, 125.2, 29.2, 29.1, 14.3, 14.0. **IR** (film, cm^{-1}) 3380, 3068, 3024, 2957, 2927, 2870, 2360, 2126, 1598, 1491, 1451, 1429, 1165, 1118, 1087, 823, 759, 736, 698, 567, 492. These spectroscopic data correspond to the previously reported data.[8a]



	Retention Time	% Area
1	42.553	21.72
2	56.164	21.53
3	58.701	28.86
4	62.833	27.90



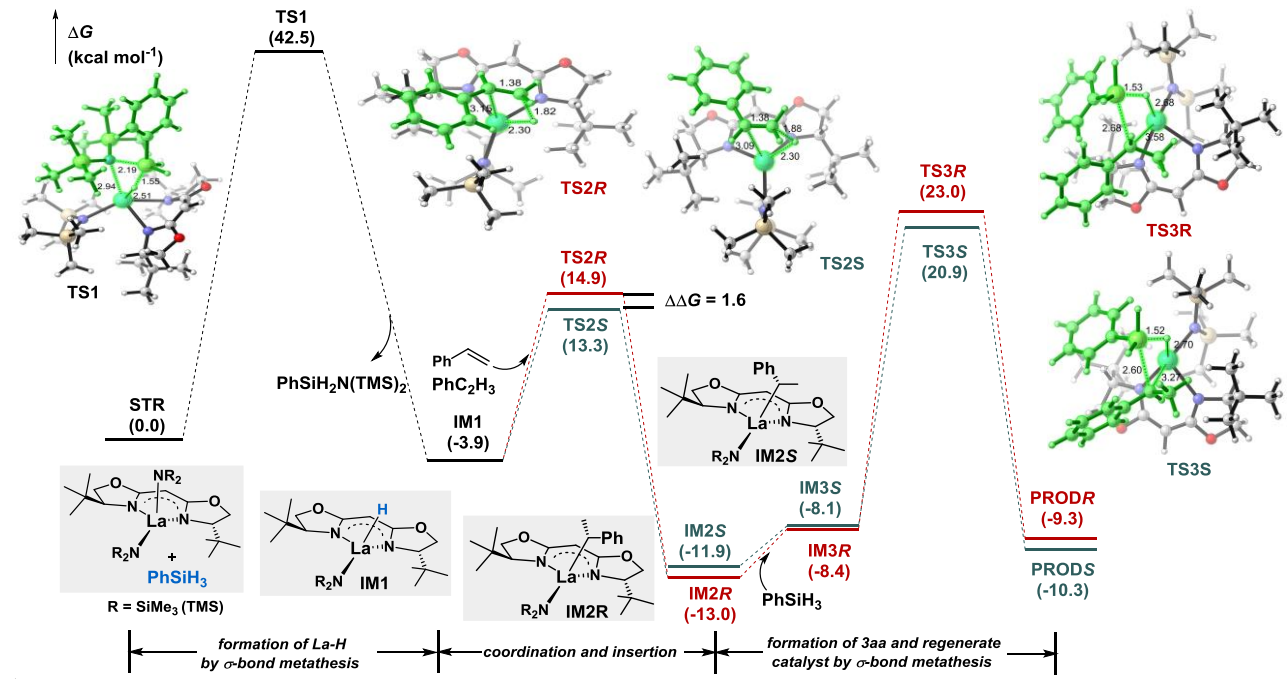
	Retention Time	% Area
1	41.766	3.80
2	54.436	38.48
3	56.861	52.97
4	61.963	4.75

9. Computational methods

All computations were carried out using the Gaussian 09 D.01 software package[9a]. The calculation of geometry optimization, frequency and Gibbs energy corrections were carried out for **STR, TS1, IM1, TS2S, TS2R, TS2me, IM2S, IM2R, IM2me, IM3S, IM3R, IM3me, TS3S, TS3R, TS3me, PROD *S*, PROD *R*, PRODme** and **$PhSiH_2N(TMS)_2$, PhC_2H_3, Add, $PhSiH_3$** at the temperature of 353.15K. All calculations were performed at B3LYP[9b] level of theory with Grimme's D3 empirical dispersion correction[9c] and SMD (toluene) implicit solvation model[9d]. The 6-311G(d) basis set[9d–9g] was used for all atoms except for the metal center La, which the MWB46 pseudo potential and its basis set were applied

. Frequency calculations for all stationary points were calculated at the same level and no imaginary frequencies were observed. The single imaginary frequency of all transition states **TS1, TS2S, TS2R, TS2me, TS3S, TS3R** and **TS3me**, which was lower than -100 cm^{-1}, was observed. Reaction paths were traced by the intrinsic reaction coordinate (IRC) method for all transition states to confirm the connectivity of the corresponding reactants and products. Single-point energies were obtained at the B3LYP[2]/6-311+G(2d,p) [9d–9g, 9j] level of theory for all non-metal atoms and B3LYP[2]/MWB46[9h, 9i] level of theory for La with GD3 empirical dispersion correction and SMD (toluene) implicit solvation model[9d]. The atomic configurations for transition states were presented by CYLview[9k] and intermolecular weak interactions were analyzed via IGMH method[9l] implemented in Multiwfn (version 3.8) [9m] and VMD[9n] was used as the visualizer.

Energy profiles



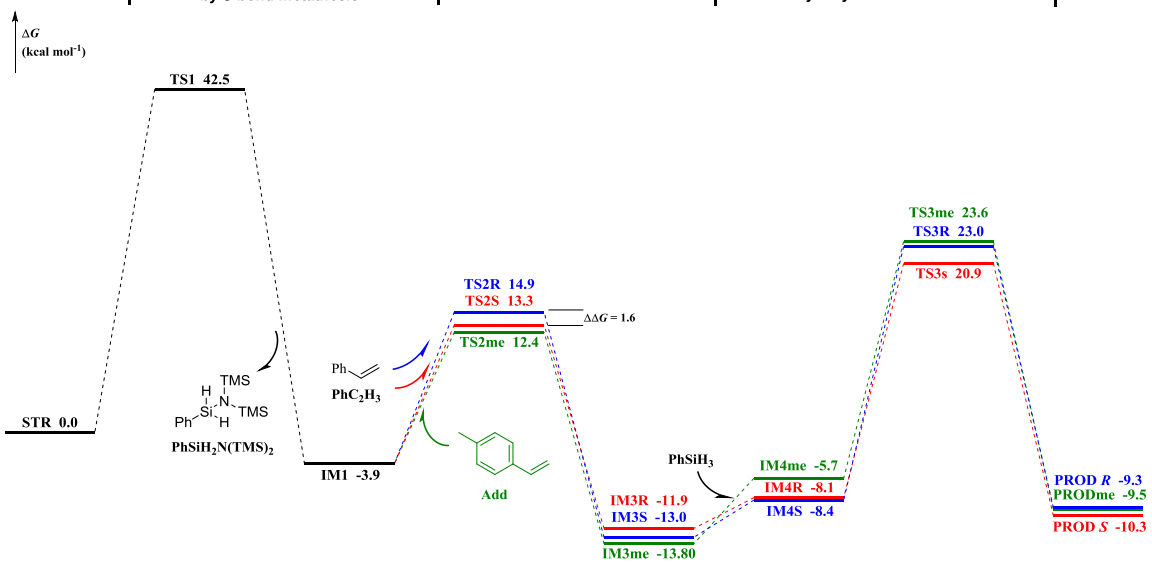
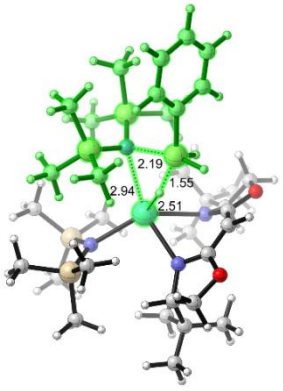
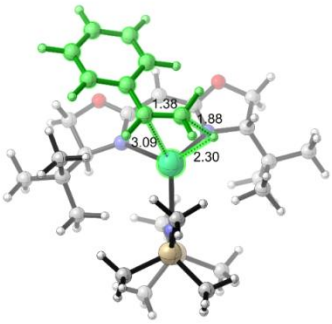


Figure S1. Energy profiles for the Si-H insertion and asymmetric metathesis reaction between PhC_2H_3 and **IM2** catalyzed by **La-Box-tBu** at the B3LYP(D3) level

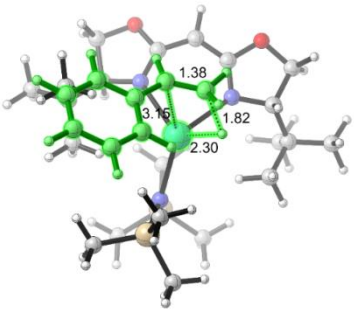
Transition states



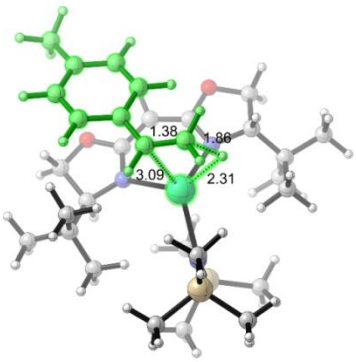
TS1



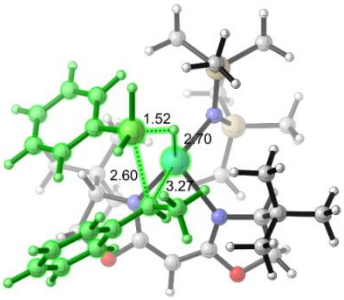
TS2S



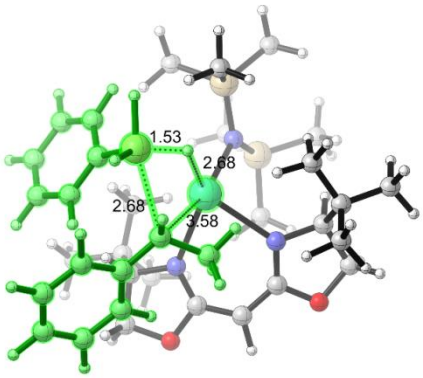
TS2R



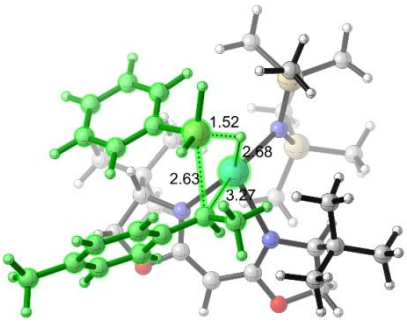
TS2me



TS3S



TS3R



TS3me

Figure S2 Optimized geometries of all transition states including La-H-N metathesis reaction (**TS1**) and PhC_2H_3 α-addition transition states (**TS2**) and La-H-C metathesis reaction (**TS3**), showing the distances between quaternary ring which undergoes bond breaking and formation, respectively.

Weak interactions

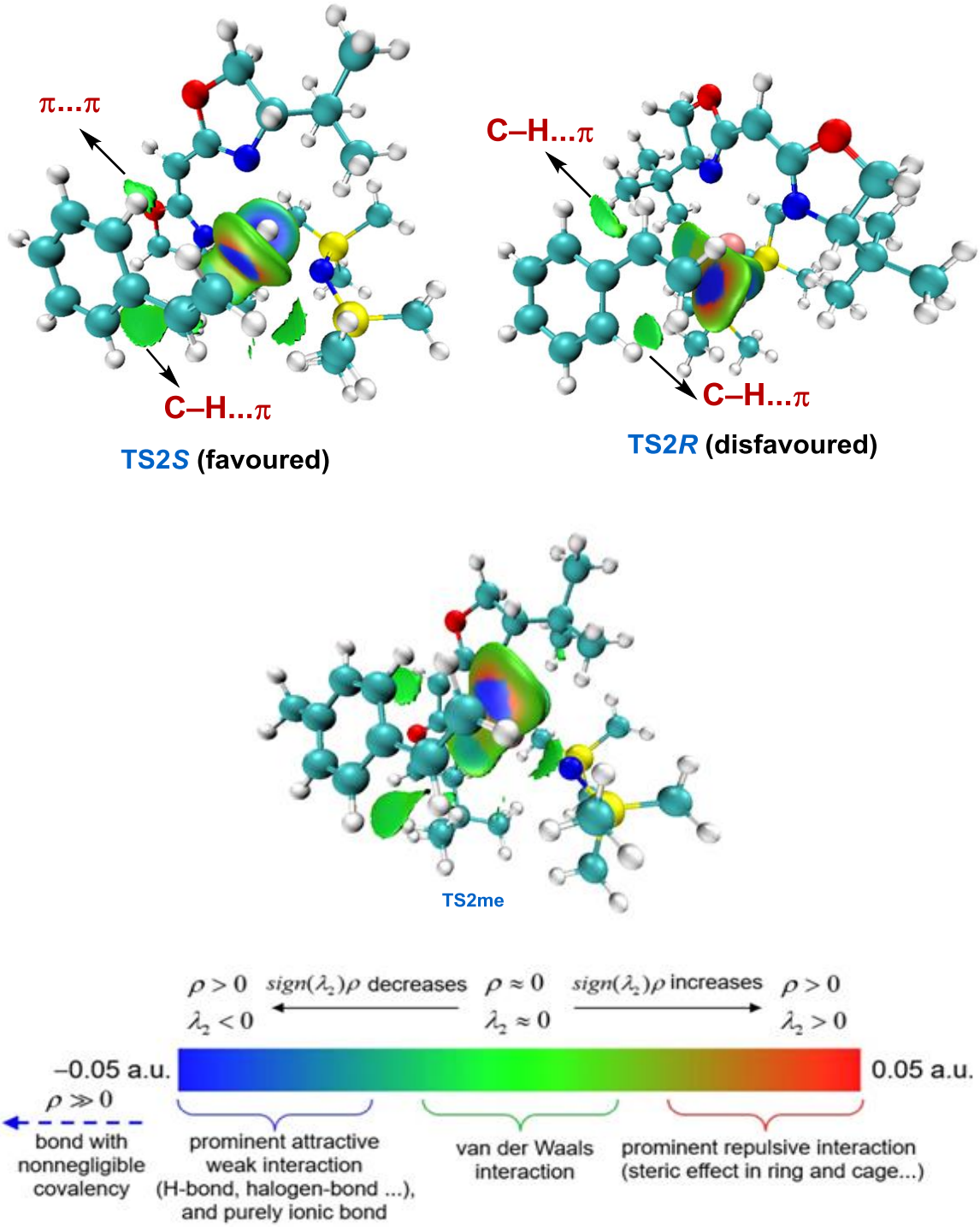


Figure S3. Weak interactions analyzed by IGMH methods of chirality determination transition states of **TS2S**, **TS2R** and **TS2me**, which showed the σ-π attractions between the substrate styrene and *tert*-butyl-oxazolidine and trimethylsilyl anion of catalysts.

Energies and coordinates

STR

La	-0.78879	-0.17894	0.00846
Si	-1.19234	-2.23617	3.07461
Si	1.02254	-0.19838	3.04525
Si	1.43941	-0.15436	-2.8154
Si	1.15824	-2.87625	-1.39845
O	-2.01462	3.46045	2.10147
O	-5.24342	0.65562	0.48543
N	-1.20959	2.30859	0.33415
N	-3.30974	0.15669	-0.57997
N	-0.27901	-1.01795	2.24793
N	0.71138	-1.22781	-1.67276
C	-2.17697	2.42174	1.23634
C	-3.33436	1.65038	1.39898
H	-3.9754	1.9121	2.22923
C	-3.89164	0.80804	0.41633
C	-0.73746	4.0671	1.78674
H	-0.0007	3.71301	2.51312
H	-0.85196	5.14443	1.88839
C	-0.43526	3.56625	0.36641
H	0.63086	3.34664	0.26221
C	-0.82474	4.54829	-0.78286
C	0.13041	5.75273	-0.73969
H	-0.08967	6.44807	-1.55509
H	1.17415	5.43921	-0.84745
H	0.04701	6.31521	0.19492
C	-0.66711	3.83365	-2.13406
H	-1.32594	2.96523	-2.19644
H	0.35868	3.49636	-2.29995
H	-0.92558	4.50655	-2.95724
C	-2.27917	5.02862	-0.64699
H	-2.98218	4.19244	-0.67916
H	-2.53137	5.70131	-1.47222
H	-2.45469	5.5761	0.28238
C	-5.61307	-0.27239	-0.55799
H	-6.53938	0.08226	-1.00617
H	-5.77781	-1.25273	-0.10251
C	-4.40541	-0.23802	-1.50348
H	-4.54698	0.59261	-2.2107
C	-4.19	-1.50681	-2.36016
C	-3.90011	-2.74658	-1.50641
H	-3.72092	-3.61675	-2.14342
H	-4.72384	-2.99833	-0.835
H	-3.01233	-2.60933	-0.89102
C	-3.02447	-1.27252	-3.33425
H	-2.9145	-2.1198	-4.01764
H	-2.06613	-1.1608	-2.82357
H	-3.18285	-0.37588	-3.94041
C	-5.47374	-1.7435	-3.17867
H	-5.34013	-2.58345	-3.86615
H	-5.73504	-0.8658	-3.77864
H	-6.33025	-1.9804	-2.54055
C	-2.85105	-2.54175	2.20759
H	-3.47035	-3.19927	2.82823
H	-2.75542	-3.04828	1.24334
H	-3.42829	-1.62349	2.05541
C	-0.29441	-3.90262	3.12728
H	-0.90862	-4.67661	3.60276
H	0.64239	-3.83984	3.6894
H	-0.04	-4.25874	2.12396
C	-1.62409	-1.77054	4.85967
H	-2.27624	-2.52843	5.30932
H	-2.15307	-0.8132	4.90782
H	-0.74201	-1.6907	5.50283
C	2.24607	-1.34198	3.9263
H	1.78693	-1.89838	4.74918
H	3.07332	-0.76357	4.35469
H	2.68064	-2.0717	3.23593
C	2.05146	0.75869	1.76697
H	2.47002	0.12336	0.98166
H	2.90482	1.21352	2.27904
H	1.52559	1.59701	1.29779
C	0.41932	1.09018	4.2975
H	0.07369	0.63251	5.22903

H	-0.42325	1.66312	3.89532
H	1.21104	1.80116	4.56216
C	2.206	1.32064	-1.8934
H	1.50729	1.87855	-1.26218
H	2.6418	2.04869	-2.5862
H	3.0066	0.96324	-1.24284
C	2.85226	-0.82302	-3.87877
H	3.28445	0.00597	-4.45195
H	2.53307	-1.58087	-4.59821
H	3.65776	-1.24889	-3.27478
C	0.14097	0.54548	-4.00806
H	0.56639	1.31872	-4.65821
H	-0.70868	1.00305	-3.48953
H	-0.26636	-0.23791	-4.6561
C	2.37258	-3.03965	0.04227
H	1.92967	-2.64769	0.96351
H	3.29607	-2.48185	-0.13813
H	2.64905	-4.08282	0.23578
C	1.88085	-3.81021	-2.88046
H	1.287	-3.6722	-3.78985
H	1.88218	-4.88401	-2.65848
H	2.91148	-3.53112	-3.11092
C	-0.36653	-3.90087	-0.91461
H	-0.87576	-3.55526	-0.00997
H	-0.07044	-4.9345	-0.70332
H	-1.10482	-3.93719	-1.72112
Si	5.27929	2.77214	-0.04647
H	6.25624	3.41572	0.87045
H	3.91787	3.08378	0.45837
H	5.43034	3.35123	-1.40491
C	5.57168	0.91797	-0.12983
C	5.59113	0.1352	1.03702
C	5.76597	0.27221	-1.36085
C	5.79388	-1.24083	0.97697
H	5.44176	0.59835	2.00851
C	5.97657	-1.10519	-1.4243
H	5.74392	0.84311	-2.28459
C	5.99074	-1.8634	-0.25574
H	5.79169	-1.82831	1.88949
H	6.12465	-1.5855	-2.3862
H	6.14481	-2.93645	-0.30431

Zero-point correction = 0.964818
Thermal correction to Enthalpy = 1.051731
Thermal correction to Gibbs Free Energy = 0.835794

TS1

La	-0.502844	0.009899	0.148675
Si	-2.379711	-3.197967	-0.459574
Si	-2.186896	-2.258926	2.365166
O	-1.665460	1.710693	-3.803590
O	0.229109	4.343264	-0.546748
N	-1.936786	0.764909	-1.777376
N	-0.915125	2.625425	0.394641
N	-1.817965	-2.005671	0.688572
C	-1.324510	1.696851	-2.491118
C	-0.420133	2.665281	-2.037411
H	0.140555	3.219746	-2.775567
C	-0.386717	3.135191	-0.719418
C	-2.592520	0.610851	-3.997742
H	-2.043703	-0.224754	-4.441550
H	-3.358946	0.947009	-4.693184
C	-3.080539	0.289152	-2.577081
H	-3.195182	-0.787014	-2.450346
C	-4.419881	0.967865	-2.148999
C	-5.574291	0.312085	-2.925043
H	-6.532328	0.754149	-2.636296
H	-5.637338	-0.762053	-2.727789
H	-5.471622	0.445449	-4.006183
C	-4.629032	0.750445	-0.640213
H	-3.871466	1.286197	-0.063092
H	-4.576805	-0.305309	-0.365892
H	-5.608501	1.126878	-0.330023
C	-4.407426	2.480693	-2.424160
H	-3.600032	2.980303	-1.883538
H	-5.348865	2.928720	-2.091984
H	-4.294388	2.713266	-3.486076
C	0.131505	4.649010	0.864612

H	0.000997	5.725046	0.960864
H	1.057585	4.337414	1.359717
C	-1.080393	3.820512	1.274395
H	-1.966826	4.359760	0.903381
C	-1.336898	3.592638	2.774275
C	-0.253495	2.744642	3.447735
H	-0.487923	2.590253	4.504532
H	0.728400	3.217700	3.392595
H	-0.164109	1.754658	2.999858
C	-2.716947	2.928974	2.917646
H	-2.920118	2.649572	3.954979
H	-2.797429	2.031641	2.302244
H	-3.510684	3.607970	2.591603
C	-1.380763	4.968542	3.467081
H	-1.697027	4.863035	4.508943
H	-2.089177	5.642341	2.974945
H	-0.401327	5.455740	3.471156
C	-1.443887	-3.057576	-2.101393
H	-1.236963	-2.033667	-2.432081
H	-2.024995	-3.528008	-2.902373
H	-0.490598	-3.588149	-2.052181
C	-2.138306	-4.990725	0.109569
H	-2.393615	-5.667151	-0.715078
H	-2.785843	-5.261425	0.949454
H	-1.108078	-5.210345	0.399204
C	-4.226221	-3.077943	-0.868626
H	-4.542293	-3.981451	-1.403796
H	-4.467896	-2.230489	-1.512263
H	-4.852952	-2.997615	0.022847
C	-1.107257	-3.561151	3.212261
H	-0.047229	-3.294614	3.176956
H	-1.204433	-4.554194	2.767163
H	-1.380879	-3.651572	4.270233
C	-3.990928	-2.710448	2.715678
H	-4.686993	-1.958425	2.330342
H	-4.157113	-2.781742	3.796831
H	-4.278815	-3.674969	2.287413
C	-1.876675	-0.671540	3.356151
H	-0.833909	-0.334092	3.387547
H	-2.129912	-0.866643	4.404086
H	-2.505622	0.166129	3.049494
Si	2.562101	-2.485862	-0.377500
Si	3.121185	-0.322081	1.643169
N	2.325251	-0.806114	0.144426
C	2.225112	-2.671771	-2.234395
H	1.239000	-2.335046	-2.553016
H	2.300697	-3.733695	-2.494917
H	2.949488	-2.149628	-2.866375
C	4.289766	-3.205320	-0.085400
H	4.387486	-4.119537	-0.683730
H	4.437619	-3.499096	0.957791
H	5.110593	-2.543479	-0.361460
C	1.420408	-3.695532	0.518440
H	1.442921	-4.669994	0.017889
H	0.381694	-3.369928	0.563253
H	1.747842	-3.864241	1.548103
C	2.854813	1.522386	1.993978
H	1.865004	1.912211	1.756954
H	3.569140	2.133484	1.437456
H	3.030241	1.711109	3.058818
C	4.991308	-0.564957	1.768210
H	5.278154	-1.593848	1.994739
H	5.368812	0.059971	2.586878
H	5.520278	-0.260862	0.863473
C	2.383272	-1.255760	3.123471
H	1.297418	-1.148947	3.219892
H	2.817730	-0.881893	4.057790
H	2.593429	-2.328316	3.084795
Si	2.439812	0.616588	-1.511567
H	2.332096	1.252137	-2.898439
H	2.045757	1.749456	-0.636978
H	1.093954	-0.097378	-1.786653
C	4.356800	0.587142	-1.528991
C	4.975909	1.763048	-1.069946
C	5.194207	-0.418375	-2.030480
C	6.362476	1.909998	-1.068868
H	4.369042	2.586922	-0.704706

C	6.582021	-0.278220	-2.037852
H	4.776070	-1.337206	-2.423657
C	7.174458	0.882846	-1.545047
H	6.807173	2.827084	-0.693106
H	7.200984	-1.081479	-2.427136
H	8.254775	0.989599	-1.541977

Zero-point correction = 0.967403
Thermal correction to Enthalpy = 1.051627
Thermal correction to Gibbs Free Energy = 0.846682

IM1

La	0.15045	0.03155	-0.96664
Si	1.9464	-2.35981	1.09099
Si	3.67007	-0.79645	-0.88035
O	-4.26778	-0.16468	-1.56701
O	-2.43978	3.76043	-0.02656
N	-2.27894	-0.59522	-0.59127
N	-0.87144	2.14438	0.16003
N	2.14969	-1.15654	-0.13177
C	-3.11417	0.33658	-1.04533
C	-3.0028	1.73004	-1.03391
H	-3.82936	2.27985	-1.462
C	-2.06177	2.48295	-0.30774
C	-4.12882	-1.60443	-1.57456
H	-3.81778	-1.91521	-2.57662
H	-5.10484	-2.03107	-1.35251
C	-3.03712	-1.86289	-0.52755
H	-2.39431	-2.69173	-0.84058
C	-3.56577	-2.18927	0.90659
C	-4.16404	-3.60577	0.89637
H	-4.52765	-3.8778	1.8917
H	-3.41817	-4.3524	0.60422
H	-5.01058	-3.69471	0.20894
C	-2.39343	-2.14813	1.89677
H	-1.97128	-1.14327	1.95586
H	-1.59576	-2.8393	1.6149
H	-2.72461	-2.42718	2.90145
C	-4.6281	-1.17737	1.3692
H	-4.23803	-0.15662	1.37247
H	-4.94481	-1.40951	2.39056
H	-5.52316	-1.19003	0.74273
C	-1.33323	4.39841	0.6441
H	-1.73353	4.97474	1.47681
H	-0.85162	5.07657	-0.06512
C	-0.43441	3.22569	1.07286
H	-0.70043	2.92975	2.09776
C	1.08511	3.53262	1.08212
C	1.6094	3.91921	-0.30992
H	2.6997	3.99654	-0.30125
H	1.22254	4.88446	-0.64459
H	1.33558	3.19032	-1.07724
C	1.85302	2.30868	1.60896
H	2.91296	2.54361	1.74047
H	1.81706	1.44615	0.93723
H	1.46432	1.97732	2.57643
C	1.32555	4.70354	2.05389
H	2.39371	4.92482	2.13337
H	0.96199	4.4694	3.05948
H	0.82904	5.6205	1.72307
C	0.80175	-3.73845	0.45205
H	-0.11841	-3.36823	-0.0153
H	0.50001	-4.43751	1.23983
H	1.32293	-4.32077	-0.31671
C	3.50887	-3.24916	1.68039
H	3.22691	-4.07256	2.34757
H	4.17587	-2.59375	2.24677
H	4.08792	-3.68856	0.86247
C	1.1795	-1.58998	2.64718
H	0.8966	-2.3478	3.38634
H	0.28352	-0.99305	2.44898
H	1.90399	-0.92254	3.12693
C	4.25816	-2.15598	-2.05781
H	3.54403	-2.30554	-2.87527
H	4.37021	-3.11846	-1.54716
H	5.22734	-1.91432	-2.50955
C	5.07846	-0.44032	0.33751
H	4.75094	0.20091	1.16293

H	5.90067	0.07814	-0.16991
H	5.49912	-1.34952	0.77492
C	3.49564	0.78711	-1.9167
H	2.75414	0.72773	-2.72184
H	4.44871	0.99961	-2.41428
H	3.27548	1.66858	-1.30415
H	0.16733	0.06923	-3.23744

Zero-point correction = 0.622820
Thermal correction to Enthalpy = 0.676258
Thermal correction to Gibbs Free Energy = 0.534336

TS2S

La	0.17801	0.10905	0.65925
Si	3.08598	-1.07558	-1.29736
Si	2.83523	-2.15959	1.50918
O	-1.32128	4.12244	-1.03502
O	-3.28003	0.25165	-2.55461
N	0.01389	2.40045	-0.43196
N	-1.48166	-0.35879	-1.32067
N	2.2425	-1.16352	0.2216
C	-1.1197	2.7736	-1.00977
C	-2.15977	2.02601	-1.57262
H	-2.97906	2.59968	-1.98256
C	-2.24169	0.64093	-1.75568
C	-0.10511	4.75317	-0.59192
H	-0.37032	5.56423	0.08582
H	0.39582	5.17083	-1.46896
C	0.68685	3.6185	0.08057
H	0.52378	3.6606	1.16563
C	2.22207	3.66645	-0.13411
C	2.734	5.014	0.40662
H	3.8237	5.07017	0.33016
H	2.47046	5.14848	1.4608
H	2.32703	5.8632	-0.15068
C	2.87619	2.53652	0.67749
H	2.6784	1.54679	0.2579
H	2.54174	2.54426	1.71915
H	3.96536	2.63674	0.68073
C	2.60676	3.52044	-1.61322
H	2.21292	2.59648	-2.03898
H	3.69491	3.50433	-1.72363
H	2.23688	4.34814	-2.22391
C	-3.30594	-1.18637	-2.52442
H	-3.60863	-1.53711	-3.50955
H	-4.0385	-1.50419	-1.77498
C	-1.86951	-1.54434	-2.14093
H	-1.26271	-1.51719	-3.05882
C	-1.68039	-2.96311	-1.54334
C	-2.27202	-3.09862	-0.13597
H	-2.17172	-4.12782	0.22162
H	-3.32974	-2.83689	-0.10599
H	-1.77221	-2.45687	0.5939
C	-0.18869	-3.33249	-1.51975
H	-0.04666	-4.33679	-1.10977
H	0.41676	-2.65268	-0.91776
H	0.23299	-3.32874	-2.52859
C	-2.39756	-3.96188	-2.47605
H	-2.18235	-4.99003	-2.17103
H	-2.06381	-3.85192	-3.51277
H	-3.48409	-3.83972	-2.45775
C	4.62106	0.03818	-1.26504
H	4.36832	1.09755	-1.35117
H	5.28407	-0.2003	-2.10514
H	5.20197	-0.08486	-0.34669
C	3.67757	-2.76824	-1.91675
H	4.06825	-2.68554	-2.93786
H	2.86802	-3.50384	-1.9363
H	4.48388	-3.18219	-1.30238
C	1.95311	-0.39318	-2.65845
H	2.54045	-0.21711	-3.5669
H	1.46832	0.55797	-2.41703
H	1.15897	-1.097	-2.92105
C	4.67367	-1.92097	1.88766
H	4.90049	-0.88029	2.14185
H	5.31422	-2.19796	1.04428
H	4.98174	-2.53917	2.7388
C	2.54148	-4.01159	1.23771

H	1.48407	-4.2271	1.04954
H	2.83638	-4.58909	2.12201
H	3.10548	-4.40829	0.38945
C	1.9037	-1.75433	3.12264
H	1.9636	-0.69843	3.40852
H	2.3558	-2.31871	3.94563
H	0.84752	-2.05144	3.1166
H	0.21971	1.37737	2.57476
C	-4.58811	1.43721	1.09585
C	-3.40485	1.16383	1.7751
C	-3.10798	-0.13684	2.22948
C	-4.06314	-1.14238	1.98517
C	-5.24934	-0.86489	1.31661
C	-5.51929	0.42732	0.86133
H	-4.77342	2.44367	0.73535
H	-2.691	1.96723	1.93081
H	-3.86464	-2.15303	2.32907
H	-5.9685	-1.66116	1.1481
H	-6.43845	0.64152	0.32619
C	-1.85519	-0.46042	2.92048
H	-1.61736	-1.5174	3.03206
C	-1.07441	0.45933	3.58298
H	-1.44414	1.45388	3.79337
H	-0.2836	0.12151	4.23986

Zero-point correction = 0.758058
Thermal correction to Enthalpy = 0.821583
Thermal correction to Gibbs Free Energy = 0.657753

IM2S

La	0.0632	-0.005	0.51728
Si	3.08066	-0.93858	-1.33939
Si	3.15687	-1.53443	1.6088
O	-1.89985	3.67551	-1.60639
O	-3.19309	-0.55963	-2.83531
N	-0.41837	2.23305	-0.69177
N	-1.44071	-0.79387	-1.42611
N	2.33482	-0.88408	0.22907
C	-1.51474	2.3803	-1.42391
C	-2.36198	1.44433	-2.02477
H	-3.19978	1.85673	-2.56891
C	-2.26727	0.04884	-2.03506
C	-0.8718	4.52451	-1.06924
H	-1.34842	5.30149	-0.47169
H	-0.34895	4.99232	-1.9066
C	0.02179	3.57597	-0.24809
H	-0.22738	3.68968	0.81767
C	1.54564	3.85136	-0.36892
C	1.8069	5.30018	0.08062
H	2.87796	5.52078	0.06431
H	1.45094	5.47329	1.10181
H	1.31776	6.02967	-0.57138
C	2.30733	2.90555	0.57254
H	2.27768	1.86966	0.22573
H	1.91811	2.95234	1.59561
H	3.36755	3.16873	0.62141
C	2.05376	3.64542	-1.8027
H	1.82669	2.641	-2.16338
H	3.13822	3.7808	-1.84575
H	1.61326	4.35586	-2.50687
C	-3.10871	-1.9705	-2.56643
H	-3.299	-2.50479	-3.4958
H	-3.87605	-2.22758	-1.82852
C	-1.68771	-2.13143	-2.02734
H	-1.01052	-2.24647	-2.88765
C	-1.45418	-3.35667	-1.11072
C	-2.1109	-3.18111	0.26392
H	-2.0218	-4.09925	0.8517
H	-3.16918	-2.92584	0.1973
H	-1.6443	-2.38473	0.85178
C	0.05727	-3.57691	-0.94304
H	0.26331	-4.39076	-0.24221
H	0.58243	-2.69125	-0.5741
H	0.52406	-3.83695	-1.89719
C	-2.04756	-4.60035	-1.79947
H	-1.78089	-5.50607	-1.24719
H	-1.66485	-4.71315	-2.81881
H	-3.13922	-4.56207	-1.85193

C	4.50723	0.29304	-1.53187
H	4.20109	1.30993	-1.26701
H	4.86052	0.32221	-2.56933
H	5.36705	0.04032	-0.90535
C	3.7597	-2.65389	-1.7783
H	4.16525	-2.66102	-2.79685
H	2.97951	-3.42023	-1.73471
H	4.5677	-2.97368	-1.11288
C	1.83731	-0.50854	-2.70346
H	2.34799	-0.54301	-3.67258
H	1.4044	0.4929	-2.61898
H	1.00311	-1.21223	-2.75995
C	5.03352	-1.28757	1.61635
H	5.29892	-0.22658	1.57146
H	5.54411	-1.79047	0.79011
H	5.45896	-1.68766	2.54412
C	2.81744	-3.38573	1.83097
H	1.75228	-3.58248	1.99985
H	3.35859	-3.79672	2.69117
H	3.11636	-3.96277	0.95026
C	2.53646	-0.68858	3.19194
H	2.68819	0.39646	3.1618
H	3.09629	-1.0584	4.05811
H	1.48008	-0.87376	3.41667
H	-0.45019	2.25853	2.4991
C	-4.48416	1.12893	1.29438
C	-3.19433	1.23415	1.81291
C	-2.57023	0.15608	2.49116
C	-3.35583	-1.01454	2.64986
C	-4.64419	-1.10955	2.14525
C	-5.22251	-0.04157	1.44946
H	-4.911	1.97444	0.76278
H	-2.65873	2.16995	1.68231
H	-2.92745	-1.86106	3.18121
H	-5.20911	-2.02583	2.29626
H	-6.22779	-0.12025	1.04866
C	-1.16887	0.19605	2.91565
H	-0.95653	-0.56531	3.67178
C	-0.61472	1.55502	3.33525
H	-1.2729	2.10434	4.02575
H	0.35311	1.44654	3.83372

Zero-point correction = 0.764554
Thermal correction to Enthalpy = 0.828034
Thermal correction to Gibbs Free Energy = 0.663746

IM3S

La	-0.79843	-0.01317	-0.45913
Si	-2.15568	2.63777	1.75609
Si	0.23345	3.41375	0.11394
O	-0.98889	-4.11311	1.90516
O	-4.92705	-2.29731	0.28814
N	-0.62156	-2.02874	1.12383
N	-3.20676	-0.93431	-0.25457
N	-0.92812	2.23057	0.60016
C	-1.48586	-3.01596	1.26867
C	-2.83323	-3.09601	0.90145
H	-3.37262	-3.9777	1.21644
C	-3.58193	-2.081	0.30215
C	0.43069	-3.91534	2.05907
H	0.94601	-4.54461	1.32927
H	0.70399	-4.24088	3.06145
C	0.64492	-2.41621	1.78307
H	1.47085	-2.29273	1.07512
C	0.98375	-1.55463	3.0344
C	2.35095	-1.99942	3.58078
H	2.64822	-1.37721	4.43046
H	3.13057	-1.9128	2.8169
H	2.34123	-3.03598	3.9294
C	1.08869	-0.08546	2.60404
H	0.12737	0.32018	2.28436
H	1.81813	0.04148	1.79537
H	1.42061	0.54643	3.43285
C	-0.09682	-1.68921	4.11639
H	-1.08339	-1.43686	3.72147
H	0.10996	-1.01586	4.95383
H	-0.1511	-2.70289	4.52271
C	-5.55643	-1.05526	-0.06678

