Supplementary material

S1 Origin and purity of used chemicals

Table S1: Used chemicals under specification of the manufacturer, purity, and type of purification

Chemical	Source	Purity	Distillation (inert gas, ambient pressure)
Iso-propylamine (**A1**)	abcr GmbH	99%	from CaH_2
N-propyamine (**A3**)	Sigma-Aldrich	≥99%	from CaH_2
Pyrrolidine (**A4**)	Sigma-Aldrich	99%	from Na
Aniline (**A5**)	Acros Organics	98%	from $SnCl_2$, then KOH, then CaH_2
Diethylamine (**A6**)	Sigma-Aldrich	≥99.5%	from CaH_2
$CDCl_3$	Deutero GmbH	99%	from CaH_2
$Cr(acac)_3$	abcr GmbH	98%	none
Trimethyl(*tert*-butylamino)silane (**M2**)	Sigma-Aldrich	98%	without additive
Trimethyl(diethylamino)silane (**M6**)	abcr GmbH	97%	without additive
Bis(diethylamino)dimethylsilane (**D66**)	abcr GmbH	97%	without additive
Triethylamine	AplliChem GmbH	99%	from CaH_2
Dichlorodimethylsilane	abcr GmbH	98%	without additive
Diethylether	VWR GmbH	99%	no distillation, use of MBRAUN SPS 800 solvent purification unit
DBU (1,8-Diazabicyclo[5.4.0]undec-7-ene)	Sigma-Aldrich	98%	no purification
Acetone-d6	Deutero GmbH	99%	from B_2O_3
Benzene-d6	Deutero GmbH	99%	from CaH_2
Hexamethyldisiloxan (HMDSO)	abcr GmbH	for synth.	no purification

S2 Data of the prepared samples for ^{29}Si NMR spectroscopy

Table S2: Quantities of substances used, and number of NMR spectra recorded

Amine	n(M2) (mmol)	n(amine) (mmol)	n($CDCl_3$) (mmol)	Number of spectra
A1	1.7	1.64	3.32	21
A3	1.75	1.77	3.16	34
A4	1.84	2.19	3.03	31
A5	1.65	2.2	3.55	52
A6	1.7	2.13	3.66	33

Table S3: Used reaction parameters for the investigation of temperature dependency

n(M2) (mmol)	n(A1) (mmol)	n($CDCl_3$) (mmol)	Temperature (°C)
1.996	2.54	3.73	5
1.707	1.68	3.92	15
1.700	1.64	3.32	25

Table S4: Used reaction parameters for the investigation of the activation volumina

n(M2) (mmol)	n(A1) (mmol)	n($CDCl_3$) (mmol)	Pressure (hPa)
1.989	1.57	3.76	115.8
1.665	1.98	3.20	115.3
2.009	1.64	3.95	79.4
1.927	1.88	3.38	78.5
1.941	2.40	3.30	64.6
1.920	1.83	3.90	64.3

Table S5: Used amount of substances for the reaction with **D11**

Amine	n(D11) (mmol)	n(amine) (mmol)	n($CDCl_3$) (mmol)
A1	1.32	1.49	4.15
A3	1.33	1.39	3.58
A4	1.20	1.52	3.53
A5	1.45	1.45	4.04
A6	1.42	1.31	4.41

Table S6: Used amount of substances for the reaction with **D33**

Amine	n(D33) (mmol)	n(amine) (mmol)	n($CDCl_3$) (mmol)
A1	1.26	1.27	3.74
A2	1.39	1.39	3.78
A4	1.22	1.92	3.61
A5	1.44	1.56	3.92
A6	1.32	1.40	3.70

Table S7: Used amount of substances for the reaction with **D44**

Amine	n(D44) (mmol)	n(amine) (mmol)	n($CDCl_3$) (mmol)
A1	1.27	1.56	3.59
A2	1.28	1.13	3.52
A3	1.26	1.54	3.72
A5	1.39	1.55	3.66
A6	1.30	1.29	4.15

Table S8: Used amount of substances for the reaction with **D55**

Amine	n(D55) (mmol)	n(amine) (mmol)	n($CDCl_3$) (mmol)
A1	1.06	0.88	4.59
A2	1.15	1.15	3.96
A3	0.99	0.86	4.15
A4	1.22	1.25	4.59
A6	1.23	1.31	4.23

Table S9: Used amount of substances for the reaction with **D66**

Amine	n(D66) (mmol)	n(amine) (mmol)	n($CDCl_3$) (mmol)
A1	1.34	1.45	4.81
A2	1.30	1.31	3.79
A3	1.24	1.25	3.63
A4	1.33	1.93	3.59
A5	1.33	1.26	3.75

S3 ^{29}Si NMR spectra all aminosilanes and experiments to exclude influence of measurement parameters

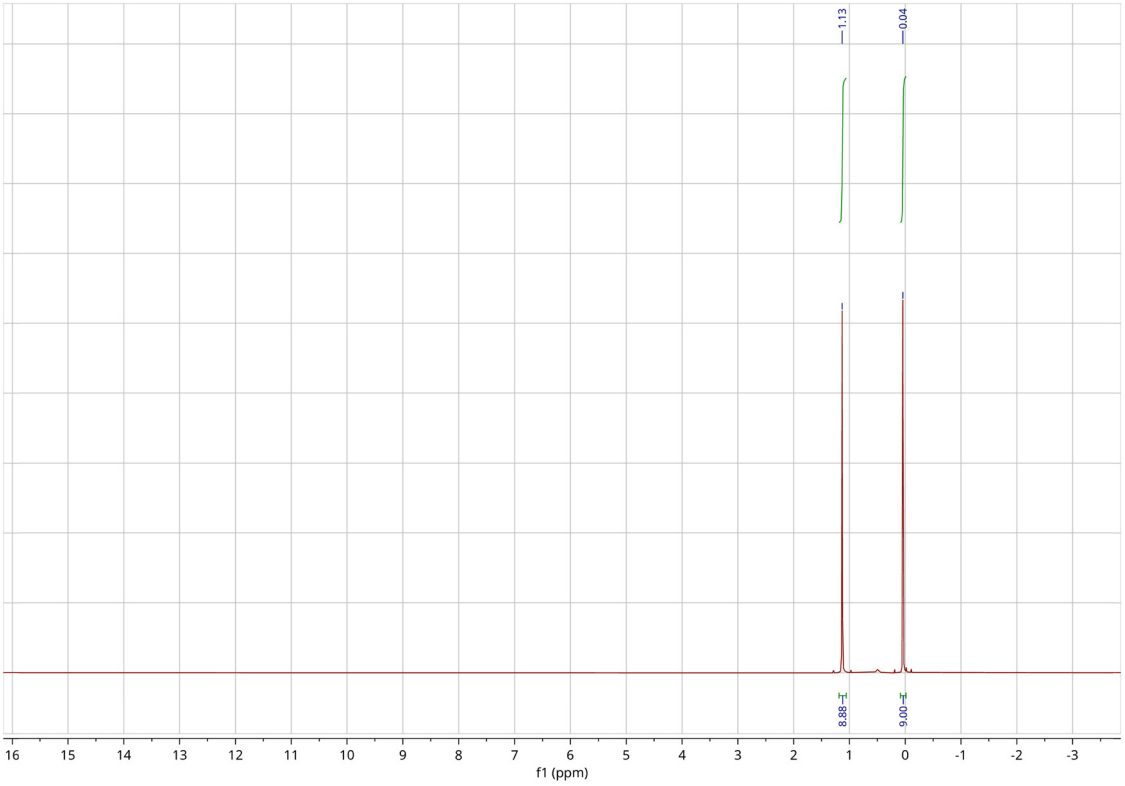

Figure S1: ^{1}H NMR spectrum of **M2**.

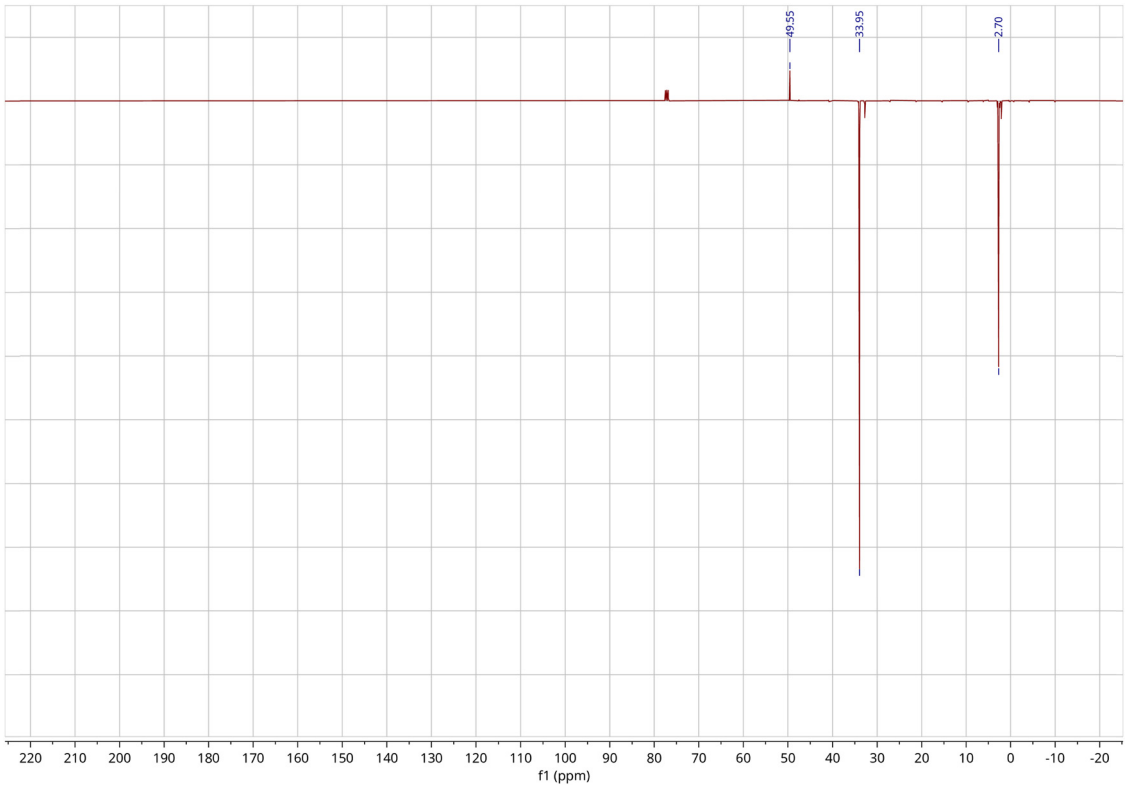

Figure S2: ^{13}C NMR APT spectrum of **M2**.

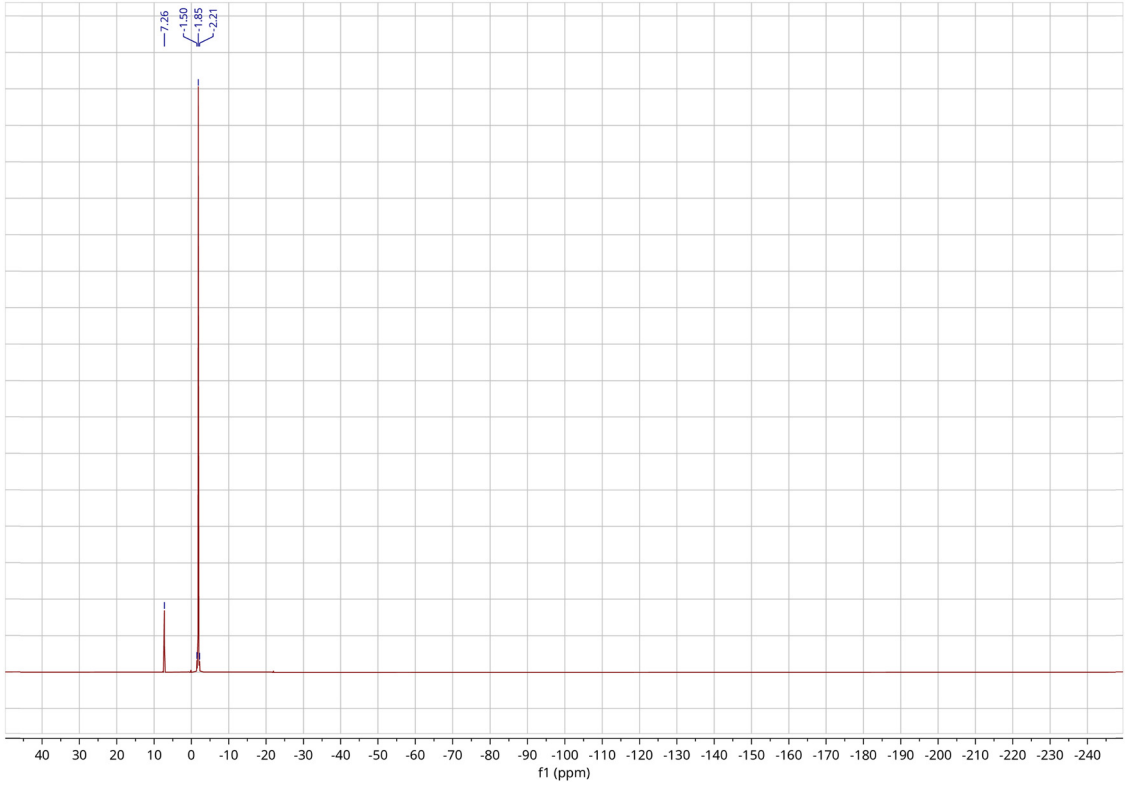

Figure S3: ^{29}Si INEPT NMR spectrum of **M2**. The Signal at 7.26 ppm is caused by hexamethyldisiloxane ($(Me_3Si)_2O$, HMDSO) as hydrolysis product.

