Supporting information for:

Molecular Structures of the Silicon Pyridine-2-(thi)olates $Me_3Si(pyX)$, $Me_2Si(pyX)_2$ and $Ph_2Si(pyX)_2$ (py = 2-Pyridyl, X = O, S), and their Intra- and Intermolecular Ligand Exchange in Solution

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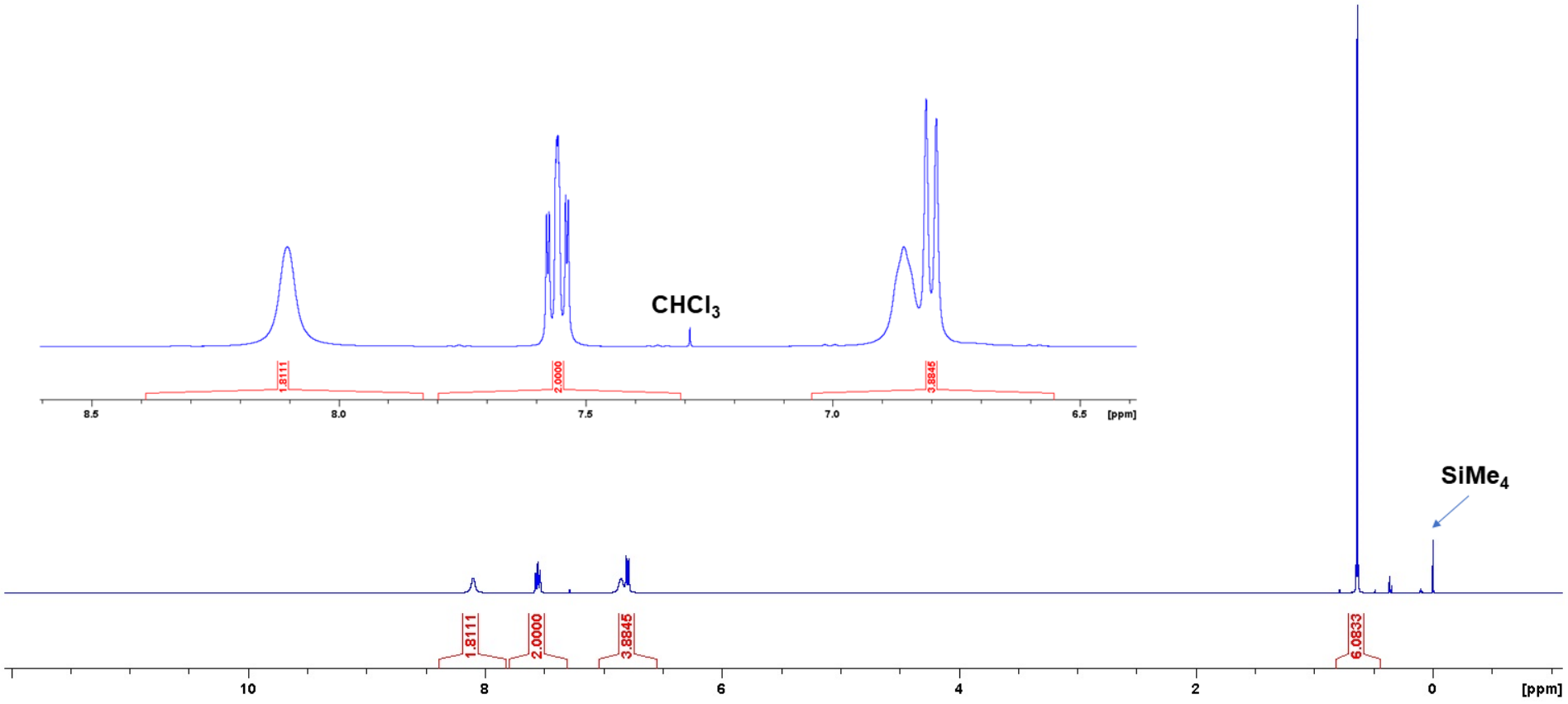

Figure S1. ^{1}H NMR spectrum of **2a** in $CDCl_3$ (full spectrum and magnified inset of group of signals).

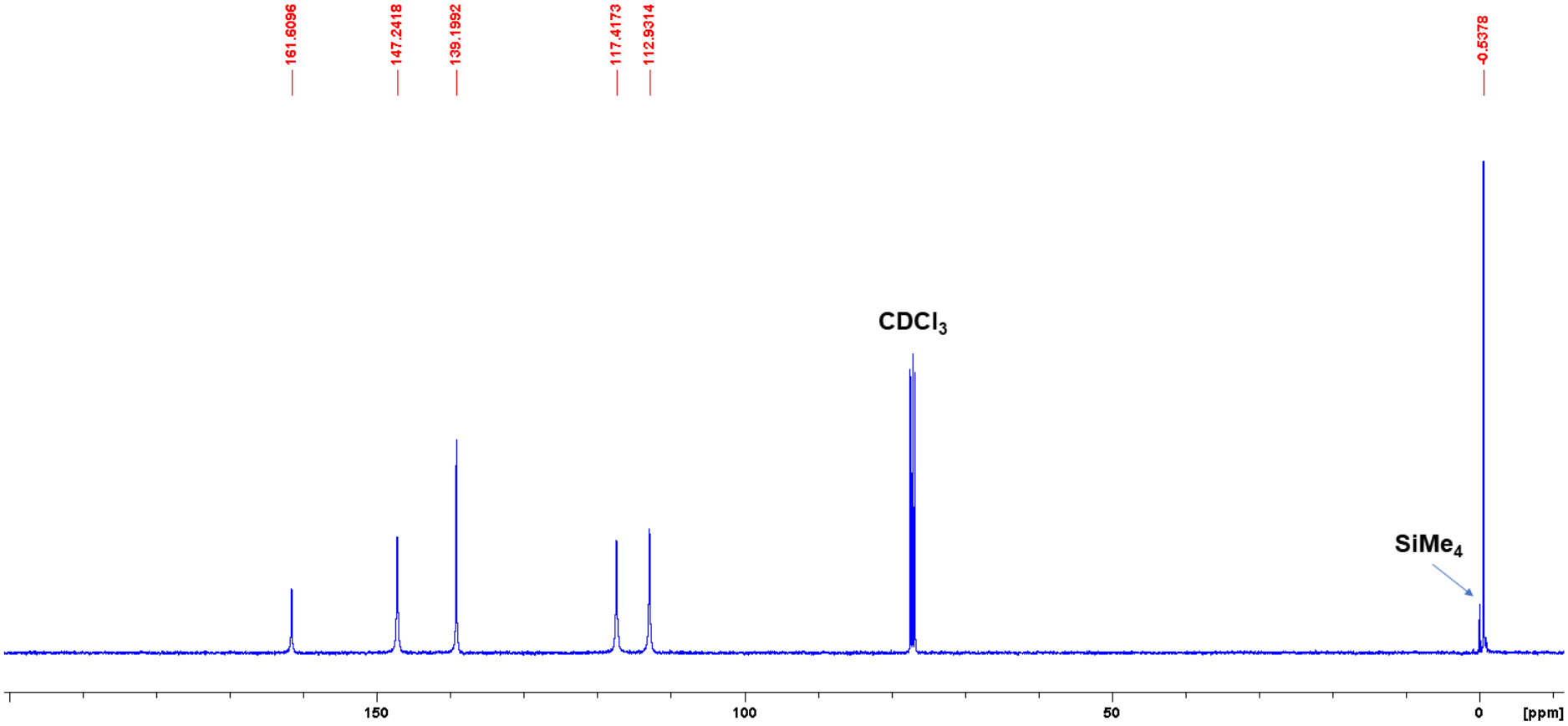

Figure S2. $^{13}C\{^{1}H\}$ NMR spectrum of **2a** in $CDCl_3$.