H	-5.94852	-0.59616	0.84552
H	-6.38839	-1.28326	-0.72994
C	-4.42843	-0.21346	-0.69592
H	-4.42994	0.78498	-0.24711
C	-4.5524	-0.0153	-2.23764
C	-4.52224	-1.36219	-2.97264
H	-4.56068	-1.21229	-4.05565
H	-5.36837	-1.99942	-2.70131
C	-3.39921	0.86575	-2.74339
H	-3.56503	1.16267	-3.7827
H	-2.44322	0.33323	-2.7465
H	-3.30061	1.78709	-2.15837
C	-5.86923	0.7257	-2.53484
H	-5.95141	0.94324	-3.60355
H	-5.92121	1.68009	-2.00036
H	-6.75194	0.14283	-2.26085
C	-2.8343	1.09659	2.62261
H	-3.69271	1.36706	3.2483
H	-2.08849	0.65294	3.28972
H	-3.1713	0.308	1.94438
C	-1.56305	3.76465	3.16164
H	-2.37178	3.91605	3.8864
H	-1.25425	4.75779	2.82135
H	-0.72043	3.324	3.70431
C	-3.61921	3.52773	0.93972
H	-4.43773	3.70514	1.64717
H	-4.03267	2.95527	0.10271
H	-3.32017	4.50159	0.53853
C	1.53158	3.77789	1.44494
H	1.96768	2.85344	1.83623
H	1.10467	4.31287	2.2973
H	2.34922	4.39628	1.05773
C	-0.5068	5.07493	-0.41461
H	-1.23852	4.95654	-1.22093
H	0.27392	5.75251	-0.78012
H	-1.01125	5.58947	0.40932
C	1.18134	2.76304	-1.39773
H	1.77309	1.86042	-1.21138
H	1.89766	3.51614	-1.74413
H	0.51767	2.57261	-2.2466
H	-3.60661	-1.91378	-2.74516
H	6.85245	-1.07963	-2.91296
C	3.08301	-2.89916	-1.1043
C	1.82397	-3.45887	-1.33947
C	0.82778	-2.73168	-1.97835
C	1.04017	-1.4067	-2.45453
C	2.33212	-0.8649	-2.19597
C	3.31884	-1.59342	-1.53592
H	1.61404	-4.4766	-1.02315
H	-0.13805	-3.19962	-2.15389
H	2.57081	0.13353	-2.54593
H	4.28379	-1.13085	-1.36001
C	-0.05365	-0.63656	-3.02464
C	0.25996	0.4016	-4.0945
H	0.64116	-0.05047	-5.02376
H	-0.63363	0.97445	-4.36677
H	1.01045	1.13168	-3.78167
Si	7.50347	-0.08591	-2.02027
H	7.89221	1.08965	-2.83948
C	6.3432	0.45092	-0.64206
C	6.33029	-0.22252	0.59049
C	5.44236	1.51309	-0.82405
C	5.44934	0.15029	1.60421
H	7.01791	-1.04492	0.76814
C	4.56015	1.88849	0.18758
H	5.42535	2.05967	-1.76329
C	4.56401	1.20835	1.40457
H	5.45844	-0.37923	2.55162
H	3.87413	2.71296	0.03045
H	3.8873	1.50764	2.19749
H	8.71536	-0.71072	-1.43242
H	-0.85938	-1.3023	-3.35822
H	3.85889	-3.46468	-0.59916

Zero-point correction = 0.880115
Thermal correction to Enthalpy = 0.956272
Thermal correction to Gibbs Free Energy = 0.761600

TS3S

La	0.32162	0.09048	-0.39062
Si	3.65008	-1.09499	0.61981
Si	3.0326	-1.40153	-2.2903
O	-2.14291	-0.28006	3.50276
O	1.15208	2.96159	3.23413
N	-0.80249	-0.66798	1.72856
N	1.06846	1.81635	1.29146
N	2.55535	-0.82342	-0.71571
C	-1.10925	0.15123	2.73351
C	-0.52381	1.35267	3.12739
H	-0.87894	1.7882	4.05025
C	0.54931	1.99561	2.49837
C	-2.72291	-1.42265	2.8362
H	-3.60888	-1.08884	2.29115
H	-3.01946	-2.13415	3.60344
C	-1.61624	-1.90228	1.8882
H	-2.05201	-2.17769	0.92485
C	-0.8056	-3.13278	2.39941
C	-1.74813	-4.34818	2.46792
H	-1.19357	-5.24434	2.76111
H	-2.21175	-4.54906	1.49752
H	-2.55016	-4.21604	3.19914
C	0.31414	-3.44974	1.39792
H	1.04722	-2.64496	1.34583
H	-0.08434	-3.62139	0.3928
H	0.85625	-4.35294	1.69096
C	-0.19339	-2.87095	3.78356
H	0.46712	-2.00194	3.77583
H	0.40015	-3.73195	4.1053
H	-0.95705	-2.70001	4.54677
C	2.34818	3.3648	2.54267
H	3.20761	2.98383	3.0995
H	2.38222	4.45263	2.55052
C	2.22938	2.73198	1.1391
H	3.11952	2.1321	0.92971
C	2.10393	3.76568	-0.01999
C	0.85732	4.64479	0.14695
H	0.76398	5.34413	-0.68828
H	0.89289	5.23932	1.06348
C	2.03652	3.0263	-1.36404
H	2.07692	3.72468	-2.20339
H	1.08628	2.49483	-1.48451
H	2.85657	2.31306	-1.48151
C	3.37537	4.63488	-0.03639
H	3.34632	5.33679	-0.87445
H	4.27708	4.024	-0.14961
H	3.48834	5.22977	0.87327
C	2.90165	-0.66065	2.30944
H	3.03087	0.39541	2.55357
H	3.43891	-1.22946	3.07724
H	1.84251	-0.88503	2.43809
C	4.19895	-2.90672	0.74347
H	4.85293	-3.04883	1.61167
H	4.75829	-3.24588	-0.13331
H	3.34526	-3.58052	0.86682
C	5.22793	-0.04547	0.51628
H	5.71719	0.00389	1.49643
H	5.01478	0.98409	0.21039
H	5.96211	-0.44379	-0.18795
C	2.52395	-3.21055	-2.54057
H	1.46284	-3.369	-2.31765
H	3.08745	-3.88355	-1.88715
H	2.69067	-3.54039	-3.5724
C	4.88479	-1.29042	-2.66577
H	5.26091	-0.2651	-2.59586
H	5.06089	-1.63078	-3.69283
H	5.50316	-1.91577	-2.01672
C	2.20378	-0.41501	-3.68166
H	1.14684	-0.63841	-3.84686
H	2.70583	-0.65962	-4.62469
H	2.29475	0.66886	-3.55331
H	-0.05309	4.04326	0.17974
H	-0.34368	0.86463	-2.88547
C	-6.13666	1.40481	0.15611
C	-5.03521	1.14679	0.97819
C	-3.74612	1.41035	0.53608

C	-3.48239	1.94312	-0.74881
C	-4.61621	2.24208	-1.54067
C	-5.90916	1.96387	-1.10077
H	-7.146	1.20114	0.49912
H	-5.18491	0.75493	1.98083
H	-2.91212	1.21514	1.20278
H	-4.4853	2.69151	-2.51825
H	-6.75063	2.1984	-1.74748
C	-2.1076	2.11044	-1.2333
C	-1.83541	3.35063	-2.0838
H	-2.04973	4.287	-1.54868
H	-0.78813	3.40113	-2.40223
H	-2.43216	3.37939	-3.00042
Si	-1.77347	0.45415	-3.20434
H	-1.40487	-0.14803	-4.55449
C	-2.2264	-1.15337	-2.30206
C	-3.4341	-1.32479	-1.60056
C	-1.39243	-2.28119	-2.45042
C	-3.796	-2.57027	-1.08836
H	-4.10599	-0.48674	-1.46787
C	-1.73865	-3.52173	-1.91216
H	-0.48406	-2.20768	-3.0446
C	-2.9504	-3.66958	-1.23922
H	-4.74247	-2.67903	-0.56833
H	-1.078	-4.37268	-2.04395
H	-3.23687	-4.63699	-0.84008
H	-2.89928	1.32575	-3.601
H	-1.44994	2.17967	-0.35057

Zero-point correction = 0.881737
Thermal correction to Enthalpy = 0.955629
Thermal correction to Gibbs Free Energy = 0.771053

PROD S

La	1.0408	-0.22978	-0.61783
Si	4.37259	-0.56133	0.90475
Si	4.34417	-0.47584	-2.11377
O	-1.78427	-1.19574	3.104
O	0.76404	2.69554	3.10101
N	-0.47592	-1.1096	1.26553
N	0.87624	1.66064	1.0977
N	3.50363	-0.46741	-0.59779
C	-0.82223	-0.52795	2.40362
C	-0.36364	0.65707	2.98371
H	-0.71365	0.8907	3.97859
C	0.42651	1.61505	2.34516
C	-2.33356	-2.18804	2.20959
H	-3.24964	-1.78418	1.77298
H	-2.5744	-3.07089	2.79822
C	-1.23823	-2.38075	1.15105
H	-1.69283	-2.44537	0.15836
C	-0.35997	-3.65567	1.35124
C	-1.22849	-4.90415	1.11915
H	-0.63607	-5.81273	1.26195
H	-1.63055	-4.92484	0.1034
H	-2.07274	-4.95832	1.81142
C	0.76698	-3.66851	0.30735
H	1.5101	-2.89049	0.50235
H	0.37527	-3.55813	-0.71145
H	1.31658	-4.61339	0.33262
C	0.25297	-3.69783	2.75902
H	0.81795	-2.79029	2.97814
H	0.93768	-4.54629	2.85368
H	-0.50892	-3.809	3.53456
C	1.72378	3.46035	2.34472
H	2.72118	3.23604	2.73367
H	1.51008	4.51519	2.50616
C	1.54361	2.96813	0.89951
H	2.52403	2.8088	0.43665
C	0.74463	3.92697	-0.03219
C	-0.64526	4.23326	0.54409
H	-1.20414	4.88852	-0.12966
H	-0.58654	4.73966	1.51104
C	0.59298	3.26633	-1.40957
H	0.11343	3.94249	-2.12178
H	-0.0385	2.37338	-1.37818
H	1.56649	2.99649	-1.8369
C	1.54411	5.22918	-0.2081

H	1.04008	5.89805	-0.91152
H	2.54794	5.03472	-0.60044
H	1.65486	5.77714	0.73138
C	3.24422	-1.12101	2.3194
H	2.36672	-0.48616	2.47834
H	3.80661	-1.09951	3.2601
H	2.90031	-2.15096	2.18946
C	5.81186	-1.79532	0.87587
H	6.26156	-1.88054	1.87208
H	6.61296	-1.50235	0.19006
H	5.48051	-2.79709	0.58329
C	5.08589	1.11322	1.43219
H	5.67256	1.02407	2.35406
H	4.28939	1.83847	1.62939
H	5.73956	1.54622	0.66911
C	4.99986	-2.18272	-2.60821
H	4.20765	-2.93962	-2.57654
H	5.80368	-2.52984	-1.95299
H	5.39591	-2.17258	-3.63062
C	5.79984	0.73579	-2.18782
H	5.48374	1.76067	-1.96571
H	6.24839	0.74394	-3.18795
H	6.59808	0.48257	-1.48307
C	3.16517	0.04037	-3.51016
H	2.33407	-0.65171	-3.68717
H	3.72493	0.07981	-4.45188
H	2.73116	1.03897	-3.37843
H	-1.23268	3.32371	0.68379
H	-0.19724	-0.15584	-2.5496
C	-5.29221	1.58907	2.02843
C	-3.98424	1.11797	1.93194
C	-3.29485	1.21754	0.72498
C	-3.88675	1.78717	-0.40888
C	-5.20115	2.26386	-0.29321
C	-5.89562	2.16601	0.91093
H	-3.4934	0.66995	2.78869
H	-2.27945	0.84275	0.66253
H	-5.69206	2.70814	-1.15306
H	-6.9128	2.54066	0.97527
C	-3.13525	1.8281	-1.7215
C	-3.14878	3.20531	-2.41023
H	-2.79069	3.98302	-1.72938
H	-2.50308	3.21044	-3.29295
H	-4.15039	3.49688	-2.73823
Si	-3.78507	0.47325	-2.89722
H	-2.95538	0.41214	-4.12629
C	-3.83595	-1.23712	-2.11345
C	-4.7102	-1.52316	-1.05056
C	-3.03978	-2.28168	-2.61201
C	-4.79476	-2.80718	-0.51482
H	-5.33515	-0.73902	-0.63425
C	-3.12691	-3.56878	-2.08198
H	-2.34533	-2.08868	-3.42371
C	-4.00862	-3.8344	-1.03497
H	-5.47955	-3.00668	0.30368
H	-2.51025	-4.3644	-2.48928
H	-4.08053	-4.83611	-0.624
H	-5.17172	0.86214	-3.27944
H	-2.09305	1.55552	-1.52684
H	-5.83354	1.51362	2.96622

Zero-point correction = 0.880979
Thermal correction to Enthalpy = 0.955646
Thermal correction to Gibbs Free Energy = 0.764716

TS2R

La	0.16434	-0.06271	-0.41704
Si	1.26351	2.75104	1.67146
Si	-0.67536	3.42919	-0.54594
O	3.12596	-3.64987	-0.57913
O	-0.05234	-3.66788	2.72962
N	2.2517	-1.56895	-0.43648
N	-0.28301	-1.71732	1.59928
N	0.2719	2.27744	0.33164
C	2.19653	-2.82508	-0.01759
C	1.35019	-3.45887	0.89883
H	1.59146	-4.48813	1.12451
C	0.34269	-2.88446	1.68181

C	4.03953	-2.83108	-1.33013
H	4.23436	-3.3242	-2.28216
H	4.97331	-2.76463	-0.76576
C	3.31464	-1.48113	-1.46861
H	2.82857	-1.43088	-2.45162
C	4.2347	-0.23563	-1.3678
C	5.3228	-0.35963	-2.45029
H	5.95914	0.52992	-2.46068
H	4.88425	-0.46319	-3.44822
H	5.97624	-1.22054	-2.28134
C	3.40822	1.02682	-1.65604
H	2.70055	1.25274	-0.85294
H	2.8492	0.93931	-2.59194
H	4.05114	1.90805	-1.73536
C	4.88597	-0.11103	0.01682
H	4.13404	-0.07692	0.80735
H	5.48044	0.80528	0.07845
H	5.55701	-0.94527	0.23794
C	-1.17739	-3.0183	3.34168
H	-1.09455	-3.14013	4.42057
H	-2.09138	-3.5084	2.99121
C	-1.05532	-1.56661	2.86629
H	-0.4239	-1.022	3.58337
C	-2.40324	-0.80438	2.79241
C	-3.29081	-1.32088	1.6558
H	-4.24102	-0.78071	1.62986
H	-3.52061	-2.38459	1.75472
H	-2.81844	-1.18942	0.68206
C	-2.14396	0.69621	2.60035
H	-3.08489	1.24909	2.53212
H	-1.5737	0.92665	1.69733
H	-1.57684	1.11285	3.43717
C	-3.13324	-0.98719	4.13757
H	-4.03668	-0.37133	4.16762
H	-2.50252	-0.68442	4.97963
H	-3.44314	-2.02235	4.30503
C	2.86531	3.62494	1.16355
H	3.52232	2.97356	0.58011
H	3.43105	3.94758	2.0456
H	2.67497	4.51571	0.5575
C	0.38893	3.90892	2.89051
H	1.01448	4.08094	3.77414
H	-0.56384	3.49785	3.23837
H	0.18078	4.89115	2.45408
C	1.79272	1.22791	2.67222
H	2.4797	1.53369	3.46935
H	2.32673	0.46396	2.09537
H	0.94764	0.73195	3.15836
C	0.26729	4.9874	-1.06119
H	1.16281	4.74721	-1.64369
H	0.58453	5.59001	-0.20422
H	-0.36437	5.63069	-1.68504
C	-2.22843	3.98945	0.3824
H	-2.84969	3.13613	0.67514
H	-2.85022	4.63982	-0.2443
H	-1.99469	4.54529	1.29503
C	-1.31822	2.63546	-2.14693
H	-0.52947	2.24724	-2.8012
H	-1.85911	3.38734	-2.73258
H	-2.04611	1.83219	-1.98062
H	0.45157	-0.39924	-2.67212
C	-1.70804	-1.97269	-2.08739
C	-0.62263	-1.84715	-2.9297
H	0.22778	-2.50686	-2.79996
H	-0.7344	-1.45524	-3.93196
H	-1.64375	-2.68046	-1.26284
C	-3.01068	-1.34828	-2.32127
C	-4.15067	-1.79334	-1.62013
C	-3.19137	-0.29217	-3.23947
C	-5.39891	-1.21675	-1.82332
H	-4.04886	-2.61226	-0.9149
C	-4.44276	0.28257	-3.44145
H	-2.34204	0.09234	-3.79352
C	-5.55612	-0.17061	-2.73438
H	-6.25588	-1.58795	-1.26904
H	-4.54512	1.09674	-4.15264
H	-6.52976	0.28191	-2.8915

Zero-point correction = 0.757565
Thermal correction to Enthalpy = 0.820354
Thermal correction to Gibbs Free Energy = 0.659138

IM2R

La	0.0507	-0.14865	0.51654
Si	1.99676	2.1716	-1.55914
Si	1.97589	2.82963	1.37701
O	-3.31444	-1.96602	-2.06854
O	0.72968	-4.1392	-1.7611
N	-1.81281	-0.49758	-1.23977
N	1.00765	-2.10816	-0.80287
N	1.47221	1.81392	0.06235
C	-2.03964	-1.73134	-1.65134
C	-1.19838	-2.85633	-1.70425
H	-1.64569	-3.7529	-2.11028
C	0.1602	-2.95351	-1.39069
C	-4.01651	-0.7069	-2.06043
H	-4.98931	-0.86407	-1.59509
H	-4.16166	-0.39669	-3.0982
C	-3.09932	0.23488	-1.26108
H	-3.47412	0.29316	-0.23255
C	-3.01389	1.6901	-1.78354
C	-4.43558	2.27977	-1.78481
H	-4.41727	3.33117	-2.08619
H	-4.88892	2.22751	-0.78959
H	-5.09729	1.75541	-2.48071
C	-2.14725	2.50734	-0.81313
H	-1.09632	2.2072	-0.83854
H	-2.51366	2.42152	0.21596
H	-2.15847	3.57005	-1.07095
C	-2.41086	1.76433	-3.19258
H	-1.41931	1.30993	-3.22521
H	-2.31506	2.80559	-3.51361
H	-3.03129	1.25534	-3.93521
C	2.04944	-4.16196	-1.19074
H	2.70858	-4.67926	-1.88545
H	2.00904	-4.71189	-0.2439
C	2.36964	-2.67847	-1.00417
H	2.75523	-2.29741	-1.96131
C	3.44934	-2.36758	0.06689
C	2.90854	-2.50877	1.49533
H	3.72159	-2.42647	2.22215
H	2.40847	-3.46441	1.66293
H	2.18937	-1.7221	1.74769
C	4.00131	-0.94718	-0.13599
H	4.77037	-0.72184	0.60882
H	3.23854	-0.17197	-0.04794
H	4.45853	-0.84187	-1.12364
C	4.61748	-3.35498	-0.13149
H	5.4585	-3.08172	0.51186
H	4.97873	-3.3419	-1.16465
H	4.34229	-4.38367	0.11634
C	1.13096	3.66738	-2.33793
H	0.06113	3.49348	-2.48242
H	1.55616	3.87833	-3.32655
H	1.23637	4.57695	-1.74091
C	3.85928	2.50855	-1.6823
H	4.15694	2.63491	-2.72987
H	4.45247	1.68529	-1.27409
H	4.15945	3.42006	-1.15594
C	1.64868	0.72051	-2.72872
H	1.90597	1.01914	-3.75169
H	0.60313	0.39983	-2.75616
H	2.24852	-0.16216	-2.49626
C	2.0595	4.67875	0.98084
H	1.09036	5.06946	0.65514
H	2.79101	4.92267	0.20509
H	2.34858	5.23859	1.87804
C	3.66554	2.31733	2.06487
H	3.65217	1.28478	2.43269
H	3.97425	2.95298	2.90298
H	4.44945	2.37712	1.30359
C	0.74231	2.67629	2.81377
H	-0.27747	2.93793	2.51005
H	1.01433	3.3692	3.61771
H	0.71546	1.68329	3.27459

C	-0.23349	-2.53382	3.18023
C	-0.6072	-1.06488	2.99742
H	-0.19067	-0.43617	3.78973
C	-2.00602	-0.75791	2.74694
C	-2.90077	-1.68303	2.14054
C	-2.53691	0.54073	2.99625
C	-4.21774	-1.34304	1.84373
H	-2.55991	-2.68891	1.91894
C	-3.85378	0.87033	2.6975
H	-1.9004	1.27865	3.47802
C	-4.71455	-0.06868	2.12126
H	-4.86448	-2.08897	1.3901
H	-4.21683	1.86785	2.92988
H	-5.74374	0.18824	1.89407
H	0.78724	-2.62912	3.55896
H	-0.89018	-3.05877	3.89169
H	-0.27009	-3.12064	2.25177

Zero-point correction = 0.764734
Thermal correction to Enthalpy = 0.828289
Thermal correction to Gibbs Free Energy = 0.666269

IM3R

La	-0.65795	-0.06197	-0.44627
Si	0.23027	2.09175	2.40198
Si	1.43744	2.93902	-0.22248
O	-3.35882	-3.51079	1.37438
O	-5.11749	0.77196	0.97549
N	-1.76234	-2.06233	0.70931
N	-3.05643	0.70042	0.05731
N	0.4493	1.85091	0.69608
C	-3.04181	-2.23803	1.00519
C	-4.09722	-1.32317	1.02791
H	-5.04215	-1.67399	1.4172
C	-4.02071	0.02541	0.6656
C	-2.20998	-4.33377	1.08796
H	-2.39349	-4.86342	0.14802
H	-2.11456	-5.06201	1.89131
C	-1.04724	-3.33567	0.96073
H	-0.44489	-3.58722	0.08488
C	-0.07759	-3.28774	2.17972
C	0.65727	-4.63731	2.27006
H	1.38264	-4.62817	3.08908
H	1.20183	-4.85542	1.34612
H	-0.02711	-5.46907	2.45734
C	0.97856	-2.19393	1.94725
H	0.55248	-1.18734	1.98635
H	1.49697	-2.33512	0.99262
H	1.73854	-2.22135	2.73236
C	-0.82816	-3.00521	3.48845
H	-1.40541	-2.08047	3.42705
H	-0.12642	-2.90321	4.32175
H	-1.52201	-3.80996	3.74521
C	-4.76143	2.1535	0.78155
H	-4.56231	2.59674	1.7616
H	-5.61743	2.65729	0.3369
C	-3.49928	2.10603	-0.10035
H	-2.73	2.76746	0.31278
C	-3.72285	2.53685	-1.582
C	-4.79975	1.67439	-2.25477
H	-4.90484	1.94409	-3.30988
H	-5.78093	1.7983	-1.78868
C	-2.40424	2.39254	-2.35629
H	-2.4933	2.80744	-3.36414
H	-2.12644	1.34347	-2.49251
H	-1.58857	2.9272	-1.86093
C	-4.13053	4.02034	-1.60912
H	-4.24626	4.36742	-2.63992
H	-3.37306	4.65191	-1.13312
H	-5.0813	4.20293	-1.10142
C	-1.31045	1.18469	3.03495
H	-2.22869	1.55282	2.56998
H	-1.40726	1.34349	4.11505
H	-1.29326	0.10066	2.88851
C	1.68804	1.44911	3.42927
H	1.53551	1.64383	4.49752
H	2.62986	1.92343	3.13962
H	1.82178	0.36932	3.31426

C	-0.01534	3.90377	2.90665
H	-0.23688	3.96765	3.97851
H	-0.85015	4.37122	2.3745
H	0.8718	4.51954	2.73001
C	3.15102	3.23093	0.51947
H	3.68258	2.29226	0.68822
H	3.10268	3.75636	1.47886
H	3.76985	3.8424	-0.14744
C	0.66083	4.65021	-0.48345
H	-0.36269	4.58819	-0.86764
H	1.24144	5.23305	-1.20839
H	0.6212	5.23492	0.43955
C	1.71566	2.25281	-1.97282
H	2.17646	1.26076	-1.98903
H	2.40786	2.91171	-2.50817
H	0.80655	2.21421	-2.58336
H	-4.54126	0.61364	-2.20739
H	4.16695	0.38532	-3.10815
C	1.59437	-4.40825	-1.7889
C	0.27561	-4.43723	-2.25208
C	-0.36774	-3.27891	-2.67045
C	0.28627	-2.01417	-2.66929
C	1.62303	-2.01429	-2.17253
C	2.25815	-3.18138	-1.75513
H	2.09364	-5.31798	-1.47391
H	-0.25956	-5.3823	-2.29178
H	-1.38712	-3.34855	-3.03318
H	2.18884	-1.0849	-2.19959
H	3.29051	-3.13786	-1.41969
C	-0.37306	-0.78086	-3.05563
C	-1.64099	-0.8931	-3.89369
H	-1.94158	0.08249	-4.28354
H	-1.52512	-1.55814	-4.76404
H	-2.50236	-1.27767	-3.33091
Si	5.49024	0.11231	-2.49492
H	6.47987	1.09568	-3.00184
C	5.40021	0.25018	-0.62256
C	4.44865	-0.47119	0.11847
C	6.29428	1.07216	0.08031
C	4.39492	-0.37804	1.50609
H	3.73526	-1.11484	-0.38672
C	6.24344	1.16787	1.47103
H	7.03773	1.65194	-0.4592
C	5.29414	0.44243	2.18634
H	3.6471	-0.93799	2.05606
H	6.94016	1.81575	1.99341
H	5.24504	0.5227	3.26719
H	5.90704	-1.25224	-2.90983
H	0.336	-0.05764	-3.46984

Zero-point correction = 0.880899
Thermal correction to Enthalpy = 0.956419
Thermal correction to Gibbs Free Energy = 0.765614

TS3R

La	0.133979	0.076768	-0.203485
Si	1.322565	-3.341406	0.179565
Si	1.893726	-2.095343	-2.498906
O	-1.498257	1.229283	3.996304
O	3.086925	0.695039	3.428628
N	-1.035684	0.201294	2.039695
N	2.012446	0.465724	1.457777
N	1.206477	-1.973459	-0.902862
C	-0.547127	0.792235	3.130306
C	0.774023	0.986288	3.529442
H	0.937481	1.339935	4.537248
C	1.905475	0.702664	2.758817
C	-2.764065	1.138186	3.305767
H	-2.991976	2.118536	2.876819
H	-3.524412	0.880099	4.039477
C	-2.508241	0.085240	2.223929
H	-3.015740	0.366673	1.296477
C	-2.982835	-1.353073	2.589436
C	-4.521083	-1.365371	2.609258
H	-4.892357	-2.369501	2.833647
H	-4.932641	-1.071016	1.639227
H	-4.934909	-0.693186	3.366205
C	-2.498993	-2.324607	1.506711

H	-1.419467	-2.457238	1.553523
H	-2.776311	-1.984768	0.505652
H	-2.944064	-3.314597	1.638043
C	-2.434555	-1.809084	3.950365
H	-1.342976	-1.770368	3.976349
H	-2.730202	-2.843925	4.148339
H	-2.810075	-1.200293	4.776628
C	4.078894	0.156080	2.531832
H	4.241078	-0.893455	2.792924
H	5.004210	0.705076	2.691924
C	3.453573	0.317670	1.136838
H	3.593055	-0.594283	0.549368
C	4.033178	1.504757	0.308492
C	3.907575	2.831959	1.070297
H	4.273563	3.660495	0.457386
H	4.489891	2.834783	1.995205
C	3.282203	1.605147	-1.026624
H	3.740250	2.349669	-1.682970
H	2.248143	1.937957	-0.897737
H	3.301052	0.653732	-1.562214
C	5.511620	1.212310	-0.003637
H	5.937343	2.008826	-0.620323
H	5.627490	0.273183	-0.554335
H	6.122793	1.145218	0.900063
C	1.297872	-2.800683	1.998766
H	2.254568	-2.347820	2.274397
H	1.167450	-3.685488	2.632282
H	0.523024	-2.090880	2.296141
C	-0.090111	-4.566520	-0.123770
H	-0.132483	-5.338028	0.653462
H	0.039961	-5.079616	-1.082387
H	-1.067685	-4.078422	-0.155514
C	2.927606	-4.337252	0.031480
H	2.936932	-5.114463	0.804921
H	3.817701	-3.720047	0.185657
H	3.040071	-4.847578	-0.929114
C	1.277507	-3.607801	-3.454585
H	0.185876	-3.616240	-3.538989
H	1.575406	-4.551211	-2.987296
H	1.681161	-3.614523	-4.473546
C	3.789954	-2.168778	-2.491631
H	4.229074	-1.491139	-1.753136
H	4.191124	-1.881849	-3.470274
H	4.167240	-3.170450	-2.271262
C	1.457756	-0.607127	-3.591392
H	0.395874	-0.513783	-3.833380
H	1.966625	-0.753105	-4.551085
H	1.798119	0.368518	-3.228979
H	2.869464	3.045288	1.334952
H	-0.605217	1.407074	-2.336183
C	0.657519	5.539149	-1.752030
C	-0.678220	5.613977	-2.158391
C	-1.622986	4.705207	-1.698719
C	-1.278537	3.651472	-0.809458
C	0.079000	3.623084	-0.391141
C	1.021350	4.539449	-0.851567
H	1.388376	6.256762	-2.109913
H	-0.989514	6.400898	-2.840497
H	-2.651118	4.804888	-2.027902
H	0.378025	2.930729	0.397114
H	2.040817	4.485642	-0.483731
C	-2.214354	2.613860	-0.429254
C	-3.681510	2.994074	-0.306372
H	-4.245189	2.220849	0.224291
H	-3.831553	3.931790	0.251076
H	-4.178992	3.136041	-1.274547
Si	-2.073599	1.379713	-2.765274
H	-1.759937	0.987935	-4.197621
C	-2.935183	-0.224688	-2.209968
C	-4.191777	-0.242867	-1.577992
C	-2.369231	-1.468336	-2.551048
C	-4.855100	-1.441078	-1.319264
H	-4.673209	0.689674	-1.310926
C	-3.011157	-2.672858	-2.257791
H	-1.426310	-1.506877	-3.087960
C	-4.263915	-2.660783	-1.650786
H	-5.836084	-1.423827	-0.854986

H	-2.537498	-3.613723	-2.518777
H	-4.776285	-3.592779	-1.435426
H	-2.917291	2.575212	-2.978633
H	-1.883011	2.110791	0.484441

Zero-point correction = 0.881737
Thermal correction to Enthalpy = 0.955629
Thermal correction to Gibbs Free Energy = 0.771053

PROD R

La	1.2512	-0.00205	0.68261
Si	4.4678	0.4504	-0.99899
Si	4.43017	0.91592	1.99435
O	-1.66203	0.82138	-2.98849
O	0.56202	-3.26023	-2.68149
N	-0.26122	0.8213	-1.21982
N	0.88943	-2.0399	-0.81265
N	3.6495	0.41429	0.52887
C	-0.74012	0.13808	-2.24933
C	-0.44409	-1.15288	-2.69447
H	-0.88182	-1.46399	-3.6318
C	0.33925	-2.0916	-2.0173
C	-2.0418	1.982	-2.21679
H	-2.9813	1.76032	-1.70597
H	-2.19843	2.8052	-2.91091
C	-0.88273	2.16989	-1.22442
H	-1.28473	2.38446	-0.23055
C	0.10918	3.32022	-1.58091
C	-0.62496	4.66533	-1.44466
H	0.0451	5.49348	-1.69354
H	-0.97928	4.82208	-0.42224
H	-1.48834	4.73698	-2.11138
C	1.27617	3.31474	-0.58106
H	1.92843	2.44696	-0.71731
H	0.91941	3.34034	0.45587
H	1.91608	4.19058	-0.71553
C	0.66073	3.16745	-3.00565
H	1.13396	2.19449	-3.15061
H	1.41398	3.93431	-3.20972
H	-0.12024	3.2708	-3.7634
C	1.55345	-3.99292	-1.93536
H	2.51917	-3.86848	-2.43383
H	1.27838	-5.04564	-1.9588
C	1.53507	-3.3432	-0.54019
H	2.56365	-3.17523	-0.19726
C	0.81202	-4.17022	0.5659
C	-0.62009	-4.52739	0.14045
H	-1.1513	-5.02691	0.95584
H	-0.6362	-5.20483	-0.71723
C	0.77215	-3.34665	1.86373
H	0.36269	-3.93221	2.69077
H	0.12433	-2.46771	1.77369
H	1.77629	-3.02759	2.17003
C	1.61803	-5.45211	0.8361
H	1.15322	-6.03798	1.63427
H	2.64261	-5.22385	1.14852
H	1.67527	-6.09786	-0.04436
C	3.29465	-0.04245	-2.4034
H	3.00041	-1.09399	-2.34861
H	3.80282	0.09451	-3.36469
H	2.37248	0.54367	-2.46081
C	5.1328	2.17415	-1.42513
H	5.63486	2.17945	-2.39946
H	5.85779	2.53864	-0.68983
H	4.32357	2.9107	-1.47278
C	5.90982	-0.77367	-1.12264
H	6.26061	-0.85479	-2.1583
H	5.60574	-1.77739	-0.80405
H	6.7706	-0.48683	-0.51322
C	4.06455	2.74159	2.35027
H	2.99522	2.90502	2.53061
H	4.35088	3.37833	1.50635
H	4.59564	3.10788	3.2363
C	6.30738	0.68523	2.03768
H	6.59307	-0.36428	1.91847
H	6.69484	1.01714	3.00801
H	6.83312	1.2618	1.27097
C	3.75689	-0.07948	3.46411

H	2.68963	0.07725	3.66272
H	4.27604	0.20759	4.38563
H	3.92043	-1.15548	3.33115
H	-1.19021	-3.63793	-0.13477
H	0.21113	0.64296	2.64418
C	-5.54535	-1.42786	-2.18781
C	-4.25176	-1.01109	-1.88427
C	-3.79023	-1.05008	-0.56841
C	-4.60789	-1.5108	0.47194
C	-5.90684	-1.93207	0.14677
C	-6.37248	-1.891	-1.16429
H	-5.90368	-1.39899	-3.21192
H	-3.59192	-0.65088	-2.6653
H	-2.77997	-0.7171	-0.36115
H	-6.55987	-2.29641	0.93524
H	-7.38063	-2.2267	-1.38796
C	-4.15105	-1.51628	1.91691
C	-2.63273	-1.65051	2.10994
H	-2.38233	-1.81333	3.16105
H	-2.24577	-2.49732	1.53846
H	-2.08828	-0.75502	1.79763
Si	-4.81881	0.04348	2.79729
H	-4.2744	0.09851	4.1805
C	-4.34433	1.61918	1.89083
C	-5.07386	2.03493	0.76367
C	-3.26935	2.41767	2.31478
C	-4.75213	3.21308	0.09349
H	-5.90369	1.43488	0.40204
C	-2.94645	3.59876	1.64667
H	-2.67507	2.12052	3.17367
C	-3.69134	4.00107	0.53896
H	-5.33153	3.51728	-0.77269
H	-2.11587	4.20533	1.99443
H	-3.44491	4.92232	0.02159
H	-6.30162	-0.04875	2.85422
H	-4.63576	-2.36255	2.42033

Zero-point correction = 0.879425
Thermal correction to Enthalpy = 0.954565
Thermal correction to Gibbs Free Energy = 0.76216

TS2me

La	0.3102	0.1047	0.69881
Si	3.28004	-0.63767	-1.33887
Si	3.27381	-1.79491	1.45757
O	-1.82201	3.78143	-1.16072
O	-3.09921	-0.41089	-2.55248
N	-0.21876	2.32579	-0.50339
N	-1.22152	-0.6623	-1.30664
N	2.51832	-0.85866	0.21075
C	-1.38456	2.49012	-1.11197
C	-2.2661	1.56811	-1.68451
H	-3.16544	1.98418	-2.11587
C	-2.12726	0.18178	-1.79057
C	-0.7604	4.62179	-0.67536
H	-1.1928	5.36136	-0.00163
H	-0.31974	5.1362	-1.53283
C	0.21192	3.64945	0.01589
H	0.02759	3.66361	1.09851
C	1.71389	3.99103	-0.17909
C	1.94277	5.43322	0.31132
H	3.00537	5.68905	0.26695
H	1.61761	5.55921	1.34937
H	1.40918	6.16864	-0.29792
C	2.5647	3.05073	0.68838
H	2.50733	2.01209	0.35274
H	2.25769	3.08385	1.73702
H	3.6229	3.32301	0.64101
C	2.1441	3.86499	-1.64723
H	1.97478	2.85696	-2.02731
H	3.20942	4.08943	-1.7533
H	1.60384	4.55644	-2.29962
C	-2.9168	-1.82981	-2.41046
H	-3.18851	-2.30003	-3.35382
H	-3.57569	-2.18768	-1.61142
C	-1.437	-1.94068	-2.04968
H	-0.86425	-1.87495	-2.98734
C	-1.01599	-3.27158	-1.37548