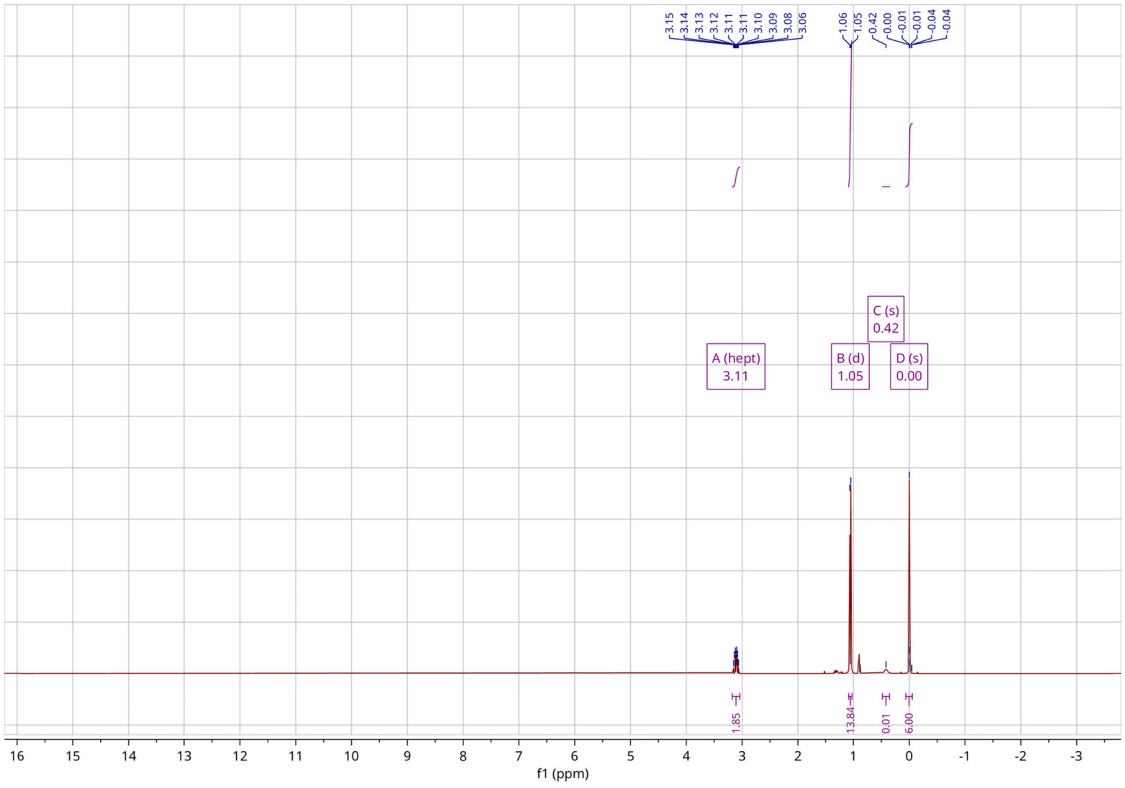

Figure S4: ^{1}H NMR spectrum of **D11**.

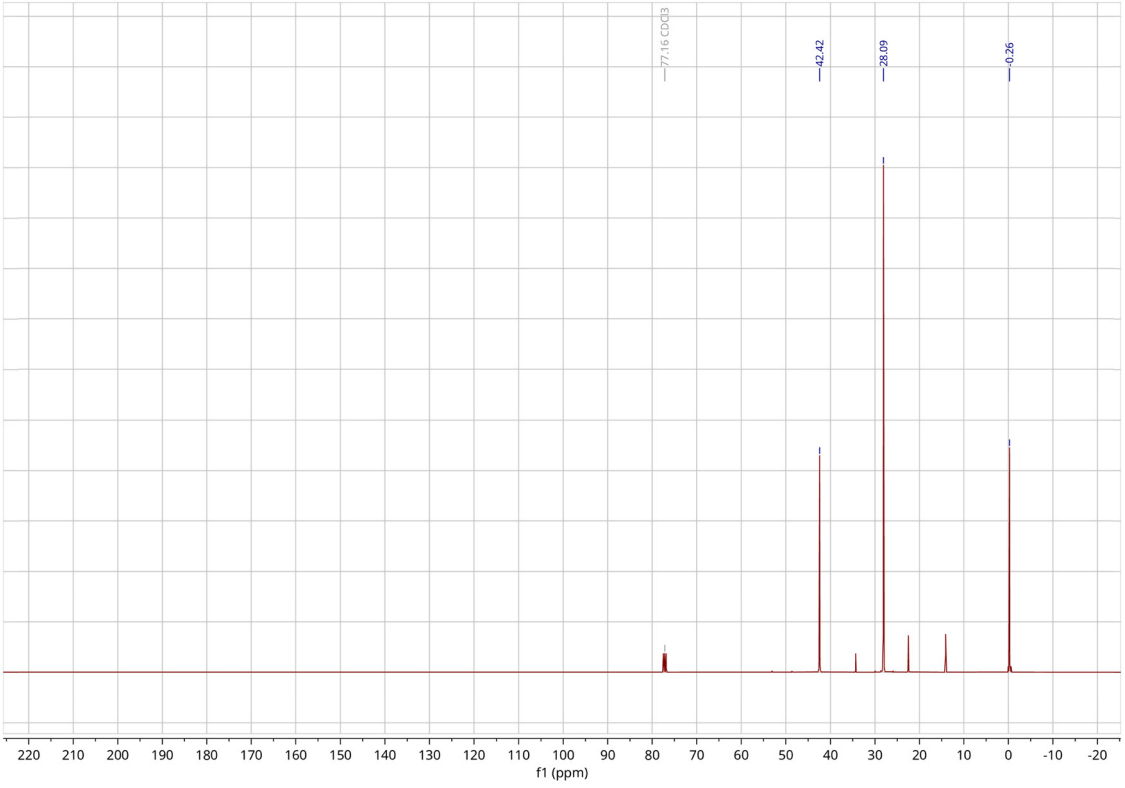

Figure S5: ^{13}C NMR spectrum of **D11**. The impurity is *n*-pentane.

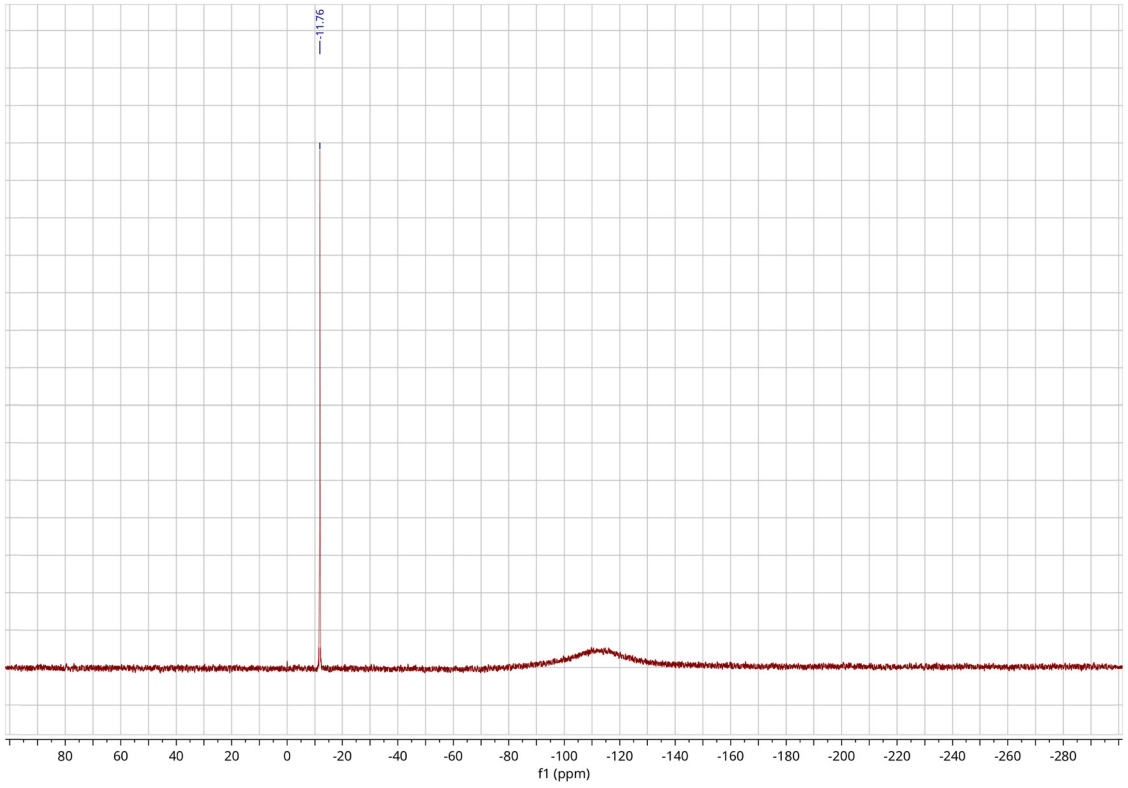

Figure S6: ^{29}Si NMR spectrum of **D11**.

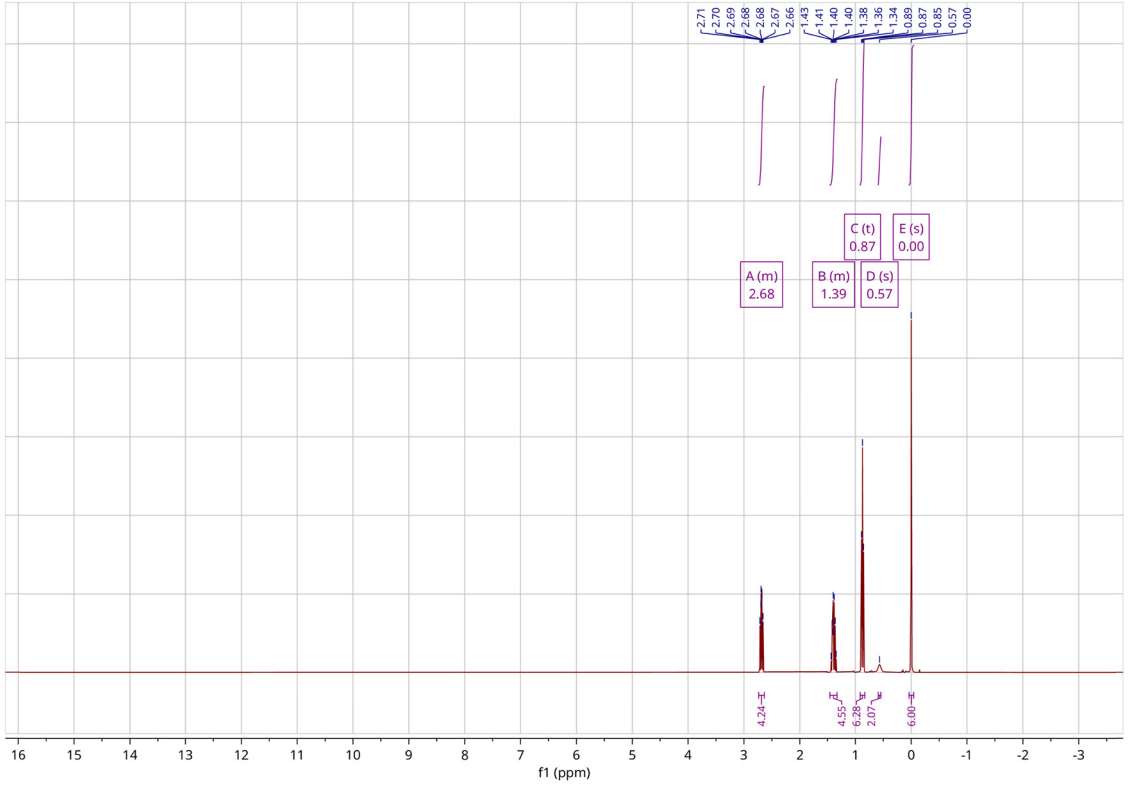

Figure S7: ^{1}H NMR spectrum of **D33**.

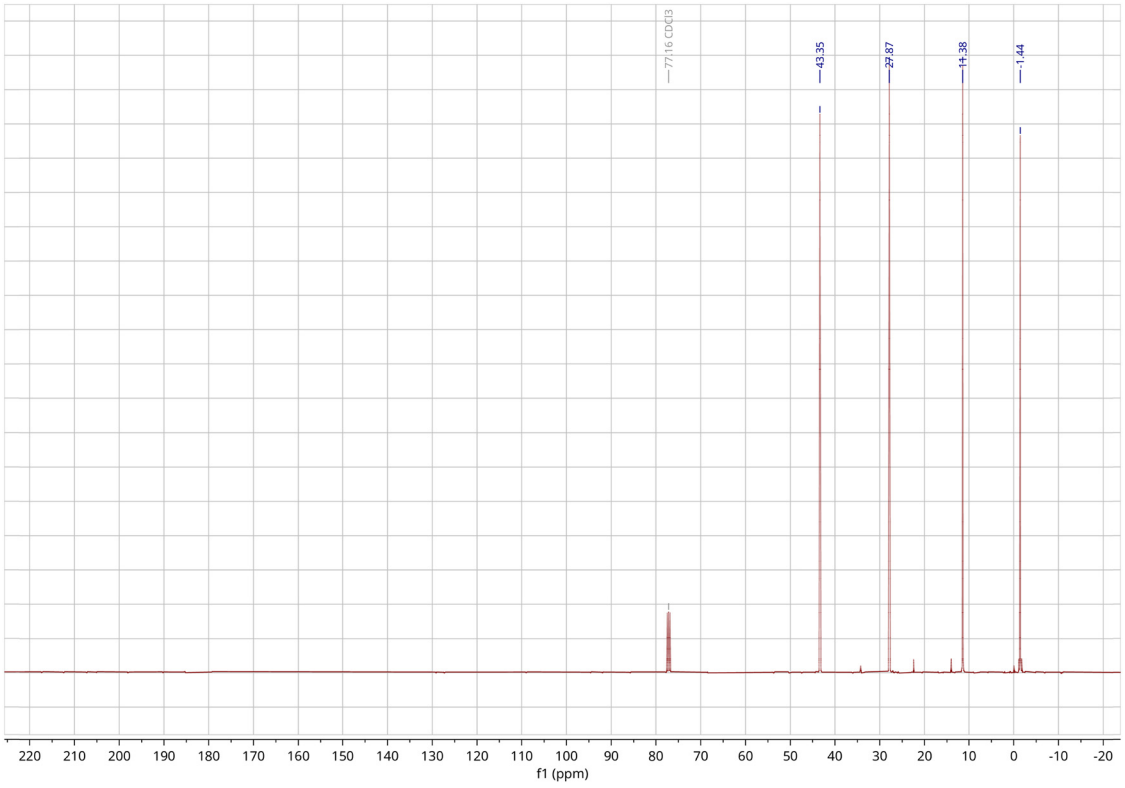

Figure S8: ^{13}C NMR spectrum of **D33**.