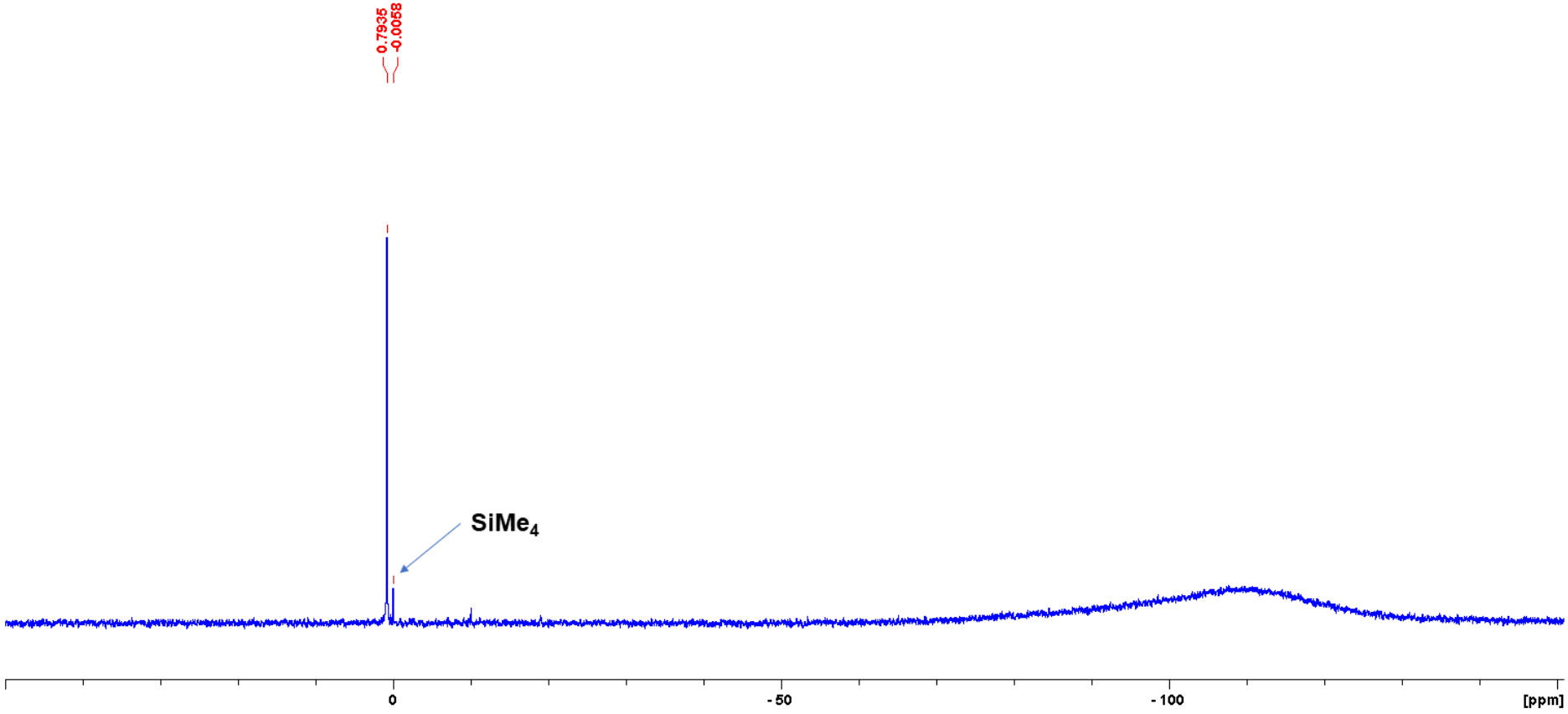

Figure S3. $^{29}Si\{^{1}H\}$ NMR spectrum of **2a** in $CDCl_3$.