C	-1.47426	-3.35097	0.08399
H	-1.20377	-4.31563	0.52307
H	-2.55183	-3.22267	0.18542
H	-1.00815	-2.57608	0.70092
C	0.50903	-3.43985	-1.45525
H	0.81903	-4.38887	-1.00812
H	1.05065	-2.64817	-0.93733
H	0.84859	-3.44174	-2.49478
C	-1.65797	-4.43224	-2.1629
H	-1.28452	-5.39257	-1.79599
H	-1.41501	-4.3735	-3.22858
H	-2.74706	-4.4501	-2.06663
C	4.63666	0.68514	-1.3366
H	4.23254	1.69632	-1.24458
H	5.20456	0.6524	-2.27414
H	5.34995	0.54412	-0.51896
C	4.09338	-2.21	-2.01735
H	4.44622	-2.033	-3.04029
H	3.39846	-3.05366	-2.05699
H	4.96418	-2.52467	-1.43317
C	2.01691	-0.11047	-2.65074
H	2.54546	0.16576	-3.57058
H	1.40091	0.75277	-2.38044
H	1.32852	-0.91999	-2.9062
C	5.0671	-1.29962	1.79782
H	5.15386	-0.23353	2.03091
H	5.71983	-1.5016	0.94237
H	5.47617	-1.85641	2.6487
C	3.24308	-3.66396	1.14952
H	2.21744	-4.04234	1.08405
H	3.73096	-4.19976	1.97258
H	3.75378	-3.95421	0.22786
C	2.31746	-1.57273	3.08954
H	2.25501	-0.53048	3.42126
H	2.83382	-2.11849	3.88687
H	1.30224	-1.98912	3.06719
H	0.31446	1.40372	2.60535
C	-4.39911	1.0558	1.10087
C	-3.23795	0.90054	1.84947
C	-2.83134	-0.36688	2.31363
C	-3.66617	-1.45701	2.0046
C	-4.82765	-1.29191	1.26116
C	-5.2147	-0.03432	0.78179
H	-4.6606	2.04463	0.7357
H	-2.62869	1.77557	2.05644
H	-3.39342	-2.4467	2.35907
H	-5.4449	-2.15959	1.04218
C	-1.58002	-0.57302	3.04579
H	-1.2586	-1.60453	3.18356
C	-0.86253	0.42401	3.66894
H	-1.30499	1.392	3.86167
H	-0.0432	0.16373	4.32684
C	-6.42259	0.13215	-0.1033
H	-6.94463	1.07289	0.0929
H	-6.12984	0.1413	-1.15968
H	-7.14016	-0.68176	0.03035

Zero-point correction = 0.785699
Thermal correction to Enthalpy = 0.851601
Thermal correction to Gibbs Free Energy = 0.680658

IM2me

La	-0.1767	0.062	0.62103
Si	-2.71186	-1.65291	-1.44278
Si	-3.19331	-1.78277	1.52839
O	3.30801	-0.02863	-2.50036
O	-0.09257	3.04233	-3.04607
N	1.63106	-0.52712	-1.07316
N	-0.42848	1.96278	-1.08874
N	-2.25065	-1.23754	0.18138
C	2.09175	0.3063	-1.98999
C	1.52816	1.46495	-2.53774
H	2.0427	1.88544	-3.39019
C	0.34315	2.10387	-2.15977
C	3.74608	-1.24363	-1.86662
H	4.71213	-1.05517	-1.39851
H	3.87275	-1.9963	-2.64605
C	2.64136	-1.58294	-0.84159

H	3.04574	-1.46146	0.16948
C	2.09468	-3.03692	-0.93217
C	3.26819	-4.00453	-0.69372
H	2.91895	-5.04105	-0.68984
H	3.75234	-3.81549	0.27038
H	4.03384	-3.9272	-1.47084
C	1.05615	-3.26253	0.17966
H	0.12652	-2.71216	-0.00055
H	1.45593	-2.98996	1.16445
H	0.76312	-4.31441	0.23716
C	1.44321	-3.32027	-2.29244
H	0.61611	-2.63654	-2.48836
H	1.04845	-4.3398	-2.3245
H	2.15339	-3.22491	-3.11821
C	-1.24774	3.6862	-2.48651
H	-2.02833	3.70537	-3.24743
H	-0.97161	4.71293	-2.2371
C	-1.61486	2.83323	-1.25437
H	-2.47999	2.20088	-1.49711
C	-2.02672	3.66982	-0.00823
C	-0.87677	4.548	0.50307
H	-1.16944	5.06229	1.42328
H	-0.58305	5.3164	-0.21629
H	0.00857	3.94748	0.72369
C	-2.48313	2.73683	1.12656
H	-3.03175	3.29297	1.89187
H	-1.63455	2.28944	1.65908
H	-3.14256	1.94259	0.76432
C	-3.22648	4.54869	-0.40911
H	-3.57923	5.13004	0.44734
H	-4.0655	3.94082	-0.76332
H	-2.97365	5.26142	-1.19896
C	-2.45303	-3.49185	-1.83702
H	-1.47394	-3.84873	-1.50428
H	-2.51179	-3.67439	-2.91633
H	-3.20538	-4.12778	-1.36198
C	-4.53156	-1.27	-1.81917
H	-4.75815	-1.47022	-2.87307
H	-4.76994	-0.21771	-1.63014
H	-5.22461	-1.87419	-1.22489
C	-1.71859	-0.69101	-2.73686
H	-1.95361	-1.08916	-3.73061
H	-0.63345	-0.75458	-2.62468
H	-1.97647	0.37061	-2.7542
C	-3.76521	-3.5855	1.42534
H	-2.92943	-4.26846	1.24283
H	-4.50195	-3.75141	0.63348
H	-4.23713	-3.8896	2.36695
C	-4.73212	-0.7272	1.85076
H	-4.47025	0.31745	2.05279
H	-5.29356	-1.09206	2.71902
H	-5.41708	-0.72772	0.99714
C	-2.13786	-1.65646	3.10518
H	-1.20734	-2.23434	3.04211
H	-2.68682	-2.06231	3.96191
H	-1.88272	-0.62838	3.38436
H	0.5276	-0.52483	4.25842
C	4.29515	-0.13301	2.14637
C	3.04751	0.02287	2.74786
C	2.16254	1.07009	2.37755
C	2.63416	1.92532	1.34355
C	3.87313	1.7509	0.74413
C	4.73973	0.71956	1.13174
H	4.94016	-0.94332	2.47986
H	2.76418	-0.65947	3.54323
H	2.00722	2.75134	1.01598
H	4.17266	2.43003	-0.04966
C	0.8077	1.19589	2.90625
H	0.47332	2.23948	2.87088
C	0.52417	0.57291	4.2687
H	1.25034	0.87158	5.04201
H	-0.46455	0.86638	4.6339
C	6.10328	0.56654	0.50491
H	6.45427	-0.469	0.54073
H	6.10363	0.88428	-0.54156
H	6.85516	1.17504	1.02189

Zero-point correction = 0.791845

Thermal correction to Enthalpy = 0.857636
Thermal correction to Gibbs Free Energy = 0.689927

IM3me

La	0.52779	0.04196	-0.35292
Si	2.60494	-2.57049	1.35621
Si	0.36005	-3.5247	-0.41066
O	-0.08797	3.7988	2.36591
O	4.05996	3.08593	0.46456
N	0.03352	1.70461	1.53528
N	2.7033	1.37339	-0.10696
N	1.30511	-2.23573	0.2537
C	0.61626	2.88725	1.63844
C	1.84996	3.33219	1.15183
H	2.1621	4.31968	1.4608
C	2.80883	2.55231	0.49237
C	-1.36642	3.20953	2.67623
H	-2.12235	3.66915	2.03504
H	-1.5927	3.44213	3.71533
C	-1.18431	1.71011	2.37226
H	-2.03594	1.35248	1.78062
C	-1.0762	0.78686	3.62458
C	-2.39263	0.86727	4.41635
H	-2.38288	0.16104	5.25154
H	-3.25437	0.62118	3.78831
H	-2.56332	1.86082	4.83927
C	-0.87363	-0.66365	3.15974
H	0.09731	-0.80428	2.68373
H	-1.65398	-0.97613	2.45846
H	-0.90658	-1.35825	4.0042
C	0.10262	1.20176	4.51655
H	1.04524	1.16821	3.96556
H	0.19245	0.52605	5.37257
H	-0.016	2.21408	4.91311
C	4.96233	2.04562	0.04838
H	5.49635	1.68558	0.93214
H	5.68057	2.48655	-0.63985
C	4.05426	0.95636	-0.56222
H	4.29011	-0.00965	-0.10603
C	4.21438	0.77794	-2.10288
C	3.91071	2.08537	-2.84737
H	3.95058	1.93117	-3.92965
H	4.62424	2.87758	-2.60565
C	3.27041	-0.32414	-2.6134
H	3.52924	-0.60591	-3.63798
H	2.23554	0.0223	-2.66421
H	3.32268	-1.23256	-2.00649
C	5.65804	0.32192	-2.38637
H	5.80374	0.16043	-3.45819
H	5.88515	-0.62152	-1.8788
H	6.40237	1.05681	-2.0694
C	3.01304	-1.07614	2.45223
H	4.0034	-1.20748	2.90382
H	2.30383	-0.98036	3.27996
H	3.02641	-0.1179	1.92641
C	2.24442	-3.97767	2.57611
H	3.06291	-4.06013	3.30124
H	2.1462	-4.95604	2.09547
H	1.32695	-3.79568	3.14504
C	4.19833	-3.05516	0.4475
H	5.00017	-3.30588	1.152
H	4.57417	-2.25215	-0.19439
H	4.04293	-3.92897	-0.19314
C	-0.82916	-4.30388	0.84069
H	-1.38135	-3.53841	1.39416
H	-0.302	-4.91672	1.5773
H	-1.56438	-4.95064	0.3488
C	1.37025	-4.92975	-1.17713
H	2.03742	-4.56761	-1.96642
H	0.71252	-5.68303	-1.6266
H	1.98926	-5.44969	-0.43919
C	-0.7212	-2.8418	-1.81871
H	-1.47998	-2.11228	-1.50963
H	-1.29071	-3.6649	-2.26331
H	-0.13823	-2.40482	-2.63589
H	2.91161	2.45372	-2.60286
H	-3.28487	-1.8021	-3.39401

C	-3.61555	3.31683	-1.3644
C	-2.30444	3.62826	-0.97589
C	-1.21275	2.92337	-1.46365
C	-1.3522	1.83932	-2.37399
C	-2.6816	1.55012	-2.76896
C	-3.7688	2.27317	-2.28203
H	-2.13033	4.45674	-0.29316
H	-0.21563	3.24009	-1.16342
H	-2.86217	0.76737	-3.49684
H	-4.76542	2.02045	-2.63732
C	-0.18849	1.0616	-2.80333
C	-0.34551	0.2075	-4.0554
H	-0.69433	0.77907	-4.93145
H	0.60619	-0.25261	-4.34117
H	-1.05723	-0.61539	-3.92536
Si	-4.6042	-1.84532	-2.71729
H	-5.27214	-3.11838	-3.08965
C	-4.43469	-1.77006	-0.84455
C	-4.4895	-0.54637	-0.1552
C	-4.28312	-2.94489	-0.09058
C	-4.40566	-0.50201	1.23554
H	-4.60333	0.38285	-0.70235
C	-4.19663	-2.90297	1.30031
H	-4.2397	-3.90955	-0.58808
C	-4.26248	-1.68078	1.9669
H	-4.46412	0.45382	1.74587
H	-4.07721	-3.82372	1.86145
H	-4.20103	-1.64749	3.04968
H	-5.41378	-0.6961	-3.19141
H	0.68325	1.72369	-2.89429
C	-4.79627	4.07065	-0.80479
H	-5.01597	3.77583	0.22917
H	-4.62002	5.15107	-0.79429
H	-5.70289	3.8917	-1.38904

Zero-point correction = 0.907751
Thermal correction to Enthalpy = 0.985898
Thermal correction to Gibbs Free Energy = 0.787973

TS3me

La	0.50966	0.07824	-0.42062
Si	3.8565	-0.86437	0.72741
Si	3.35685	-1.42936	-2.16644
O	-2.07108	-0.32954	3.38971
O	0.99041	3.13316	3.12858
N	-0.63991	-0.68633	1.68124
N	1.06262	1.93582	1.21808
N	2.78489	-0.77175	-0.65077
C	-1.03902	0.1449	2.64299
C	-0.55436	1.39768	3.01408
H	-0.97465	1.83378	3.90909
C	0.48877	2.10372	2.40122
C	-2.55264	-1.52598	2.73939
H	-3.43395	-1.2647	2.14901
H	-2.83493	-2.23187	3.51725
C	-1.3812	-1.96387	1.85149
H	-1.75958	-2.29591	0.88254
C	-0.51867	-3.12478	2.43474
C	-1.39039	-4.3911	2.5168
H	-0.79593	-5.24155	2.86325
H	-1.80456	-4.65421	1.53896
H	-2.22518	-4.27965	3.21378
C	0.65167	-3.41185	1.48376
H	1.33513	-2.56563	1.41504
H	0.29871	-3.65247	0.47574
H	1.23882	-4.2652	1.8341
C	0.02565	-2.77704	3.82808
H	0.63207	-1.86956	3.81016
H	0.65753	-3.5876	4.20326
H	-0.775	-2.62511	4.55666
C	2.19172	3.58574	2.4771
H	3.04664	3.24561	3.06678
H	2.17756	4.67372	2.47854
C	2.15005	2.93723	1.07667
H	3.08917	2.4079	0.88884
C	1.96312	3.94986	-0.09283
C	0.66567	4.75432	0.06649
H	0.5126	5.41319	-0.79245

H	0.67887	5.38532	0.95899
C	1.9389	3.19892	-1.43394
H	2.00916	3.89512	-2.27353
H	0.99488	2.66901	-1.58749
H	2.77237	2.49505	-1.52353
C	3.18021	4.89379	-0.11228
H	3.10119	5.6019	-0.94188
H	4.11535	4.33841	-0.24055
H	3.26794	5.48405	0.80339
C	3.03107	-0.38733	2.36892
H	3.05451	0.68963	2.54317
H	3.60541	-0.85123	3.17928
H	1.99655	-0.70645	2.49939
C	4.54452	-2.61198	0.99272
H	5.20387	-2.63136	1.86846
H	5.13162	-2.97901	0.14617
H	3.74472	-3.33661	1.17537
C	5.344	0.3071	0.59862
H	5.80831	0.4398	1.58321
H	5.05046	1.30069	0.2435
H	6.12213	-0.05773	-0.0759
C	2.98189	-3.28086	-2.29833
H	1.9093	-3.4849	-2.2031
H	3.48362	-3.85224	-1.51146
H	3.30354	-3.69332	-3.26148
C	5.20756	-1.20533	-2.49419
H	5.50022	-0.15097	-2.48956
H	5.44631	-1.60302	-3.48729
H	5.84825	-1.73062	-1.78132
C	2.50272	-0.59626	-3.63972
H	1.45239	-0.8661	-3.78104
H	3.01171	-0.89973	-4.56154
H	2.55728	0.49728	-3.59855
H	-0.20328	4.09762	0.13832
H	-0.15294	0.71976	-2.94184
C	-6.02553	1.01047	-0.02332
C	-4.92508	0.89283	0.83706
C	-3.64501	1.24649	0.43201
C	-3.37144	1.74052	-0.86424
C	-4.49927	1.91316	-1.70003
C	-5.77834	1.5397	-1.29327
H	-5.07712	0.52965	1.85121
H	-2.82726	1.14575	1.13805
H	-4.37559	2.327	-2.69405
H	-6.60831	1.67261	-1.98422
C	-1.99621	1.98007	-1.32177
C	-1.79975	3.19632	-2.22573
H	-2.08407	4.13897	-1.73563
H	-0.75844	3.308	-2.54453
H	-2.38998	3.1419	-3.14526
Si	-1.56575	0.23921	-3.24179
H	-1.17385	-0.41362	-4.56001
C	-1.97858	-1.33928	-2.26731
C	-3.20067	-1.52239	-1.59331
C	-1.11986	-2.4532	-2.36721
C	-3.54908	-2.76333	-1.06168
H	-3.89648	-0.69947	-1.50143
C	-1.45216	-3.68841	-1.80889
H	-0.19992	-2.37669	-2.94338
C	-2.6777	-3.84783	-1.16476
H	-4.5071	-2.88005	-0.56516
H	-0.77036	-4.52735	-1.90498
H	-2.95472	-4.81217	-0.7518
H	-2.70975	1.0635	-3.67809
H	-1.35807	2.12387	-0.43141
C	-7.42038	0.64958	0.42455
H	-7.4103	-0.14213	1.17966
H	-7.93872	1.50823	0.86877
H	-8.03604	0.30185	-0.41037

Zero-point correction = 0.910175
Thermal correction to Enthalpy = 0.985806
Thermal correction to Gibbs Free Energy = 0.798307

PRODme

La	1.07755	-0.02153	-0.45119
Si	4.47502	0.11043	0.88022
Si	4.26252	-1.09282	-1.88195

O	-1.86869	-0.79239	3.20846
O	0.15965	3.36321	2.75092
N	-0.41021	-0.82654	1.4873
N	0.66317	2.0645	0.97319
N	3.52713	-0.33991	-0.50094
C	-0.96062	-0.10906	2.45287
C	-0.75616	1.22368	2.81994
H	-1.25737	1.56899	3.71248
C	0.03031	2.15449	2.13734
C	-2.12003	-2.04342	2.53422
H	-3.05336	-1.94787	1.9734
H	-2.23402	-2.81249	3.29566
C	-0.91109	-2.21696	1.60154
H	-1.24981	-2.56588	0.62183
C	0.16873	-3.22218	2.10954
C	-0.43608	-4.63663	2.12428
H	0.29902	-5.36482	2.47926
H	-0.75165	-4.94445	1.12367
H	-1.30583	-4.71	2.78283
C	1.35918	-3.22563	1.13722
H	1.92685	-2.29112	1.168
H	1.03701	-3.41962	0.10683
H	2.07464	-4.01134	1.3951
C	0.6638	-2.84692	3.51415
H	1.04488	-1.82379	3.54325
H	1.47445	-3.51228	3.8261
H	-0.12782	-2.92562	4.26384
C	1.17835	4.09442	2.04336
H	2.10867	4.0289	2.61516
H	0.86671	5.13595	1.99439
C	1.28368	3.38041	0.6846
H	2.3388	3.23283	0.42681
C	0.6261	4.14112	-0.50648
C	-0.86006	4.4199	-0.23718
H	-1.32063	4.90786	-1.10098
H	-1.00807	5.07706	0.62383
C	0.75575	3.29418	-1.77935
H	0.41982	3.84942	-2.65929
H	0.12677	2.39965	-1.743
H	1.79427	2.99609	-1.96943
C	1.38561	5.4604	-0.72884
H	0.97865	5.99586	-1.59129
H	2.44842	5.28202	-0.92442
H	1.31404	6.1339	0.12932
C	3.39284	0.30186	2.42498
H	2.64745	1.0984	2.35118
H	4.02574	0.54341	3.28644
H	2.85773	-0.61816	2.68297
C	5.80438	-1.15414	1.3554
H	6.31072	-0.84221	2.27634
H	6.57995	-1.27148	0.59236
H	5.37291	-2.14308	1.54144
C	5.35073	1.7735	0.63409
H	5.89234	2.08454	1.53518
H	4.63689	2.57067	0.39516
H	6.07621	1.73782	-0.18493
C	4.70408	-2.91055	-1.57453
H	3.85067	-3.46049	-1.16077
H	5.53168	-3.02779	-0.86913
H	4.99606	-3.41386	-2.50385
C	5.82959	-0.21665	-2.484
H	5.63734	0.83481	-2.72193
H	6.21859	-0.6913	-3.39223
H	6.63305	-0.24238	-1.74129
C	3.05073	-1.11038	-3.34106
H	2.16092	-1.72975	-3.17675
H	3.55014	-1.53152	-4.22122
H	2.69682	-0.11513	-3.63083
H	-1.41057	3.49606	-0.0456
H	-0.08095	-0.05007	-2.40102
C	-5.66826	0.75676	1.22603
C	-4.27794	0.74758	1.36212
C	-3.44788	0.96573	0.26388
C	-3.96981	1.19958	-1.01205
C	-5.36652	1.22126	-1.14387
C	-6.19543	1.00262	-0.04795
H	-3.82886	0.56466	2.33302

H	-2.37298	0.94764	0.40733
H	-5.81365	1.39273	-2.11794
H	-7.27361	1.01905	-0.18558
C	-3.05123	1.35082	-2.20432
C	-3.32628	2.60791	-3.05024
H	-3.29202	3.50746	-2.42703
H	-2.57777	2.72311	-3.8401
H	-4.30796	2.58173	-3.53162
Si	-3.1155	-0.22714	-3.27784
H	-2.13432	-0.16943	-4.38813
C	-2.8768	-1.8376	-2.32279
C	-3.79389	-2.24359	-1.3382
C	-1.82149	-2.71114	-2.63682
C	-3.66968	-3.47893	-0.70266
H	-4.61996	-1.59499	-1.064
C	-1.6971	-3.94977	-2.00724
H	-1.09124	-2.42145	-3.38574
C	-2.62638	-4.33884	-1.04241
H	-4.3937	-3.77376	0.05073
H	-0.88196	-4.61482	-2.27741
H	-2.53883	-5.30662	-0.55944
H	-4.48177	-0.26395	-3.87631
H	-2.02188	1.4089	-1.8397
C	-6.57679	0.54331	2.4111
H	-6.04802	0.07568	3.24527
H	-6.98294	1.4938	2.77518
H	-7.42994	-0.09254	2.15639

Zero-point correction = 0.907893
Thermal correction to Enthalpy = 0.985104
Thermal correction to Gibbs Free Energy = 0.788944

$PhSiH_2N(TMS)_2$

Si	-2.01144	-1.29141	0.08963
Si	-1.08913	1.67578	0.09772
N	-0.85637	-0.02296	-0.36326
C	-1.1315	-2.93073	0.39799
H	-0.73876	-3.40023	-0.50657
H	-1.83923	-3.63902	0.84425
H	-0.30058	-2.82428	1.1029
C	-2.90095	-0.88066	1.70088
H	-3.61488	-1.68446	1.91441
H	-3.47228	0.05003	1.68614
H	-2.20788	-0.83794	2.5459
C	-3.28736	-1.51645	-1.27714
H	-4.0058	-2.30633	-1.03104
H	-2.81409	-1.79079	-2.22585
H	-3.85541	-0.59676	-1.45056
C	0.15663	2.78034	-0.78705
H	0.02162	2.80203	-1.87143
H	1.19773	2.51428	-0.58192
H	0.01855	3.80622	-0.42638
C	-0.82843	1.93283	1.94522
H	-1.58122	1.44052	2.5644
H	-0.86183	3.00166	2.18532
H	0.15362	1.56369	2.25819
C	-2.81081	2.25902	-0.40111
H	-2.9684	2.13645	-1.47747
H	-2.93178	3.32492	-0.17633
H	-3.61975	1.73248	0.112
Si	0.48185	-0.43504	-1.40693
H	0.25885	-1.80002	-1.94728
C	2.12529	-0.36398	-0.49254
C	2.18769	-0.55838	0.89566
C	3.32471	-0.11866	-1.17901
C	3.40437	-0.51752	1.57483
H	1.27312	-0.73378	1.45429
C	4.5443	-0.07798	-0.50534
H	3.31062	0.05256	-2.25279
C	4.58553	-0.27739	0.87421
H	3.43077	-0.66905	2.6497
H	5.46085	0.11579	-1.0543
H	5.53411	-0.24193	1.40096
H	0.59179	0.47135	-2.57921

Zero-point correction = 0.339301
Thermal correction to Enthalpy = 0.37098
Thermal correction to Gibbs Free Energy = 0.274104

PhC_2H_3

C	-0.40712	-1.28063	0.00000
C	0.51451	-0.2215	-0.0001
C	0.00929	1.09015	-0.00012
C	-1.35956	1.32797	-0.00004
C	-2.26214	0.26242	0.00007
C	-1.77944	-1.04392	0.00009
H	-0.0402	-2.30312	0.00003
H	0.69103	1.93367	-0.00024
H	-1.72689	2.3495	-0.00007
H	-3.33069	0.45214	0.00014
H	-2.47117	-1.88044	0.00017
C	1.95433	-0.52956	-0.00014
H	2.19117	-1.5927	-0.00047
C	2.97222	0.33557	0.00019
H	2.83527	1.41255	0.00057
H	3.99896	-0.01465	0.00011

Zero-point correction = 0.132878
Thermal correction to Enthalpy = 0.143332
Thermal correction to Gibbs Free Energy = 0.093622

Add

C	0.1806	1.33939	-0.002
C	1.03265	0.22612	-0.00092
C	0.4344	-1.04644	-0.00499
C	-0.94524	-1.18779	-0.00907
C	-1.79502	-0.07161	-0.00859
C	-1.20445	1.19336	-0.00604
H	0.60995	2.33742	-0.00167
H	1.05338	-1.93738	-0.00768
H	-1.37772	-2.18474	-0.01383
H	-1.83352	2.07905	-0.00731
C	2.48862	0.43607	0.00249
H	2.79578	1.48106	0.00152
C	3.44808	-0.49405	0.0074
H	3.24054	-1.55974	0.00911
H	4.49566	-0.21198	0.01
C	-3.29212	-0.24663	0.01209
H	-3.61762	-1.00838	-0.70266
H	-3.63839	-0.56845	1.00076
H	-3.81311	0.68258	-0.23047

Zero-point correction = 0.160448
Thermal correction to Enthalpy = 0.173213
Thermal correction to Gibbs Free Energy = 0.117914

$PhSiH_3$

Si	2.34556	0.00017	0.00632
H	2.84764	1.28868	-0.53476
H	2.86433	-1.12215	-0.81665
H	2.87708	-0.16266	1.38527
C	0.46674	0.00007	-0.01375
C	-0.25603	-1.20438	-0.01066
C	-0.25571	1.20404	-0.0107
C	-1.64916	-1.20617	0.00337
H	0.26906	-2.15597	-0.02401
C	-1.64966	1.20565	0.00323
H	0.27002	2.15498	-0.02392
C	-2.34849	0.00002	0.01133
H	-2.18885	-2.14812	0.00441
H	-2.18924	2.14766	0.004
H	-3.434	-0.00022	0.02013

Zero-point correction = 0.115044
Thermal correction to Enthalpy = 0.125703
Thermal correction to Gibbs Free Energy = 0.075617

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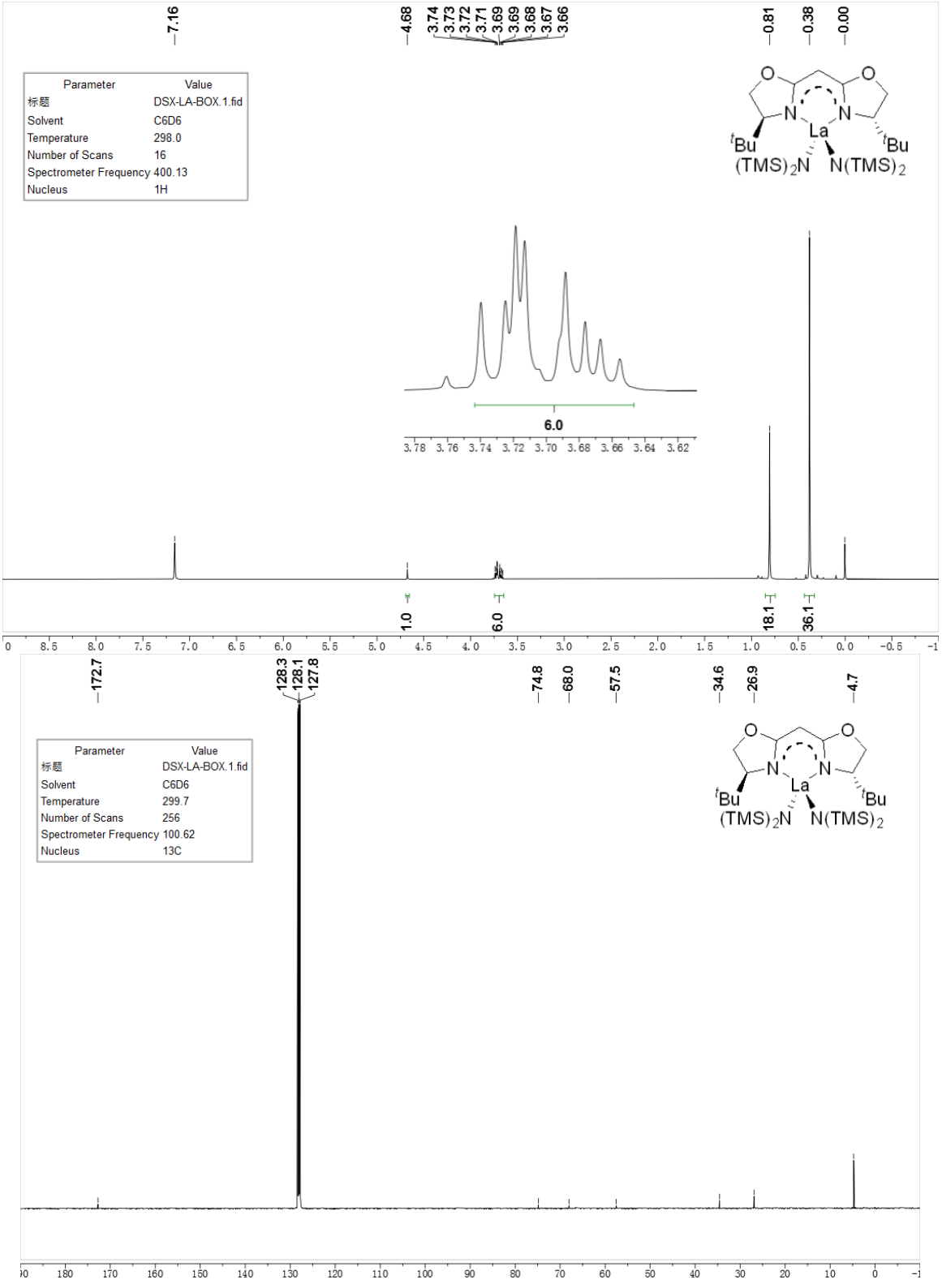
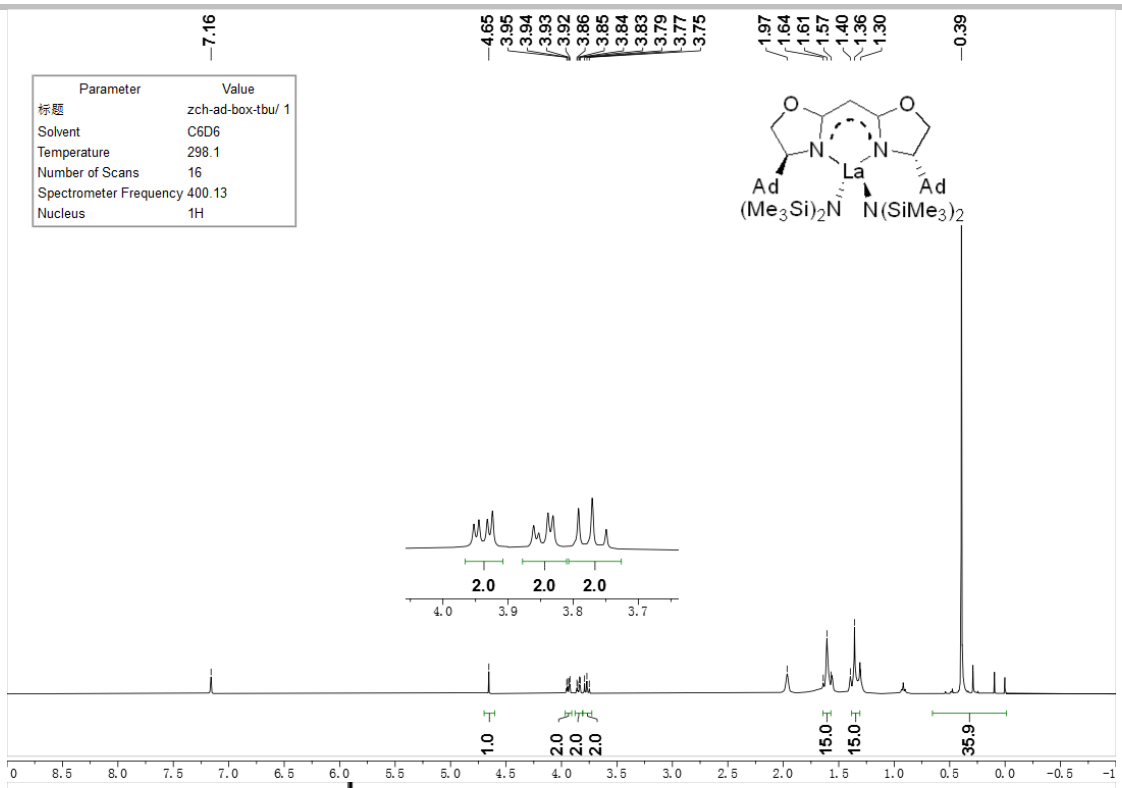
11. Copies of NMR spectra for products