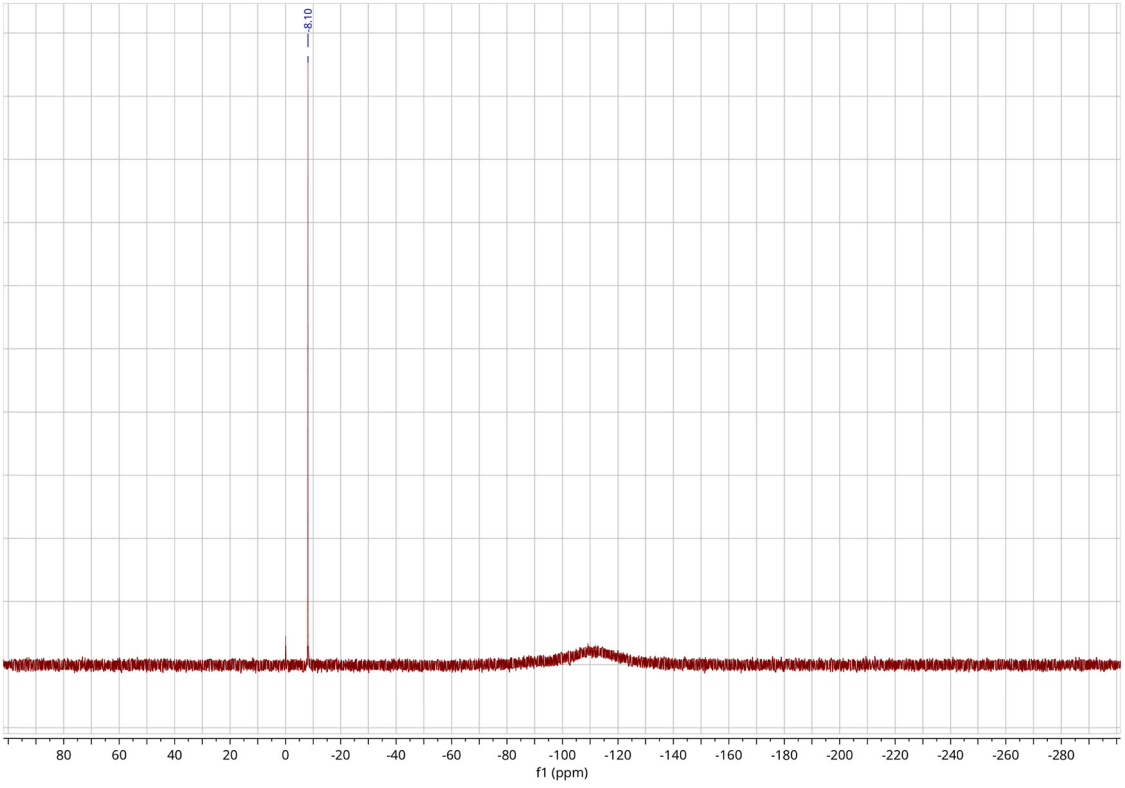

Figure S9: ^{29}Si NMR spectrum of **D33**.

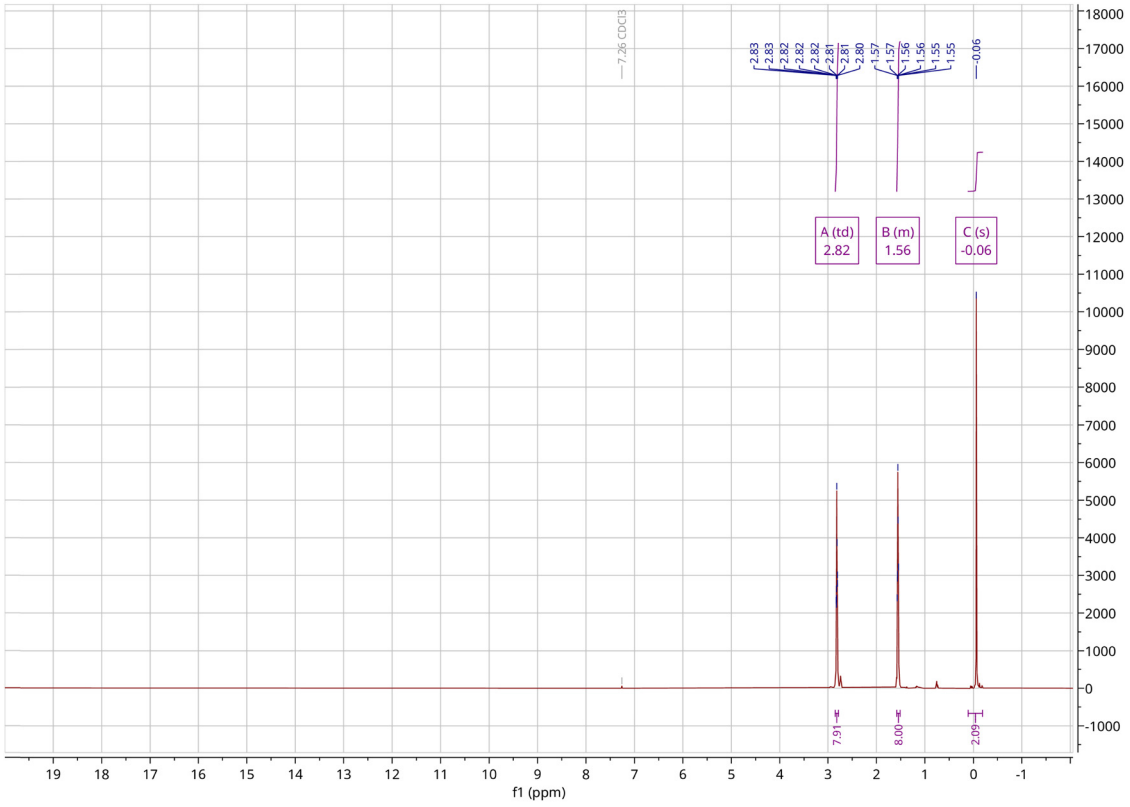

Figure S10: ^{1}H NMR spectrum of **D44**.

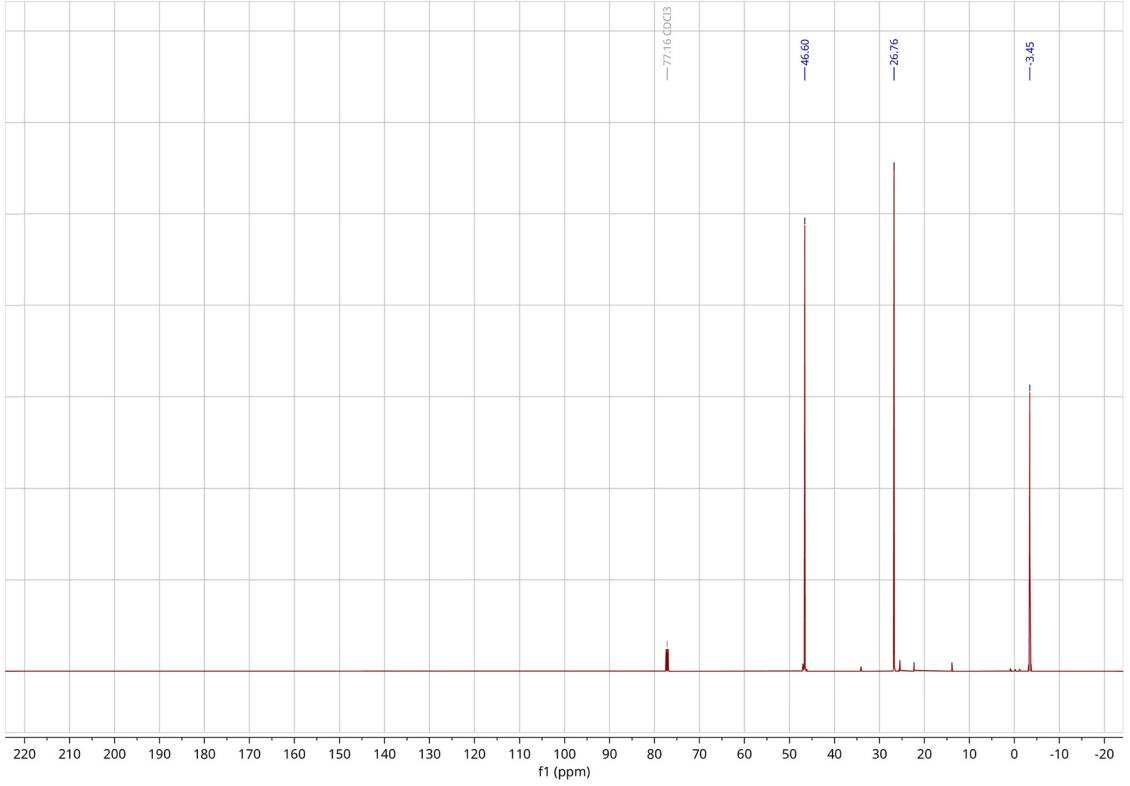

Figure S11: ^{13}C NMR spectrum of **D44**.

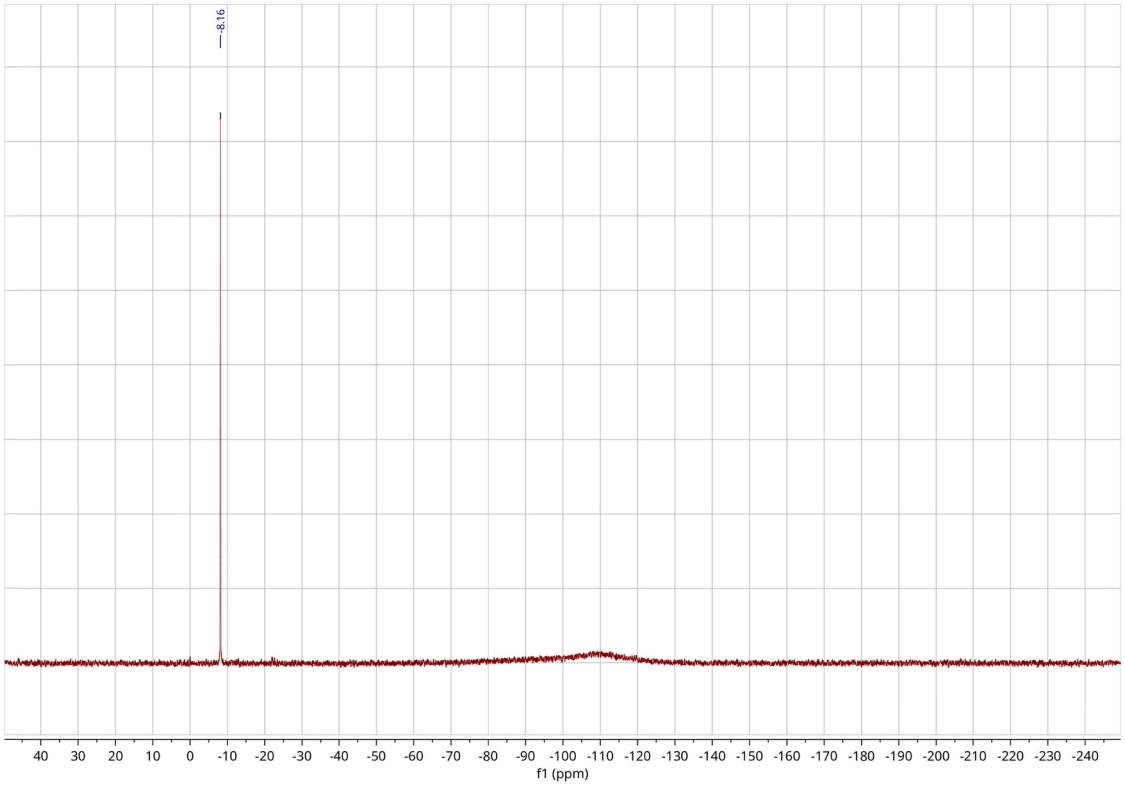

Figure S12: ^{29}Si NMR spectrum of **D44**.

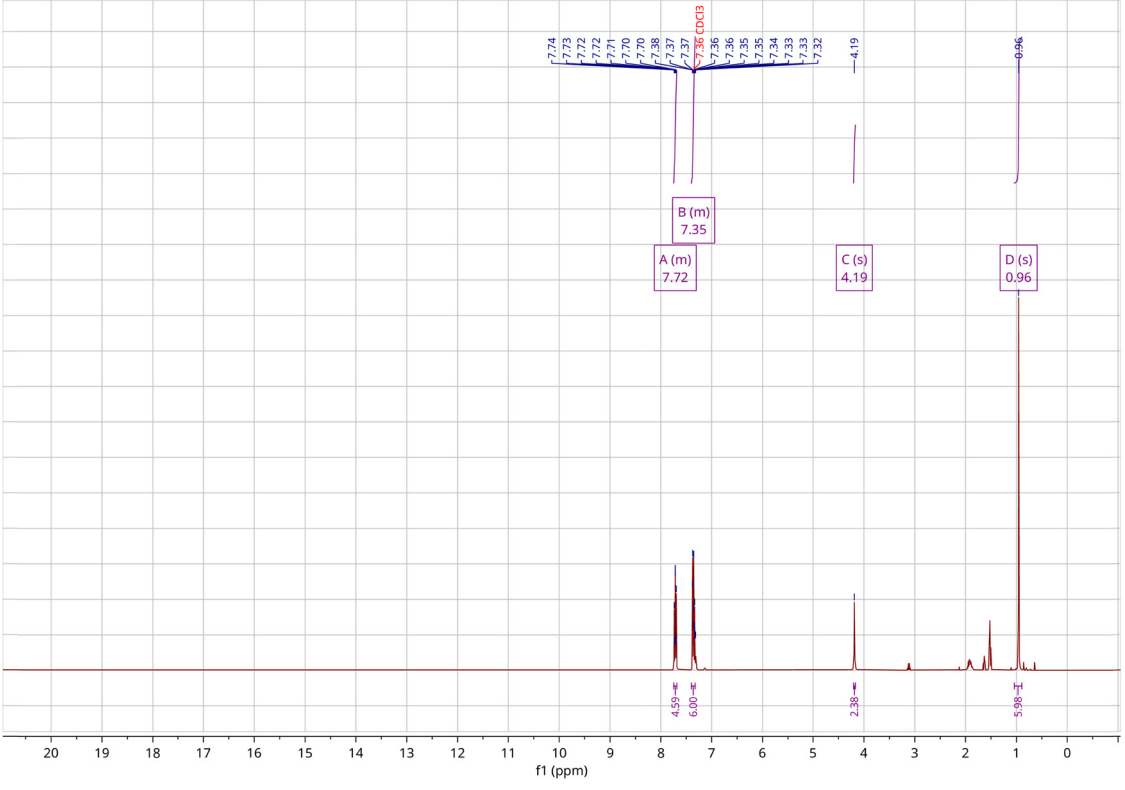

Figure S13: ^{1}H NMR spectrum of **D55**.