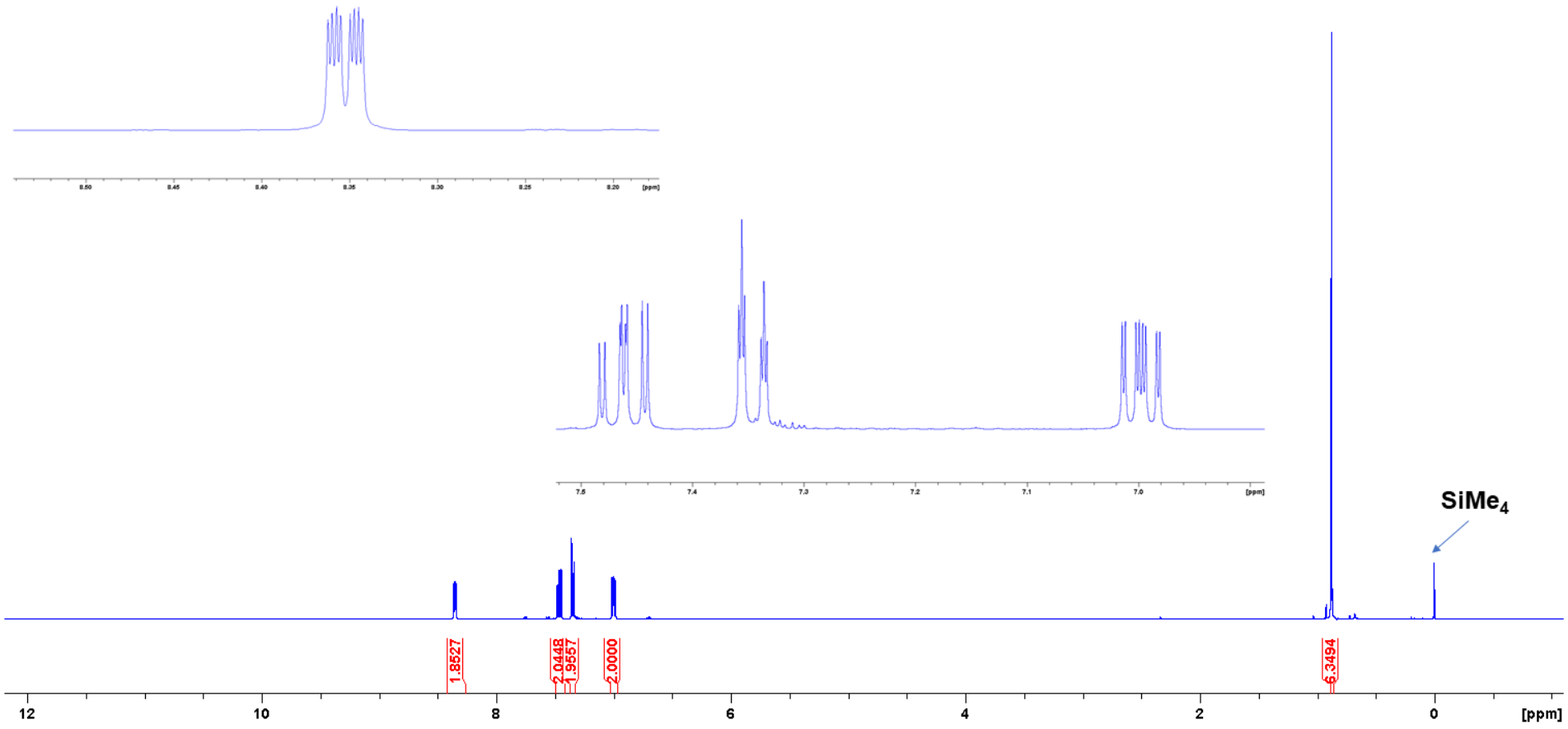

Figure S4. ^{1}H NMR spectrum of **2b** in $CDCl_3$ (full spectrum and magnified insets of group of signals).

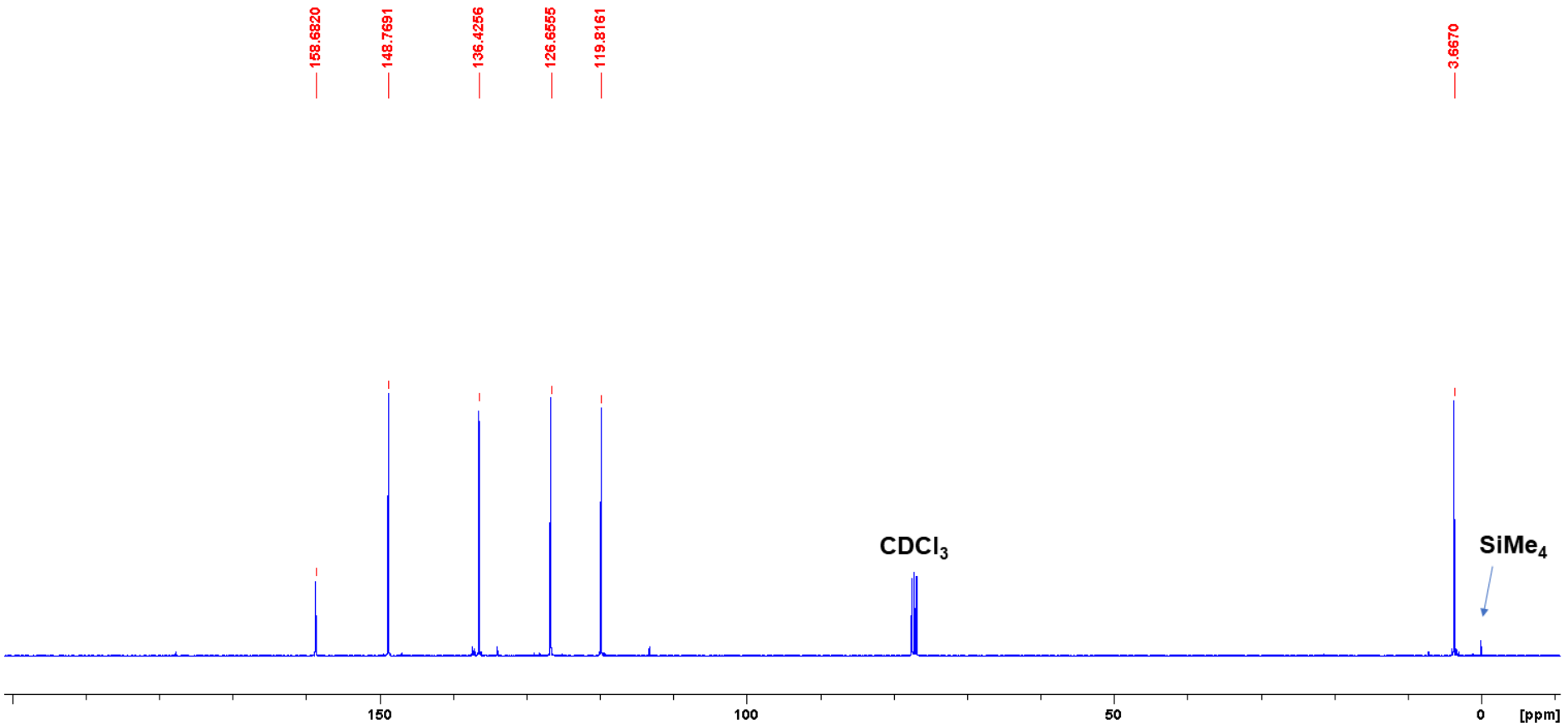

Figure S5. $^{13}C\{^{1}H\}$ NMR spectrum of **2b** in $CDCl_3$.