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1.97
1.64
1.61
1.57
1.40
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Nucleus 1H
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O
N
N
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Ad
Ad
(Me3Si)2N
N(SiMe3)2
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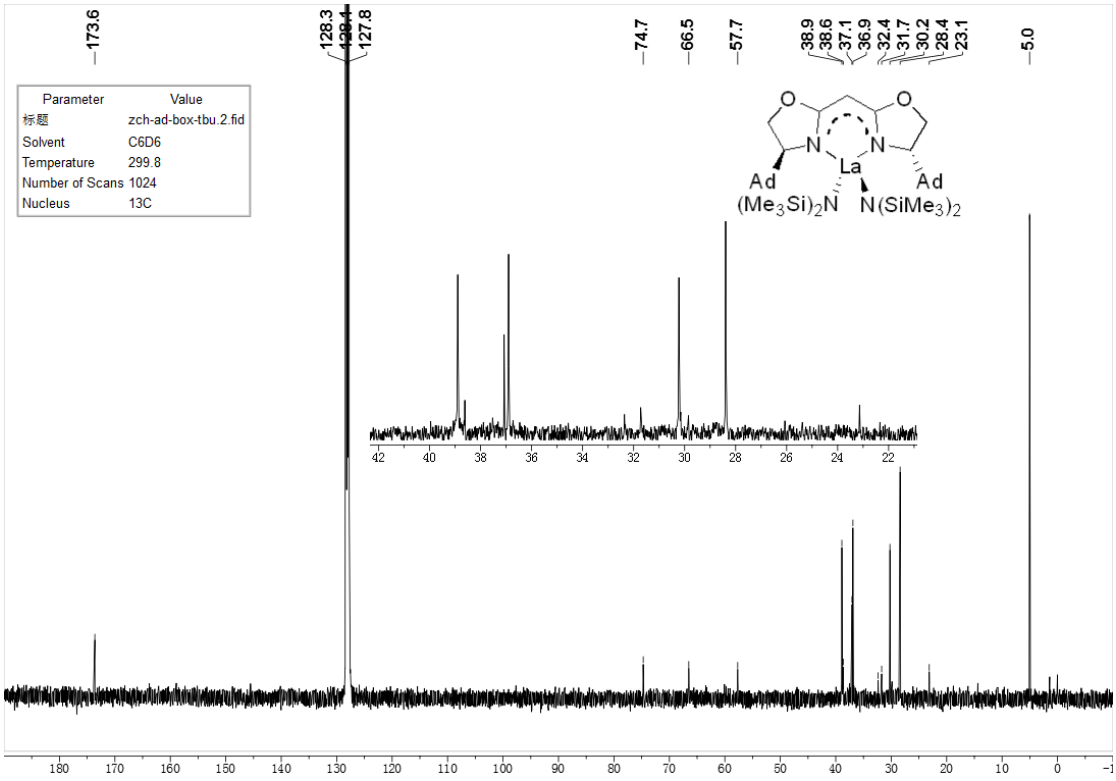
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30.2
28.4
23.1
5.0
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N
N
La
Ad
Ad
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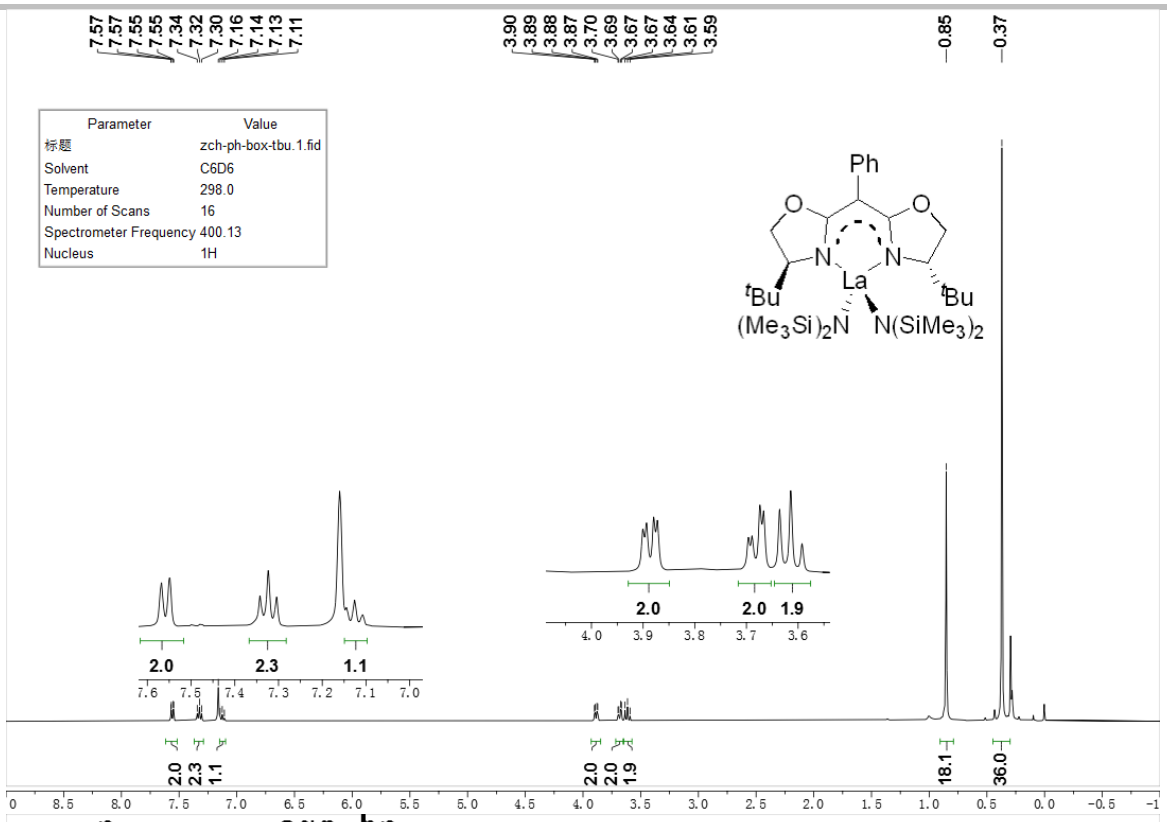
N(SiMe3)2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3.87
3.70
3.69
3.67
3.67
3.64
3.61
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0.85
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O
N
N
La
tBu
tBu
(Me3Si)2N
N(SiMe3)2
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2.3
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18.1
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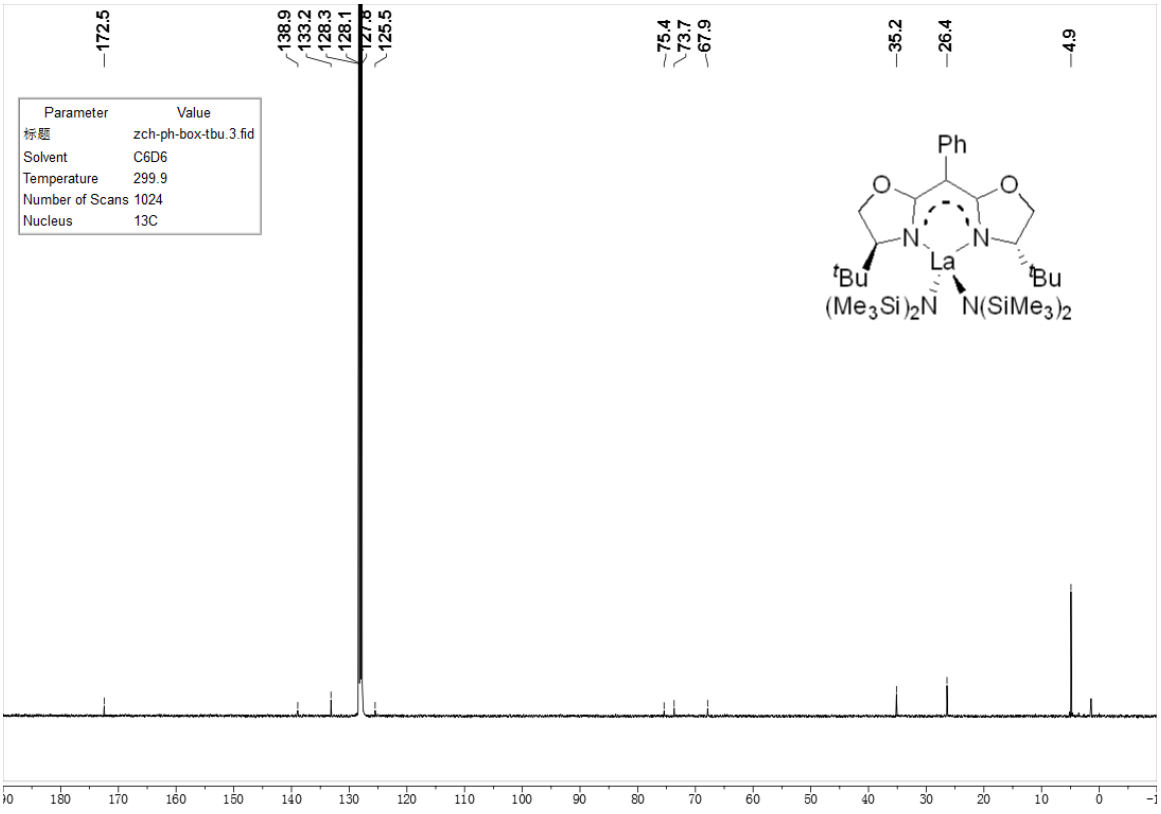
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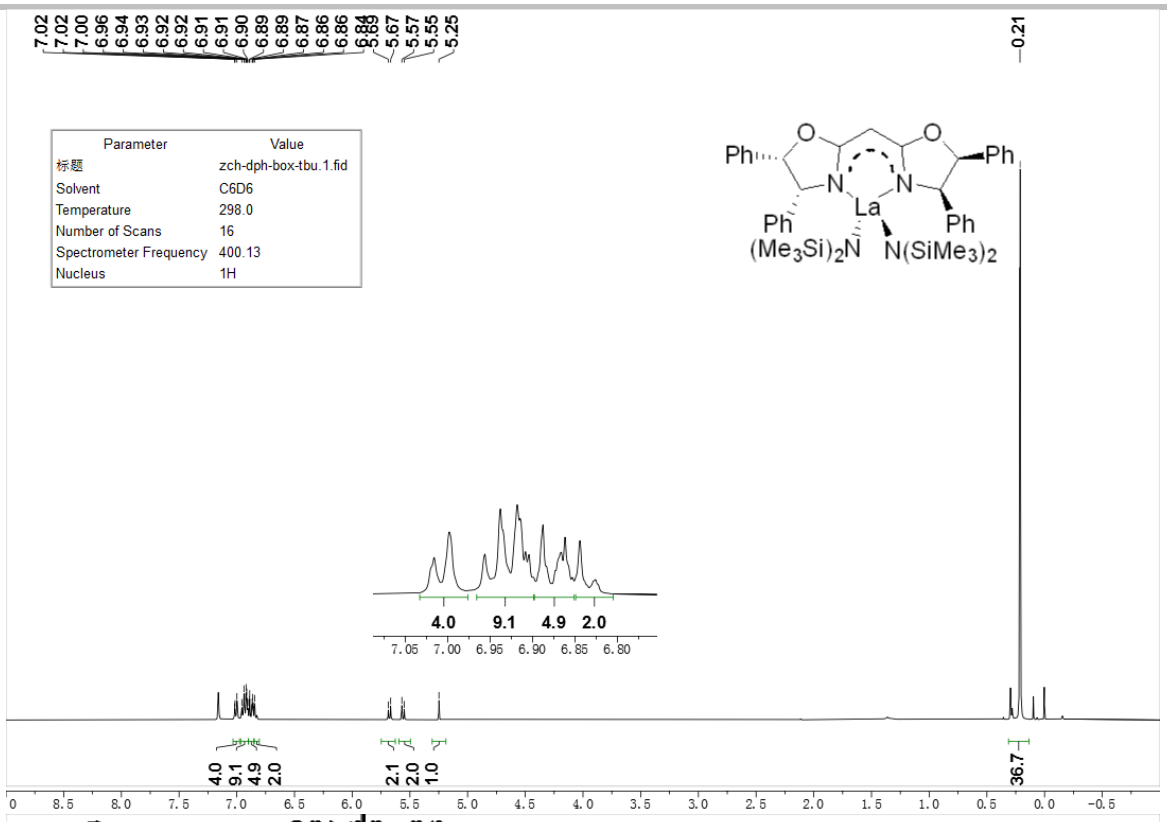
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7.05 7.00 6.95 6.90 6.85 6.80
4.0 9.1 4.9 2.0 2.1 2.0 1.0 36.7
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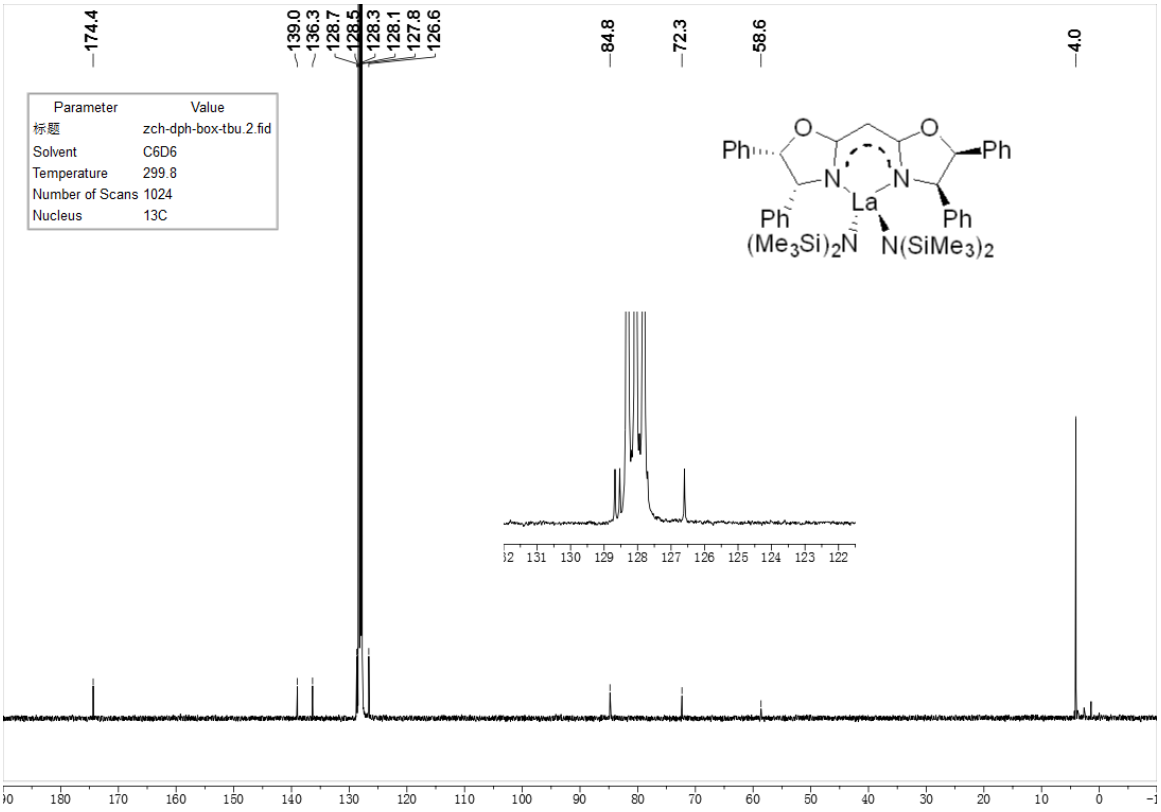
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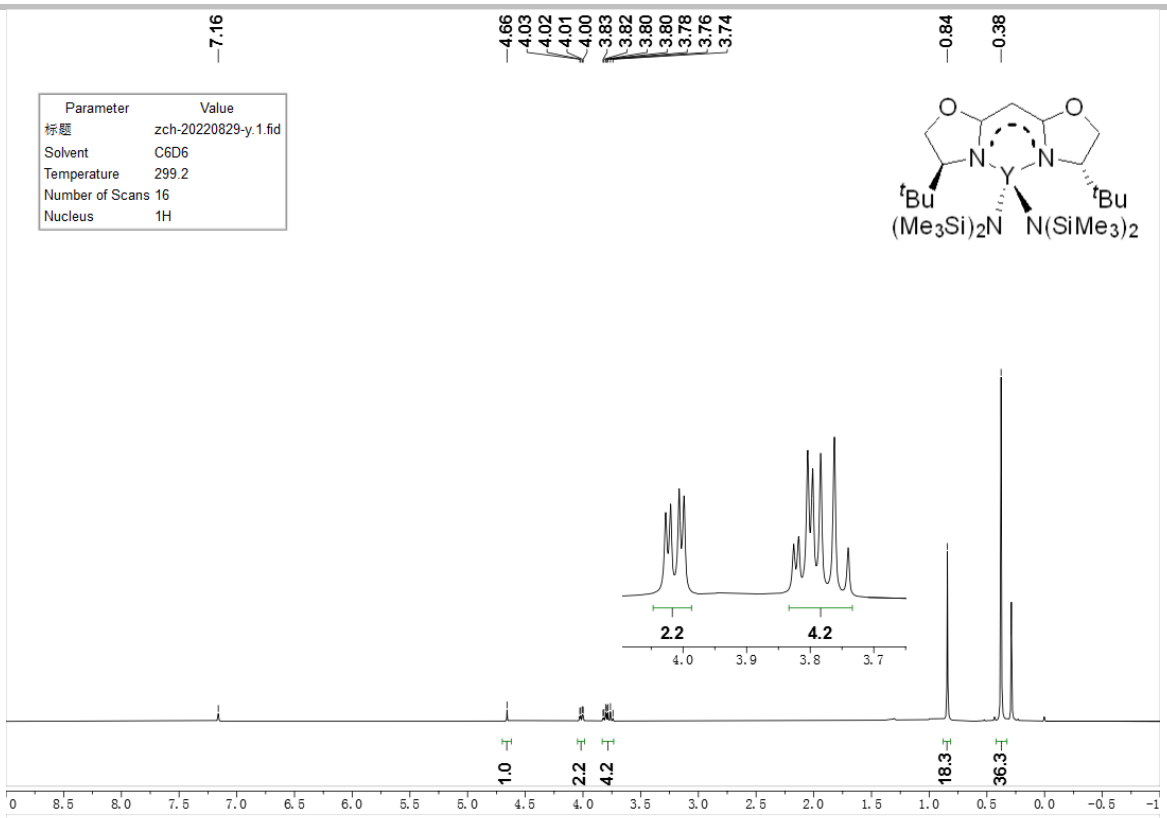
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3.74
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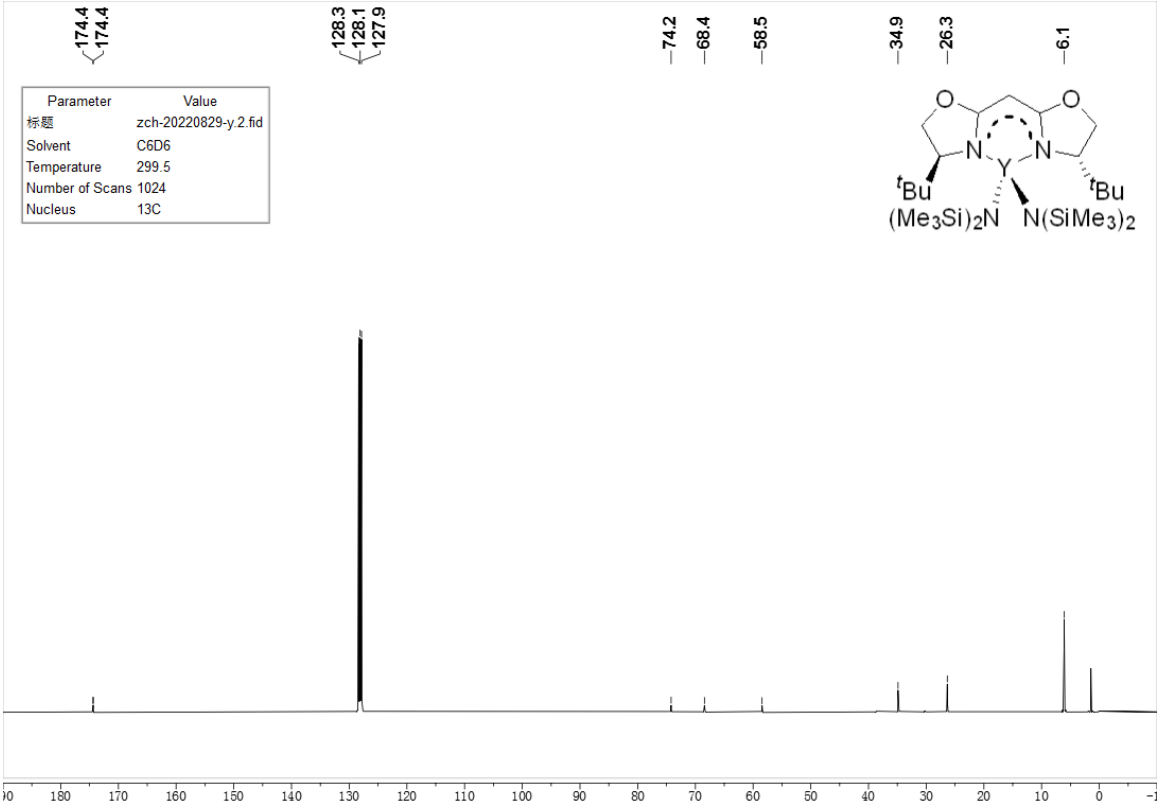
4.2
18.3
36.3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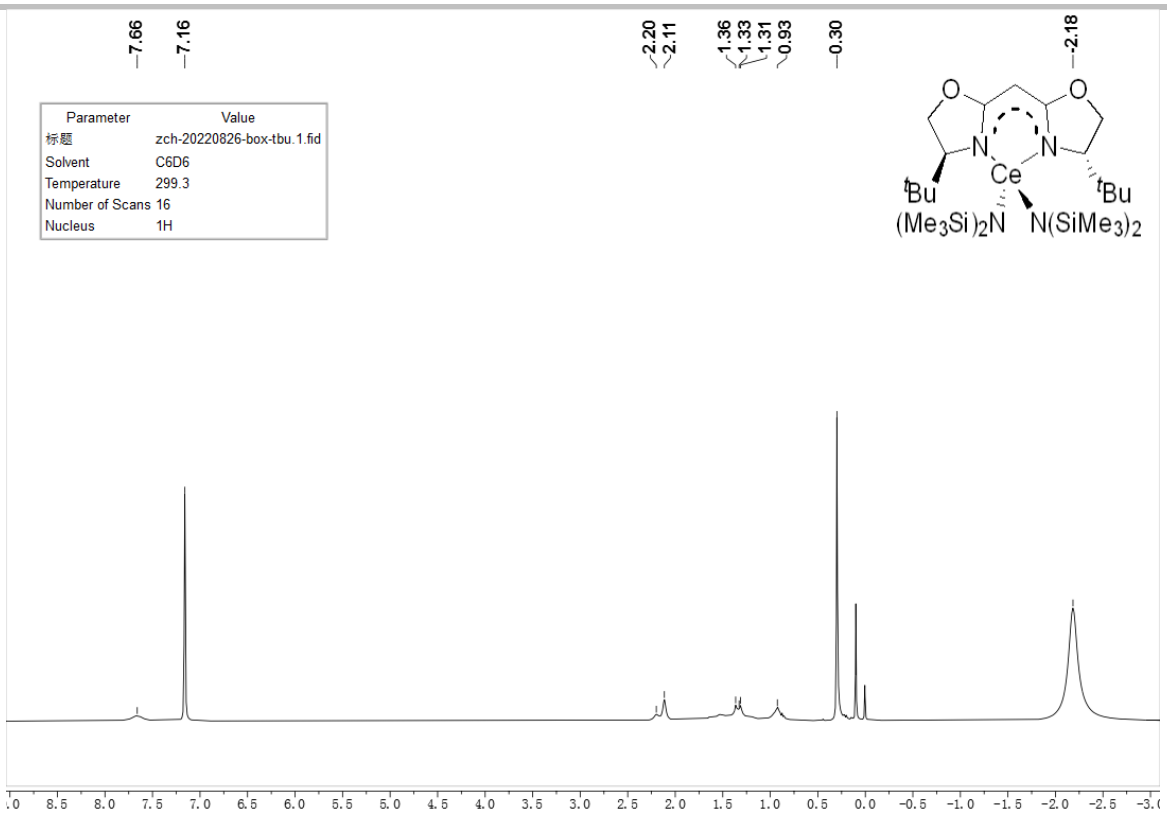
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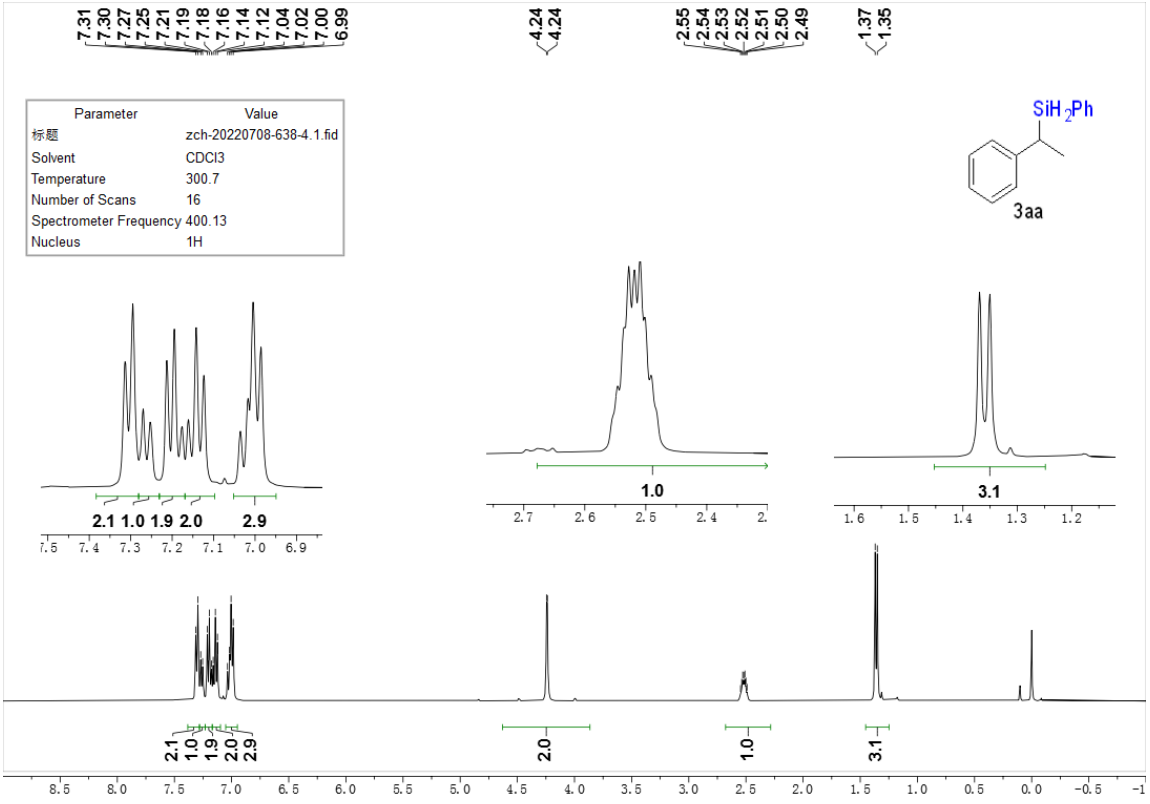
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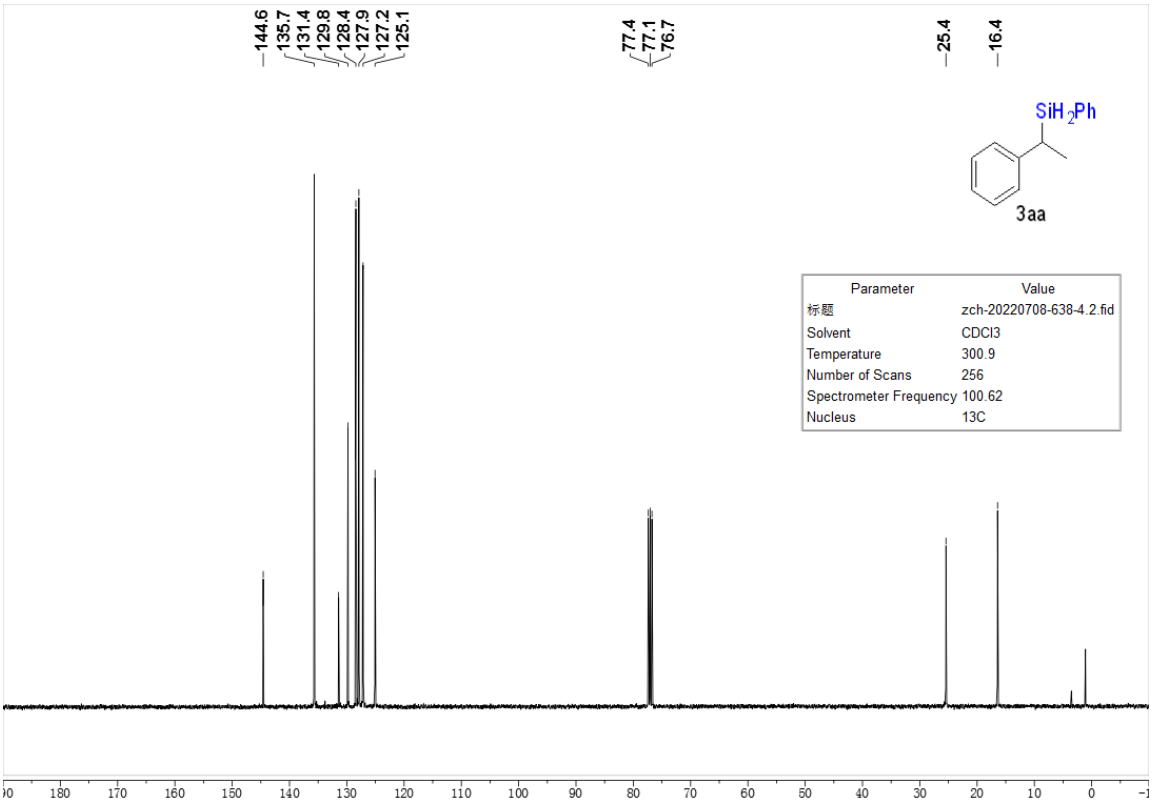
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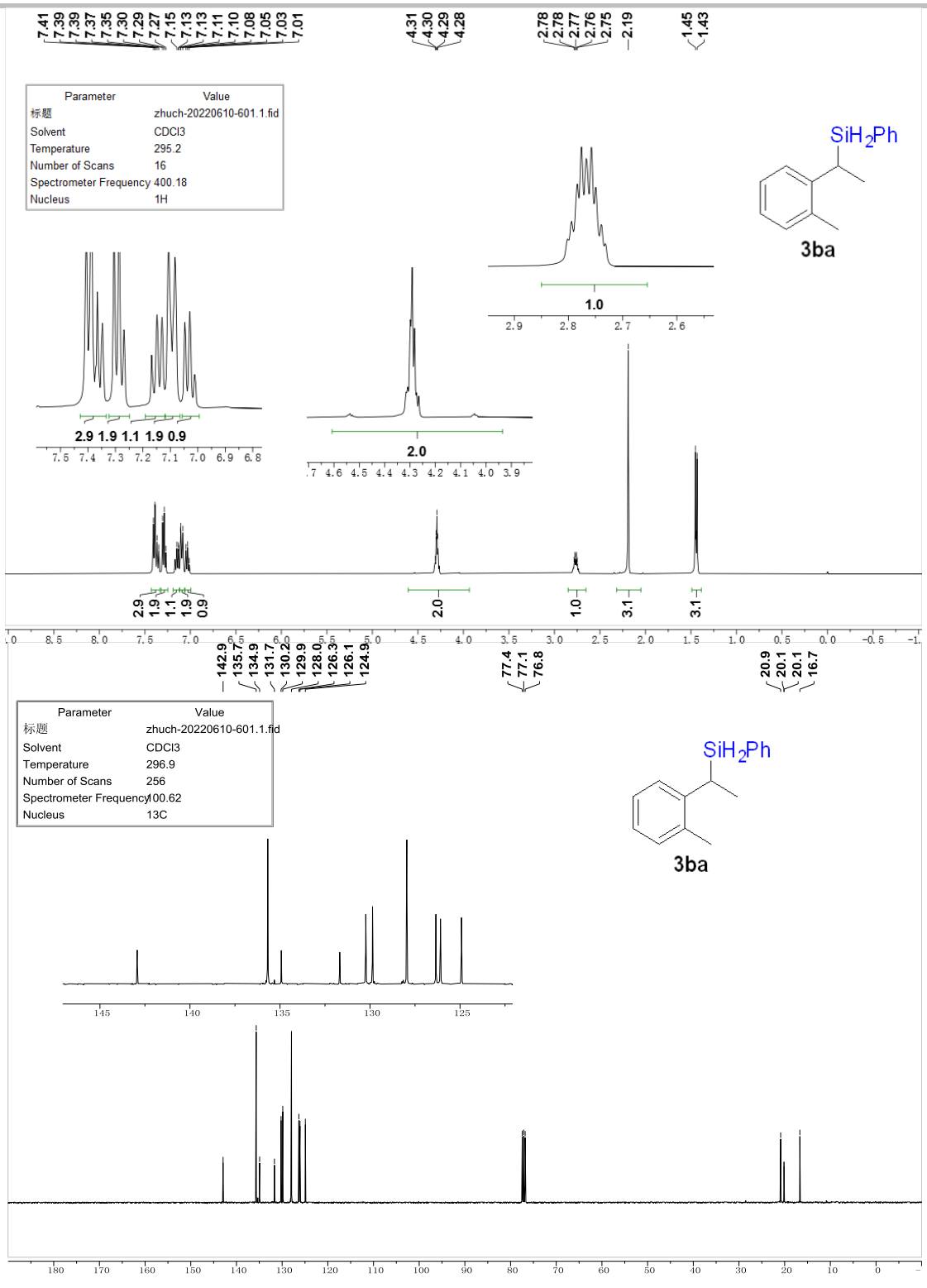
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2.78 2.78 2.77 2.76 2.75
2.19
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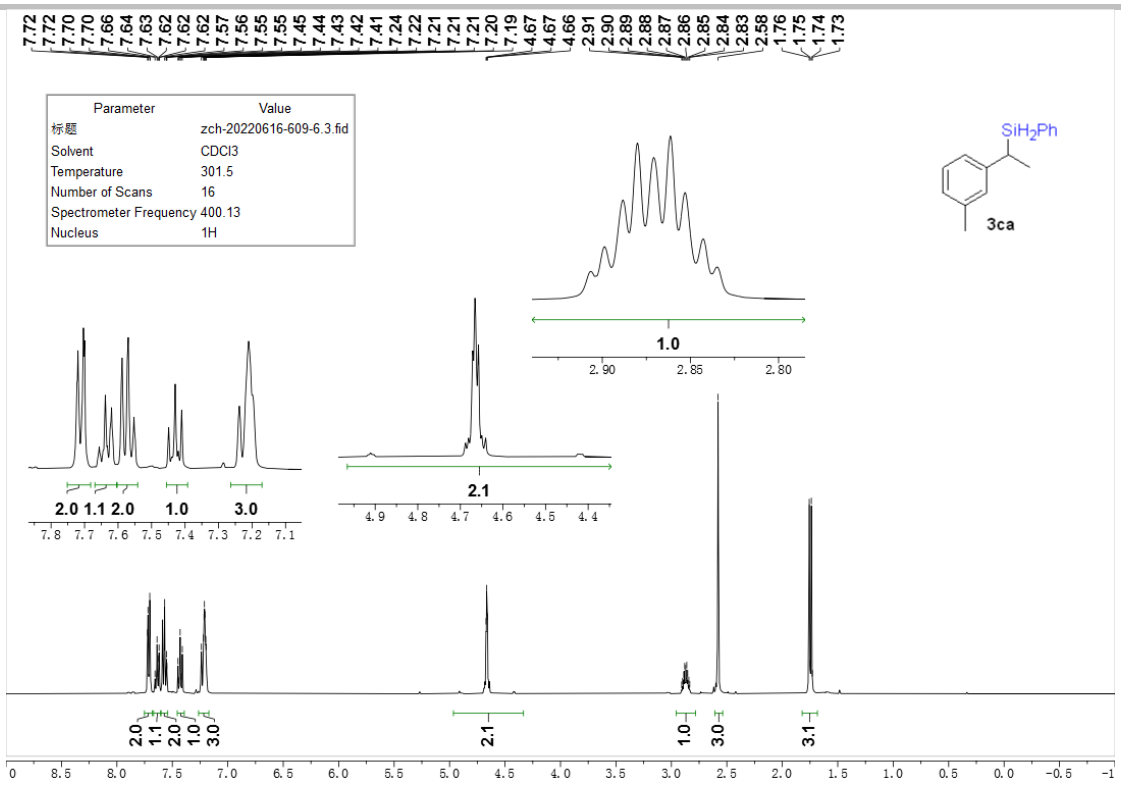
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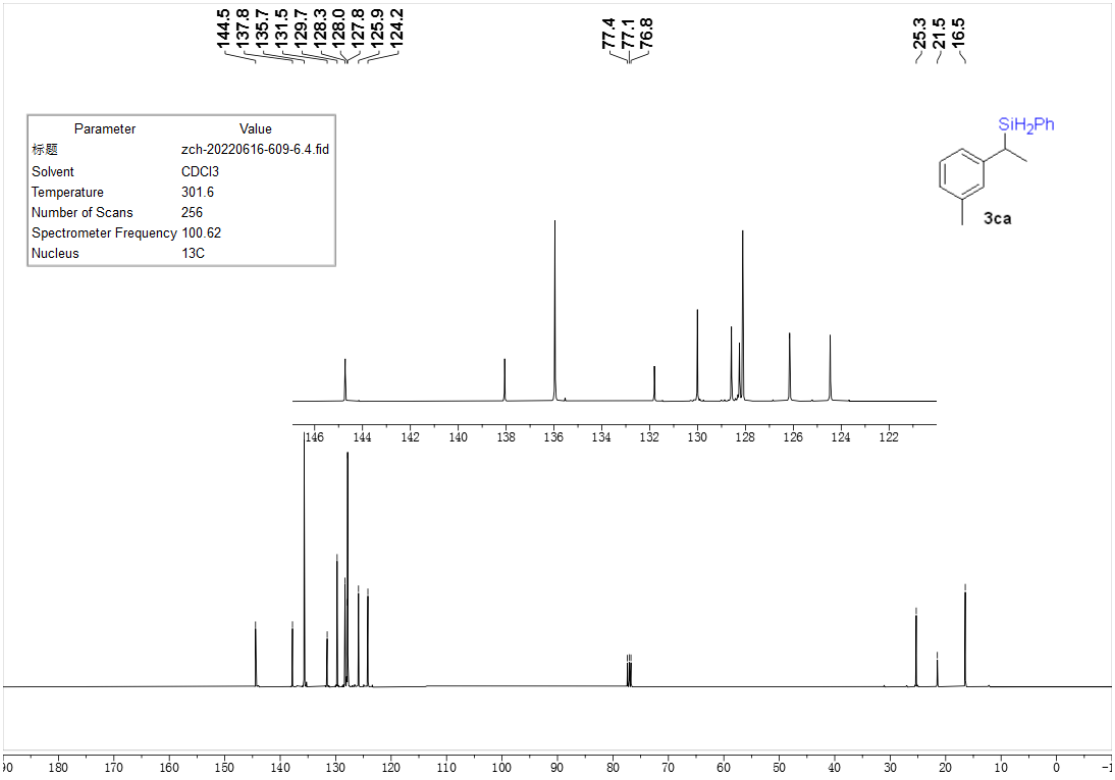
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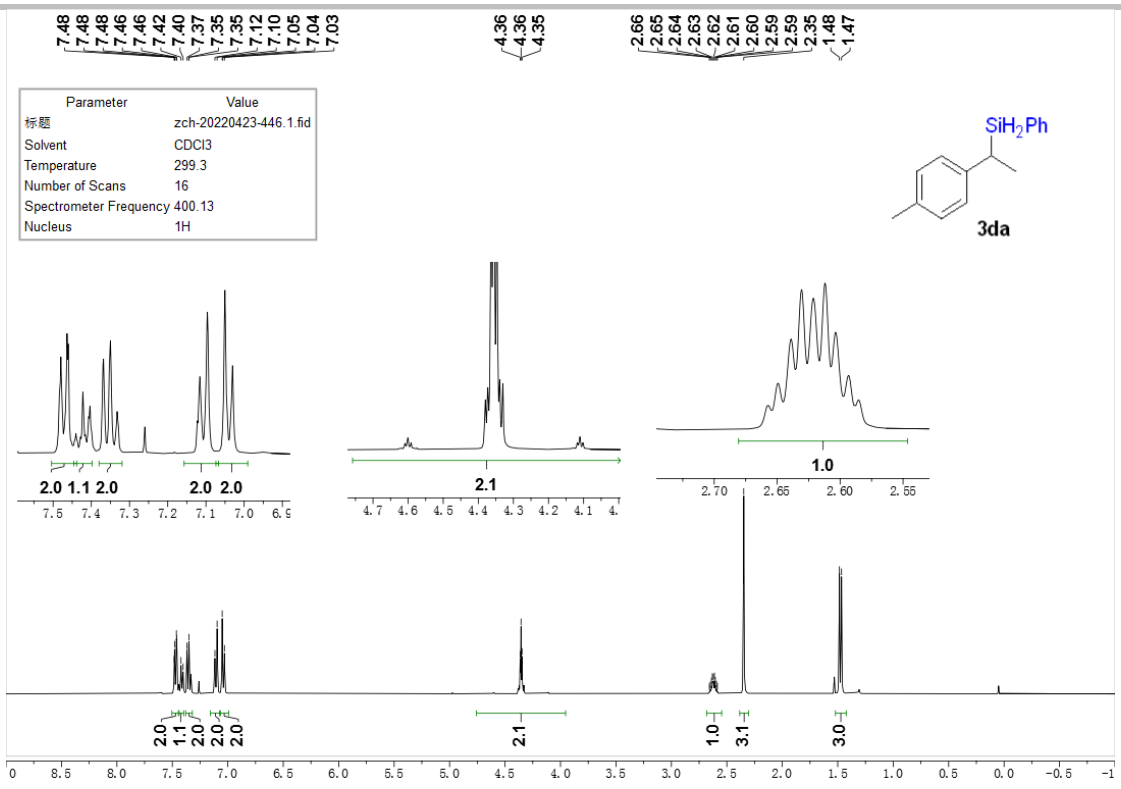
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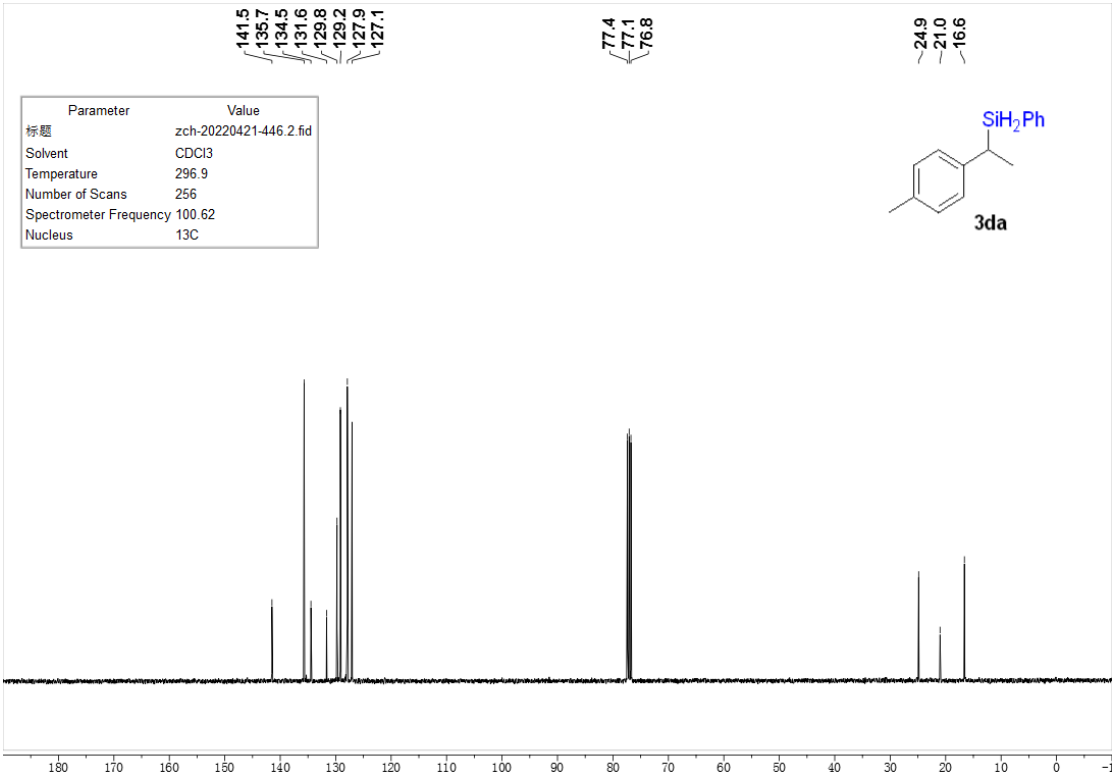
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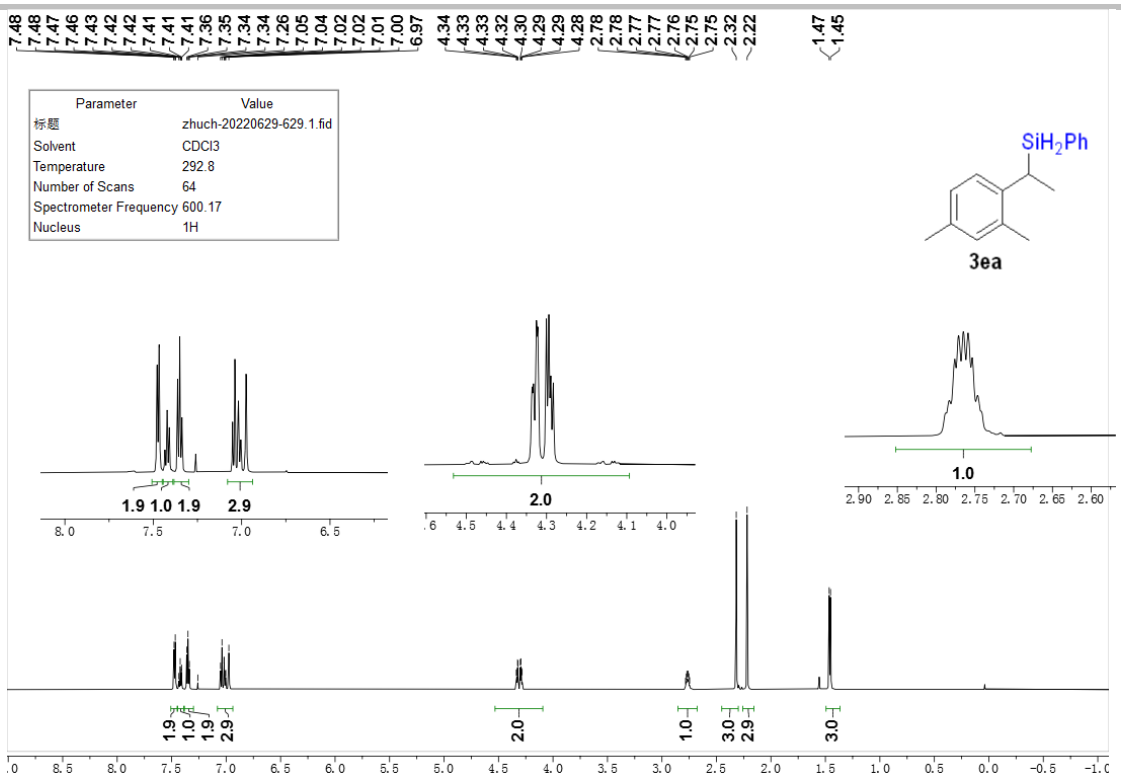
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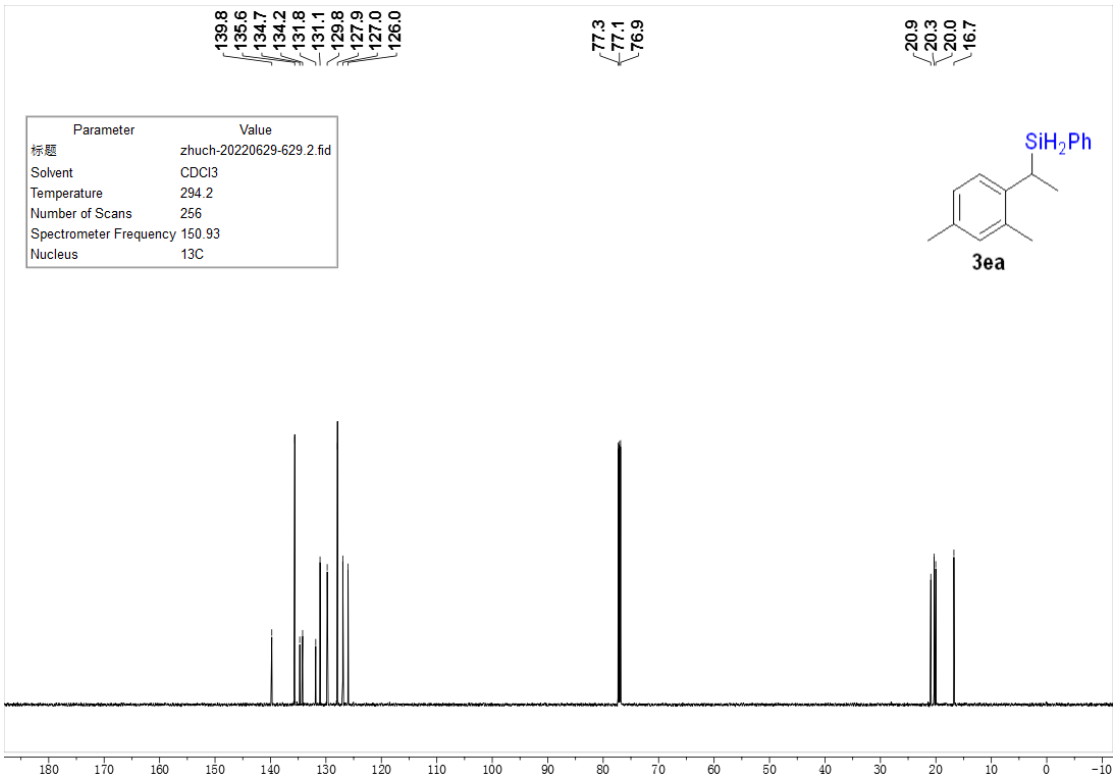
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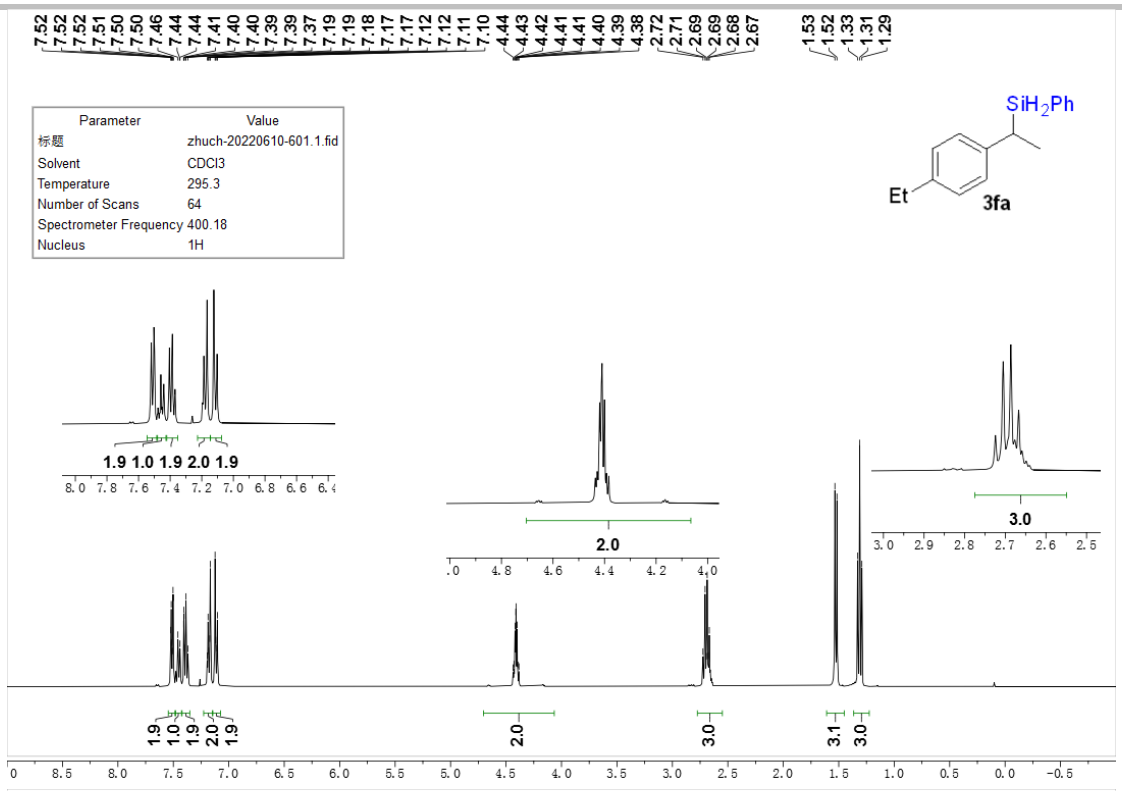
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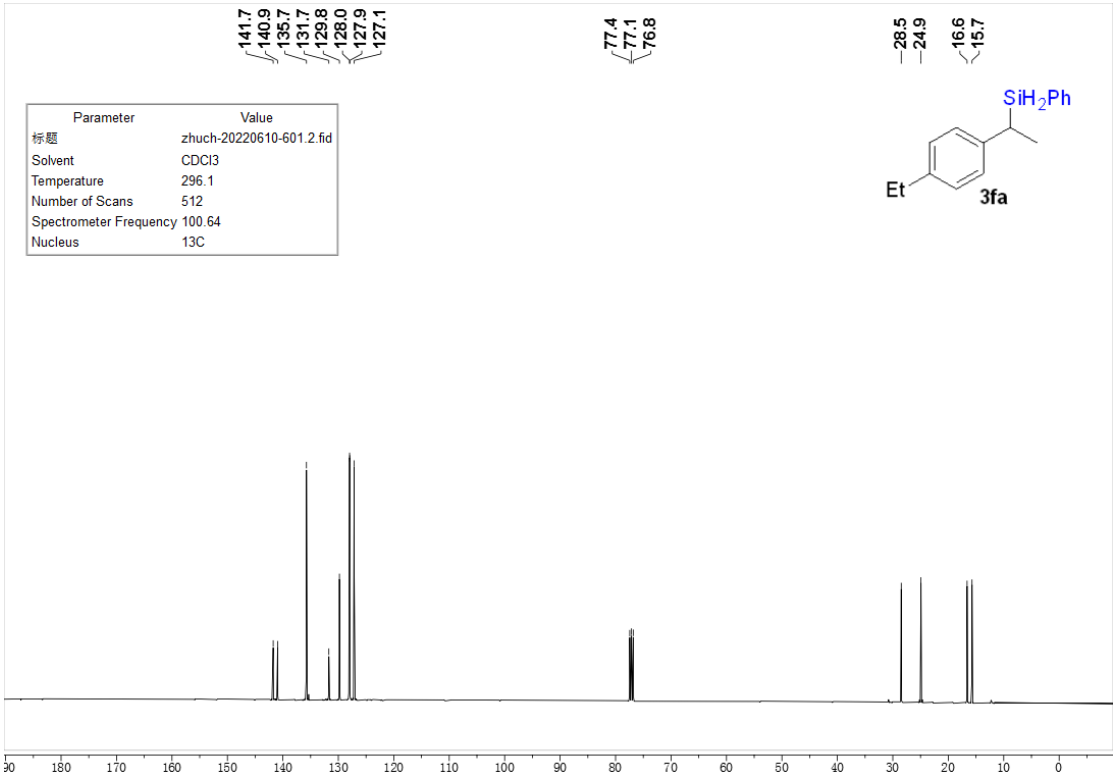
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標題 zhuch-20220610-601.2.fid
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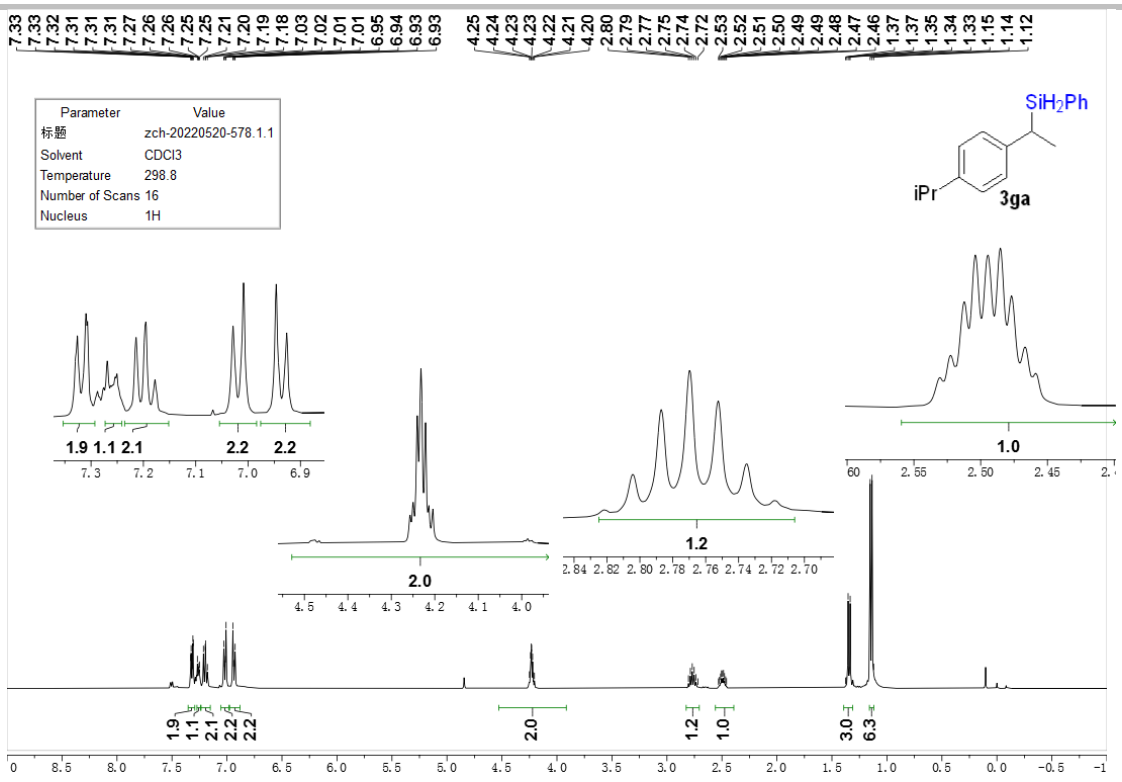
Temperature 296.1
Number of Scans 512
Spectrometer Frequency 100.64
Nucleus 13C
SiH2Ph
Et
3fa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4.25 4.24 4.23 4.23 4.22 4.21 4.20 2.80 2.79 2.77 2.75 2.74 2.72 2.53 2.52 2.51 2.50 2.49 2.49 2.48 2.47 2.46 1.37 1.37 1.35 1.34 1.33 1.15 1.14 1.12
Parameter Value
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Solvent CDCl3
Temperature 298.8
Number of Scans 16
Nucleus 1H
SiH2Ph
iPr
3ga
1.9 1.1 2.1 2.2 2.2
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1.2
1.0
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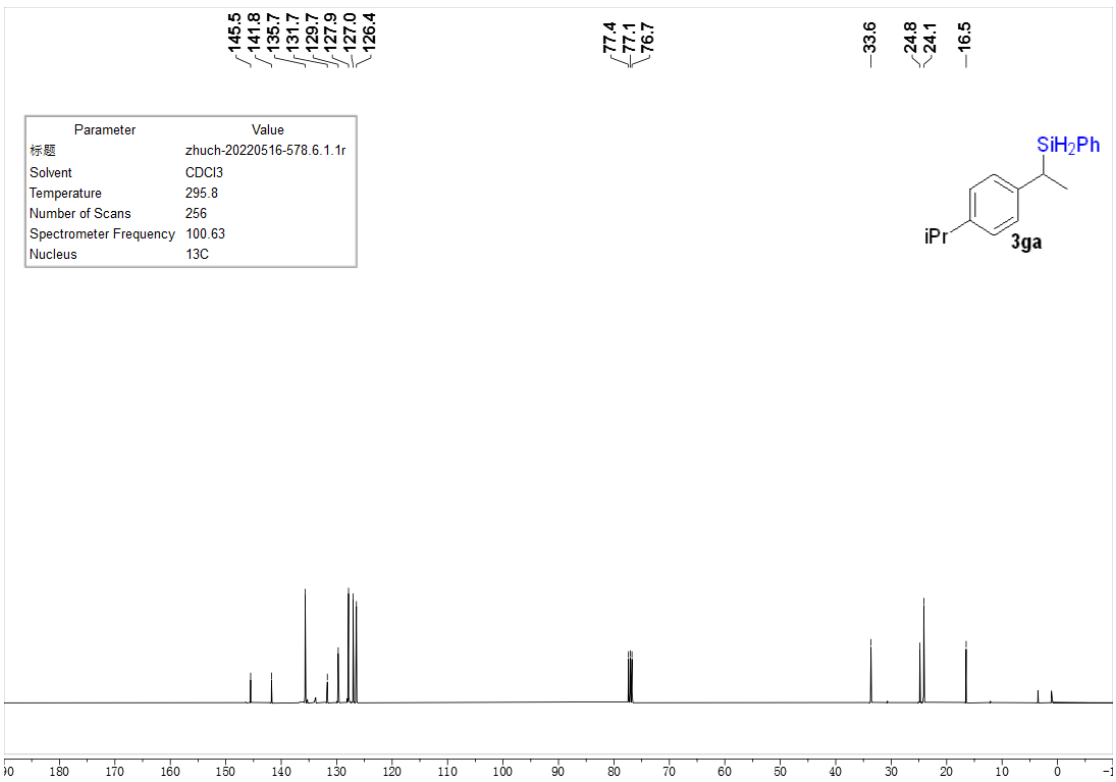
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Parameter Value
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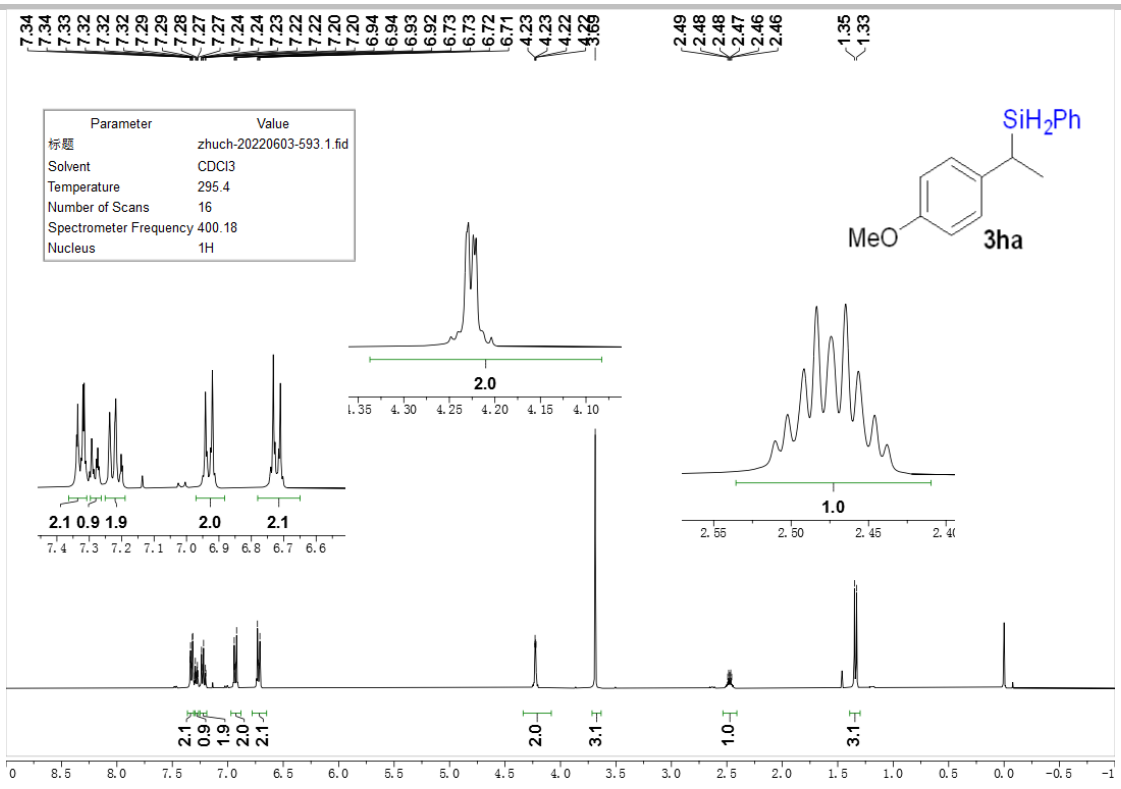
Solvent CDCl3
Temperature 295.8
Number of Scans 256
Spectrometer Frequency 100.63
Nucleus 13C
SiH2Ph
iPr
3ga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2.49 2.48 2.48 2.47 2.46 2.46
1.35 1.33
Parameter Value
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Solvent CDCl3
Temperature 295.4
Number of Scans 16
Spectrometer Frequency 400.18
Nucleus 1H
SiH2Ph
MeO
3ha
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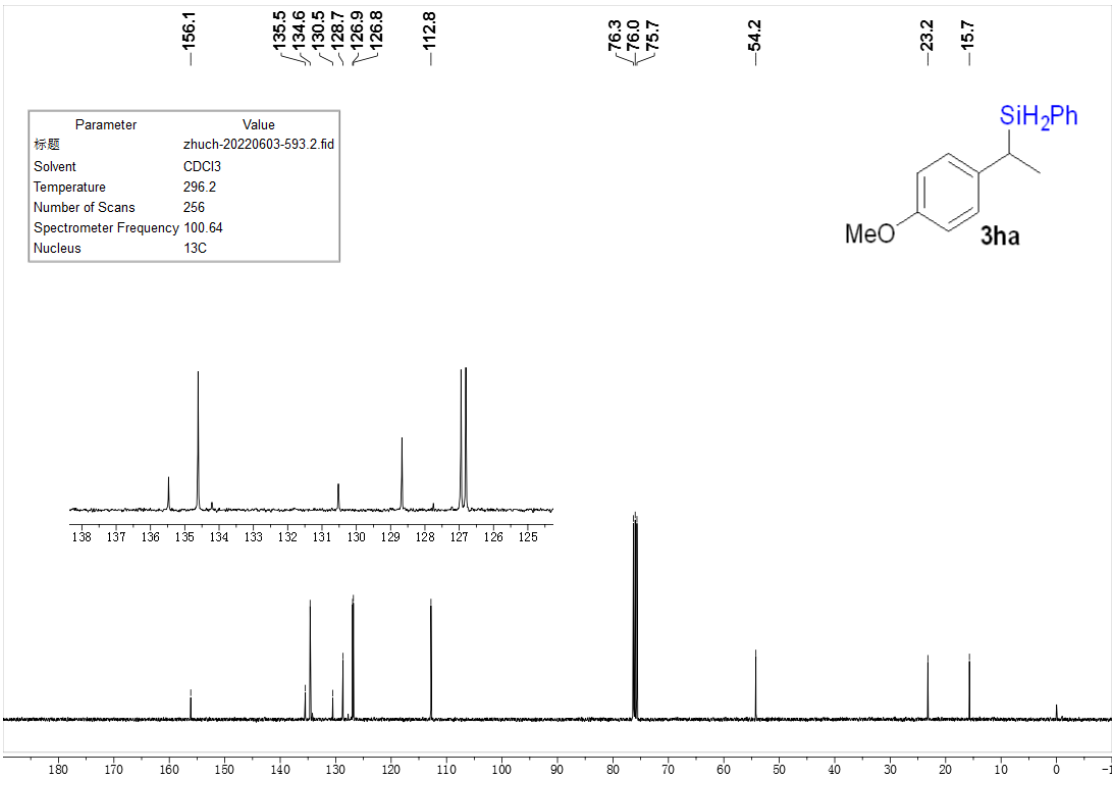
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Parameter Value
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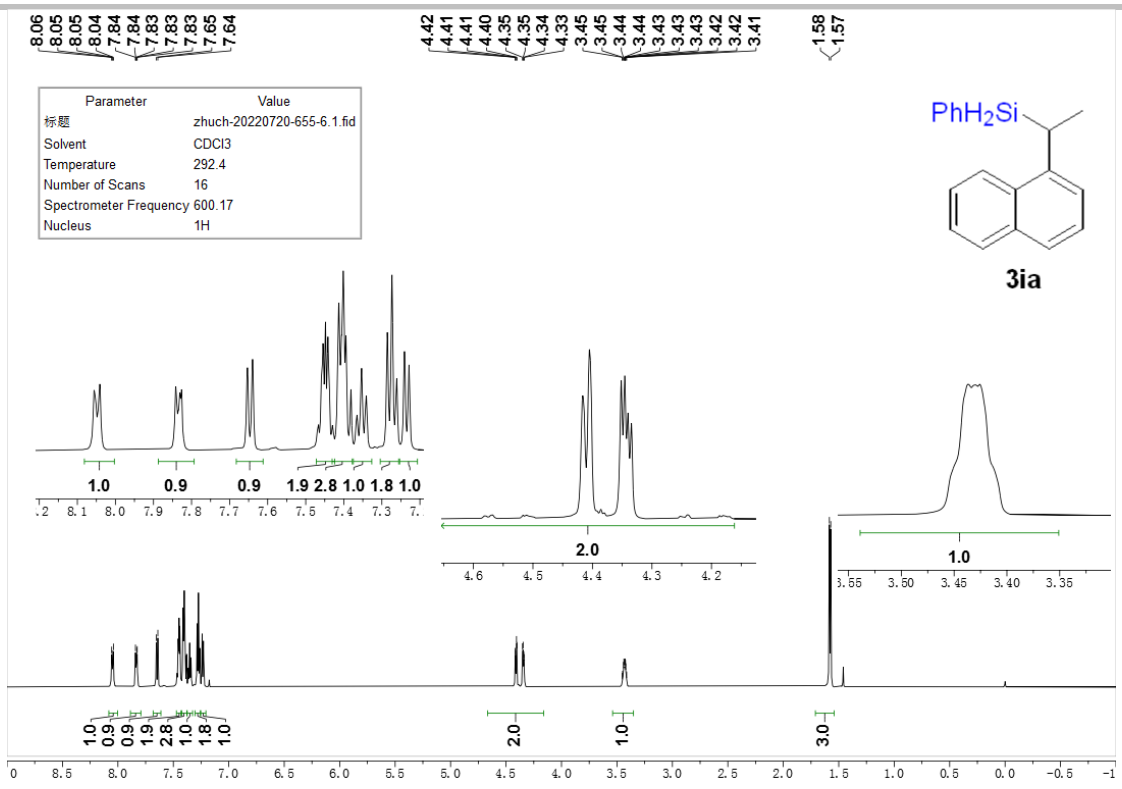
Temperature 296.2
Number of Scans 256
Spectrometer Frequency 100.64
Nucleus 13C
SiH2Ph
MeO
3ha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4.42 4.41 4.41 4.40 4.35 4.35 4.34 4.33 3.45 3.45 3.44 3.44 3.43 3.43 3.42 3.42 3.41
1.58 1.57
Parameter Value
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Solvent CDCl3
Temperature 292.4
Number of Scans 16
Spectrometer Frequency 600.17
Nucleus 1H
PhH2Si
3ia
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1.0
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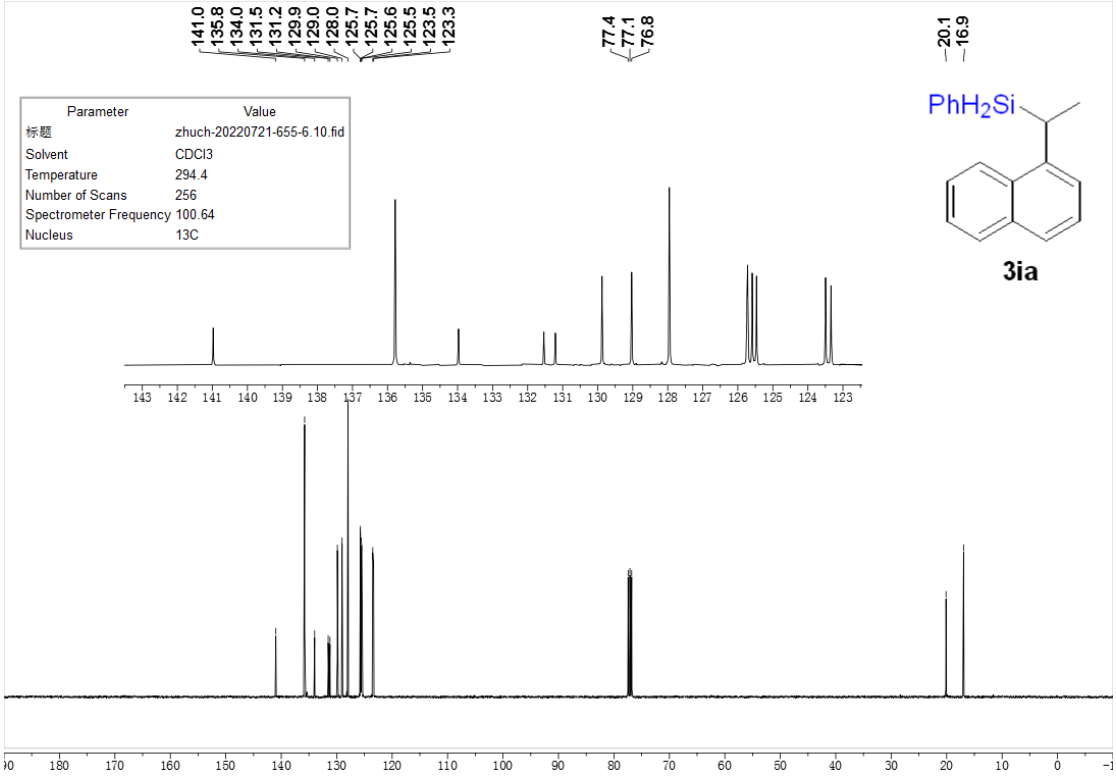
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77.4 77.1 76.8
20.1 16.9
Parameter Value
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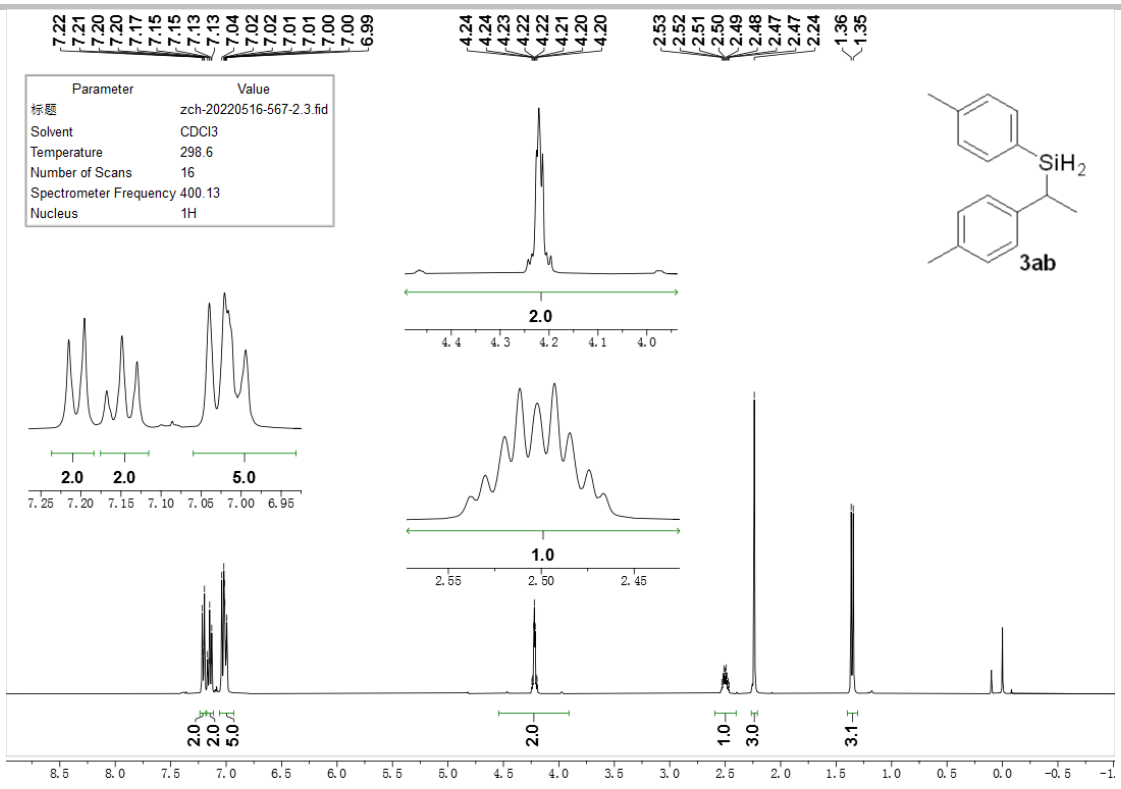
Temperature 294.4
Number of Scans 256
Spectrometer Frequency 100.64
Nucleus 13C
PhH2Si
3ia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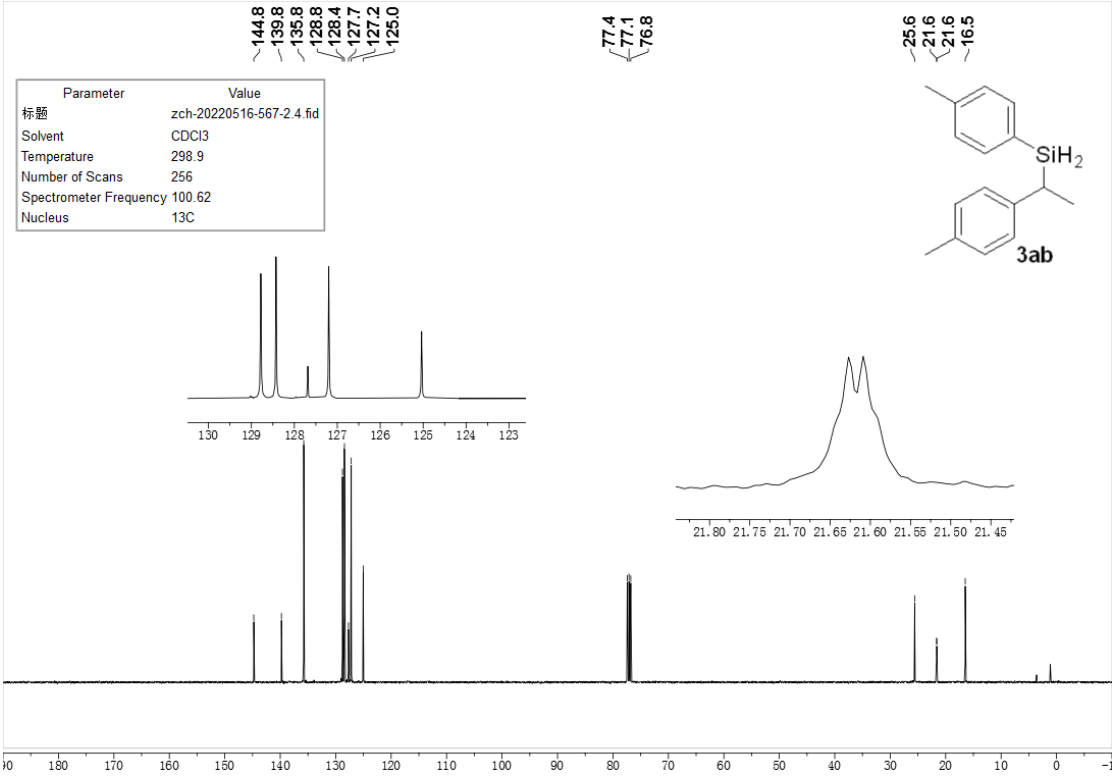
4.24 4.24 4.23 4.22 4.22 4.21 4.20 4.20
2.53 2.52 2.51 2.50 2.49 2.48 2.47 2.47 2.24
1.36 1.35
Parameter Value
标题 zch-20220516-567-2.3.fid
Solvent CDCl3
Temperature 298.6
Number of Scans 16
Spectrometer Frequency 400.13
Nucleus 1H
SiH2
3ab
2.0
2.0 2.0 5.0
1.0
2.0 2.0 5.0 2.0 1.0 3.0 3.1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77.4 77.1 76.8
25.6 21.6 21.6 16.5
Parameter Value
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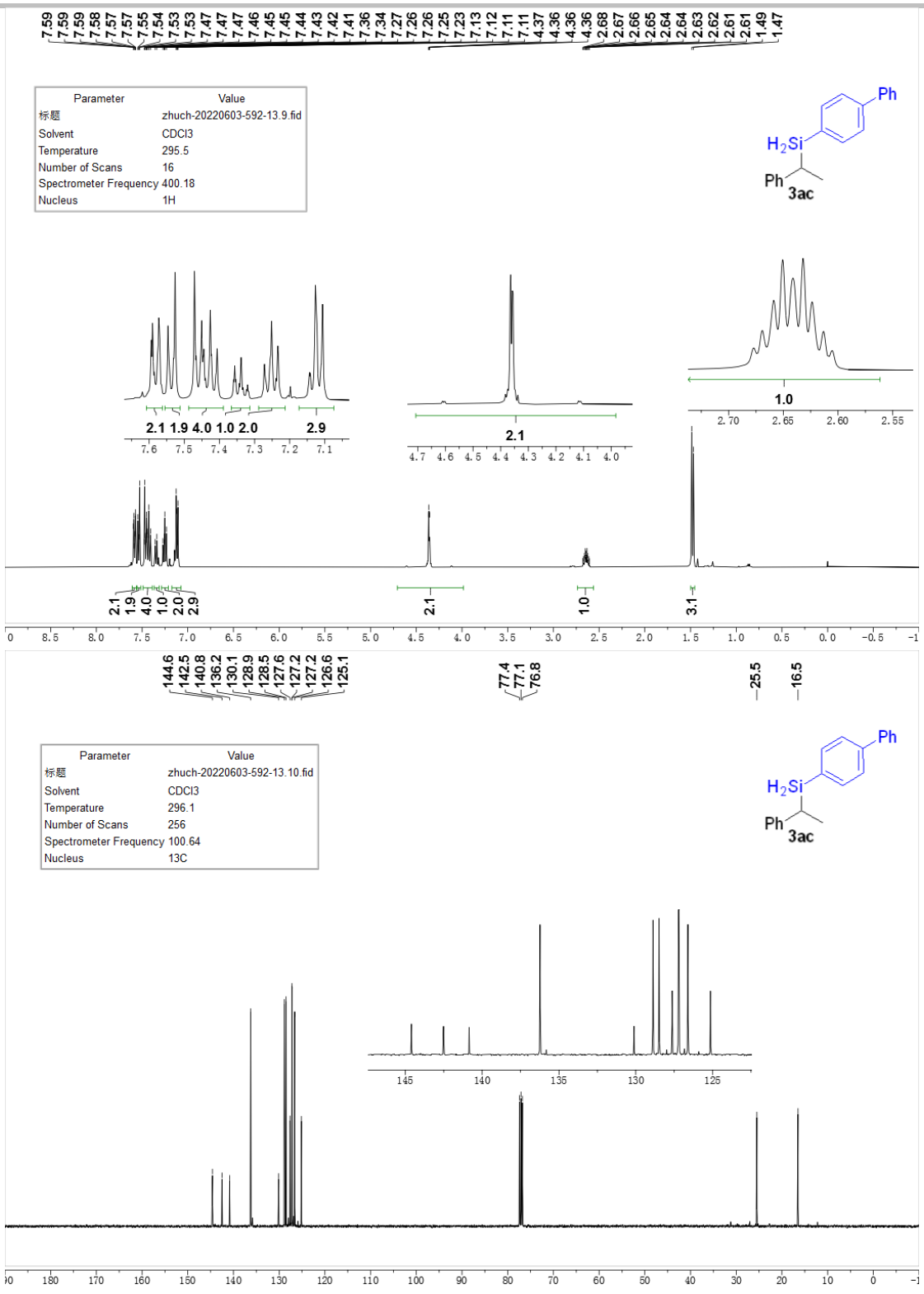
Solvent CDCl3
Temperature 298.9
Number of Scans 256
Spectrometer Frequency 100.62
Nucleus 13C
SiH2
3ab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Parameter Value
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Solvent CDCl3
Temperature 295.5
Number of Scans 16
Spectrometer Frequency 400.18
Nucleus 1H
Ph
H2Si
Ph
3ac
2.1 1.9 4.0 1.0 2.0 2.9
2.1
1.0
144.6 142.5 140.8 136.2 130.1 128.9 128.5 127.6 127.2 127.2 126.6 125.1
77.4 77.1 76.8
25.5
16.5
Parameter Value
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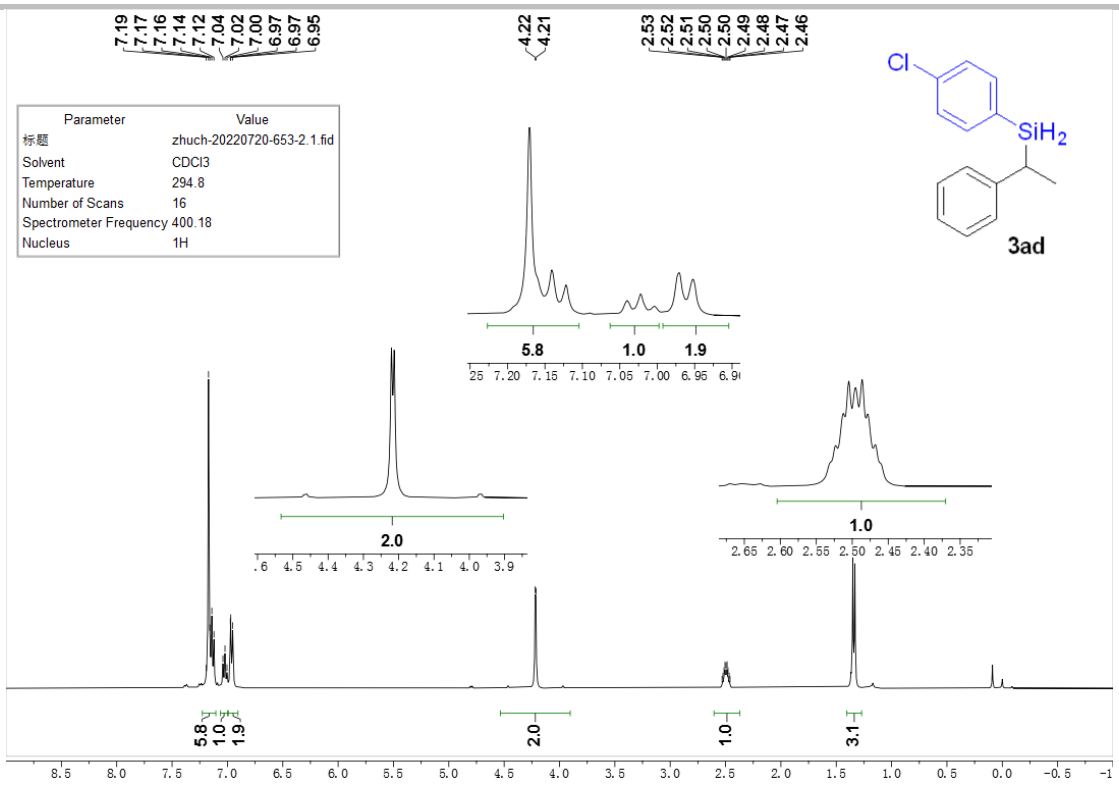
Temperature 296.1
Number of Scans 256
Spectrometer Frequency 100.64
Nucleus 13C
Ph
H2Si
Ph
3ac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6.95
4.22
4.21
2.53
2.52
2.51
2.50
2.50
2.49
2.48
2.47
2.46
Parameter Value
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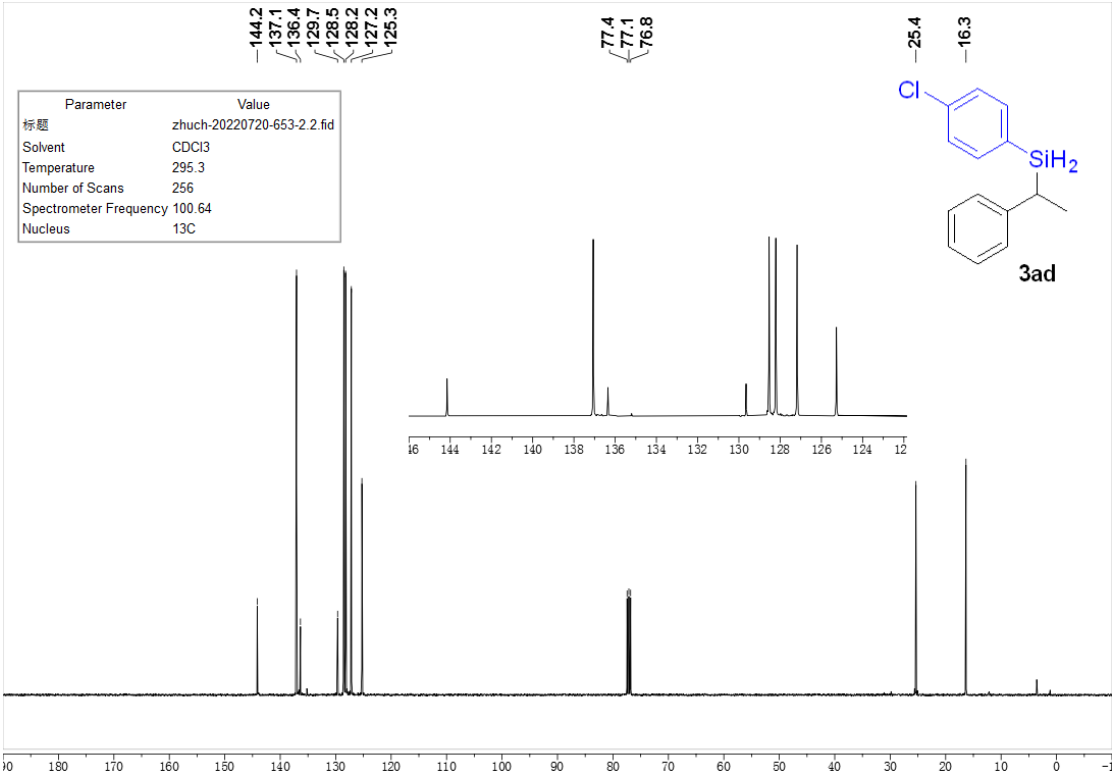
Solvent CDCl3
Temperature 294.8
Number of Scans 16
Spectrometer Frequency 400.18
Nucleus 1H
Cl
SiH2
3ad
5.8
1.0
1.9
2.0
1.0
5.8
1.0
1.9
3.1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137.1
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128.2
127.2
125.3
77.4
77.1
76.8
25.4
16.3
Parameter Value
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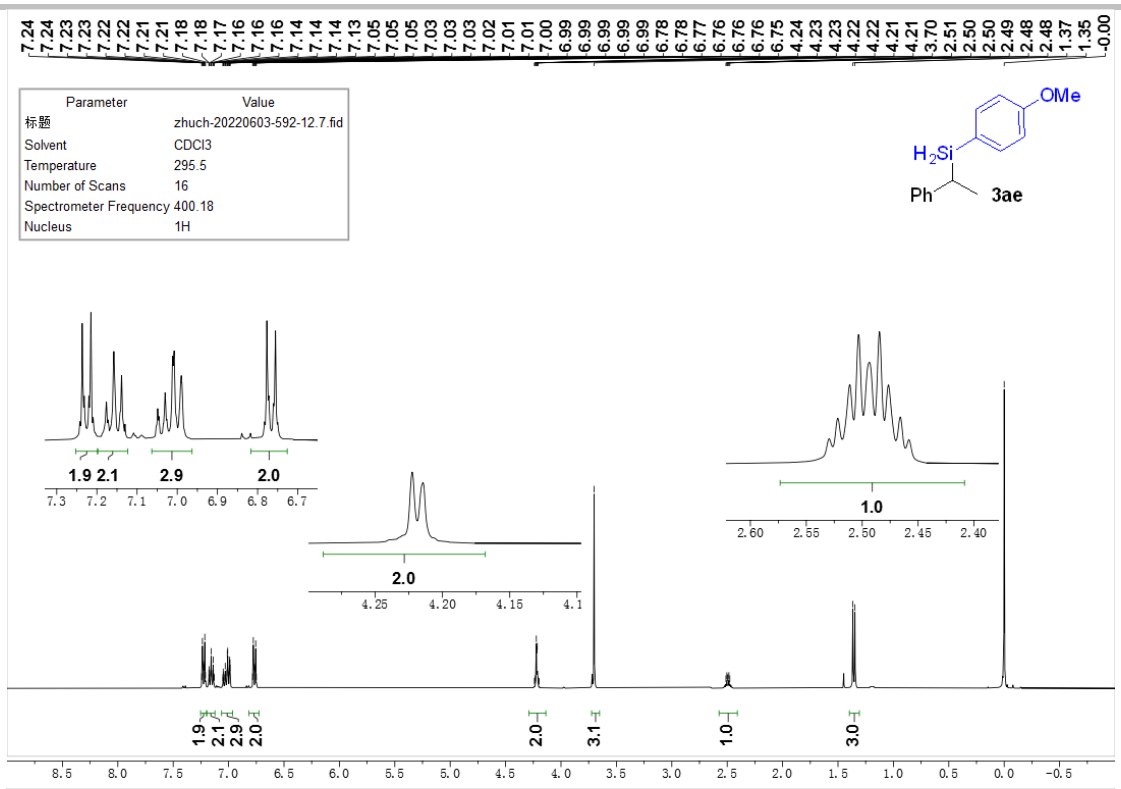
Solvent CDCl3
Temperature 295.3
Number of Scans 256
Spectrometer Frequency 100.64
Nucleus 13C
Cl
SiH2
3ad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Parameter Value
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Temperature 295.5
Number of Scans 16
Spectrometer Frequency 400.18
Nucleus 1H
OMe
H2Si
Ph
3ae
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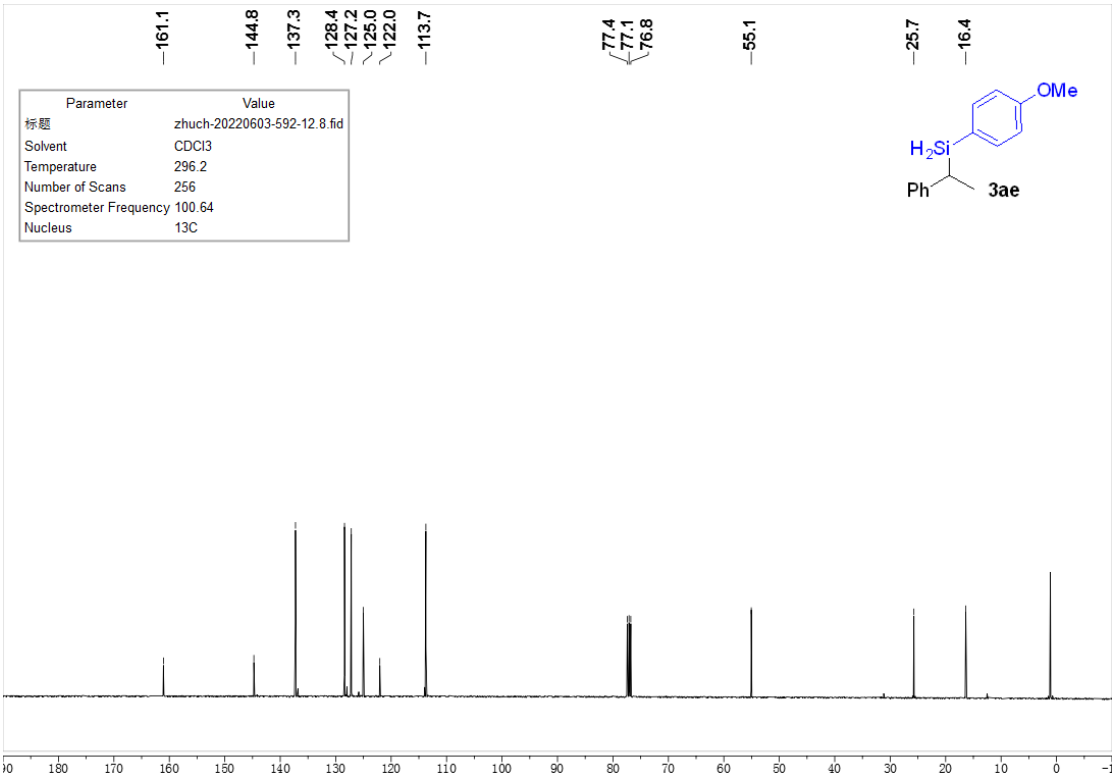
2.0
1.0
1.9 2.1 2.9 2.0 2.0 3.1 1.0 3.0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Parameter Value
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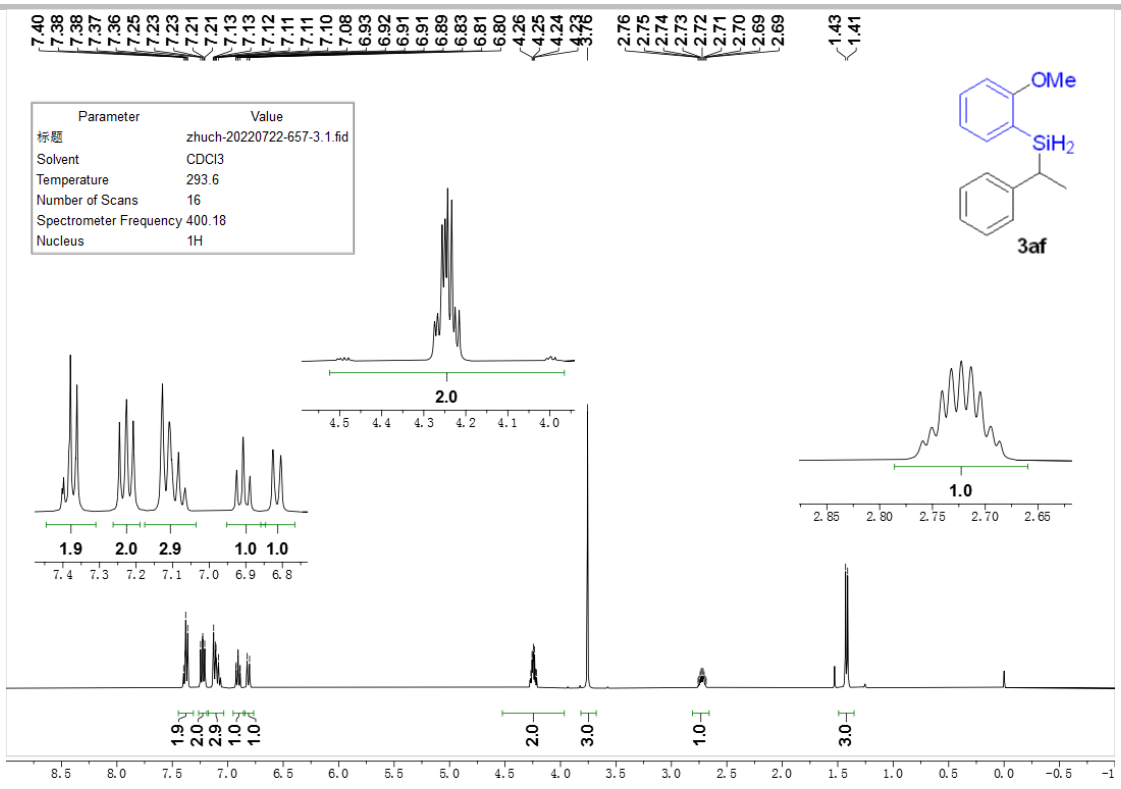
Temperature 296.2
Number of Scans 256
Spectrometer Frequency 100.64
Nucleus 13C
OMe
H2Si
Ph
3ae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Parameter Value
标题 zhuch-20220722-657-3.1.fid
Solvent CDCl3
Temperature 293.6
Number of Scans 16
Spectrometer Frequency 400.18
Nucleus 1H
OMe
SiH2
3af
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1.0
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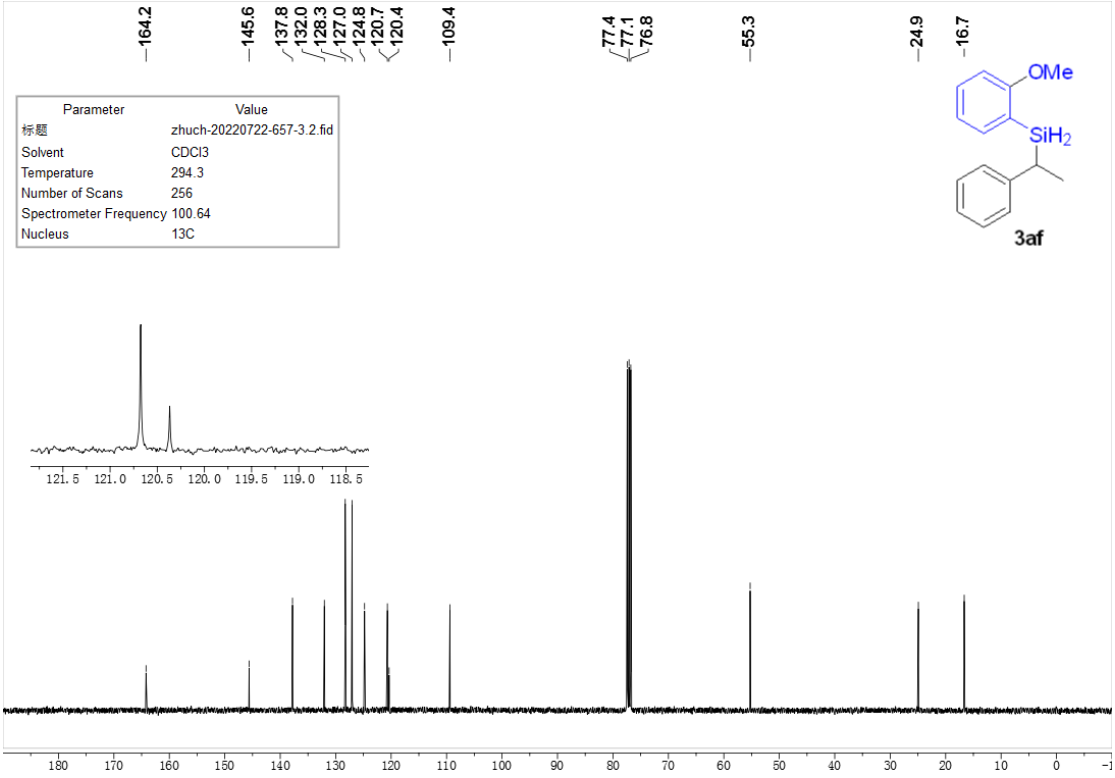
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Parameter Value
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Temperature 294.3
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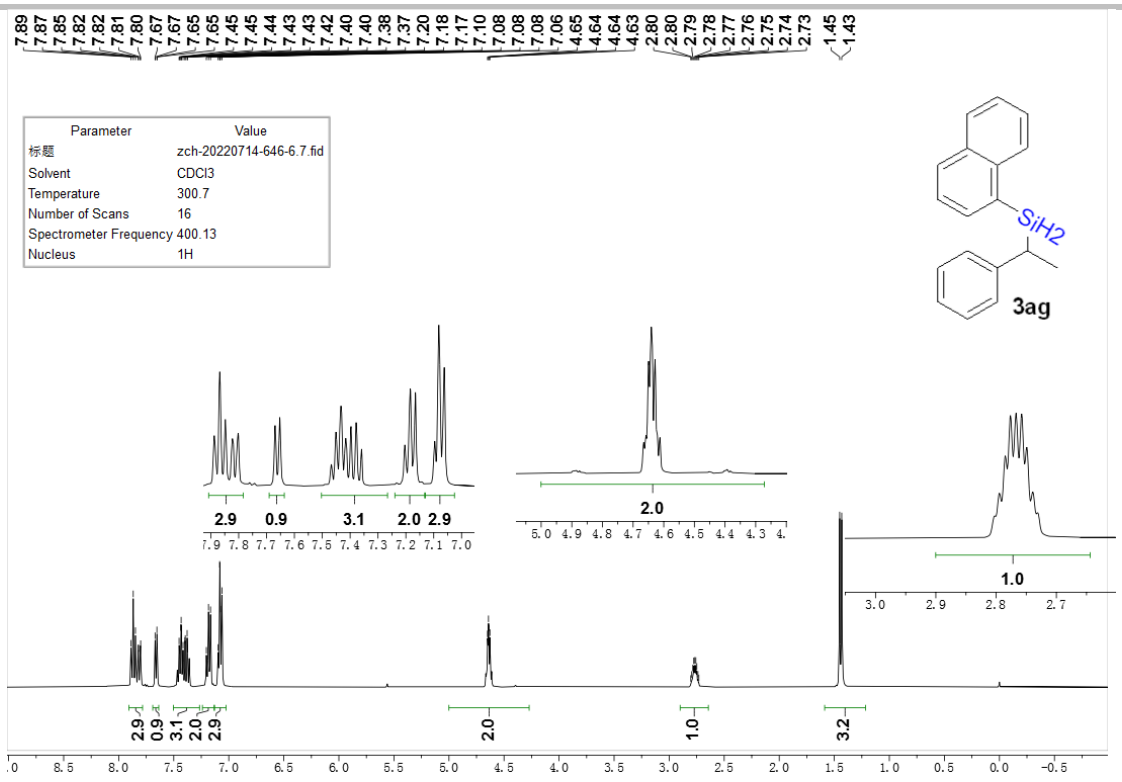
Spectrometer Frequency 100.64
Nucleus 13C
OMe
SiH2
3af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Parameter Value
标题 zch-20220714-646-6.7.fid
Solvent CDCl3
Temperature 300.7
Number of Scans 16
Spectrometer Frequency 400.13
Nucleus 1H
SiH2
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1.0
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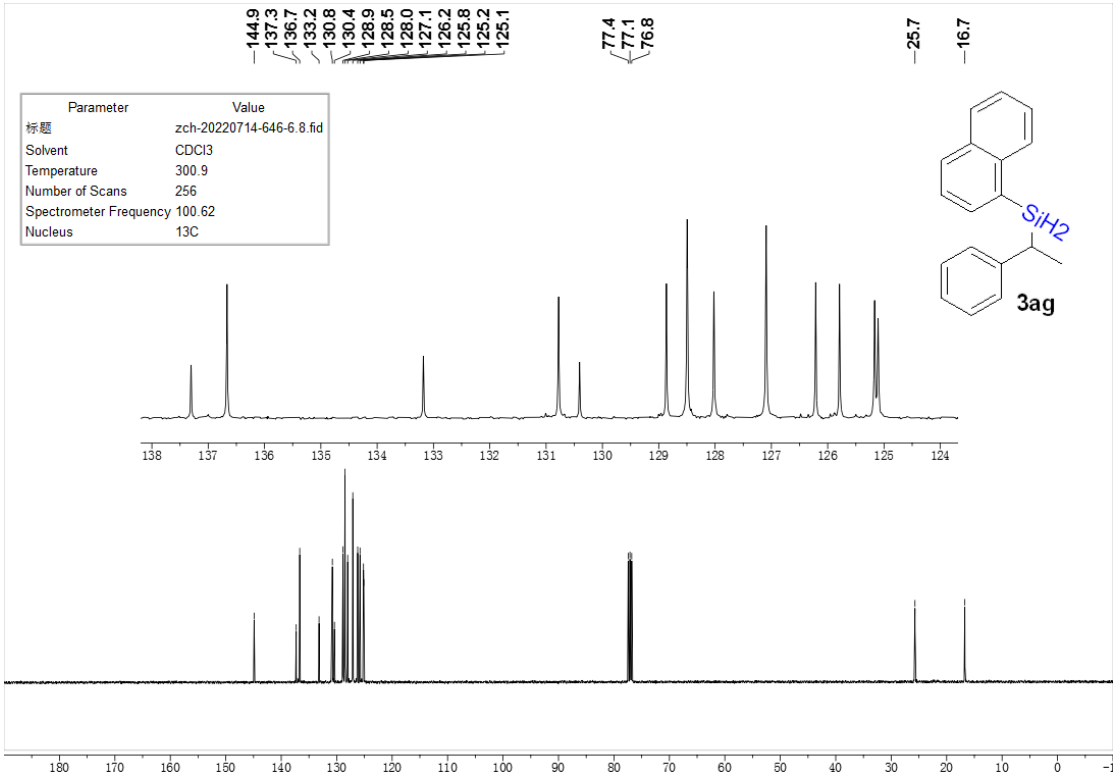
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77.4 77.1 76.8
25.7 16.7
Parameter Value
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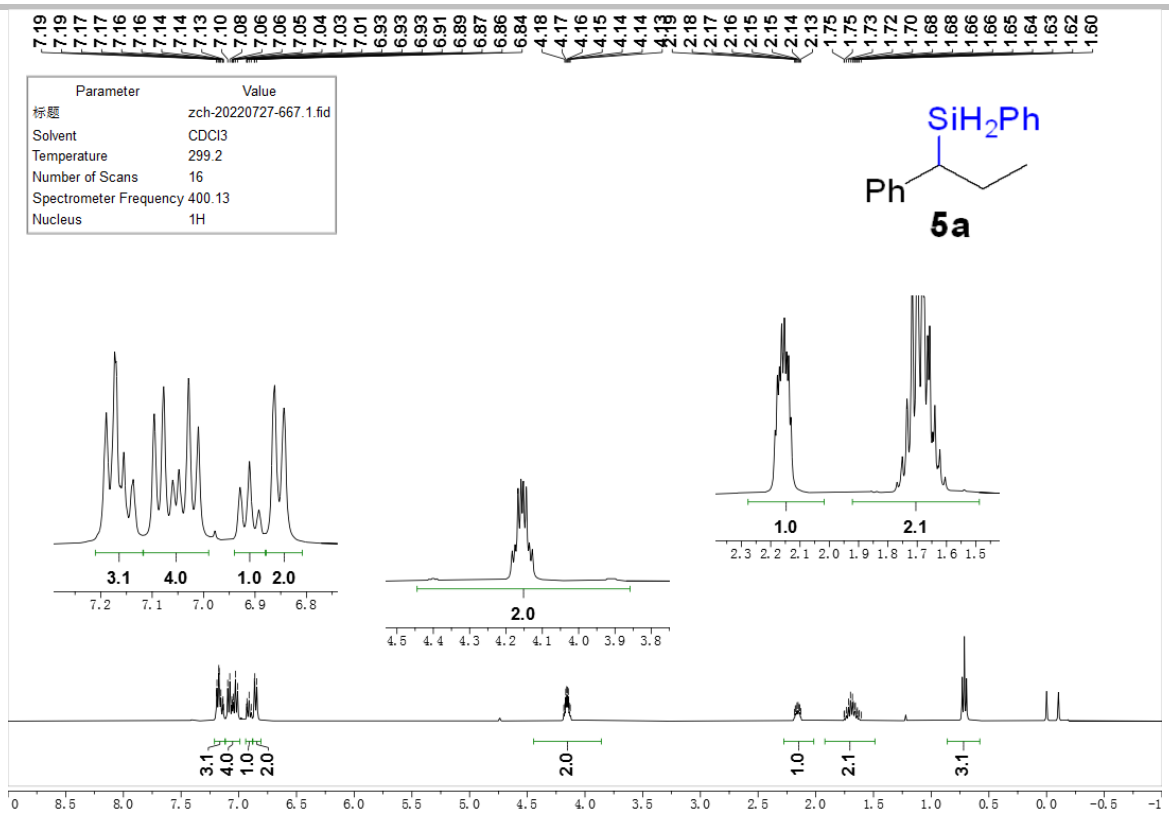
Solvent CDCl3
Temperature 300.9
Number of Scans 256
Spectrometer Frequency 100.62
Nucleus 13C
SiH2
3ag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Number of Scans 16
Spectrometer Frequency 400.13
Nucleus 1H
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Ph
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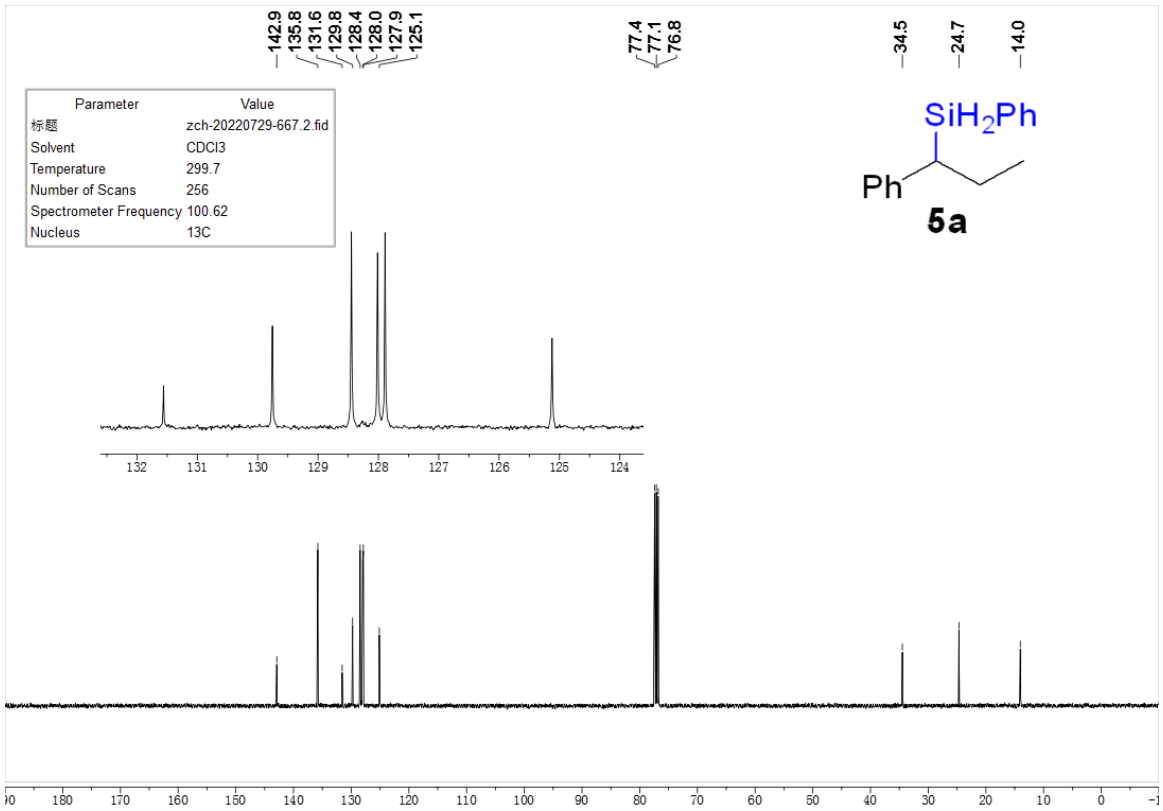
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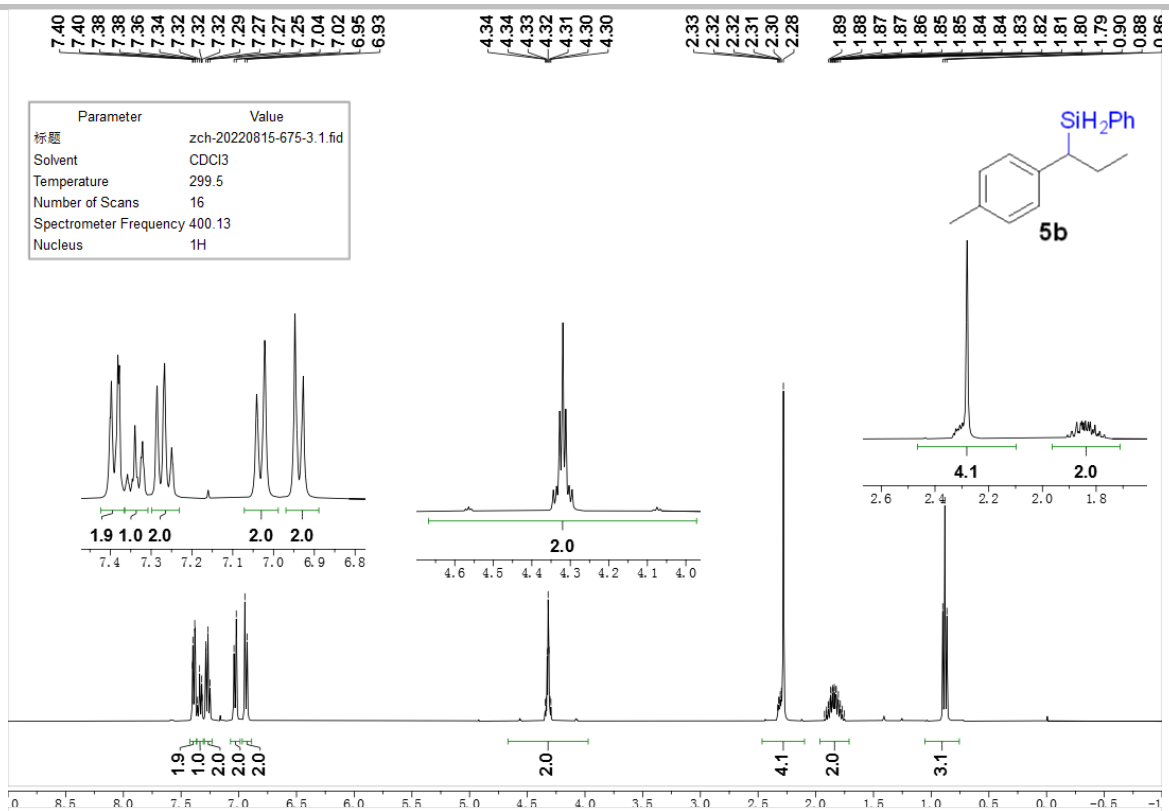
Spectrometer Frequency 100.62
Nucleus 13C
SiH2Ph
Ph
5a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Temperature 299.5
Number of Scans 16
Spectrometer Frequency 400.13
Nucleus 1H
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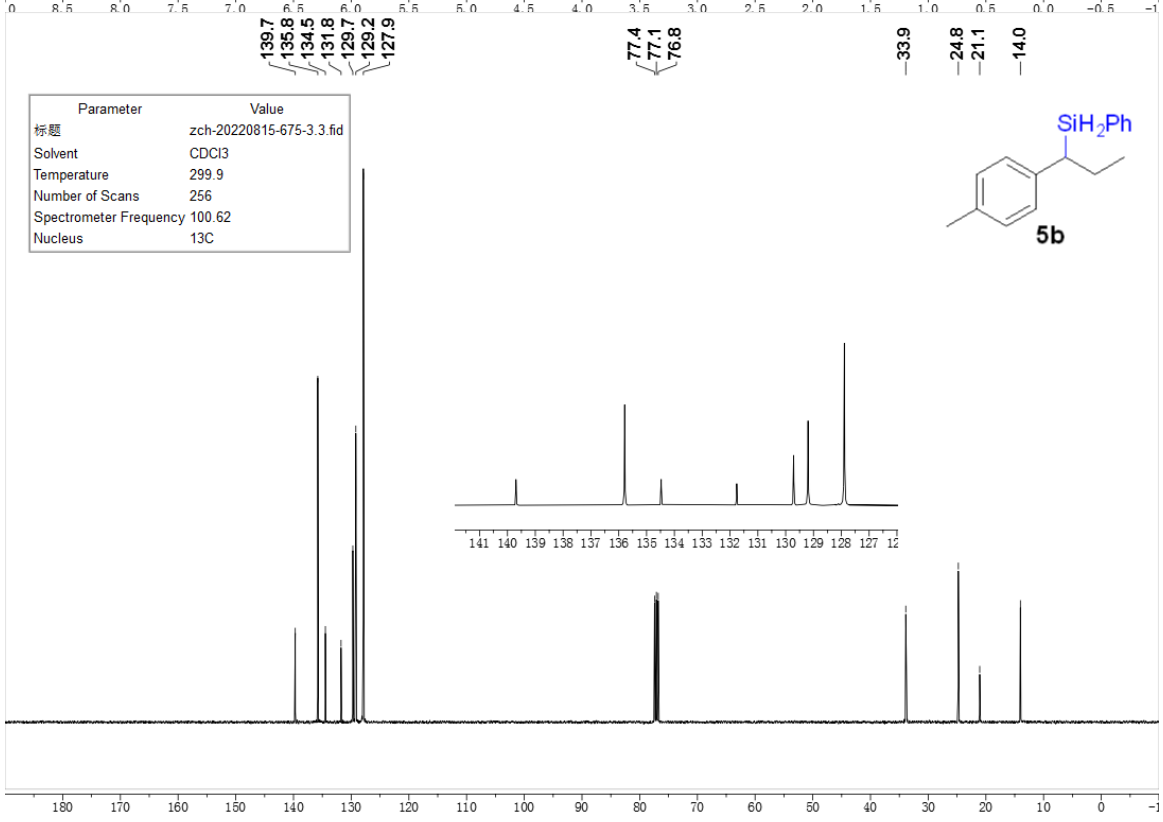
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Number of Scans 256
Spectrometer Frequency 100.62
Nucleus 13C
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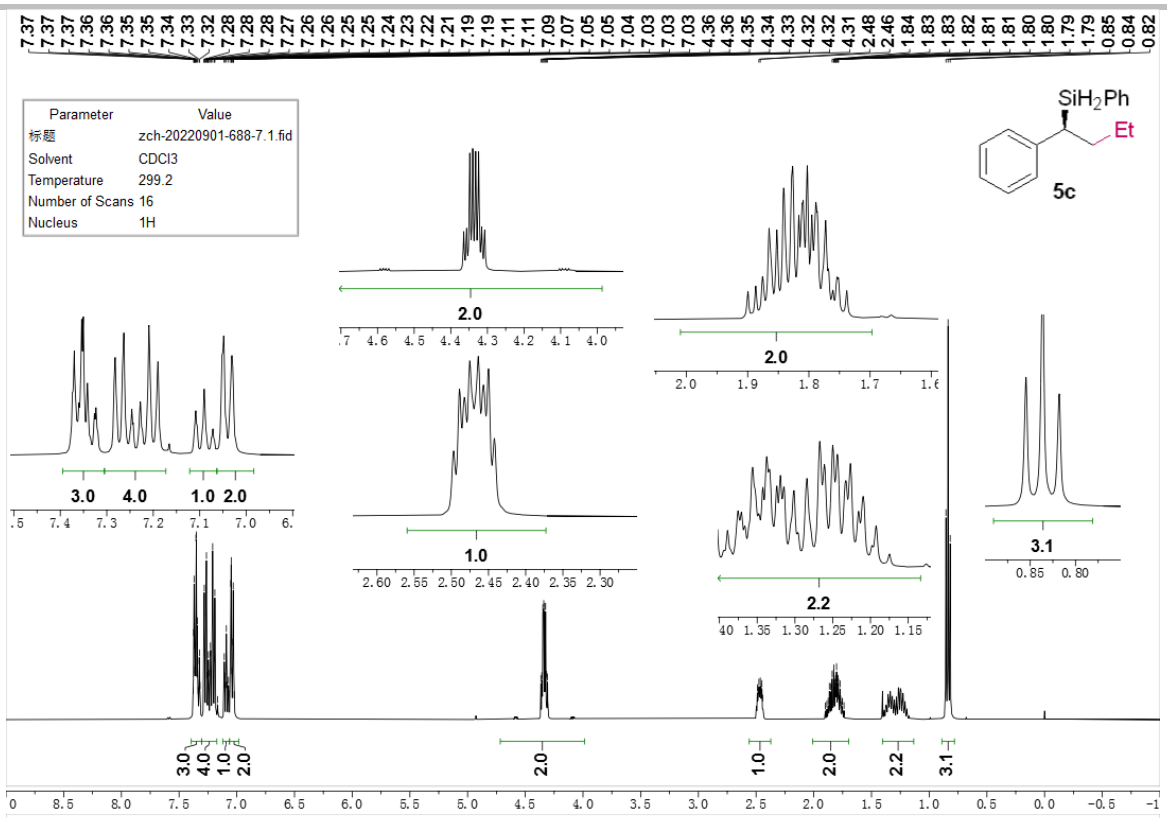
5b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Temperature 299.2
Number of Scans 16
Nucleus 1H
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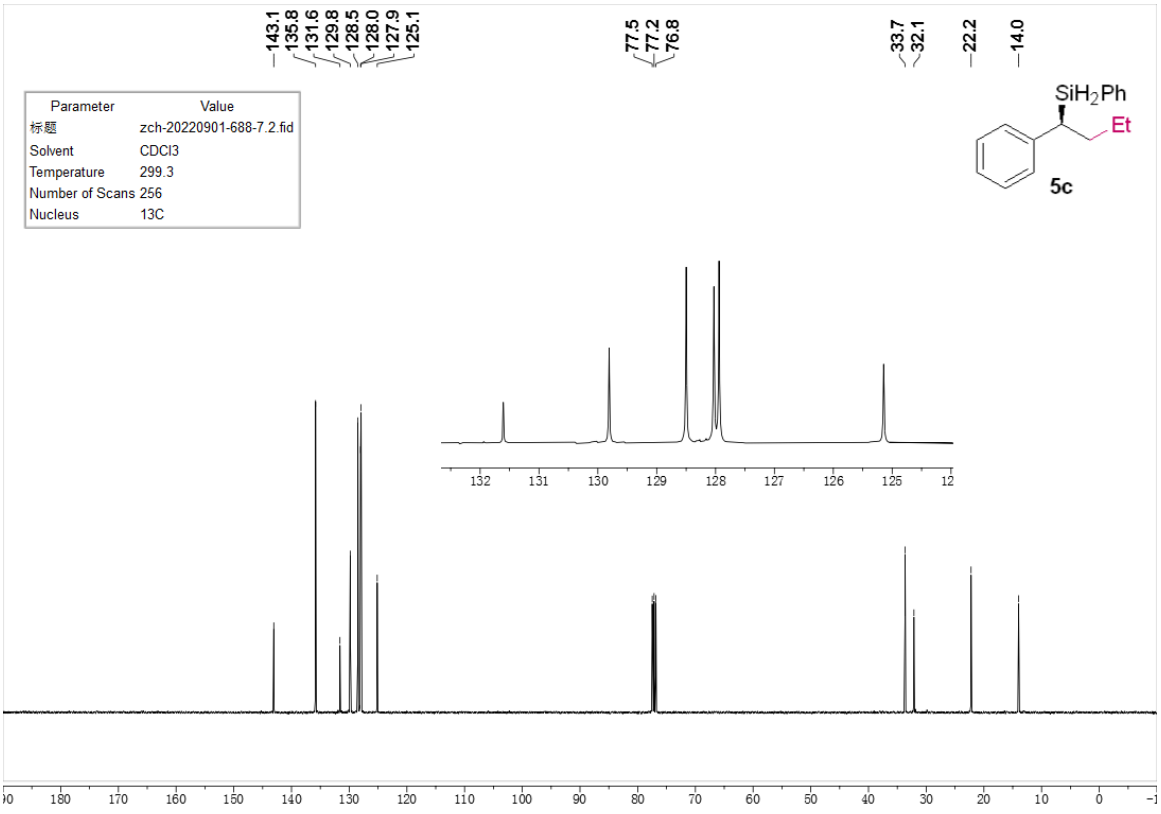
Et
5c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Number of Scans 256
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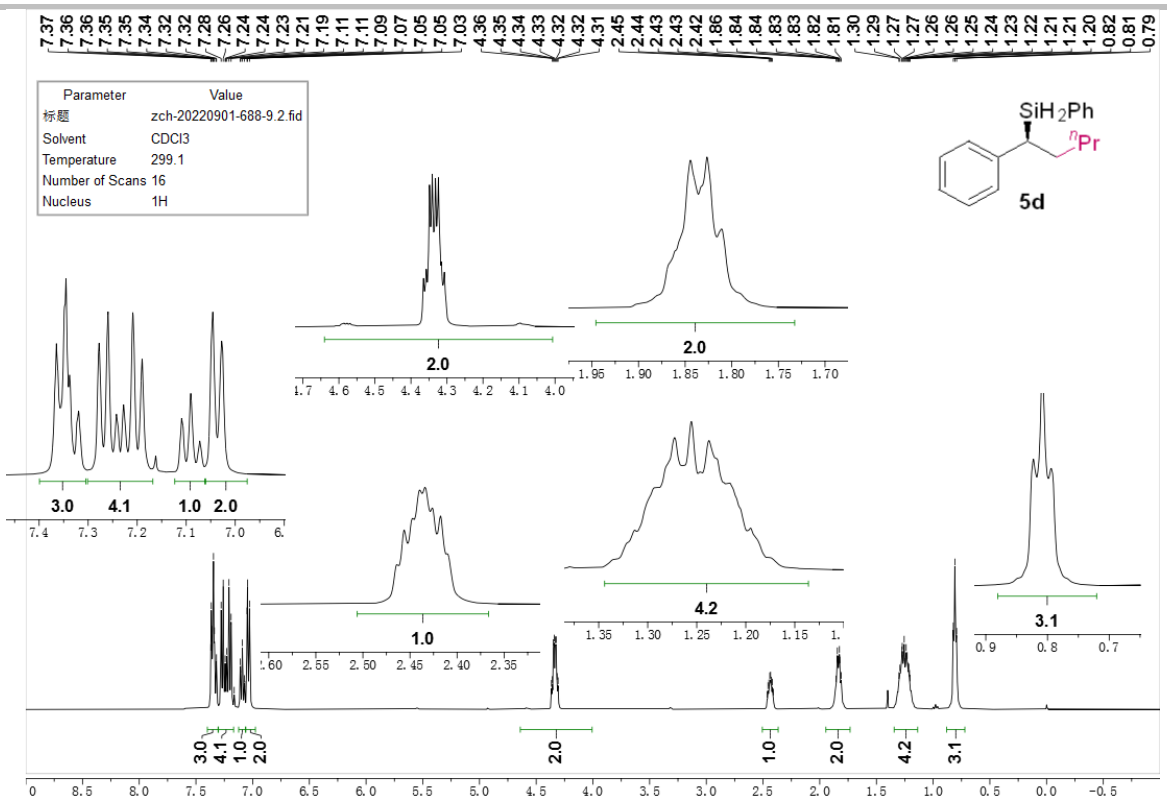
Et
5c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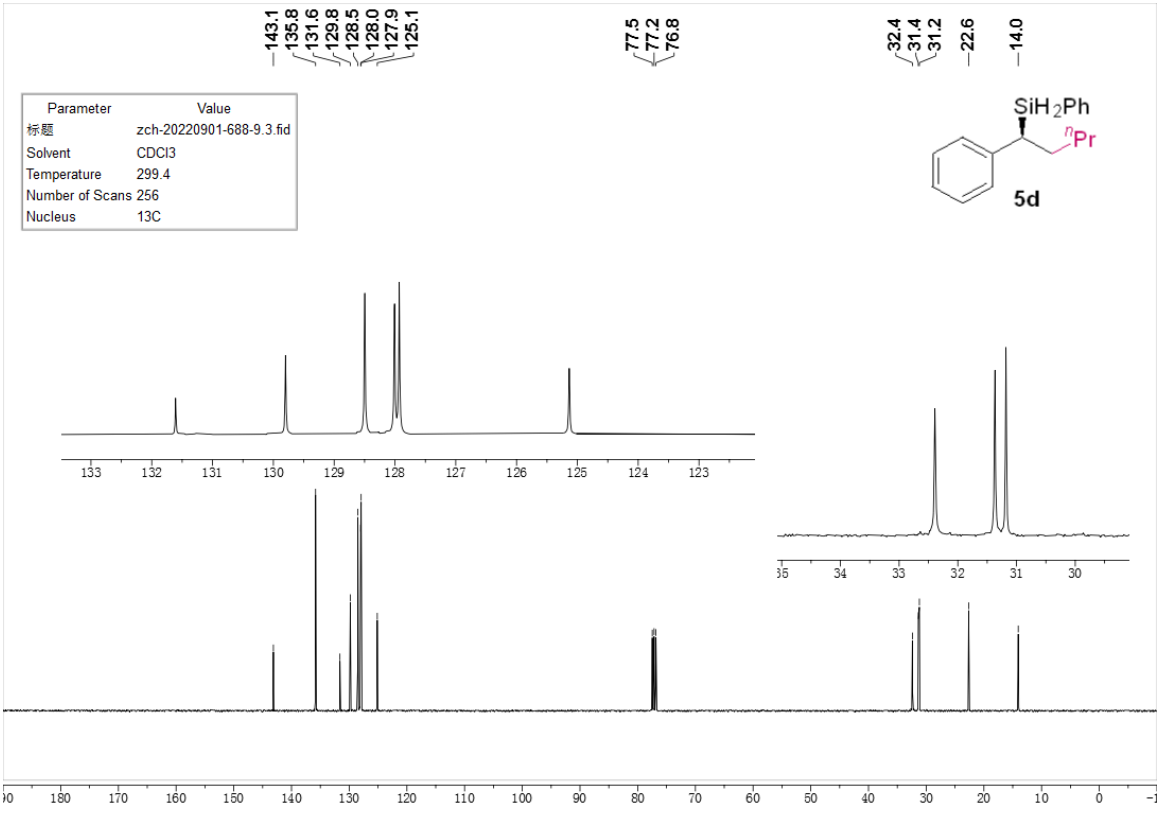
Number of Scans 16
Nucleus 1H
SiH2Ph
nPr
5d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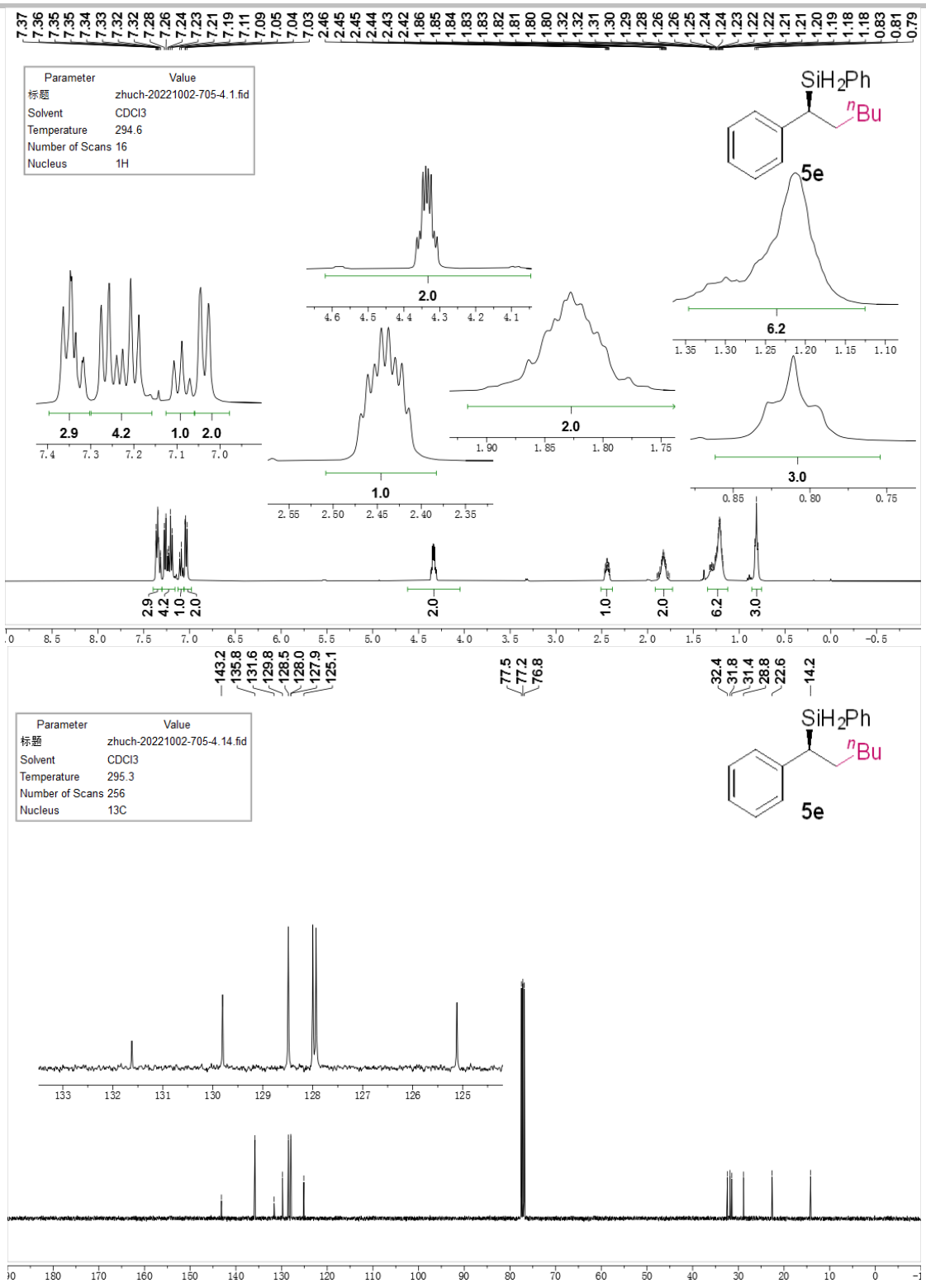
Number of Scans 256
Nucleus 13C
SiH2Ph
nPr
5d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Temperature 294.6
Number of Scans 16
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SiH2Ph
nBu
5e
Parameter Value
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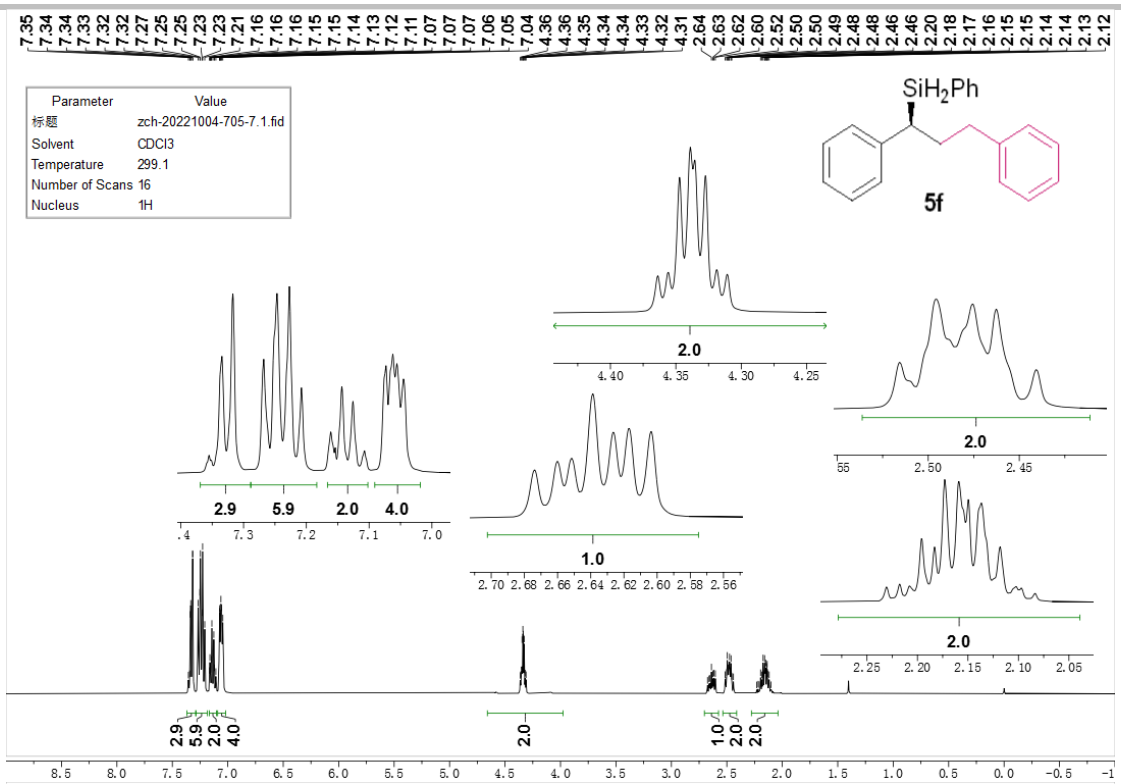
Temperature 295.3
Number of Scans 256
Nucleus 13C
SiH2Ph
nBu
5e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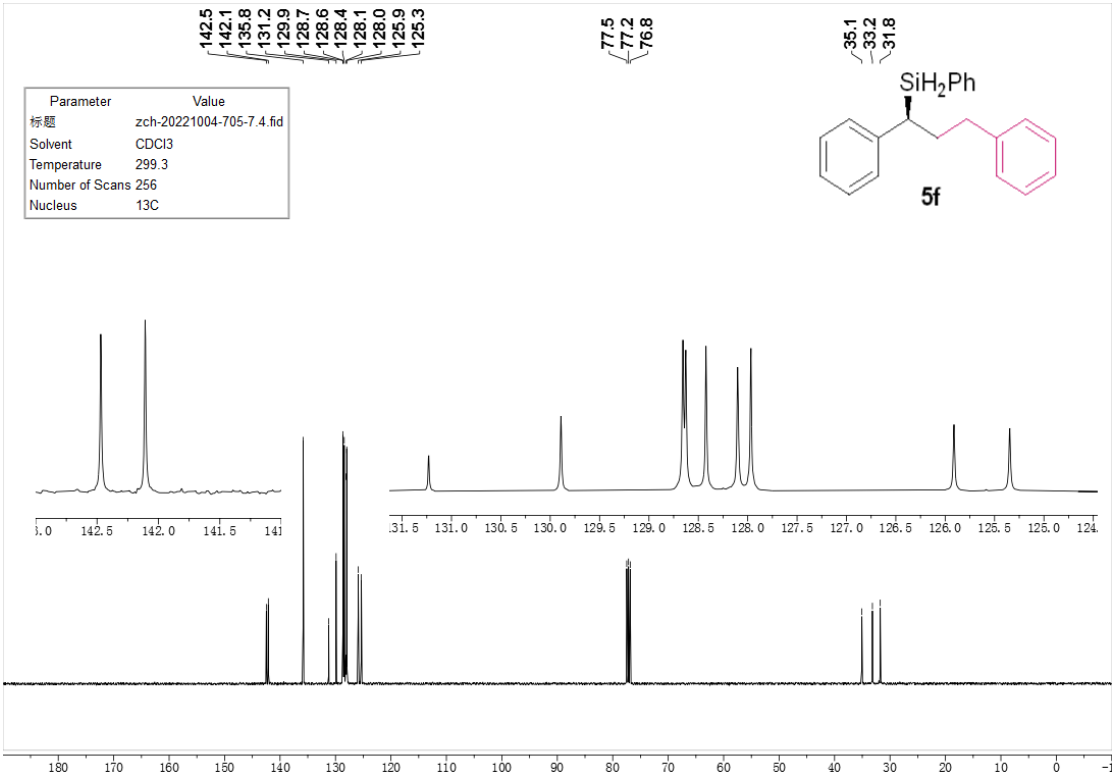
Number of Scans 16
Nucleus 1H
SiH2Ph
5f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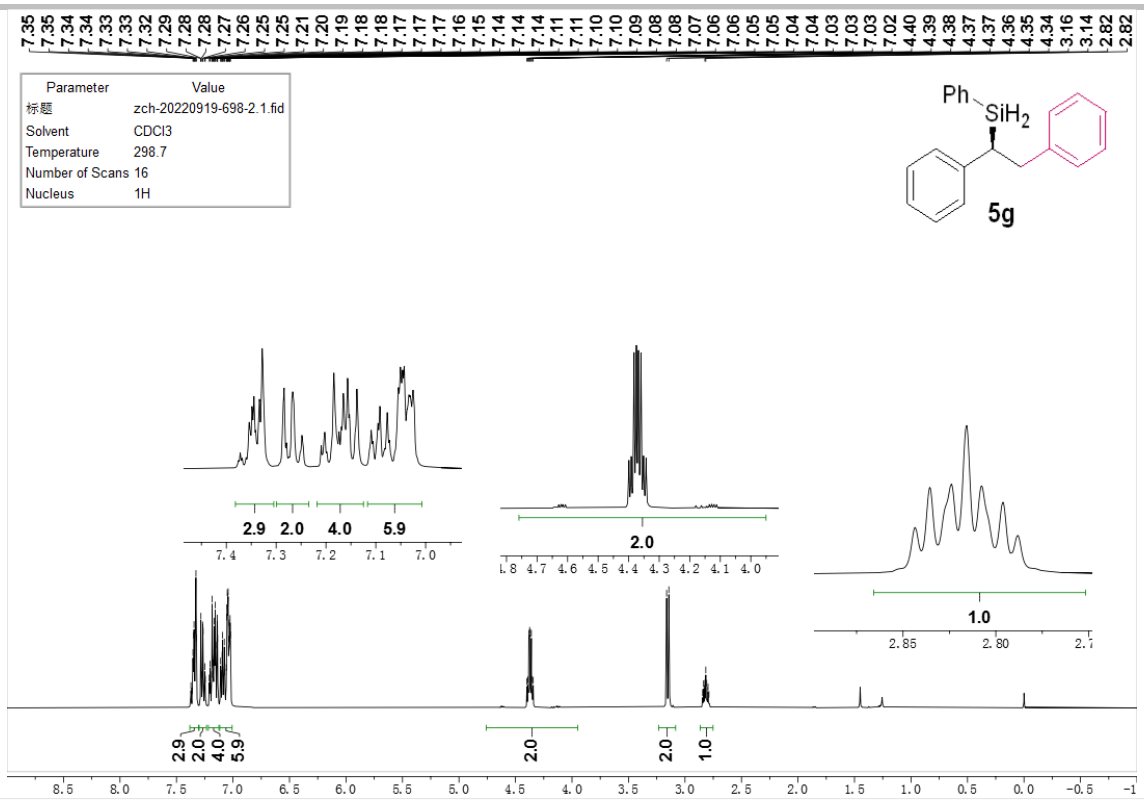
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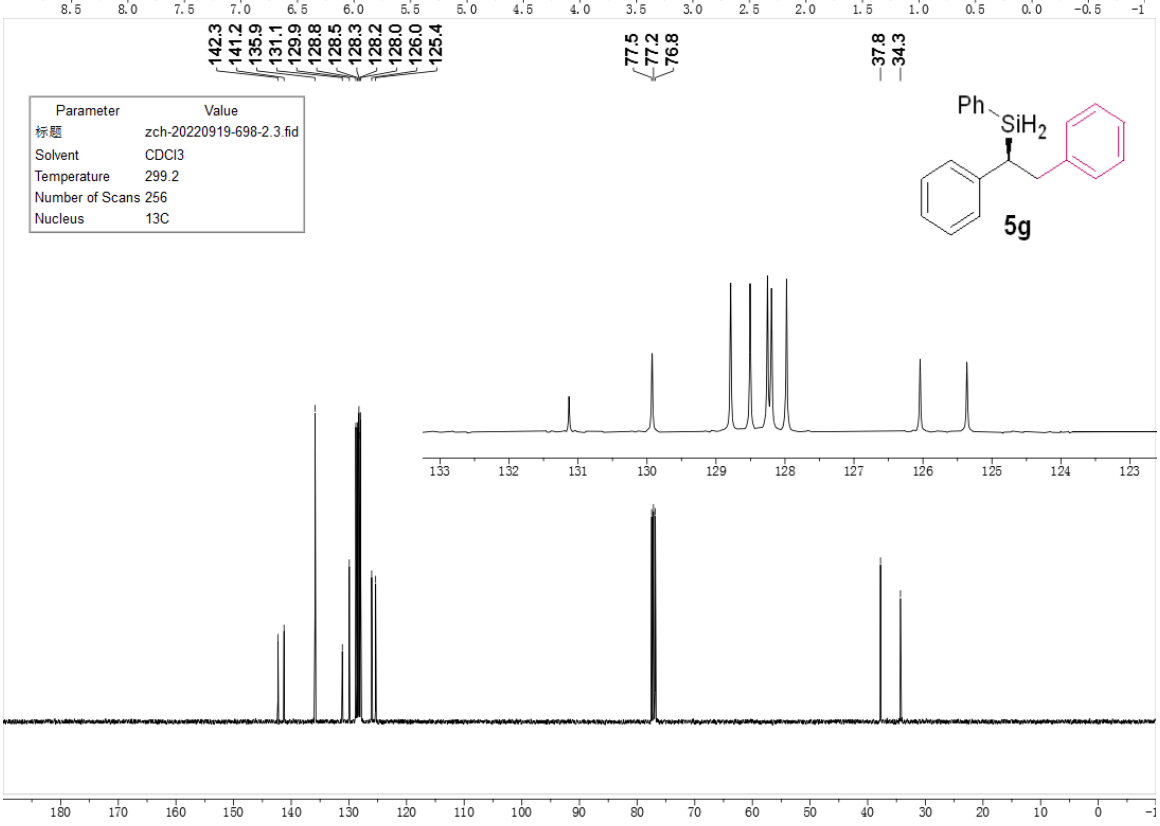
Solvent CDCl3
Temperature 298.7
Number of Scans 16
Nucleus 1H
Ph SiH2
5g