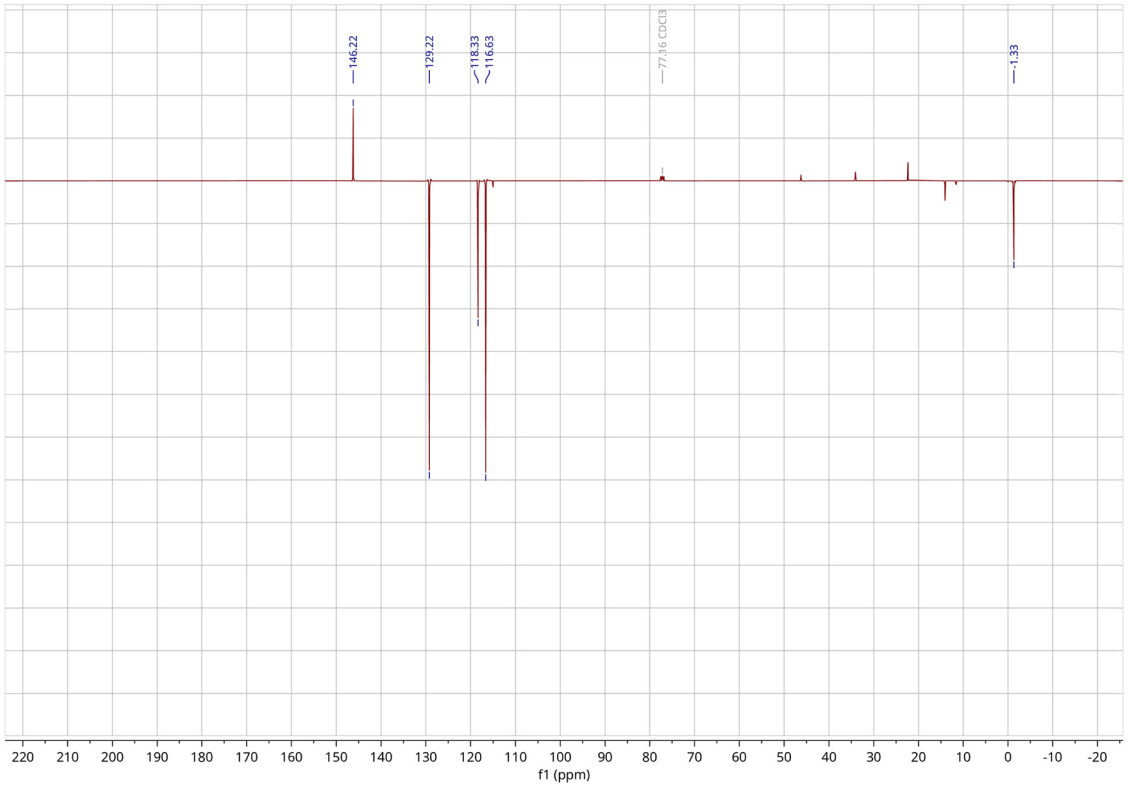

Figure S14: ^{13}C NMR APT spectrum of **D55**.

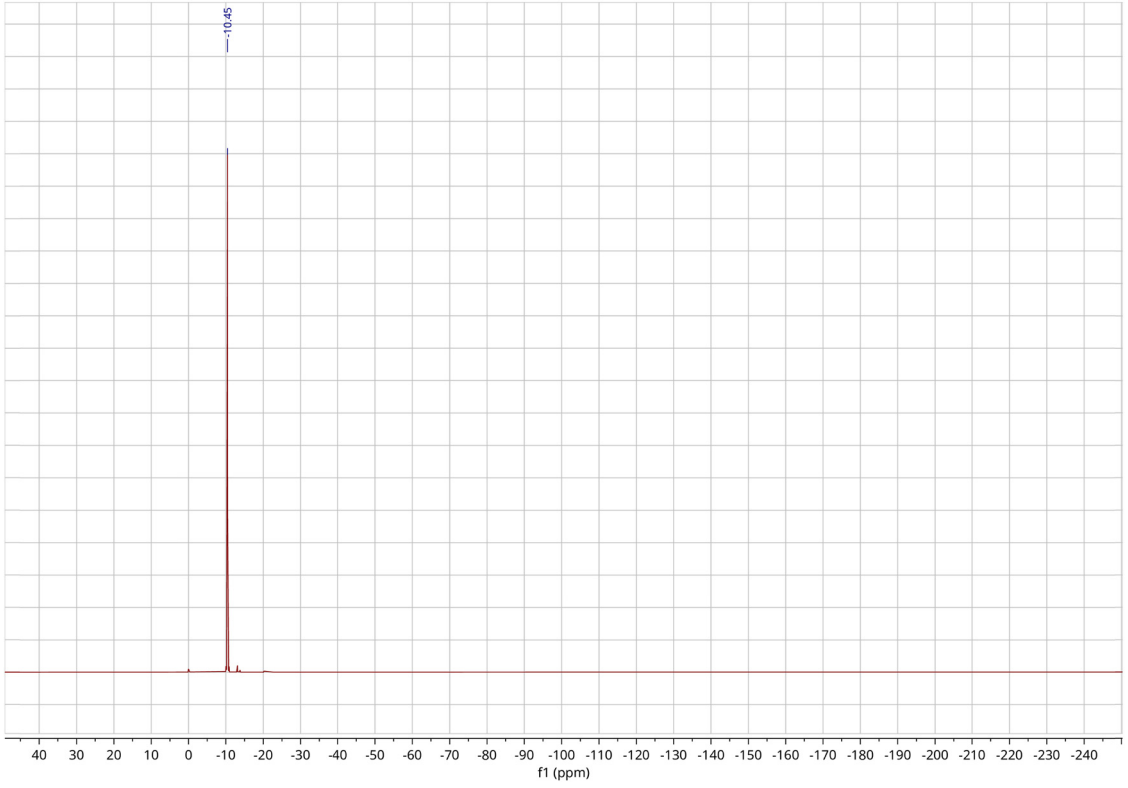

Figure S15: ^{29}Si INEPT NMR spectrum of **D55**.

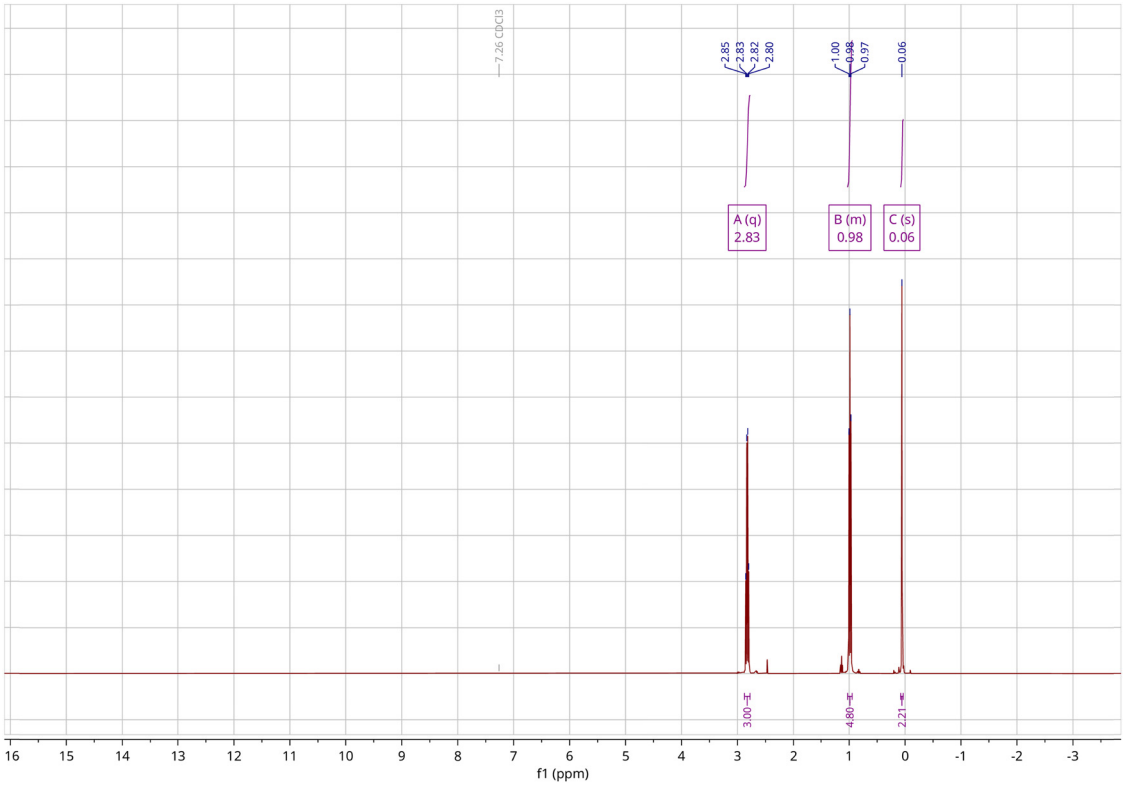

Figure S16: ^{1}H NMR spectrum of **D66**.

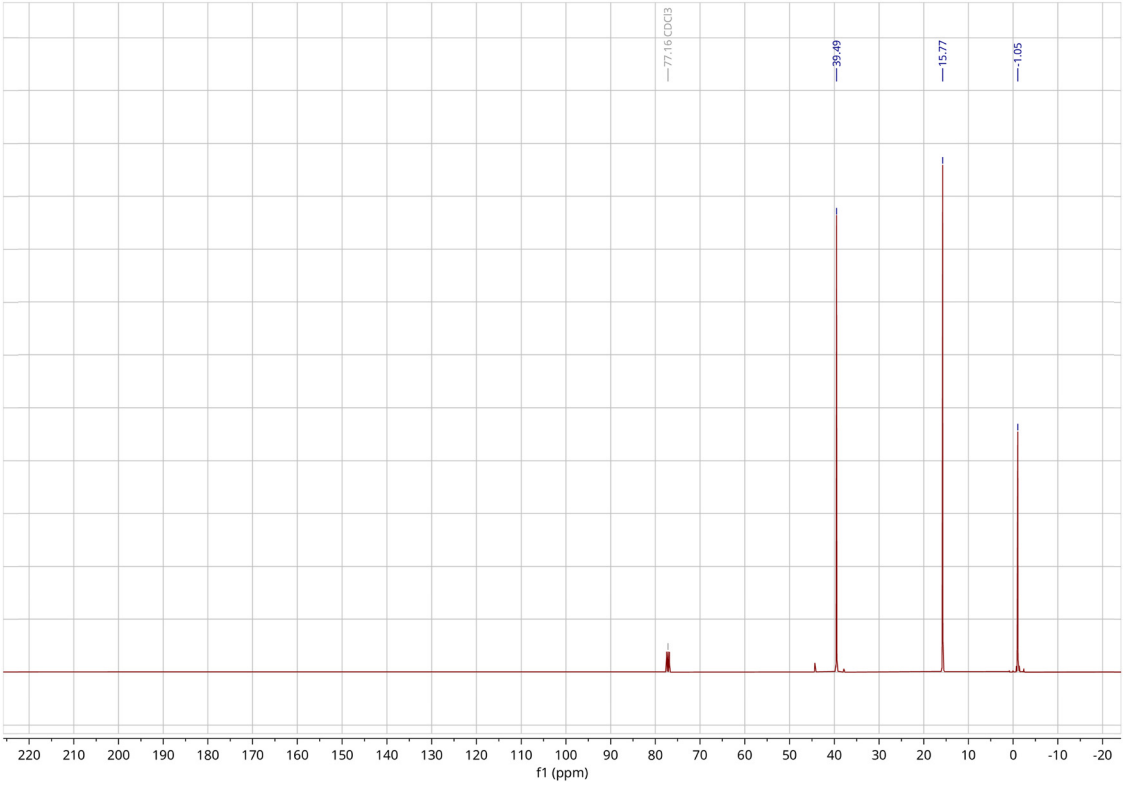

Figure S17: ^{13}C NMR spectrum of **D66**.

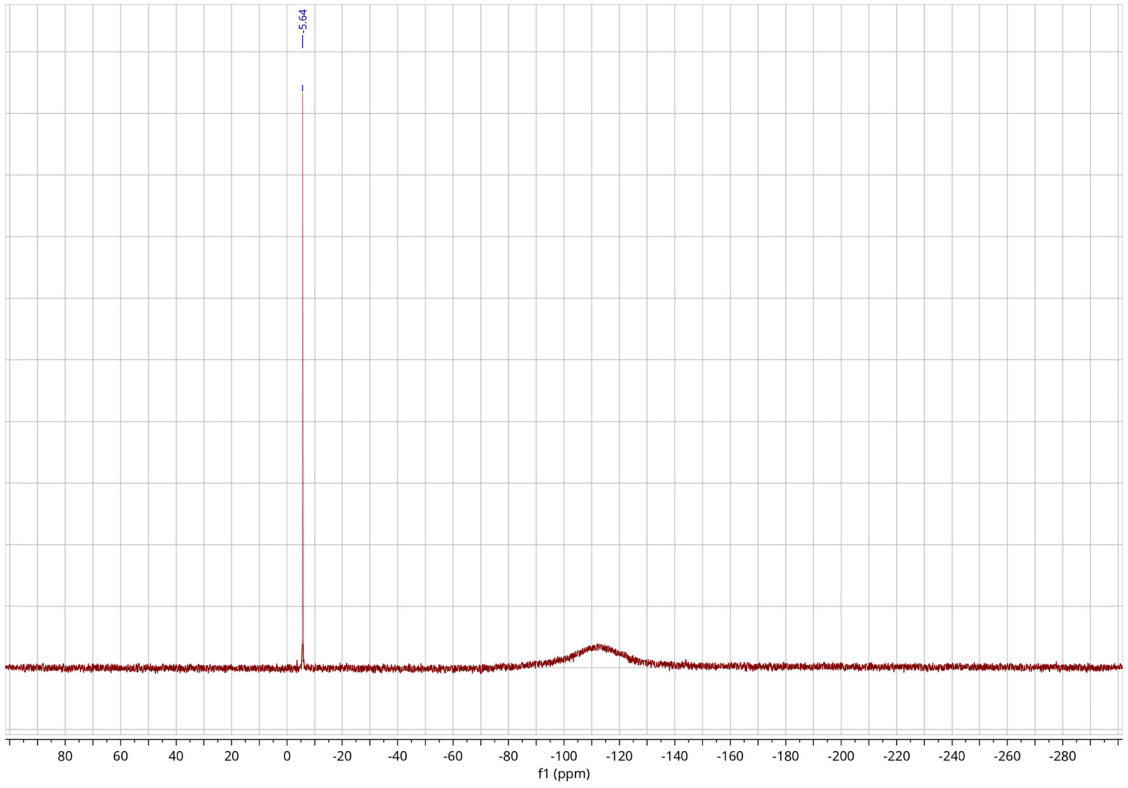

Figure S18: ^{29}Si NMR spectrum of **D66**.