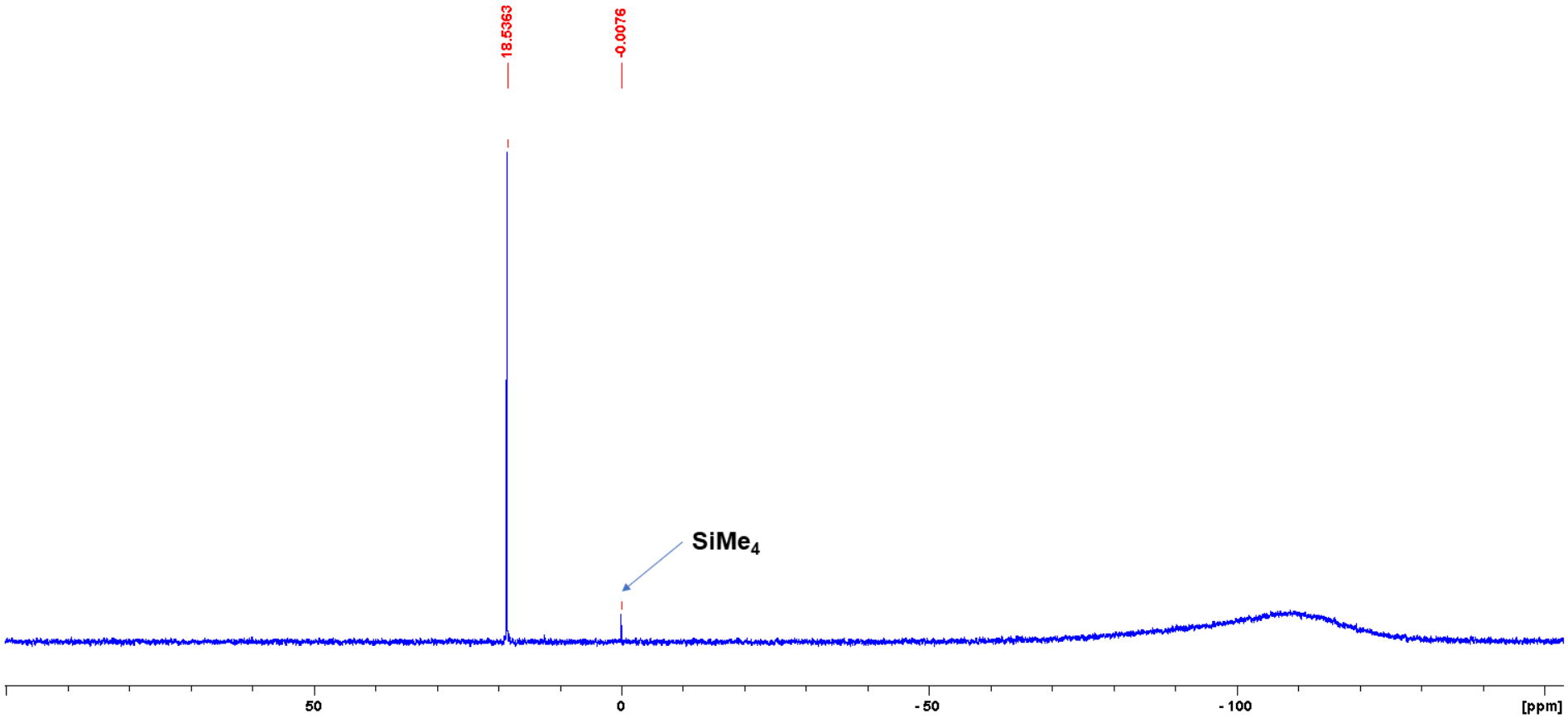

Figure S6. $^{29}Si\{^{1}H\}$ NMR spectrum of **2b** in $CDCl_3$.

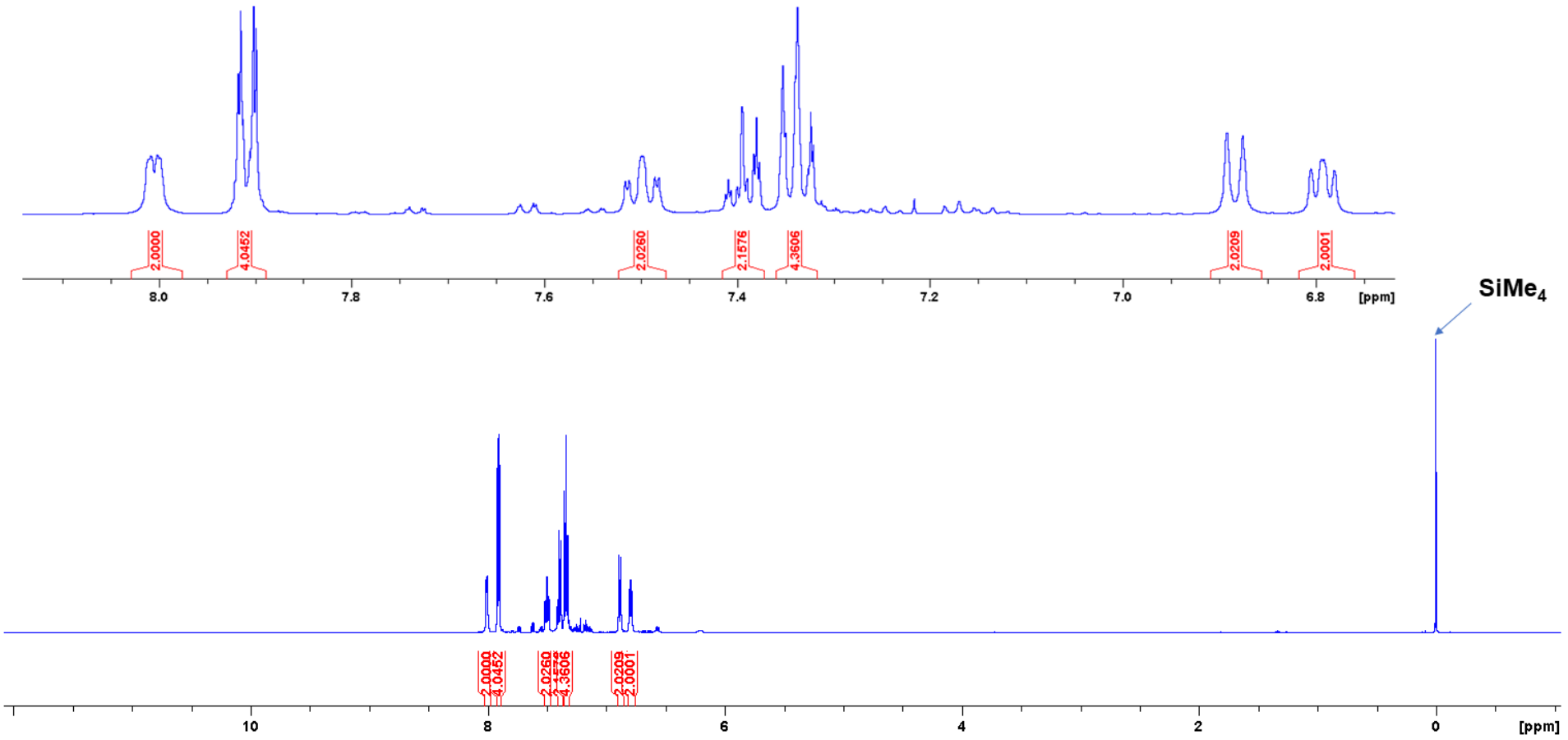

Figure S7. ^{1}H NMR spectrum of **3a** in $CDCl_3$ (full spectrum and magnified insets of group of signals).