Parameter Value
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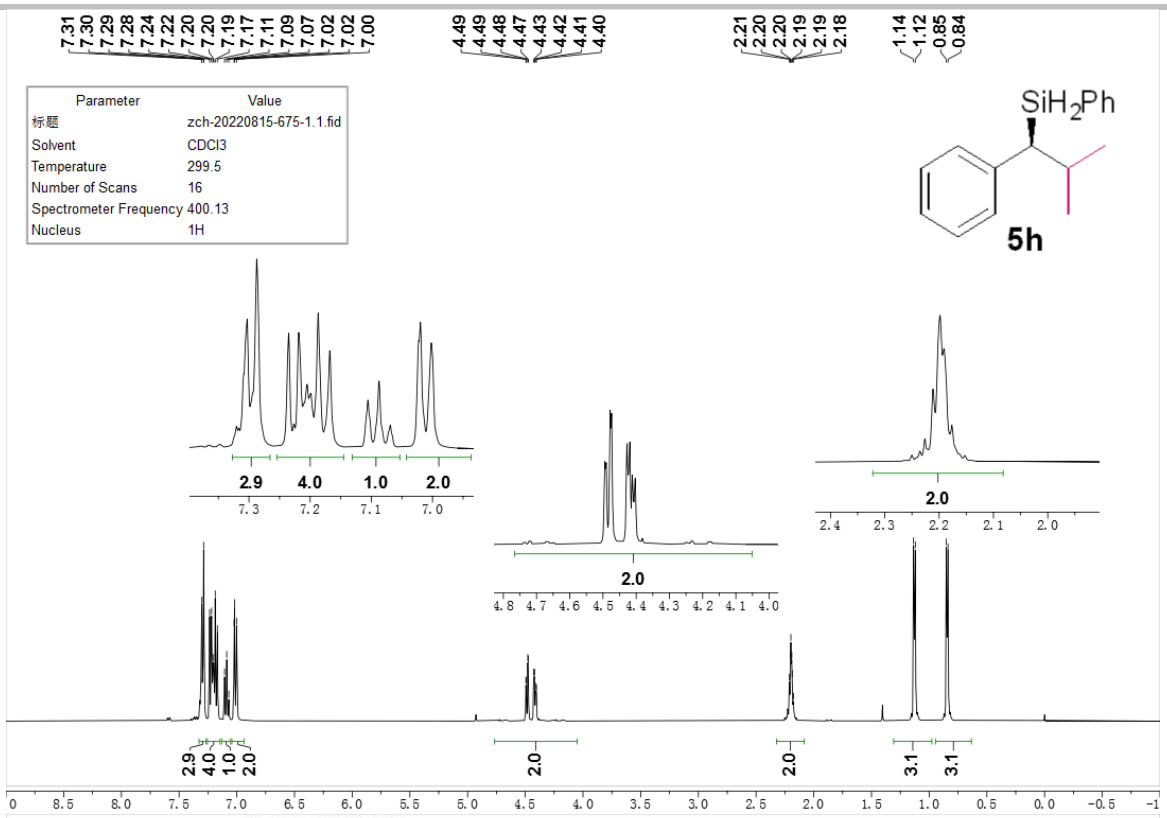
Solvent CDCl3
Temperature 299.2
Number of Scans 256
Nucleus 13C
Ph SiH2
5g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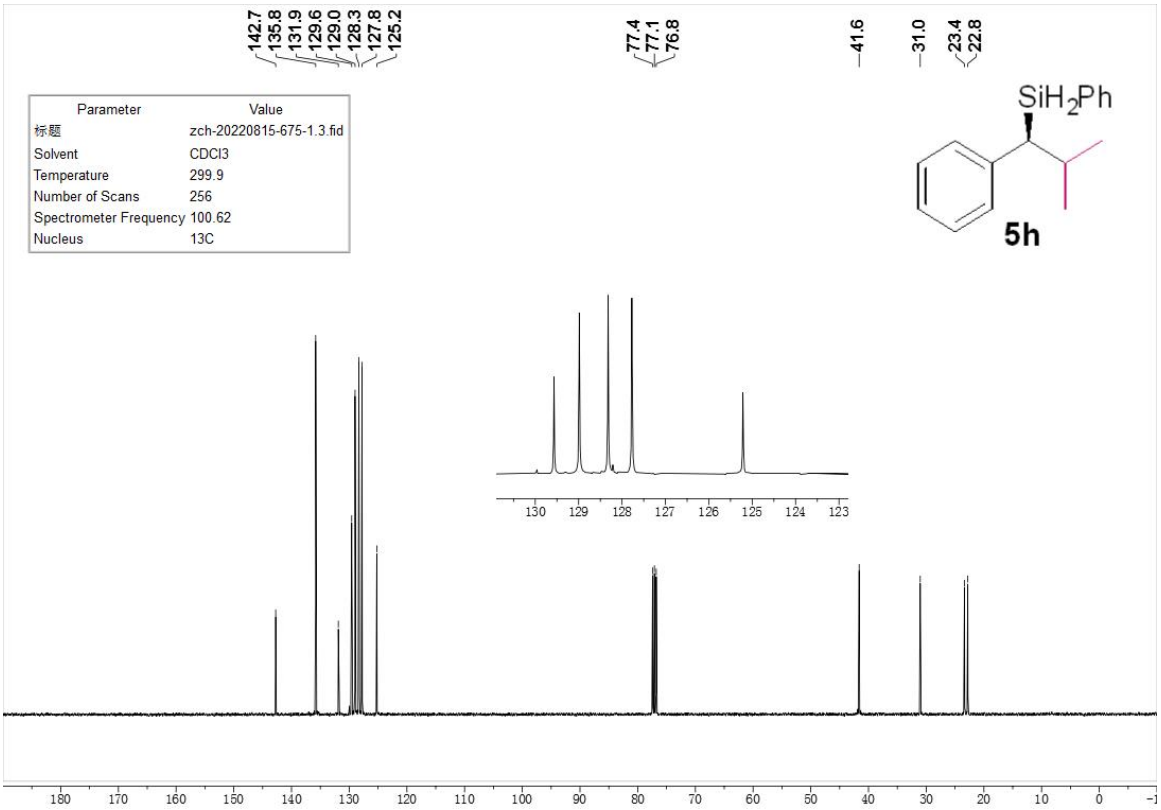
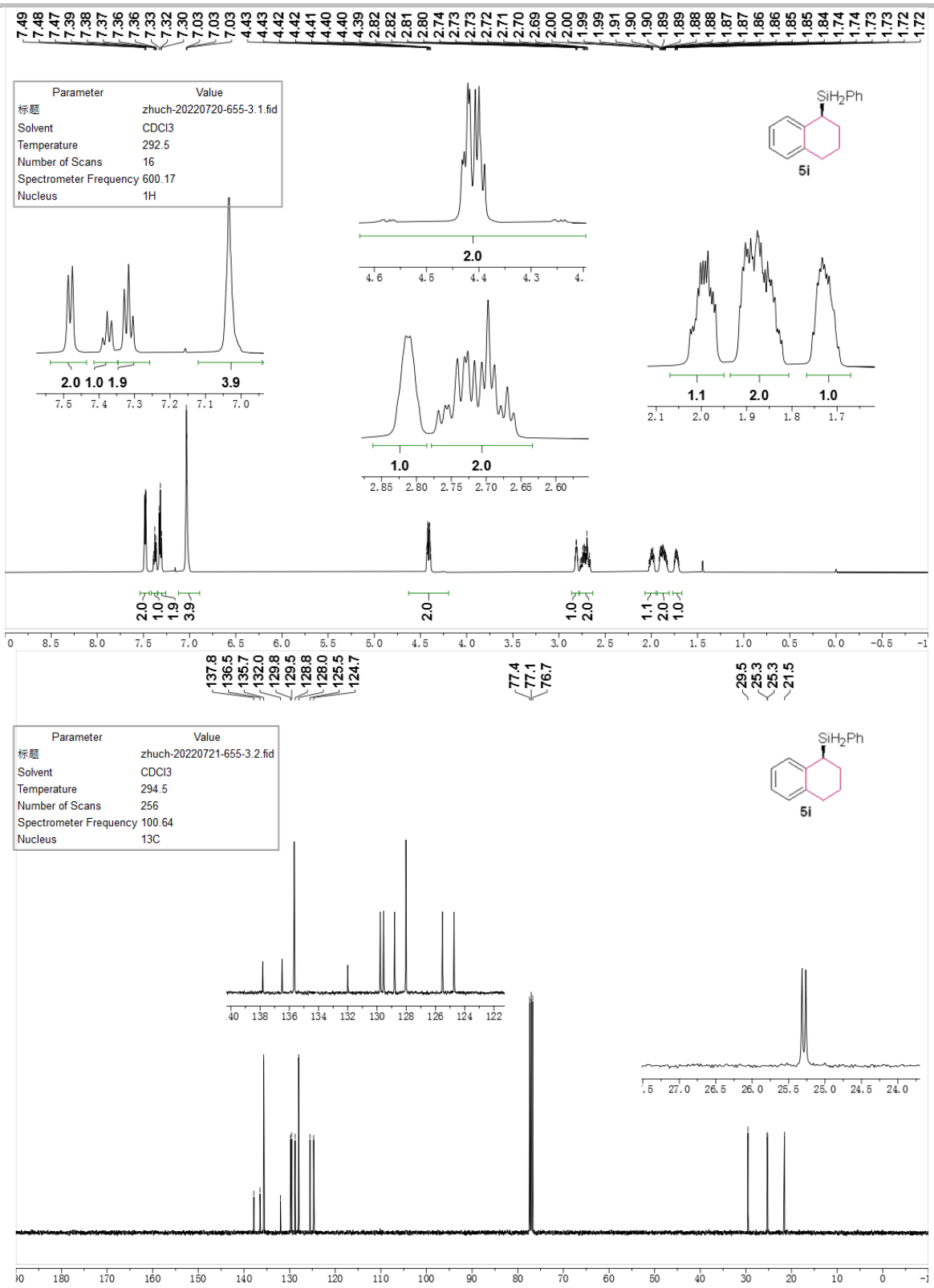
4.49 4.49 4.48 4.47 4.43 4.42 4.41 4.40
2.21 2.20 2.20 2.19 2.19 2.18
1.14 1.12 0.85 0.84
Parameter Value
标题 zch-20220815-675-1.1.fid
Solvent CDCl3
Temperature 299.5
Number of Scans 16
Spectrometer Frequency 400.13
Nucleus 1H
SiH2Ph
5h
2.9 4.0 1.0 2.0
2.0
2.0
2.0 4.0 1.0 2.0 2.0 3.1 3.1