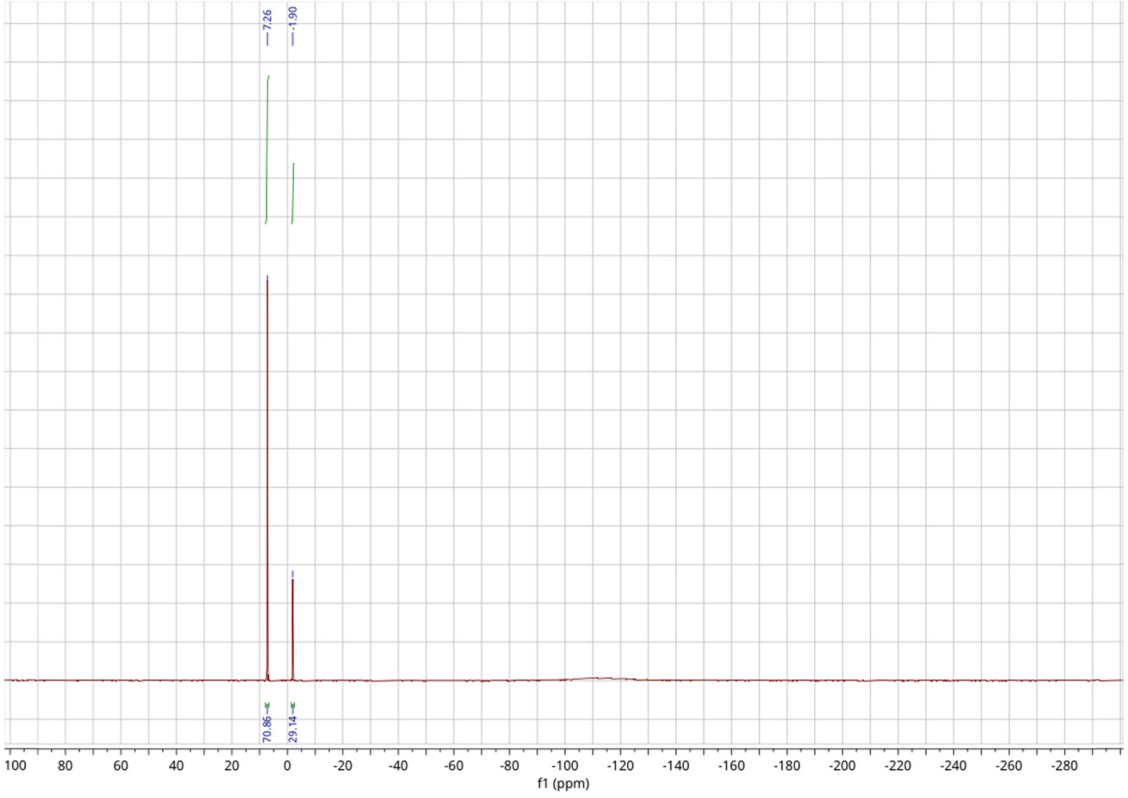

Figure S19: ^{29}Si NMR of the mixture of 0.291 g **M2** with 0.220 g HMDSO in 0.433 g $CDCl_3$ (sat. with $Cr(acac)_3$). The ration $n_{M2}\ I_{HMDSO}/n_{HMDSO}\ I_{M2} = 3.6$.

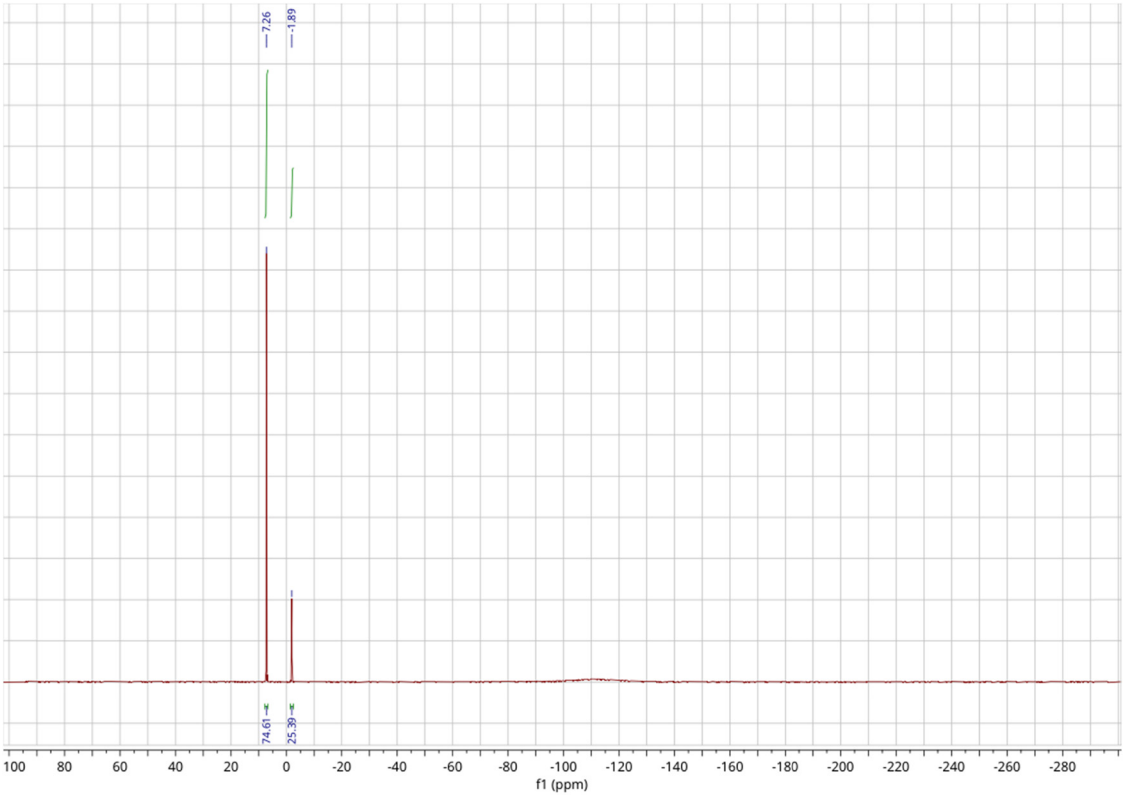

Figure S20: ^{29}Si NMR of the mixture of 0.276 g **M2** with 0.257 g HMDSO in 0.412 g $CDCl_3$. The ration $n_{M2}\ I_{HMDSO}/n_{HMDSO}\ I_{M2}$ = 3.5.

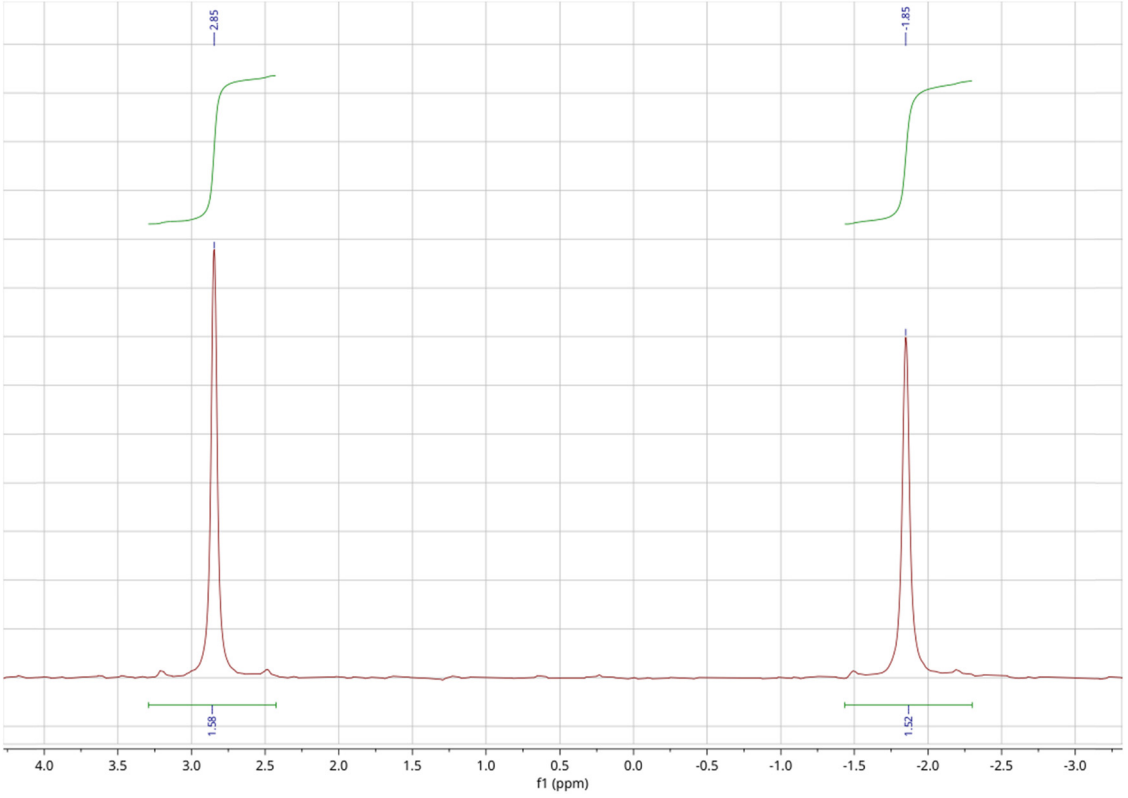

Figure S21: ^{29}Si NMR of the mixture of **M2** (0.230 g/1.583 mmol) and **M5** (0.254 g/1.537 mmol).

S4 Quantum chemical calculations

Initial geometries for reactants and products were optimized using the B97-3c (Brandenburg et al., 2018) method as implemented in the ORCA software package version 4 (Neese, 2017). Final electronic energies were calculated using the optimized structures and Martin's double hybrid functional DSD-BLYP-D3BJ/def2-QZVPP (Kozuch and Martin, 2013) making use of the RIJK (Weigend, 2007) approximation with the def2/JK (Weigend and Ahlrichs, 2005; Weigend, 2007) auxillary basis set as well as the RI-MP2 (Hellweg et al., 2007) approximation with the corresponding def2-QZVPP/C (Hellweg et al., 2007) auxillary basis set. As solvent model the CPCM (chloroform) (Barone and Cossi, 1998) keyword was used.

S4.1Atomic coordinates of optimized structures without solvent model

iso-propylamine (**A1**)

C −2.11226337490552 1.43889065313726 0.32394698140103
C −0.88758233993789 0.54993211257505 0.20681649281439
H −0.63838996665961 0.38734335283373 −0.84110639931614
H −0.02938875978530 1.00120288041560 0.70296875702984
H −1.05948366445228 −0.42460940022268 0.66587331131852
H −1.64917859566000 2.69212796681741 −1.36434768108741
H −2.75244779348394 3.43954708477890 −0.21031927454332
H −1.04131328335767 3.31121649211720 0.17806206981967
C −1.87364726998149 2.80004397415423 −0.30384509845937
H −4.07263091084206 1.35364784977062 −0.25142486885380
H −3.43604712987000 −0.10034552803789 0.07931976308658
N −3.23679379929919 0.79126333097620 −0.35853601275482
H −2.31193311176503 1.59483923068438 1.39669195954483

tert-butylamine (**A2**)

C −2.76544050564560 0.99025007408716 −0.20505641135429
C −3.30479705098285 2.36632133933342 −0.57559619330085
H −2.62290659503652 2.88264001786484 −1.25313806258715
H −4.26810383970105 2.27568522510377 −1.07297936815559
H −3.42612257775817 2.99024861804980 0.30863660473533
H −4.71371551307357 0.16905173698331 0.23494517208608
H −3.38404608922285 −0.71793299351667 0.97825365360525
H −3.88012154142175 0.83198552948856 1.64725094984697
C −3.74566759967335 0.27842576989906 0.71918070213074
H −1.48455282386288 1.71968467674892 1.40938175806694
H −1.00215338565869 0.15771551711576 0.75110279462172
C −1.40932096738794 1.13566594284020 0.49109603868664
H −0.69172642081490 1.63387510325487 −0.16205926956916
N −2.67708273191800 0.20242809934167 −1.44568099609204
H −2.29531009158901 −0.71286091330889 −1.23270042627609
H −2.01113226625285 0.64121625671422 −2.07243694644452

n-propylamine (**A3**)

N 2.18315990338068 0.86796250557691 0.26019493131802
H −1.08684747675277 3.16714566904203 0.18388014555914
H −0.48995750635288 2.40340931760427 −1.28514221087546
H −0.43886128769770 1.52554083842656 0.23414576296270
C 2.19721000258294 2.15615306689963 −0.43182502955180