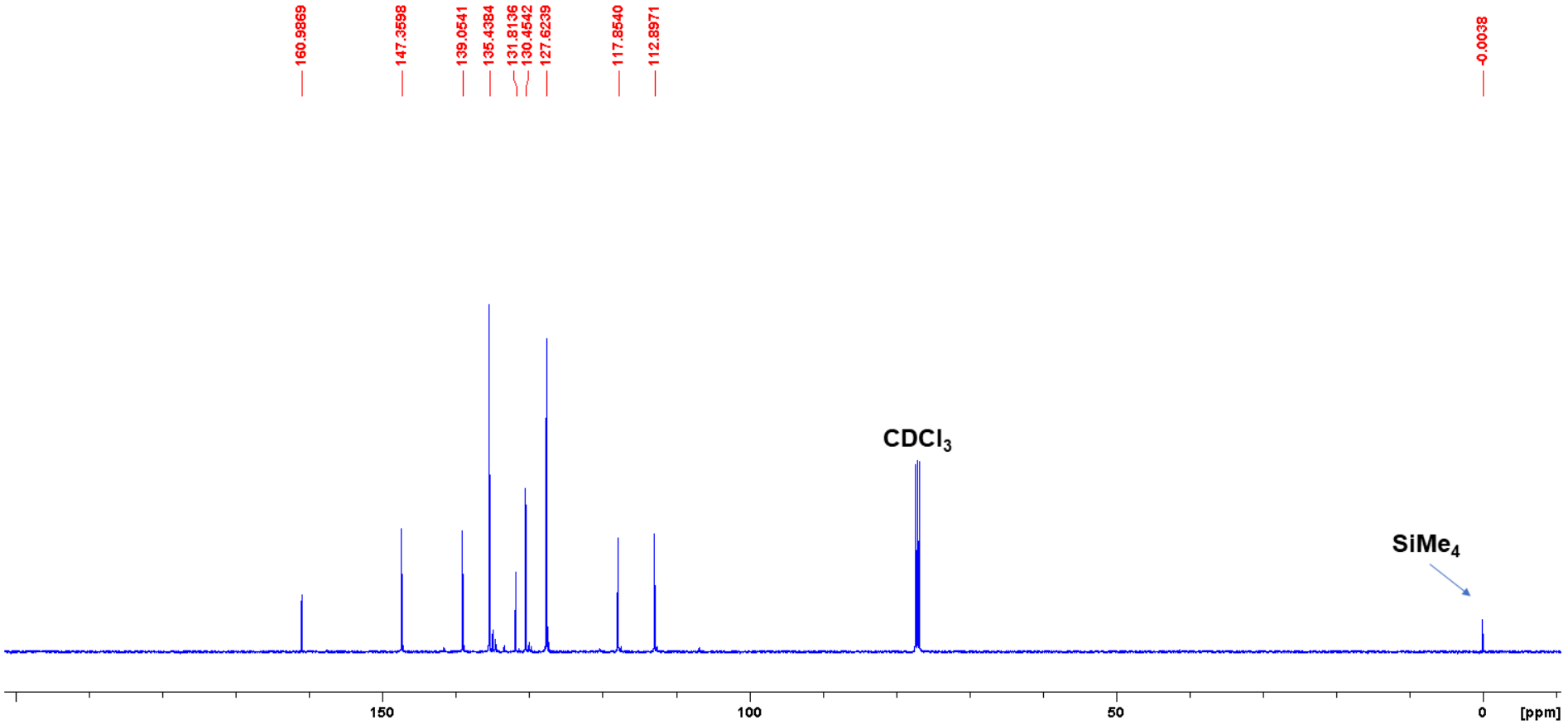

Figure S8. $^{13}C\{^{1}H\}$ NMR spectrum of **3a** in $CDCl_3$.

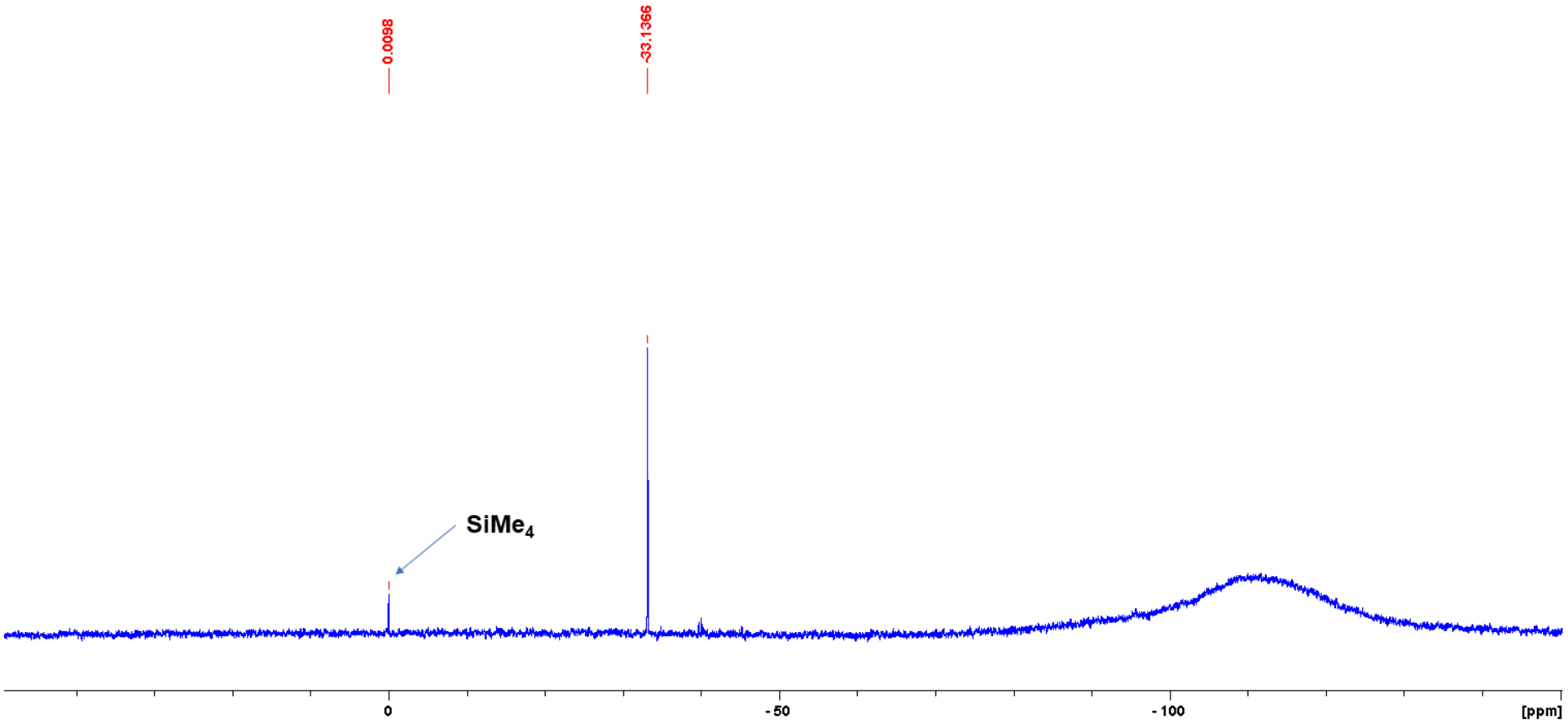

Figure S9. $^{29}Si\{^{1}H\}$ NMR spectrum of **3a** in $CDCl_3$.