142.7 135.8 131.9 129.6 129.0 128.3 127.8 125.2
77.4 77.1 76.8
41.6
31.0
23.4 22.8
Parameter Value
标题 zch-20220815-675-1.3.fid
Solvent CDCl3
Temperature 299.9
Number of Scans 256
Spectrometer Frequency 100.62
Nucleus 13C
SiH2Ph
5h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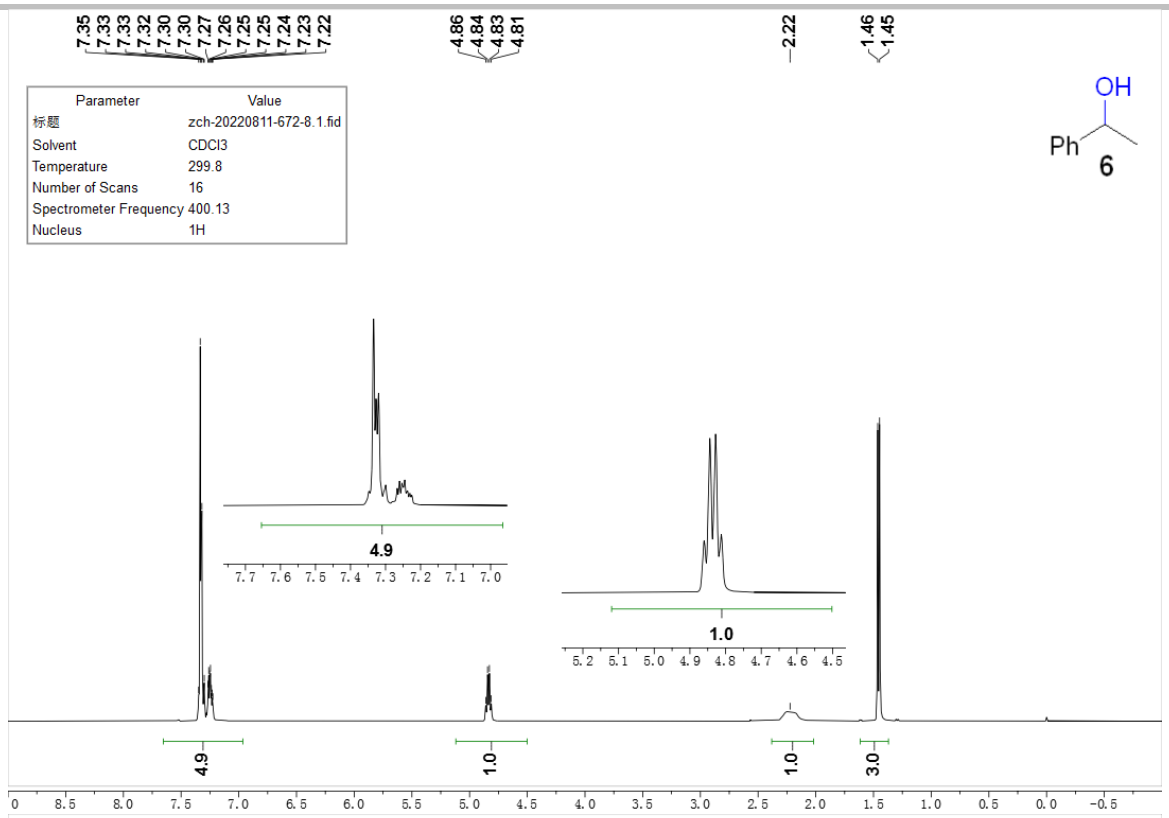
Parameter Value
标题 zhuch-20220720-655-3.1.fid
Solvent CDCl3
Temperature 292.5
Number of Scans 16
Spectrometer Frequency 600.17
Nucleus 1H
SiH2Ph
5i
2.0 1.0 1.9 3.9
2.0
1.0 2.0
1.1 2.0 1.0
2.0 1.0 1.9 3.9 2.0 1.0 2.0 1.1 2.0 1.0
137.8 136.5 135.7 132.0 129.8 129.5 128.8 128.0 125.5 124.7
77.4 77.1 76.7
29.5 25.3 25.3 21.5
Parameter Value
标题 zhuch-20220721-655-3.2.fid
Solvent CDCl3
Temperature 294.5
Number of Scans 256
Spectrometer Frequency 100.64
Nucleus 13C
SiH2Ph
5i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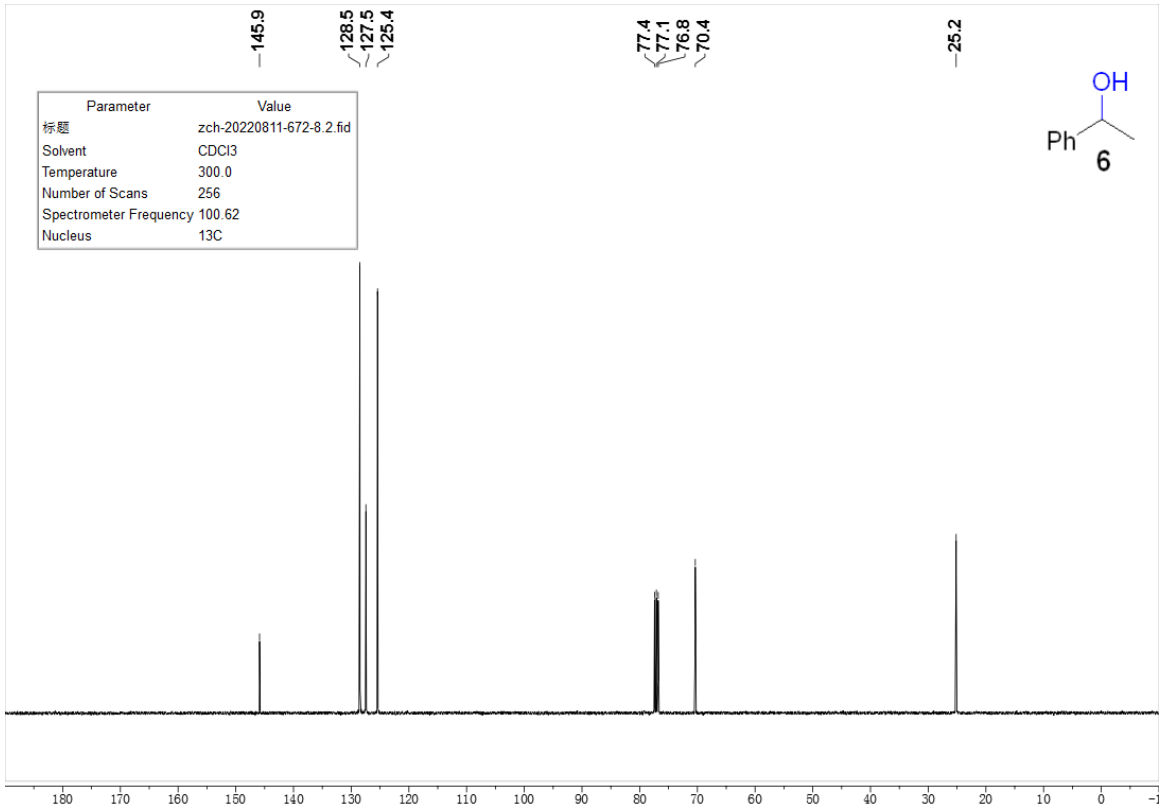
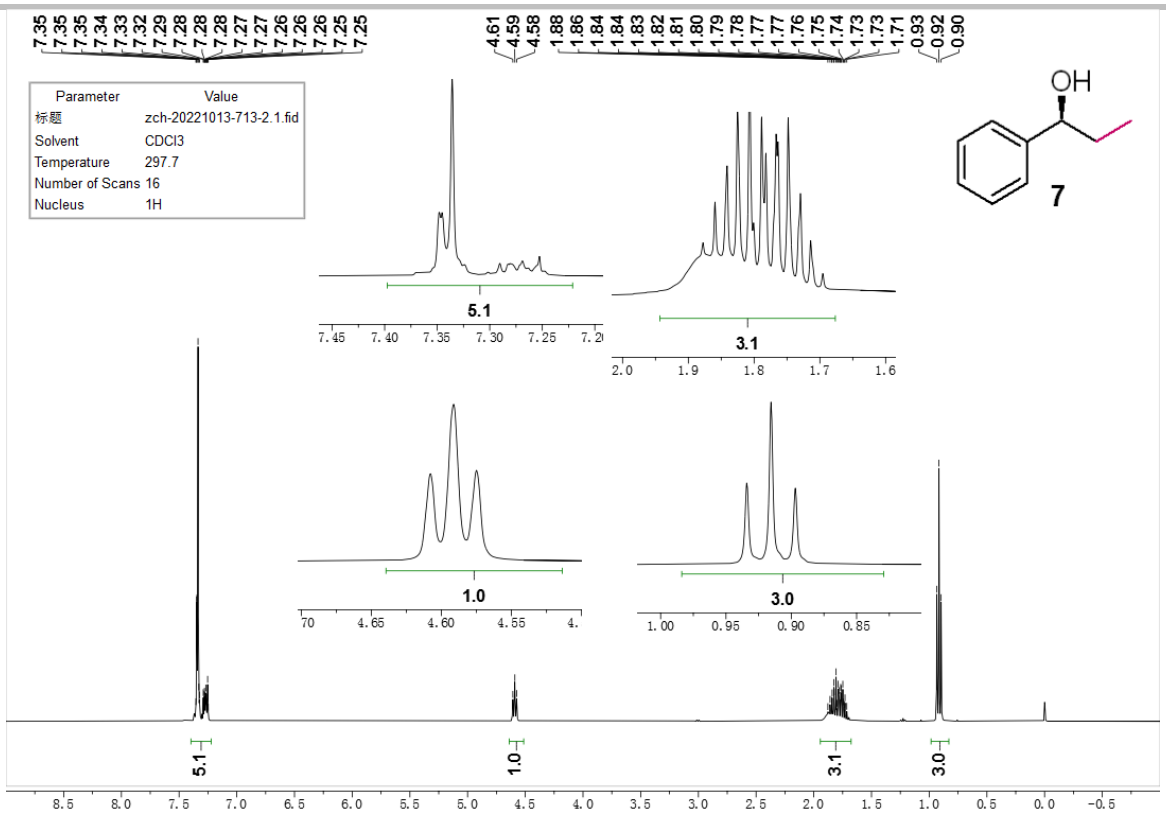
7.33
7.33
7.32
7.30
7.30
7.27
7.26
7.25
7.25
7.24
7.23
7.22
4.86
4.84
4.83
4.81
2.22
1.46
1.45
Parameter Value
标题 zch-20220811-672-8.1.fid
Solvent CDCl3
Temperature 299.8
Number of Scans 16
Spectrometer Frequency 400.13
Nucleus 1H
OH
Ph
6
4.9
1.0
4.9
1.0
1.0
3.0