H 2.42070903684267 1.00607252426005 1.23549460028783
H 2.89649196816635 0.26038191220984 −0.12185964126060
C 1.07449484603845 3.05733832928572 0.05812872122436
H 3.15088501801757 2.69666848106067 −0.33683790777200
H 2.05724281198325 1.96157903225794 −1.49771997641859
C −0.31497900549985 2.50857276500583 −0.21346052288519
H 1.20267879496093 3.22931017584353 1.13165723360140
H 1.19077289433035 4.03586538252701 −0.41365610618980
pyrrolidine (**A4**)
N 2.52928244164380 −1.64342949419824 0.79694330611942
C 1.31528985411480 −1.71440967598135 −0.02074279010016
H 3.00943056536359 0.81531800830213 −0.67465776983066
H 3.89133248382519 −2.08312808948323 −0.71522980009376
H 3.34037705303577 −0.18336993260459 −2.07695668948421
C 1.41207880116986 −0.60543514330313 −1.09455773127263
H 0.76755977074865 0.23760082143681 −0.84994494763325
H 1.09893516476372 −0.97100659261323 −2.07162363422940
C 3.56033654158588 −1.21102281830586 −0.14664196001005
H 0.42956023184285 −1.63382092665090 0.60628434365525
H 1.28301123523524 −2.69481271340257 −0.49940400714472
C 2.89622010546529 −0.18942772702845 −1.08224951868625
H 4.42747516393802 −0.82040643984421 0.38272414126487
H 2.40799158726733 −0.91635127632316 1.49319305744554
aniline (**A5**)
C 3.32789832806770 −1.25904158968495 −0.03965310640985
C 2.92857703674798 0.06637475646600 −0.02833746135088
C 2.38411264819992 −2.28656741613290 0.04675567923386
N 2.77527405875011 −3.62004471809013 −0.02790457891422
H 4.37995619656174 −1.50584204395852 −0.11880015293879
C 1.03238815708217 −1.94231743053166 0.13814777180258
H 3.67853774415507 0.84406065467829 −0.09322384705106
H 2.13355852775177 −4.26971259465889 0.39542794933872
C 1.58498352533234 0.40293926653559 0.06510508055600
H 1.27724446509586 1.43931415171069 0.07494520270117
H −0.40901826502917 −0.37263497414518 0.22334379699627
C 0.64345840483778 −0.61380979868534 0.14866059468479
H 3.71943799562117 −3.79765062880608 0.27226505344322
H 0.28519117682555 −2.72466763469690 0.19826801790819
diethylamine (**A6**)
N 1.97527681279788 −1.22961130102064 0.06786898146994
C 0.67707339463250 −0.85094165821246 0.61370176147846
H −1.05334633945864 0.33829315846212 0.13039718221251
H 0.46230870361045 1.11528982232976 −0.28835127195325
H −0.13630703369680 −0.21486401117386 −1.27618771520284
H 5.11219002030056 0.04493334549450 −0.17631143093538
H 4.67976531366295 −1.56579627462647 0.37814595183833
H 4.30851200235222 −1.08139743890127 −1.27507614816993
C 3.00321158216611 −0.20838742067179 0.20036336172343
H 0.75748088362273 −0.45053521515284 1.63912318389356
H 0.07692344007220 −1.75962413387902 0.68042071169833
C 4.35208264599335 −0.73188003960295 −0.24512661731526

H 2.72743995414460 0.64369093740297 −0.42139683236850
H 3.07703301219333 0.17642751619132 1.23285485429105
C −0.05106145161706 0.15575752632663 −0.25596120232734
H 2.29371705922361 −2.06665481296599 0.54093522966689
iso-propylaminotrimethylsilane (**M1**)
C −1.59617788049026 0.93428327688277 0.85845690909687
C −0.16511706716055 0.43040889007497 0.78320142959531
H 0.23715531206491 0.57785514474136 −0.21812908010061
H 0.46438622542770 0.96297780662109 1.49488942026306
H −0.09530729371680 −0.62952171762034 1.02120373080285
H −1.26986540125972 2.67330868571220 −0.37333425061266
H −2.67238157936629 2.80802343368862 0.68988607142319
H −1.05314965727384 2.96929863117001 1.35715200470759
C −1.64983501970587 2.43416492031087 0.61954031435162
H −0.29366548579058 −2.17549581306611 −0.82603945672736
H −1.46261111657472 −3.28767636420146 −1.51775163536435
N −2.43973208688818 0.25244501144881 −0.11778502029598
H −1.95499858069075 0.74941012494218 1.88320249553178
Si −2.64198749364108 −1.46920723831937 −0.30282869110576
H −1.16614261781940 −1.72882745857297 −2.28298695005213
H −3.27300983328712 0.78393082818567 −0.31821734684839
C −1.26067387925970 −2.23362625456036 −1.32239895766123
H −3.55242854580640 −1.98690045443883 1.96124746853411
H −2.88552780620865 −3.43274833622690 1.21159384939496
C −2.72996797619278 −2.36258690159471 1.35282101709491
H −1.81521370964416 −2.24652451009409 1.93380740771222
H −5.11235022855475 −1.31359978635880 −0.63904721427579
C −4.26659912776224 −1.67635324539442 −1.22320668739605
H −4.25854400142922 −1.13653043369019 −2.17001370353007
H −4.45525514896953 −2.72520823964002 −1.45036312453808
tert-buytlaminotrimethylsilan (**M2**)
N 2.48663807645892 0.54229497211152 0.80432827156579
H 5.03134400911523 1.49373838450699 0.74921408252059
C 4.45658378970777 1.67789848701055 −0.15848912550451
H 4.82861515414072 2.59849947145789 −0.61012093253596
C 2.96177388599741 1.77070789817064 0.16569623736569
H 0.26497242096019 −0.26383561348027 −1.58392312354004
H −0.10482191873284 −1.84507034585044 −0.92132967766628
C 2.17663570446594 2.01979829235138 −1.11555218023219
H 3.06740499731886 3.87487353276386 0.70581436207468
H 1.66648091115555 3.01936939391830 1.36676120782051
H 4.65039464112043 0.85844197080768 −0.84737084960571
H 1.11089119159772 2.08611637396525 −0.90895513667557
H 2.49559533578056 2.95135494566413 −1.57934509726328
Si 1.97122401301557 −0.96957219367579 0.11682066652460
H −0.44680816182231 −0.39517724160889 0.01825580210582
H 2.84724452310309 0.45969450789539 1.74298135143752
C 0.26611451129021 −0.85102468594473 −0.66745144006956
H 4.14791970419330 −1.82518754181143 −0.76256437298850
H 2.79181479403754 −2.66043577330252 −1.51117310811194
C 3.14728750227280 −1.68660781877675 −1.17066669739354

H 3.23673172108414 −1.05419003512389 −2.05348211874978
H 1.53485298356414 −3.12384112502364 1.27607413907092
C 1.89133233772477 −2.14127288805674 1.58401599115724
H 2.86986316742778 −2.28208362692504 2.04343548147378
H 1.21120395898314 −1.77423716504995 2.35219938355657
C 2.72504343348056 2.93158683092832 1.13026817613518
H 3.26779378482169 2.77469711733806 2.06380049939995
H 2.33517352773709 1.22546387574011 −1.84354179187197
n-propylaminotrimethylsilane (**M3**)
C −2.18167692620088 0.86608791837099 −0.46570753951990
C −0.98533615592560 1.37038391567977 0.31924990774961
H 3.32969176890055 −1.19103822277420 1.52504009555352
H 3.47656634196818 0.19966770284949 0.45496782259634
H 2.31940716967420 0.21653866329701 1.78161682975549
H −2.36037127048779 1.48024734442434 −1.35017528741922
H −2.02763050324642 −0.15974763592464 −0.79878247929736
H −3.09065496711019 0.88032563093821 0.13401382982681
C 0.30957244896820 1.39369868898417 −0.49073529043547
H −0.84022758439067 0.74977178841835 1.20635309348742
H −1.17962610056664 2.38329716579837 0.68361782429517
N 0.74322020079364 0.11735426950853 −1.03157339228680
H 0.19761871549299 2.10316275327106 −1.31630319855234
H 1.11030630909020 1.79217296277234 0.13434919574927
Si 1.47866778741076 −1.16904711625290 −0.12319654226238
H 3.02477341565376 −1.81202349626460 −1.96404108219948
H 2.73038420403422 −3.17904547876107 −0.89135673918130
C 2.76720465664164 −0.41122696263640 1.01157247842745
H −0.51530516572306 −2.60733145471234 0.32079306764149
H 0.79345145578762 −3.00880167512179 1.42364711299052
C 0.28305145962119 −2.18087714534986 0.92884110498667
H −0.18686803979833 −1.57797739208957 1.70536480560703
H 1.52199763615418 −2.71904766982211 −2.07533646346062
C 2.26239756614233 −2.32367693739915 −1.37861483524904
H 0.23337657711590 −0.14593061720399 −1.85962731880288
pyrrolidinotrimethylsilane (**M4**)
N 2.65142639758585 −2.11116462168442 0.13650984664596
C 1.31936071740260 −1.79514266557656 −0.37119065747376
C 1.71645239954727 −4.58247386686457 1.39291749336462
H 2.01233326429065 −5.57297020707184 1.73875043855857
H 1.36310194892830 −4.02184616617134 2.25754590465892
H 0.87301970438321 −4.71687320507631 0.71632588382936
H 1.22812550921866 0.25112136288314 0.28695239331990
H 0.62063421961861 0.02922701878893 −1.35464937396464
C 3.60598867991506 −1.07367641885338 −0.26824487374356
H 0.54915770979154 −2.05513764293443 0.35593975725890
H 1.07952739008780 −2.33247796070366 −1.30154353231965
C 2.80163824081458 −0.11527582572375 −1.14468325773599
H 4.00904146268641 −0.55486597765765 0.60803090314014
H 4.46269430805082 −1.48052441549126 −0.81495854075217
C 1.37599432594597 −0.29948431531002 −0.64286818973680
H 5.47289919668721 −3.09086314753668 1.24548398226744

Si 3.15590924600143 −3.71567216629846 0.55782397242620
H 4.36943760237534 −3.01257457590347 2.61258195616536
H 4.96055907028927 −4.56919694068528 2.03871189138500
C 4.62389164813241 −3.58257123988259 1.71985020422700
H 2.85242054070512 −4.81520884280823 −1.66431835462090
H 4.50369097749054 −4.24182587928150 −1.48051351824852
C 3.67427934008688 −4.71587941852633 −0.95488223065874
H 3.99536482985141 −5.72264257301204 −0.68403542688187
H 2.86580519912628 −0.42154278928418 −2.18965296695721
H 3.15724607098672 0.91134248066599 −1.07758370415357
anilinotrimethylsilane (**M5**)
C 3.46494410756429 −1.31488355482900 −0.75516654903515
C 2.33993257054621 −0.60291695126658 −1.13575856995692
C 3.51993916580055 −1.95791007515848 0.48783221964099
N 4.63179584943654 −2.67737875506914 0.89333149851093
H 4.30583879690397 −1.37055354994642 −1.43108197597640
C 2.40116002723623 −1.85337247650445 1.32558666760457
H 0.43507717153873 −1.07929898062772 1.60798191312244
H 2.32851128501747 −0.11736261407233 −2.10319379733454
C 1.23789134069646 −0.50636639267853 −0.29831410417761
H 0.36230947378074 0.05088269474343 −0.60106650334574
H 5.37478663986423 −4.86551269015771 −1.33616658777508
C 1.28208106131705 −1.13988846051851 0.93666274992659
C 7.09064795628840 −1.39550968230786 −0.24848227984699
H 4.52667766837854 −3.08250808469151 1.80921231667483
Si 6.15724775563706 −2.98804390326145 0.08204598402305
H 6.59523326023160 −4.98248964067342 1.51464815170374
H 8.09073857339050 −4.30607029770313 0.89629760816696
H 7.27113651886661 −0.85479605990020 0.67978829893341
H 8.05859477948914 −1.60330866143104 −0.70576471405187
H 6.55377361225136 −0.72388881107471 −0.91564594483470
C 7.11186664900368 −4.04753243774428 1.29888989177265
H 7.27871943527872 −3.52959979982761 2.24310479645073
H 5.31163553729517 −3.36658400050298 −2.24535653050960
C 5.89742735664632 −3.92757385630491 −1.51975074203908
H 6.85351529127101 −4.16541977238744 −1.98718436224643
H 2.41781811626936 −2.34171318610400 2.29325056459920
diethylaminotrimethylsilane (**M6**)
N 2.54518011614460 −1.83923666447868 0.45738442483241
C 1.17102299271670 −1.44330965835411 0.20939258675959
H −0.21354579162936 −0.77738198936978 −1.31327664070527
H 1.37735338904789 −0.04431205464618 −1.44291352447813
H 1.14482480557626 −1.71786139522774 −1.93921993649121
H 4.99925704476213 0.26060773482074 −0.75536053340141
H 4.87565471411598 −1.46059093096760 −1.09578215923758
H 3.63156208835263 −0.36719183480637 −1.67794485448944
C 3.53074310340677 −0.76982120843895 0.45751908513375
H 0.89186583216990 −0.65380409695883 0.91781206743685
H 0.52443354328657 −2.28856173049903 0.44714590392335
C 4.29874279467216 −0.57160582840633 −0.84416704780592
H 3.01887262859454 0.16031678154676 0.71945156621296

H 4.25142130237247 −0.94378909707319 1.25989603031295
C 0.85508161441480 −0.96882263491995 −1.20370570397693
H 5.47930834079100 −3.14978718040150 0.70804813263423
Si 3.00871095176239 −3.51703419382017 0.44686017976904
H 4.68805533768554 −3.27823405888295 2.27462788490188
H 4.98474606611884 −4.71846225557164 1.31247504962149
C 4.69582943249432 −3.66884433511881 1.25773008640644
H 2.12962816488404 −4.20591536316601 −1.78577876831905
H 3.81717379346746 −3.73576745218694 −1.91067766208581
C 3.09607133177368 −4.25919246060156 −1.28391845935364
H 3.38669574353566 −5.31053624263525 −1.25242364714008
H 0.78973459194257 −4.59535240321841 0.93131124552061
C 1.75721778626684 −4.52311858728650 1.42654327277561
H 2.12127601698512 −5.54281947704711 1.55675364930140
H 1.59418226428845 −4.10047138228387 2.41701777194190