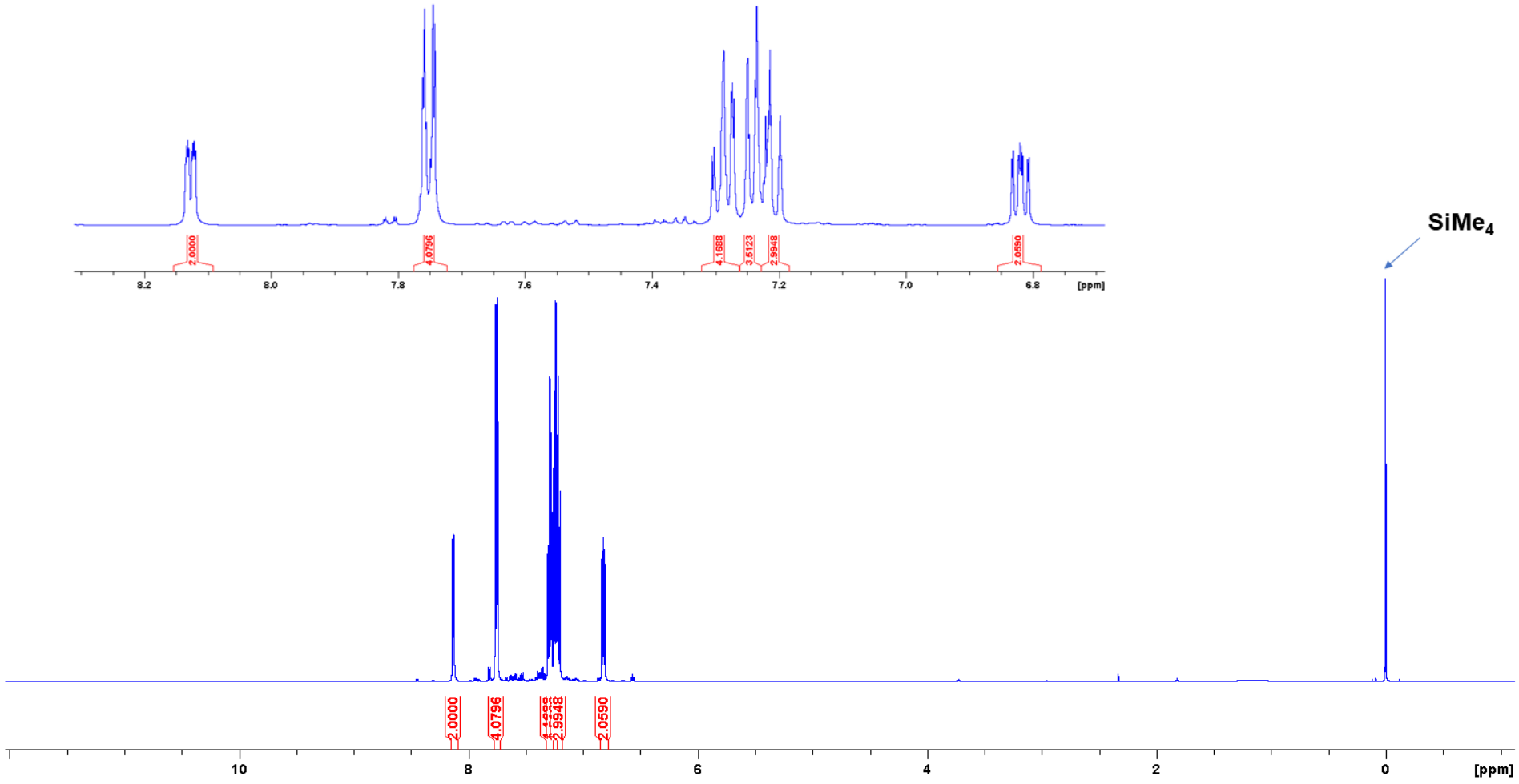

Figure S10. ^{1}H NMR spectrum of **3b** in $CDCl_3$ (full spectrum and magnified inset of group of signals).

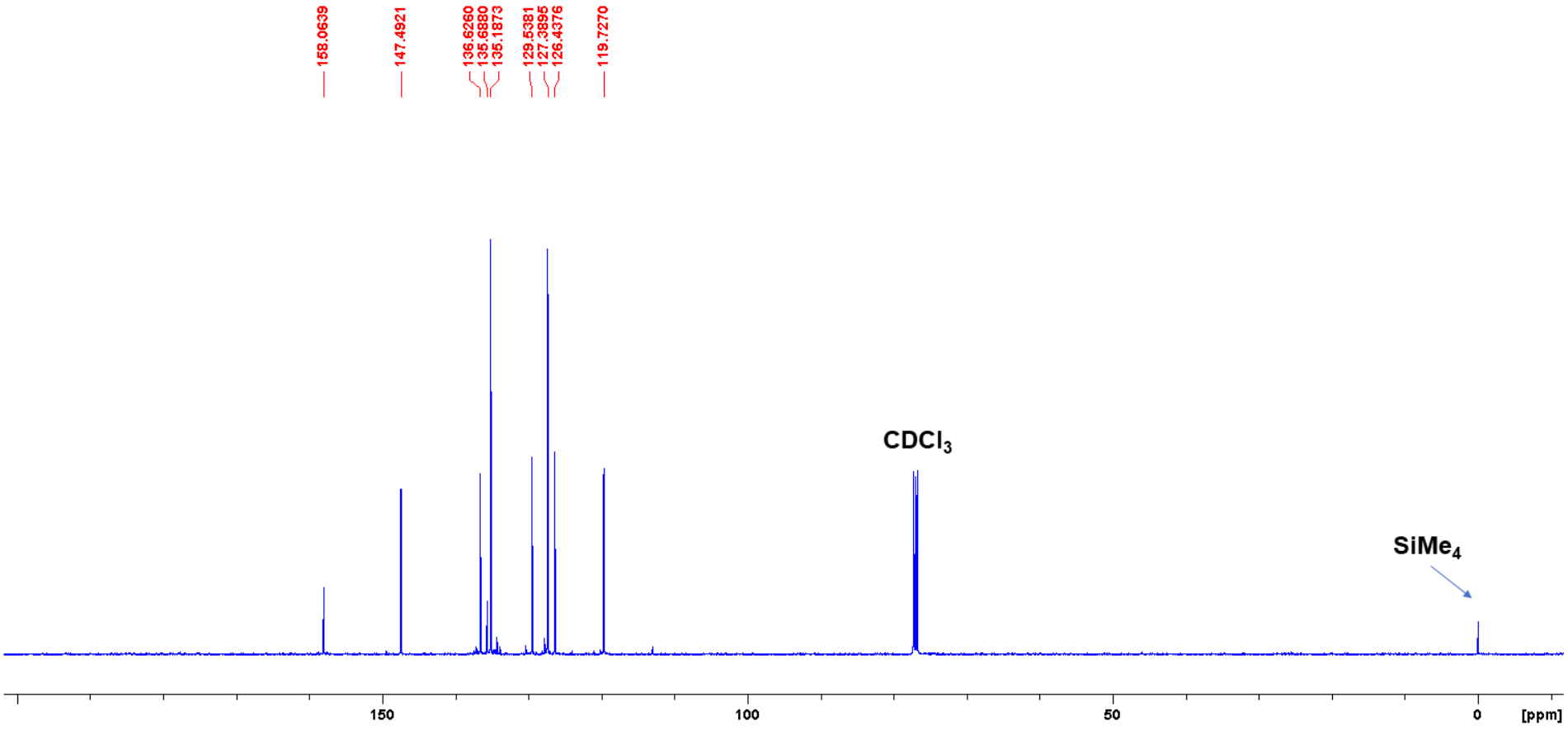

Figure S11. $^{13}C\{^{1}H\}$ NMR spectrum of **3b** in $CDCl_3$.