145.9
128.5
127.5
125.4
77.4
77.1
76.8
70.4
25.2
Parameter Value
标题 zch-20220811-672-8.2.fid
Solvent CDCl3
Temperature 300.0
Number of Scans 256
Spectrometer Frequency 100.62
Nucleus 13C
OH
Ph
6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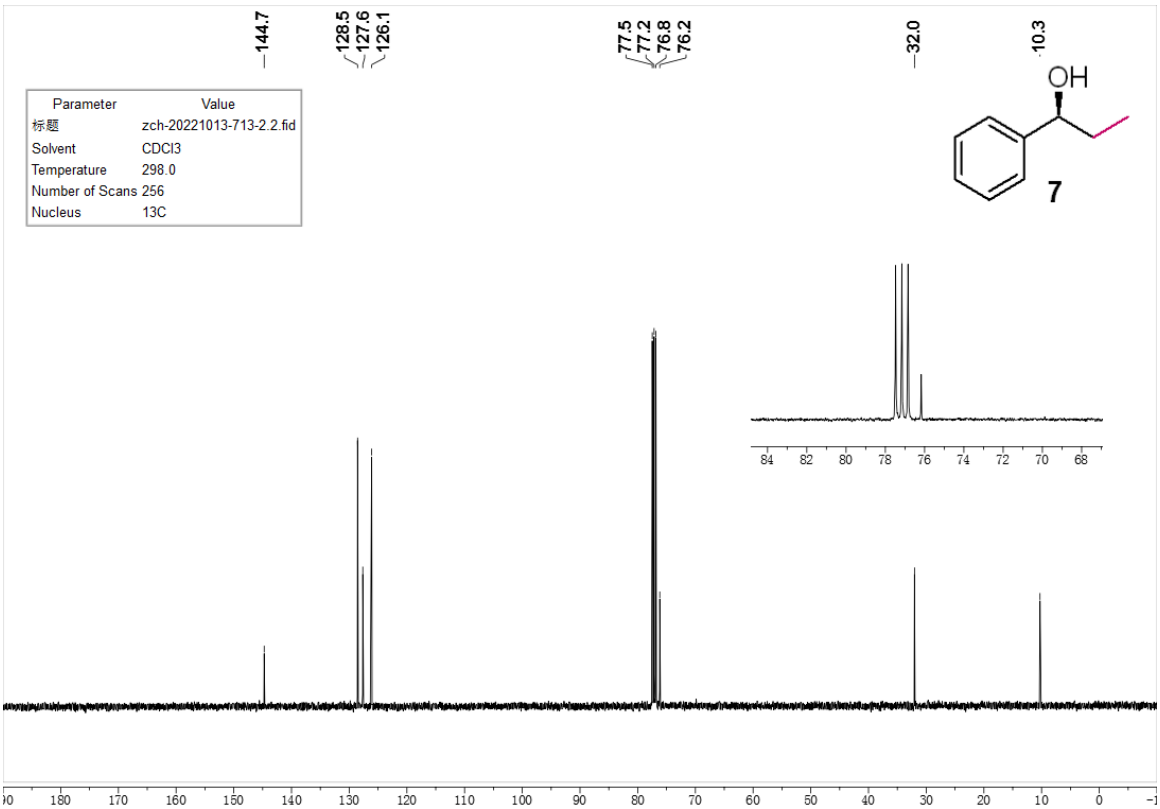
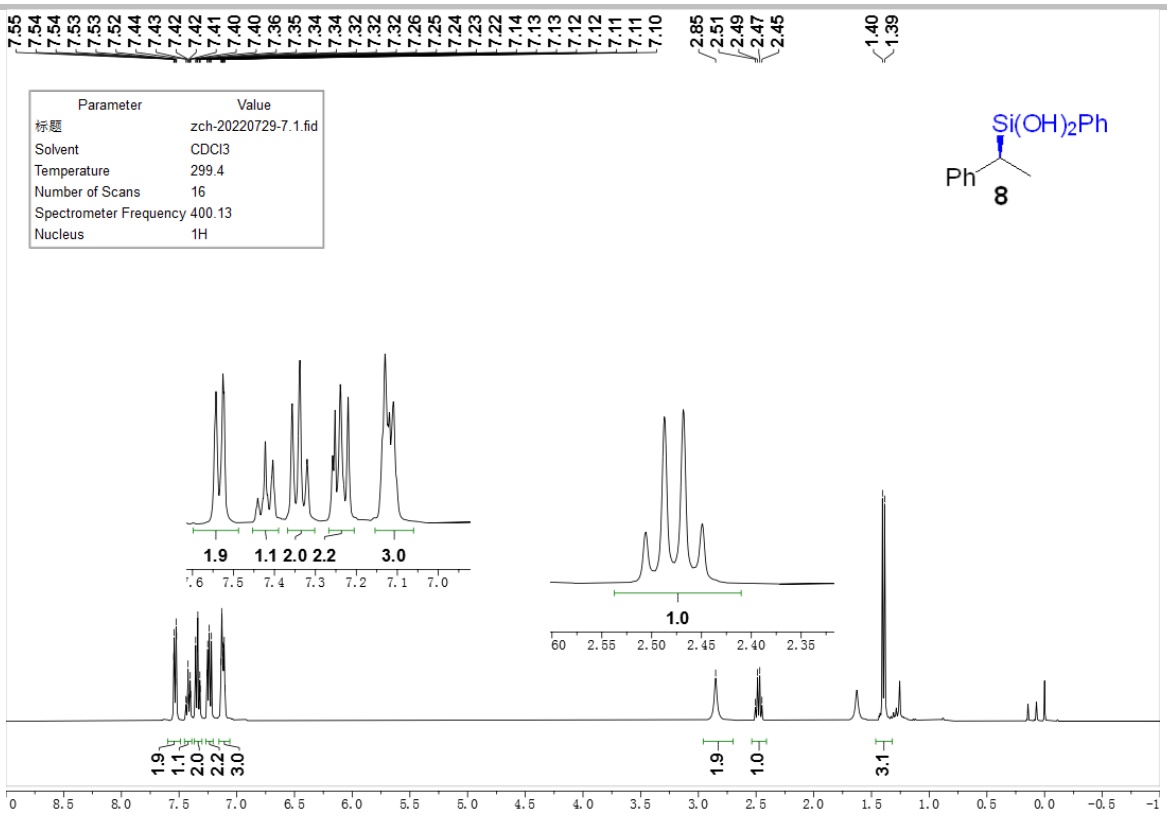
4.61 4.59 4.58 1.88 1.86 1.84 1.84 1.83 1.82 1.81 1.80 1.79 1.78 1.77 1.77 1.76 1.75 1.74 1.73 1.73 1.71 0.93 0.92 0.90
Parameter Value
标题 zch-20221013-713-2.1.fid
Solvent CDCl3
Temperature 297.7
Number of Scans 16
Nucleus 1H
OH
7
5.1
3.1
1.0
3.0
5.1 1.0 3.1 3.0