S4.2Atomic coordinates of optimized structures with CPCM (chloroform)

iso-propylamine (**A1**)
C −2.11083608801925 1.43777648063650 0.31576030753736
C −0.88559080688068 0.54913315204976 0.20366525825693
H −0.62014386389696 0.39599157650432 −0.84271661512383
H −0.03367534520715 0.99850240140294 0.71219614231024
H −1.06571941964624 −0.42809762796467 0.65313224580820
H −1.63259531584524 2.69893380575780 −1.36636825937571
H −2.75644877358535 3.43364150842377 −0.22049499547194
H −1.04633712693391 3.31229276154237 0.18418477915506
C −1.87260671776642 2.80071242567165 −0.30767178777106
H −4.07491989765368 1.35269353548934 −0.23115752584614
H −3.44163646425825 −0.09394316583634 0.09921878446737
N −3.24322405936317 0.78736548363915 −0.36153878873676
H −2.31736612094368 1.59009766268342 1.38589045479029
tert-butylamine (**A2**)
C −2.77052598829622 0.99078209234988 −0.20682314676305
C −3.30796998178087 2.36736060519055 −0.57689488669423
H −2.62999304561440 2.87606903569361 −1.26352972880651
H −4.28021018343866 2.28304693809001 −1.05998658019674
H −3.41595010851596 2.99140815907315 0.30893275403056
H −4.72486370712037 0.18246265402799 0.24660486678569
H −3.39040863174875 −0.72187631208872 0.96575522830856
H −3.86947647545963 0.82866717211709 1.65114039785789
C −3.74860093511842 0.27855747947076 0.71921630514397
H −1.49099098097410 1.71576402909822 1.40561092850115
H −1.00901733131760 0.15376664169276 0.74172724710720
C −1.41342546775795 1.13388422751621 0.48641132228674
H −0.69887680393631 1.63379248564021 −0.16852627208330
N −2.67036326718538 0.19855667376189 −1.44966888733854
H −2.27371209746016 −0.70764571160487 −1.22175531982283
H −1.98781499427520 0.63980382997125 −2.05801422831658

n-propylamine (**A3**)
N 2.20291925663465 0.85189671880670 0.25573968004560
H −1.08865278458373 3.20556020526486 0.15391592787822
H −0.48710467348508 2.39430800441467 −1.28858880645870
H −0.49123555719522 1.55224488363264 0.25454364961915
C 2.19040225160304 2.14666488379091 −0.43496398799686
H 2.44101761216213 1.00657700051185 1.22931212916898
H 2.95386252727580 0.28404217607354 −0.11820404509538
C 1.07010648496275 3.04427041771272 0.06544871204589
H 3.14168516351162 2.68829331801488 −0.34019290462277
H 2.04643336703248 1.95476473028397 −1.50056799719506
C −0.32750322757245 2.51921188623169 −0.21655134278546
H 1.19794835326097 3.20221957096258 1.14067153024693
H 1.19312122639302 4.02594620429898 −0.39756254485053
pyrrolidine (**A4**)
N 2.52944677817764 −1.64378940084842 0.80074322950730
C 1.31365417784982 −1.71744825037555 −0.02245391975174
H 3.01001421277097 0.81204160260516 −0.66726491874946
H 3.89000593856020 −2.08493490000319 −0.71902204257353
H 3.34053898032742 −0.18514707180813 −2.07379432593664
C 1.41238126227090 −0.60620140578573 −1.09149613626492
H 0.76907826271579 0.23578307940014 −0.84134706839397
H 1.09946910356802 −0.97160955997059 −2.06848082346962
C 3.56289602759363 −1.21302581372472 −0.14841420209259
H 0.42847380398150 −1.63526854290618 0.60478699604510
H 1.28487776876445 −2.69619678217330 −0.50412901873191
C 2.89666705202127 −0.19050539483462 −1.07915049524349
H 4.42885129786525 −0.82053301417726 0.38123018949560
H 2.40252633353312 −0.89686654539759 1.47592853615986
aniline (**A5**)
C 3.32950914662229 −1.25881367029068 −0.03861857791078
C 2.92940023815466 0.06766928309714 −0.02887622588639
C 2.38459723181500 −2.28884471481638 0.04541236047874
N 2.77472009895906 −3.62047356011320 −0.03215936295787
H 4.38121492803621 −1.50753801123088 −0.11151963180392
C 1.03091903985688 −1.94294658462216 0.13894586057381
H 3.67972425744996 0.84540226434932 −0.09192404060657
H 2.13404694530026 −4.27043333433936 0.39489117254528
C 1.58408282045677 0.40538599775219 0.06244520700483
H 1.27615722800338 1.44192981909364 0.07105006222892
H −0.41059621830841 −0.37211017271449 0.22444461594521
C 0.64195842159218 −0.61317002293443 0.14797643970070
H 3.71988218249546 −3.79915892166722 0.26802506218871
H 0.28598367956627 −2.72649837156348 0.20490705849934
diethylamine (**A6**)
N 1.97491761099470 −1.23446240401239 0.05610236130250
C 0.67741667541049 −0.84586249349146 0.60922616435030
H −1.04803506429370 0.35582676858113 0.14784174687637
H 0.46674051462111 1.10220290342268 −0.33243601271345
H −0.18355109900354 −0.23933105821744 −1.27262556557514
H 5.11830695159724 0.04456789986414 −0.14681033226052

H 4.67399153983379 −1.58182127042006 0.35817302511871
H 4.32646328742104 −1.04726456229279 −1.28593788949343
C 3.00735120232622 −0.21251250857063 0.20398569501144
H 0.77553417724660 −0.43377895288514 1.62675873275727
H 0.07862528397693 −1.75329653064355 0.69629523583418
C 4.35799014312301 −0.72904604406522 −0.24463092673046
H 2.73231601579910 0.65081425003169 −0.40192327292541
H 3.07559495128348 0.14867445466798 1.24351140196974
C −0.05972070764940 0.15171700751736 −0.26314888904333
H 2.28835851731290 −2.06172745948630 0.55101852552125
iso-propylaminotrimethylsilane (**M1**)
C −1.58360682632131 0.91503551448167 0.83475394253224
C −0.14277338560393 0.44557717769595 0.73624110135269
H 0.25561280215752 0.65058074368007 −0.25726976121521
H 0.47449913836920 0.96065706286629 1.47117084711214
H −0.04845555547412 −0.62231504773265 0.92410368365379
H −1.28439087401091 2.72465517455497 −0.30119191987513
H −2.70168573211024 2.76807056278877 0.75163466838624
H −1.09001652854436 2.93047883929919 1.44442885677286
C −1.66961176470276 2.42396973065325 0.67349033436835
H −0.30167188205667 −2.23099308889418 −0.79841287862996
H −1.49169708638958 −3.31847778736927 −1.49837323298717
N −2.41647174559436 0.26372150905533 −0.17995822494998
H −1.94075047284100 0.67086215982354 1.84676713945892
Si −2.64131995560343 −1.46934098266024 −0.31833821595780
H −1.14198382961885 −1.77633208752408 −2.27637565698235
H −3.28887572473088 0.76387718716923 −0.28559059984498
C −1.26108004516733 −2.26860855014397 −1.31147681491484
H −3.56269243387055 −1.90804384731282 1.95500217384985
H −2.90320617384540 −3.38414065397003 1.25289699432753
C −2.74108774676096 −2.31119232506131 1.36258927378987
H −1.82372496257884 −2.17666259081065 1.93561576165904
H −5.10354151961773 −1.28480763656293 −0.67558344664213
C −4.26186911183402 −1.68322769874308 −1.24247380237522
H −4.23626693276249 −1.17447103108893 −2.20625461461855
H −4.46233165048695 −2.73757233419412 −1.43249560827016
tert-buytlaminotrimethylsilan (**M2**)
N 2.44738964405469 0.55810815559119 0.82647540722958
H 5.01506672100016 1.45953728933929 0.72805634297045
C 4.43174746131944 1.64697425140970 −0.17388341558670
H 4.81165620089506 2.55860779368690 −0.63687519439844
C 2.94420915252495 1.77381523812541 0.16965919047215
H 0.27815884741755 −0.26788204486601 −1.59694362736876
H −0.06809477051094 −1.86477858177020 −0.95221012364513
C 2.14781418803144 2.03479315456146 −1.10184150662403
H 3.12181153243255 3.87423370482813 0.69929367729810
H 1.69697483888763 3.07118586971317 1.37311149963079
H 4.59944052177109 0.82090271682313 −0.86156810311751
H 1.08568846169259 2.12314160344029 −0.88212667944356
H 2.48040480125056 2.96071310048894 −1.56735105931776
Si 1.97083109878187 −0.96558252841771 0.12074825649122

H −0.45589755953879 −0.42998259128893 −0.00477037572278
H 2.89471984342267 0.44283096284033 1.72585041694074
C 0.27544893948743 −0.86388234877532 −0.68605770853905
H 4.16723741868112 −1.79752459738915 −0.72745507408431
H 2.82686291734173 −2.64863848101775 −1.49217364028981
C 3.17098767049258 −1.67083255755103 −1.15072156338499
H 3.26232560518989 −1.03339123733503 −2.02976996557505
H 1.54480698392601 −3.12842287095543 1.26192213727915
C 1.88041264492098 −2.14237346608511 1.58311552448355
H 2.85283596071360 −2.26665788304759 2.06041702467014
H 1.18006241851670 −1.78456352494114 2.33769627988120
C 2.75142803258258 2.94528478440548 1.13198440476662
H 3.29384440480190 2.76959357736346 2.06199462963484
H 2.28112601991289 1.23679051082353 −1.83087675465064

n-propylaminotrimethylsilane (**M3**)

C −2.14744158597440 0.83469383277754 −0.36668323540985
C −0.91330491893575 1.37717357054586 0.33040692595574
H 3.24035850336018 −1.16673575383214 1.57065983534712
H 3.42876268207153 0.22111323443889 0.50171571398783
H 2.21043494322389 0.24078043652983 1.77465650759242
H −2.38872179762092 1.42243995071879 −1.25418183220906
H −1.99952657228735 −0.19714162015732 −0.68376179032718
H −3.01689188088189 0.85361317704090 0.28961915449569
C 0.33037530476837 1.40140527839643 −0.55570041566620
H −0.70458605485812 0.78528462466848 1.22437925574538
H −1.10242247047644 2.39712147821217 0.67737594268088
N 0.75958568240619 0.11942223743516 −1.09997600024965
H 0.15471890386747 2.08925383613166 −1.38812429239640
H 1.15852000054003 1.82510755318762 0.01421074388664
Si 1.46281946679082 −1.16333470061449 −0.14859889212923
H 3.10220659293017 −1.81618629035006 −1.90481582325760
H 2.74668041513125 −3.17808568912711 −0.84146542803305
C 2.69832161853212 −0.38948971423177 1.03153238558030
H −0.54077316229210 −2.60753592794343 0.20126241980805
H 0.72085853279459 −3.00349137562241 1.36299703974142
C 0.22488562430829 −2.17843135274642 0.84863648243916
H −0.28065491250299 −1.57532585495938 1.60209193888178
H 1.59977619939540 −2.71548024094681 −2.08955607580253
C 2.30827343069372 −2.32397553323099 −1.35813905522667
H 0.16173645501590 −0.18525815632099 −1.85456450543497

pyrrolidinotrimethylsilane (**M4**)

N 2.64025001690999 −2.07963969681180 0.22148290413599
C 1.32307702060063 −1.79935771826509 −0.35464824186162
C 1.72447093939893 −4.59380241349145 1.41259127929760
H 2.02916455100950 −5.59237565706648 1.72680371538689
H 1.38179588470107 −4.05552899685705 2.29590081005113
H 0.87463467785595 −4.70888948253578 0.74018878112332
H 1.20303412905722 0.27144649517999 0.21812504231906
H 0.63621871572606 −0.02351115632660 −1.42745906639094
C 3.60551547148380 −1.06582187829009 −0.23573094190960
H 0.52863079619584 −2.04356394642284 0.35104152295661

H 1.12865197282132 −2.37442166277929 −1.27246080486135
C 2.81212057494951 −0.14389716296769 −1.16152678469082
H 4.00934649144592 −0.51009125497803 0.61622093165433
H 4.46004675449314 −1.50429058867905 −0.75997018770486
C 1.37615470817071 −0.31634210770467 −0.68452177331791
H 5.47461292225212 −3.09535371424741 1.25625266040546
Si 3.15215805099373 −3.70256198451709 0.58336415902279
H 4.39163840136234 −3.06958220543664 2.64490226650265
H 4.97463708015617 −4.60492130298841 2.00453899083515
C 4.63551098431521 −3.60614840611405 1.72828517949192
H 2.80715461375481 −4.71585428719742 −1.66929342397892
H 4.46752815202767 −4.15860213552026 −1.49029806445170
C 3.64282393310054 −4.64894882774943 −0.97204849755382
H 3.96003660242005 −5.66604996410946 −0.73747778860342
H 2.89928906170771 −0.48638401044170 −2.19344692583104
H 3.16149749308996 0.88629406631792 −1.12251574202689

anilinotrimethylsilane (**M5**)

C 3.46767663934947 −1.30258616938652 −0.75147486051441
C 2.33965163833343 −0.59148745809468 −1.12936982080775
C 3.52309303806467 −1.95626053926465 0.48888441025821
N 4.63352518321102 −2.67063769539491 0.89370112855268
H 4.30919947189869 −1.34733500437074 −1.42729906487607
C 2.39748639957690 −1.86286742788936 1.32417543460133
H 0.42679128449949 −1.09923233409180 1.60601771366476
H 2.33020937589422 −0.09840830810669 −2.09318232677049
C 1.23252663398800 −0.50539516075214 −0.29466734025030
H 0.35578435471096 0.05127126714489 −0.59580482619654
H 5.36148660072710 −4.86395938844212 −1.32945522470124
C 1.27622731415683 −1.15039029876860 0.93667173993035
C 7.09614326994796 −1.39699537776046 −0.25780736507862
H 4.52931219915039 −3.08160705304035 1.80824760890556
Si 6.16367995449412 −2.98851615862076 0.08008525618131
H 6.58818175655813 −4.97444110040686 1.51856288891047
H 8.09019774913417 −4.30445198871376 0.89642704350242
H 7.25855531929665 −0.84195971541166 0.66566301359223
H 8.07246473131370 −1.61944359744000 −0.69004373655735
H 6.57351259373312 −0.74165691404503 −0.95227541077527
C 7.11249353342091 −4.04416689080437 1.30107075340308
H 7.27501331393787 −3.51954225022269 2.24228900145993
H 5.32315400068721 −3.36507088969427 −2.25049821131575
C 5.89438242668655 −3.93242997458172 −1.51788412195951
H 6.85351024421577 −4.18205868278962 −1.97314214381702
H 2.41504097301256 −2.35997088905109 2.28680846065797

diethylaminotrimethylsilane (**M6**)

N 2.54794290078343 −1.82769911177261 0.49361913664097
C 1.17262074954001 −1.42948941951540 0.24054603310506
H −0.22266086355620 −0.79481801375728 −1.28141912956233
H 1.37824644039013 −0.09032274138753 −1.46025954895284
H 1.11053886763067 −1.77674038220878 −1.89747067816276
H 4.99100197856000 0.24196856396355 −0.80119163527396
H 4.86597641506187 −1.48588979397475 −1.10684865677051

H 3.61334233261744 −0.40255364715930 −1.69637202046375
C 3.54024941257894 −0.76146081232672 0.44924971787721
H 0.90695742329038 −0.61362963458159 0.92334144729211
H 0.52245200784206 −2.26201643144659 0.51030384324054
C 4.29055021263189 −0.59268986378185 −0.86712262504784
H 3.03646224128366 0.17631277360294 0.69830789373723
H 4.27458284226177 −0.92208443770539 1.24216627785405
C 0.84514959637499 −0.99802508452566 −1.18365815166565
H 5.47634180456367 −3.15355518724463 0.73538987862030
Si 3.01141394592337 −3.50829103117781 0.45234059929985
H 4.67260062678397 −3.28627456995810 2.29760220789625
H 4.96961654308226 −4.72622736828665 1.32913601271868
C 4.68921885734469 −3.67370574550396 1.27932570781832
H 2.16839597284063 −4.14849861792402 −1.80739458978055
H 3.86918047795176 −3.70497249135729 −1.88757326281752
C 3.12376845617338 −4.22656960261897 −1.28792491029215
H 3.39776234009201 −5.28273168866888 −1.25944269827068
H 0.78211932232801 −4.57651499926500 0.88530258744350
C 1.74290217950258 −4.52664859278364 1.39636343467126
H 2.10244856118838 −5.55091195119862 1.50303165084622
H 1.57191835493417 −4.12686011743541 2.39545147799900

S5 Detailed description of the determination of the rate constant

The rate constant were determined like described in Bittrich et al. (1973).