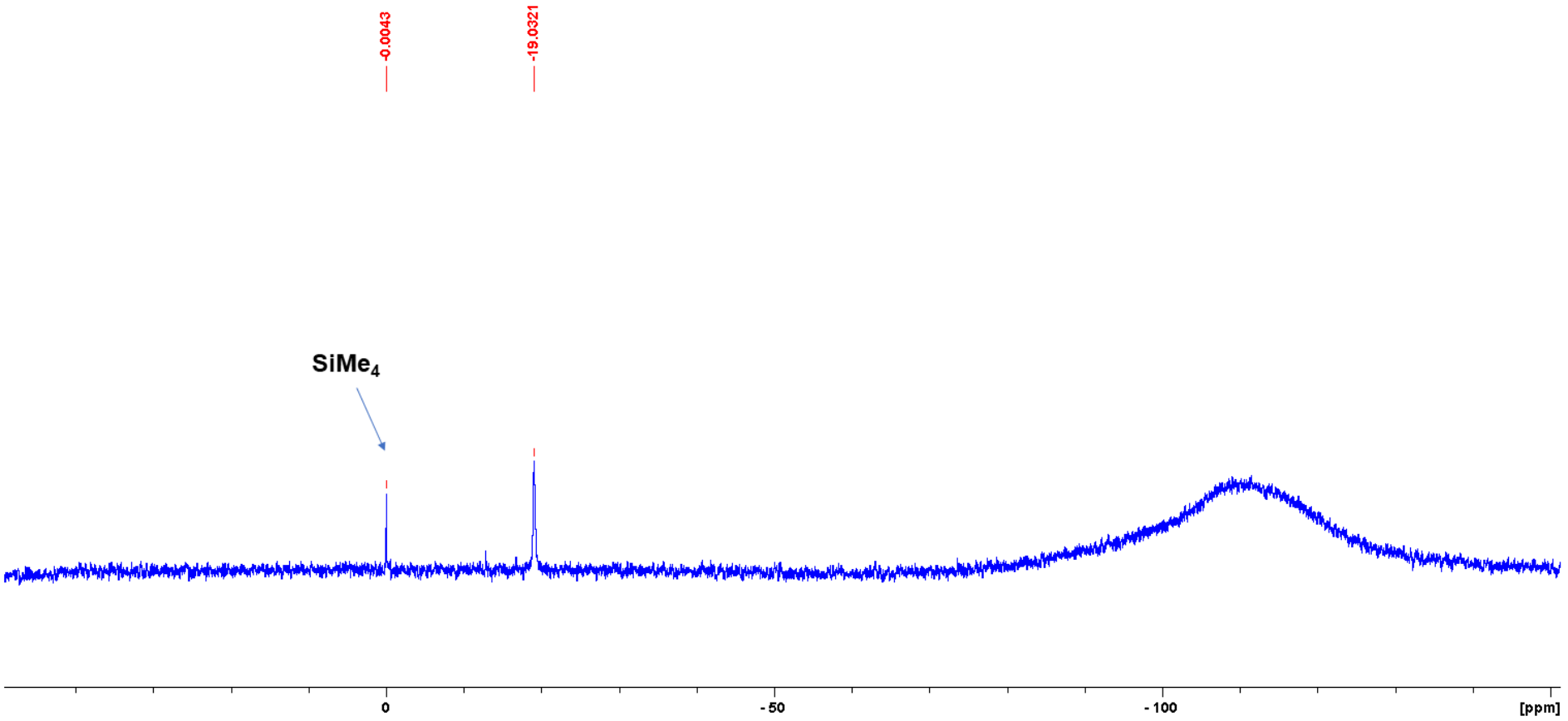

Figure S12. $^{29}Si\{^{1}H\}$ NMR spectrum of **3b** in $CDCl_3$.

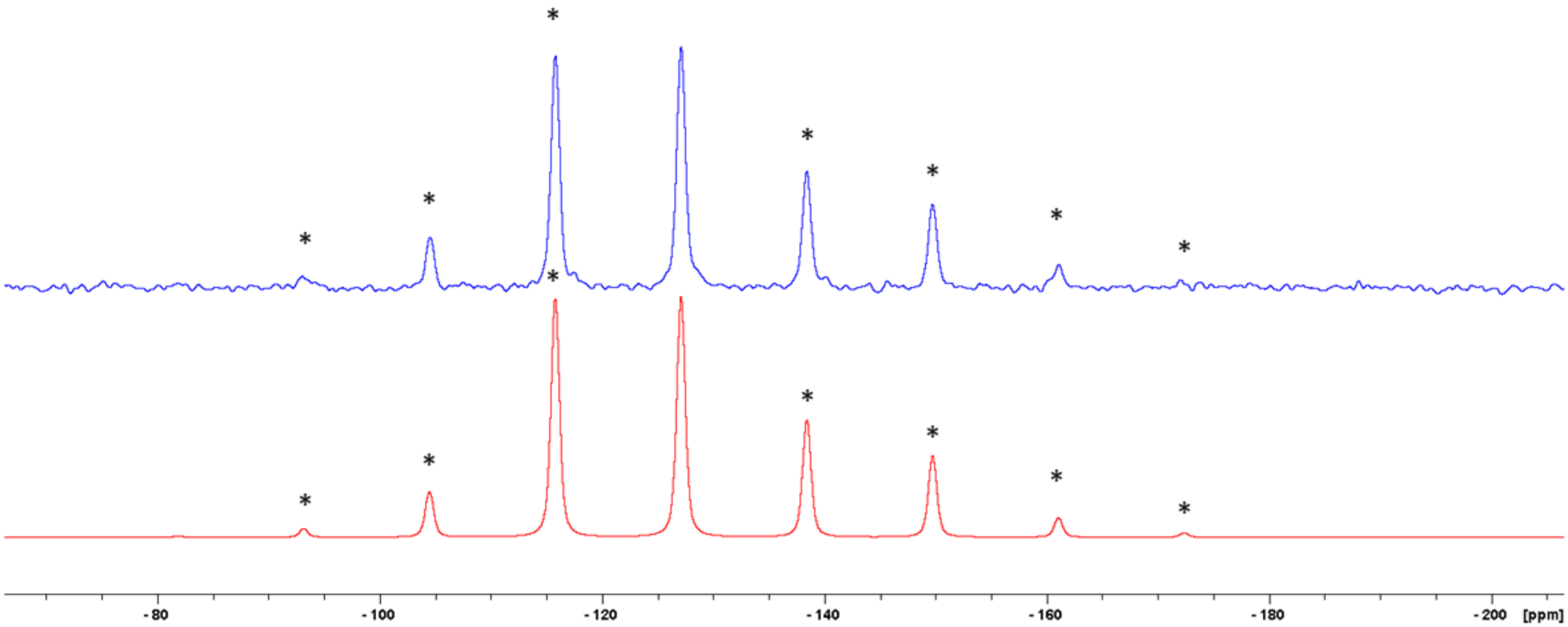

Figure S13. ^{29}Si CP/MAS NMR spectrum of **3b**[1] (MAS frequency 900 Hz, spinning side bands are asterisked) showing the experimental spectrum (top, blue trace) and the spinning side band spectrum simulated from the CSA tensor derived therefrom (bottom, red trace).