144.7
128.5 127.6 126.1
77.5 77.2 76.8 76.2
32.0
10.3
Parameter Value
标题 zch-20221013-713-2.2.fid
Solvent CDCl3
Temperature 298.0
Number of Scans 256
Nucleus 13C
OH
7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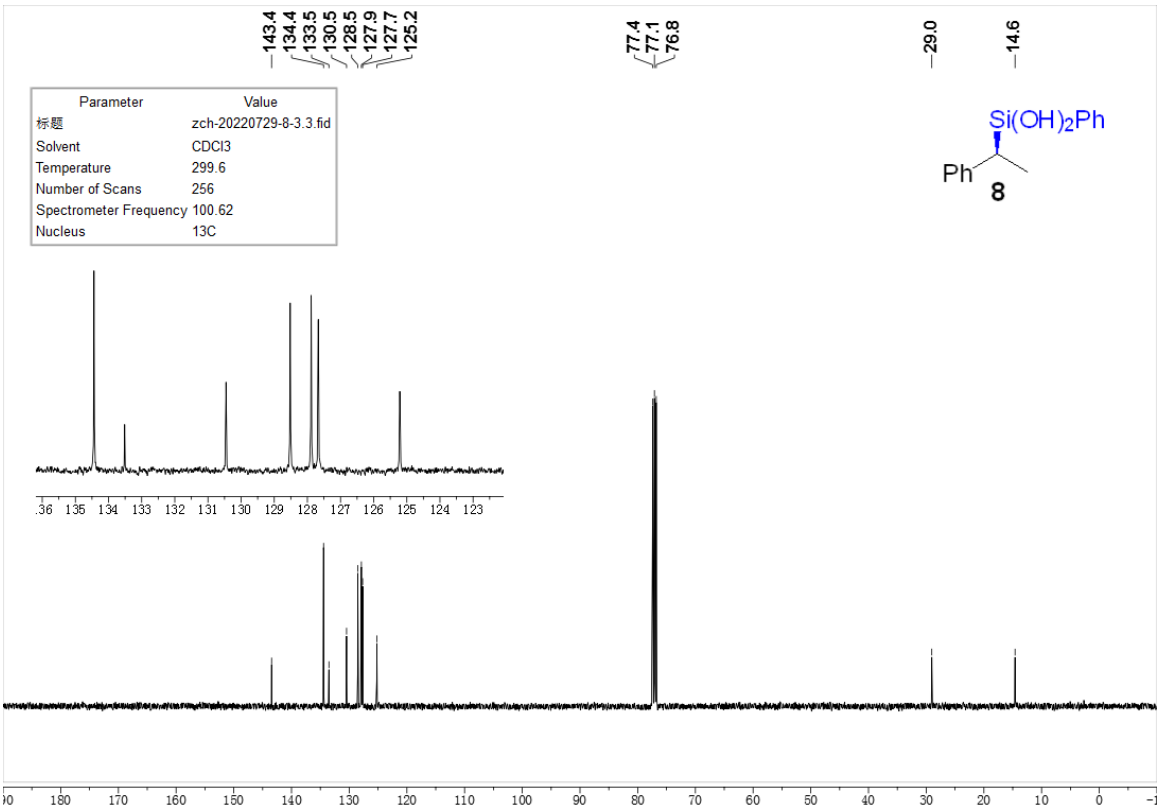
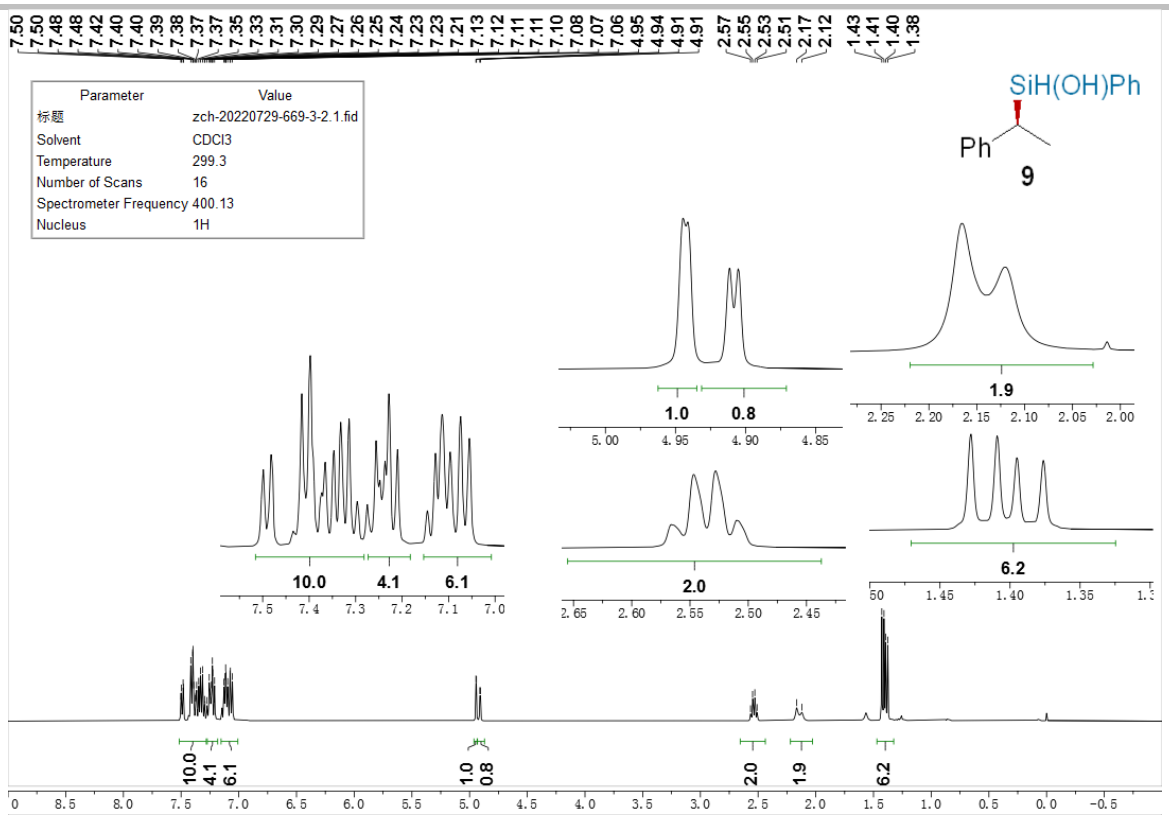
2.85 2.51 2.49 2.47 2.45
1.40 1.39
Parameter Value
标题 zch-20220729-7.1.fid
Solvent CDCl3
Temperature 299.4
Number of Scans 16
Spectrometer Frequency 400.13
Nucleus 1H
Si(OH)2Ph
Ph
8
1.9 1.1 2.0 2.2 3.0
1.0
1.9 1.1 2.0 2.2 3.0
1.9 1.0 3.1


143.4 134.4 133.5 130.5 128.5 127.9 127.7 125.2
77.4 77.1 76.8
29.0
14.6
Parameter Value
标题 zch-20220729-8-3.3.fid
Solvent CDCl3
Temperature 299.6
Number of Scans 256
Spectrometer Frequency 100.62
Nucleus 13C
Si(OH)2Ph
Ph
8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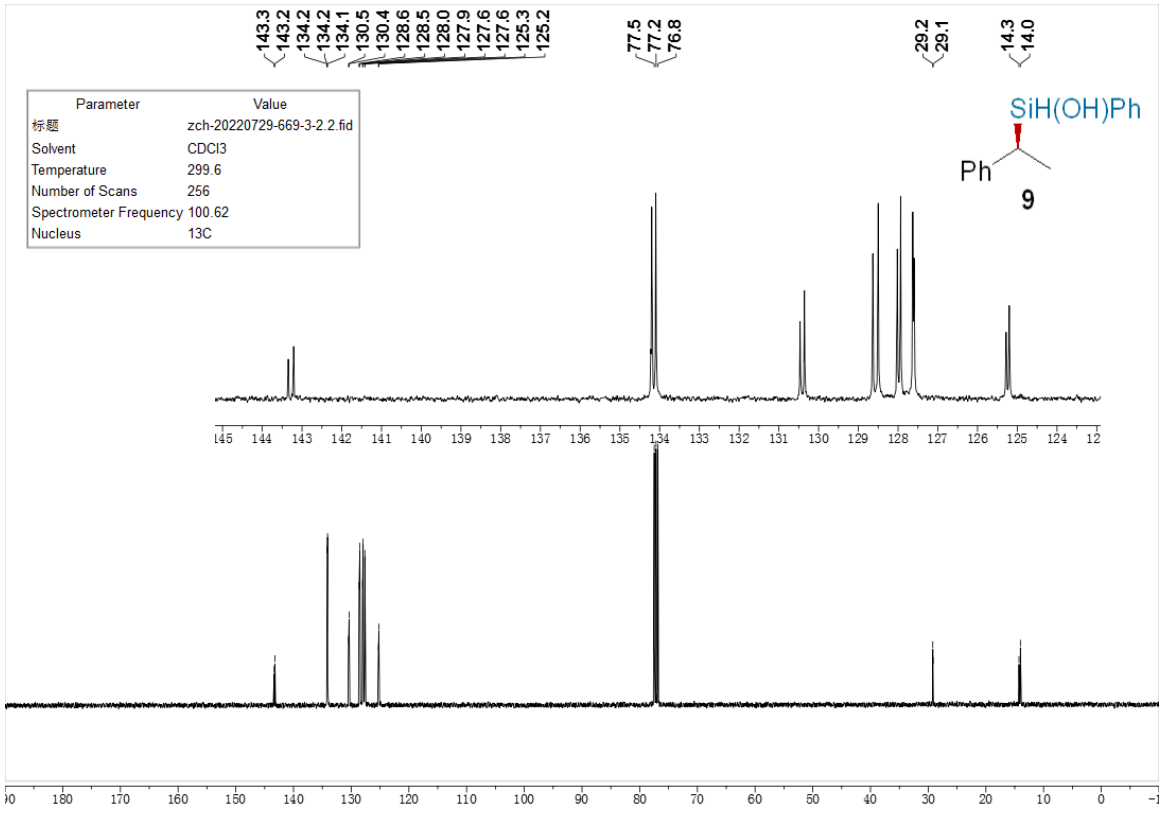
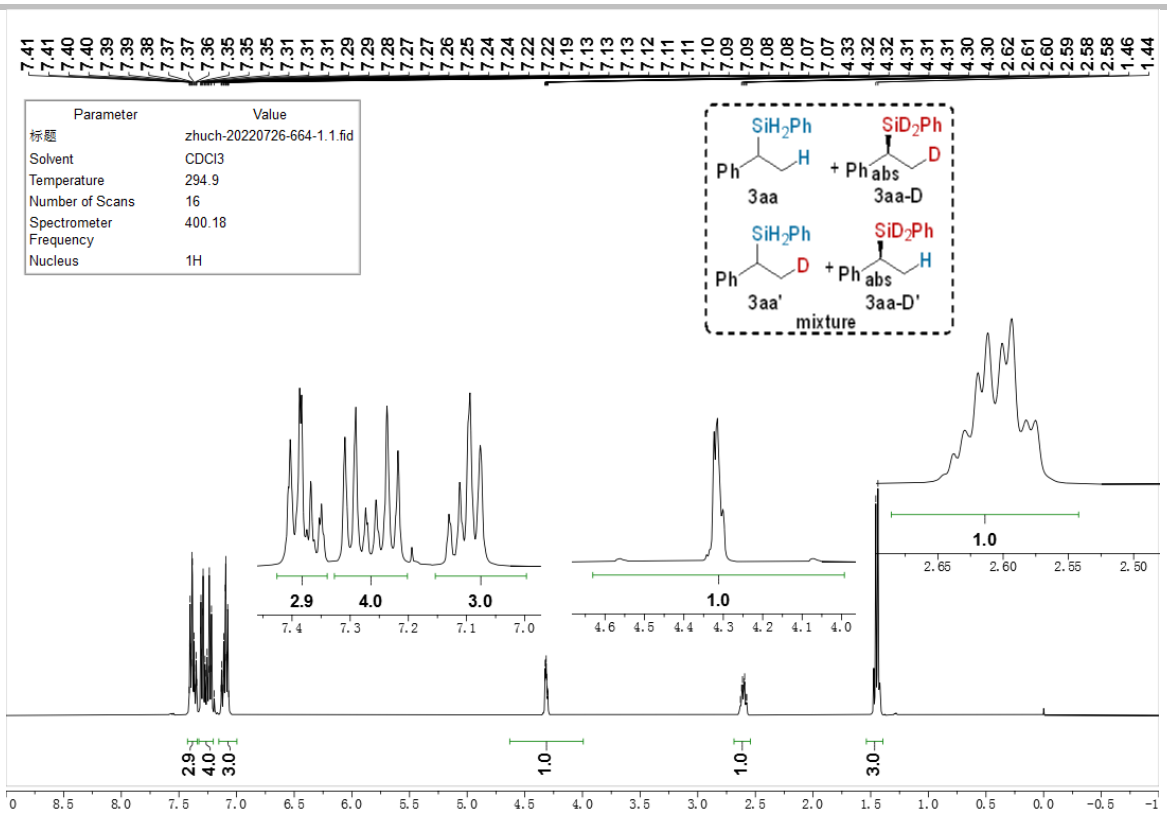
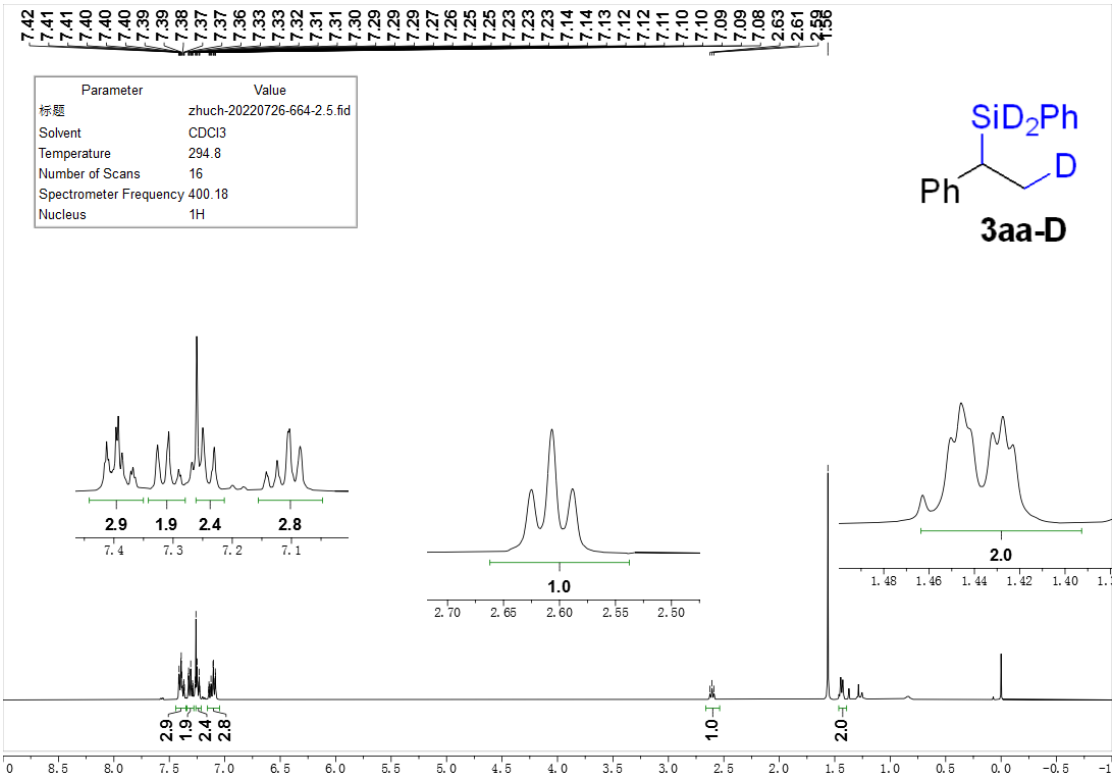
Parameter Value
标题 zch-20220729-669-3-2.1.fid
Solvent CDCl3
Temperature 299.3
Number of Scans 16
Spectrometer Frequency 400.13
Nucleus 1H
SiH(OH)Ph
Ph
9
10.0 4.1 6.1 1.0 0.8 2.0 1.9 6.2


143.3 143.2 134.2 134.2 134.1 130.5 130.4 128.6 128.5 128.0 127.9 127.6 127.6 125.3 125.2 77.5 77.2 76.8 29.2 29.1 14.3 14.0
Parameter Value
标题 zch-20220729-669-3-2.2.fid
Solvent CDCl3
Temperature 299.6
Number of Scans 256
Spectrometer Frequency 100.62
Nucleus 13C
SiH(OH)Ph
Ph
9


Parameter Value
标题 zhuch-20220726-664-1.1.fid
Solvent CDCl3
Temperature 294.9
Number of Scans 16
Spectrometer Frequency 400.18
Nucleus 1H
SiH2Ph
Ph
H
3aa
+ Ph abs
SiD2Ph
D
3aa-D
SiH2Ph
Ph
D
3aa'
+ Ph abs
SiD2Ph
H
3aa-D'
mixture
2.9
4.0
3.0
1.0
1.0
1.0
2.9
4.0
3.0
1.0
1.0


Parameter Value
标题 zhuch-20220726-664-2.5.fid
Solvent CDCl3
Temperature 294.8
Number of Scans 16
Spectrometer Frequency 400.18
Nucleus 1H
SiD2Ph
Ph
D
3aa-D
2.9
1.9
2.4
2.8
1.0
2.0
2.9
1.9
2.4
2.8
1.0
2.0