The reaction of trimethylsilymaines with amines is an equlibrium reaction:

$$\underset{SiA1}{Me_3SiNHR^1} + \underset{A2}{H_2NR^2} \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} \underset{SiA2}{Me_3SiNHR^2} + \underset{A1}{H_2NR^1}$$

To determine the rate constant, the equilibrium constant has to be known. According to this equation, the euqilibrium constant K_C can be described as:

$$K_c = \frac{[SiA2]\cdot[A1]}{[SiA1]\cdot[A2]}$$

With ^{29}Si NMR spectroscopy, the molar ration of the silicon containing species x_{SiA1} and x_{SiA2} can be determined, so the equilibrium constant can be calculated using the starting concentration (t = 0) of the aminosilan $[SiA1]_0$ and the amine $[A2]_0$ as:

$$K_C = \frac{([SiA1]_0\cdot(1 - x_{SiA1}))^2}{[SiA1]_0\cdot x_{SiA1}\cdot([A2]_0 - [SiA1]_0\cdot(1 - x_{SiA1}))}$$

Therefore, the equilibrium constant can be determined from the NMR data.

To determine the rate constants k_1 and k_{-1}, a turnover variable v is used for the time-law:

$$\frac{dv}{dt} = \dot{v} = k_1\cdot[SiA1]\cdot[A2] - k_{-1}\cdot[SiA2]\cdot[A1]$$

Assuming, the equilibrium was reached and no A1 or SiA2 were present at the start of the reaction, the time-law can be described as:

$$\dot{v} = (k_1 - k_{-1})\cdot\left(v^2 - \frac{k_1\cdot([SiA1]_0 + [A2]_0)}{k_1 - k_{-1}}\cdot v + \frac{k_1\cdot[SiA1]_0\cdot[A2]_0}{k_1 - k_{-1}}\right)$$

$$\dot{v} = \Delta k\cdot(v^2 + P\cdot v + Q) \text{ with } \Delta k = k_1 - k_{-1},\ P = \frac{-k_1\cdot([SiA1]_0 + [A2]_0)}{\Delta k} \text{ and } Q = \frac{k_1\cdot[SiA1]_0\cdot[A2]_0}{\Delta k}$$

P and Q can also be calculated from the equilibrium constant K_C:

$P = \frac{-K_C \cdot ([SiA1]_0 + [A2]_0)}{K_c - 1}$ and $Q = \frac{K_C \cdot [SiA1]_0 \cdot [A2]_0}{K_C - 1}$

In the equilibrium case, the turnover variable does not change in time ($\dot{v} = 0$), so the zero points of the quadratic equation can be determined as:

$v_{1,2} = \frac{-P}{2} \pm \sqrt{\frac{P^2}{4} - Q}$

Using this relationship, the time-law equation can be described as:

$\dot{v} = \Delta k \cdot (v - v_1) \cdot (v - v_2)$

which can be integrated to:

$\ln\left(\frac{v - v_1}{v - v_2} \cdot \frac{v_2}{v_1}\right) = (v_1 - v_2) \cdot \Delta k \cdot t$

From the slope of this equation m, the rate constants can be determined:

$\Delta k = \frac{m}{v_1 - v_2}$, $k_{-1} = \frac{\Delta k}{K_C - 1}$ and $k_1 = \Delta k + k_{-1}$

S6 Python script for spectra evaluation

```
#!/usr/bin/env python3
    # -*- coding: utf-8 -*-
    """
    Created on Mon Oct 18 15:52:38 2021
    @author: steven
    """
    import numpy as np
    import matplotlib.pyplot as plt
    from scipy.signal import find_peaks
    from pandas import *
    from uncertainties import unumpy
    Name = "sk-d4-a5" #Name of experiment and .csv of the NMR-Data
    Nummer=45 #Number of experiment (used in tables for integrals and amount of substances)
    Daten = read_csv("/home/steven/Dokumente/Uni/Hiwi/2021/GG-Diaminosilane/csv/"+Name,skiprows=1,nrows=12000,sep="\s+",names = ("x","y"))
    Datenvoll = read_csv("/home/steven/Dokumente/Uni/Hiwi/2021/GG-Diaminosilane/csv/"+Name,skiprows=1,sep="\s+",names = ("x","y"))
    Integralrange = np.loadtxt("/home/steven/Dokumente/Uni/Hiwi/2021/GG-Diaminosilane/Integrale", skiprows=0, dtype='float',delimiter='\t')
    Stoffmengen = np.loadtxt("/home/steven/Dokumente/Uni/Hiwi/2021/GG-Diaminosilane/Stoffmengen", skiprows=0, dtype='float',delimiter=',')
    """
    Explanation of the files
    Daten:
    - link to the .csv with the NMR-Data
    - only data of the noise to calculate the standard deviation
    Datenvoll:
    - link to the .csv with the NMR-Data
    - all data
    Integralrange
    - link to the .txt with the limits of the integration of the individual peaks
    - Structure:
```

```
    Number_of_experiment lower_limit_starting_material upper_limit_starting_material lower_limit_mixed_substituted_product upper_limit_mixed_substituted_product lower_limit_dual_substituted_product upper_limit_dual_substituted_product
    Stoffmengen
    - link to the .txt with the used amount of substances of the starting materials
    - Structure:
    Number_of_experiment, amount_of_substance_of_the_first_diaminosilane, amount_of_substance_of_the_second_diaminosilane_or_the_amine
    """
    st_dev = np.std(Daten["y"])
    print("Standardabweichung: " + str(st_dev)) #shows the standard deviation
    Integral1 = np.array([item for item in Integralrange
    if item[0] == Nummer])
    IntegralEdukt = unumpy.uarray(Datenvoll.loc[(Datenvoll['x'] >= Integral1[0,1]) & (Datenvoll['x'] <= Integral1[0,2])],st_dev)
    IntegralMisch = unumpy.uarray(Datenvoll.loc[(Datenvoll['x'] >= Integral1[0,3]) & (Datenvoll['x'] <= Integral1[0,4])],st_dev)
    IntegralProdukt = unumpy.uarray(Datenvoll.loc[(Datenvoll['x'] >= Integral1[0,5]) & (Datenvoll['x'] <= Integral1[0,6])],st_dev)
    IntegralEdukt1 = sum(np.trapz(IntegralEdukt))
    print(IntegralEdukt1) #shows the value of the integral of the starting material
    IntegralMisch1 = sum(np.trapz(IntegralMisch))
    print(IntegralMisch1) #shows the value of the integral of the mixed substituted product
    IntegralProdukt1 = sum(np.trapz(IntegralProdukt))
    print(IntegralProdukt1) #shows the value of the integral of the dual substituted product
    Stoffmenge = np.array([item for item in Stoffmengen
    if item[0] == Nummer])
    if len(str(Nummer)) <= 2:# in case of the investigation of the reaction of a diaminosilane and an amine
    n0Amin=Stoffmenge[0,2]
    n0AS=Stoffmenge[0,1]
    if IntegralMisch1 != 0: #in case of more than one signal in the NMR-spectra
    if IntegralProdukt1 != 0: #in case of three peaks
    #calculation of the amount of substances of all substances contained
    nAS1=IntegralEdukt1/(IntegralEdukt1+IntegralMisch1+IntegralProdukt1)*n0AS
    print("[AS1]=" + str(nAS1)) #shows the value of the calculated amount of substance
    nAS12=IntegralMisch1/(IntegralEdukt1+IntegralMisch1+IntegralProdukt1)*n0AS
    print("[AS12]=" + str(nAS12)) #shows the value of the calculated amount of substance
    nAS2=IntegralProdukt1/(IntegralEdukt1+IntegralMisch1+IntegralProdukt1)*n0AS
    print("[AS2]=" + str(nAS2)) #shows the value of the calculated amount of substance
    #calculation of K1, K2 and 1/K2
    K1 = (nAS12*(nAS12+2*nAS2))/(nAS1*(n0Amin-nAS12-2*nAS2))
    print("K1=" + str(K1))
    K2 = ((nAS2*(nAS12+2*nAS2))/(nAS12*(n0Amin-nAS12-2*nAS2)))
    print("K2=" + str(K2))
    rezK2 = 1/((nAS2*(nAS12+2*nAS2))/(nAS12*(n0Amin-nAS12-2*nAS2)))
    print("1/K2=" + str(rezK2))
    if IntegralProdukt1 == 0: #in case of two peaks
    #calculation of the amount of substances of all substances contained
    nAS1=IntegralEdukt1/(IntegralEdukt1+IntegralMisch1+IntegralProdukt1)*n0AS
    print("[AS1]=" + str(nAS1)) #shows the value of the calculated amount of substance
    nAS12=IntegralMisch1/(IntegralEdukt1+IntegralMisch1+IntegralProdukt1)*n0AS
```

```
print("[AS12]=" + str(nAS12)) #shows the value of the calculated amount of substance
#calculation of K1
K1 = (nAS12/nAS1)
print("K1=" + str(K1))
if IntegralMisch1 == 0: #in case of just one Signal
print('just starting material')
if len(str(Nummer)) >= 4: # in case of the investigation of the reaction of two aminosilanes
n0AS1=Stoffmenge[0,1]
n0AS2=Stoffmenge[0,2]
#calculation of the amount of substances of all substances contained
nAS1=IntegralEdukt1/(IntegralEdukt1+IntegralMisch1+IntegralProdukt1)*(n0AS1+n0AS2)
print("[AS1]=" + str(nAS1)) #shows the value of the calculated amount of substance
nAS12=IntegralMisch1/(IntegralEdukt1+IntegralMisch1+IntegralProdukt1)*(n0AS1+n0AS2)
print("[AS12]=" + str(nAS12)) #shows the value of the calculated amount of substance
nAS2=IntegralProdukt1/(IntegralEdukt1+IntegralMisch1+IntegralProdukt1)*(n0AS1+n0AS2)
print("[AS2]=" + str(nAS2)) #shows the value of the calculated amount of substance
#calculation of K1
K1 = (nAS12*nAS12)/(nAS1*nAS2)
print("K1 = " + str(K1))
#plotting of the NMR-spectra with the used limits of the integration
plt.figure(figsize=(50,15),dpi=150)
plt.plot(Datenvoll['x'], Datenvoll['y'])
plt.axvline(x=Integral1[0,1], ymin=0–100, ymax=5e8)
plt.axvline(x=Integral1[0,2], ymin=0–100, ymax=5e8)
plt.axvline(x=Integral1[0,3], ymin=0–100, ymax=5e8)
plt.axvline(x=Integral1[0,4], ymin=0–100, ymax=5e8)
plt.axvline(x=Integral1[0,5], ymin=0–100, ymax=5e8)
plt.axvline(x=Integral1[0,6], ymin=0–100, ymax=5e8)
plt.xlim(-4,-18)
plt.savefig("/home/steven/Dokumente/Uni/Hiwi/2021/GG-Diaminosilane/Abbildungen/" + Name + '.pdf')
plt.show()
```

References

Barone V., Cossi M., Quantum calculation of molecular energies and energy gradients in solution by a conductor solvent model. J. Phys. Chem. A, 1998, 102(11), 1995–2001. doi: 10.1021/jp9716997.

Bittrich H.J., Haberland D., Just G., Leitfaden der chemischen Kinetik. Deutscher Verlag der Wissenschaften. Berlin, 1973. doi: 10.1002/zfch.19750150424.

Brandenburg J.G., Bannwarth C., Hansen A., Grimme S., B97-3c: A revised low-cost variant of the B97-D density functional method. J. Chem. Phys., 2018, 148(6), 064104. doi: 10.1063/1.5012601.

Hellweg A., Hättig C., Höfener S., Klopper W., Optimized accurate auxiliary basis sets for RI-MP2 and RI-CC2 calculations for the atoms Rb to Rn. Theor. Chem. Acc., 2007, 117(4), 587–597. doi: 10.1007/s00214-007-0250-5.

Kozuch S., Martin J.M.L., Spin-component-scaled double hybrids: An extensive search for the best fifth-rung functionals blending DFT and perturbation theory. J. Comput. Chem., 2013, 2327–2344. doi: 10.1002/jcc.23391.

Neese F., Software update: the ORCA program system, version 4.0. WIREs Comput. Mol. Sci., 2017, 8(1). doi: 10.1002/wcms.1327.

Weigend F., Hartree-Fock exchange fitting basis sets for H to Rn. J. Comput. Chem., 2007, 29(2), 167–175. doi: 10.1002/jcc.20702.

Weigend F., Ahlrichs R., Balanced basis sets of split valence, triple zeta valence and quadruple zeta valence quality for H to Rn: Design and assessment of accuracy. Phys. Chem. Chem. Phys., 2005, 7(18), 3297. doi: 10.1039/b508541a.