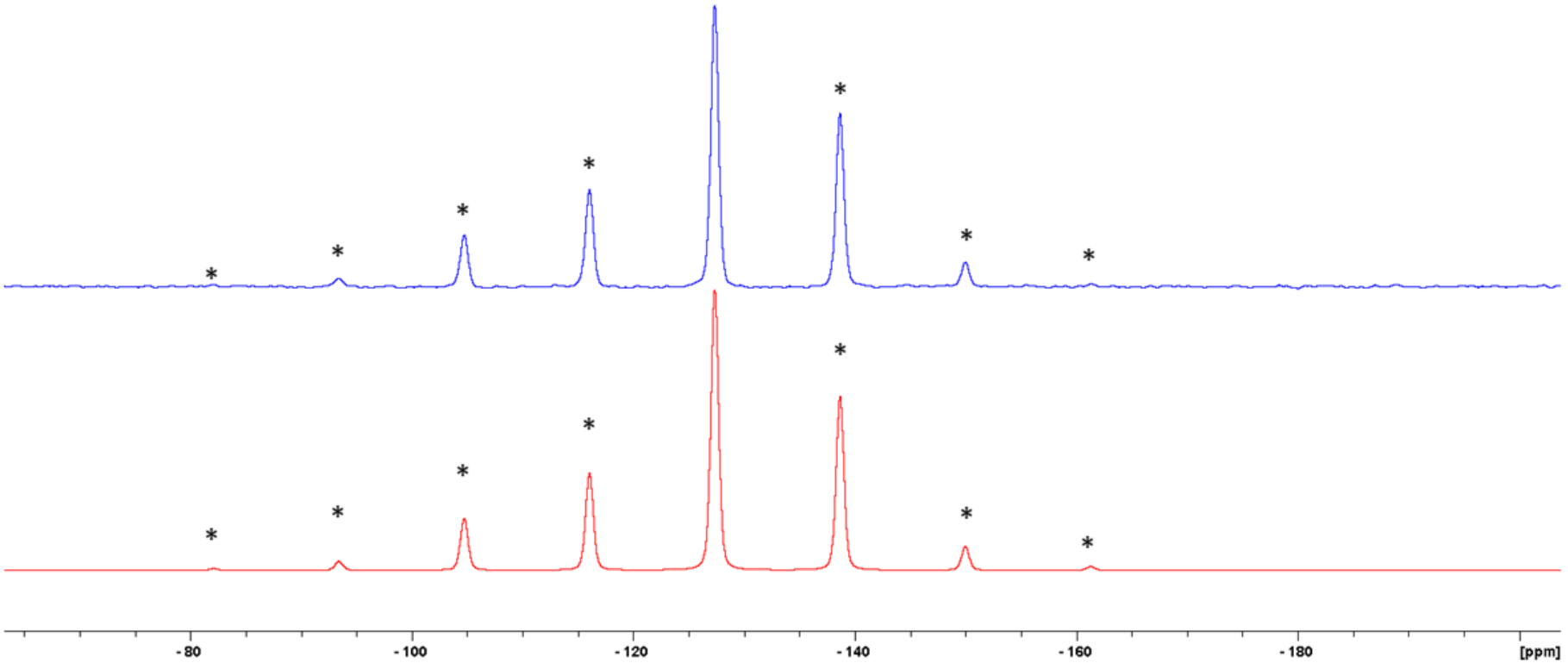

Figure S14. ^{29}Si CP/MAS NMR spectrum of **3b²** (MAS frequency 900 Hz, spinning side bands are asterisked) showing the experimental spectrum (top, blue trace) and the spinning side band spectrum simulated from the CSA tensor derived therefrom (bottom, red trace).

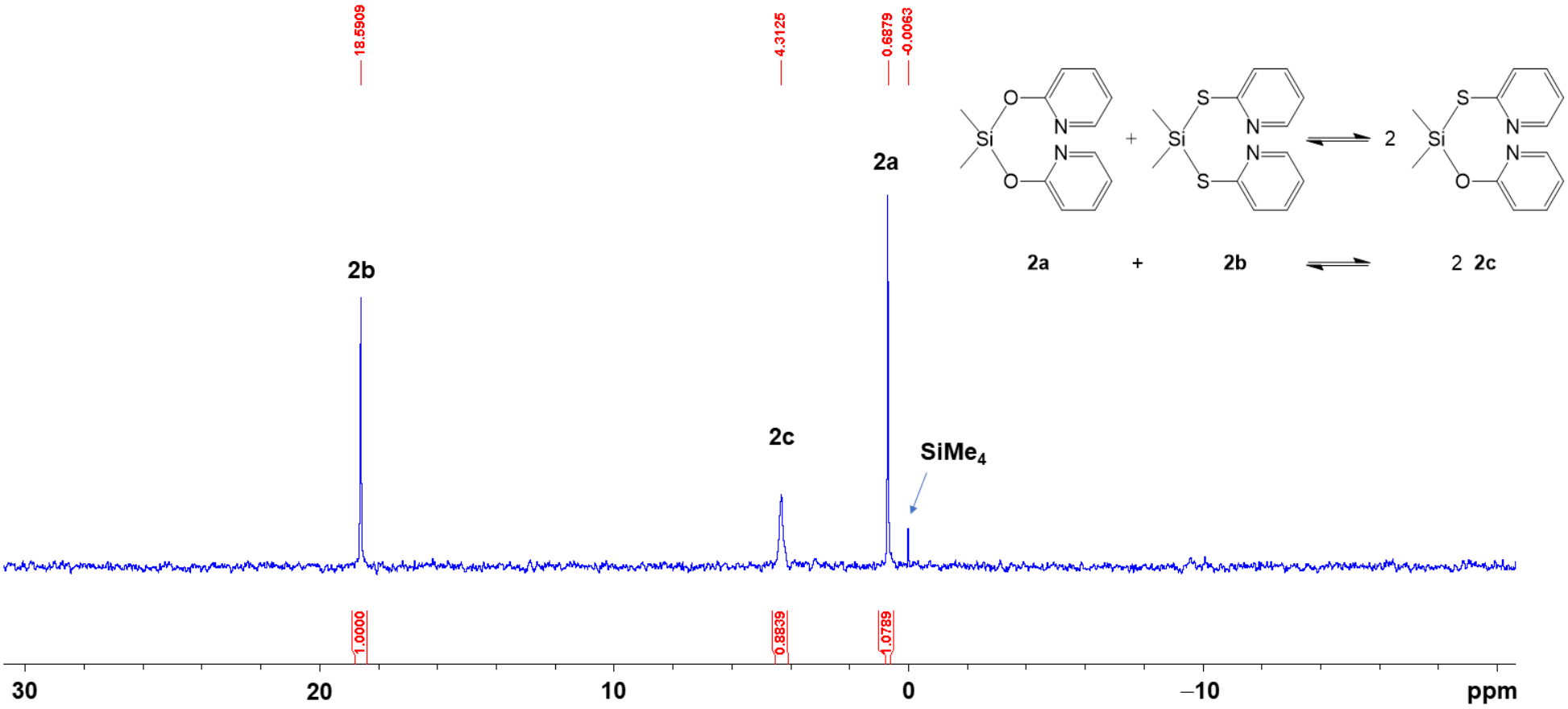

Figure S15. $^{29}Si\{^{1}H\}$ NMR spectrum of an equimolar mixture of **2a** and **2b** in $CDCl_3$ (with integrals of the signal intensities of **2a**, **2b** and **2c**).

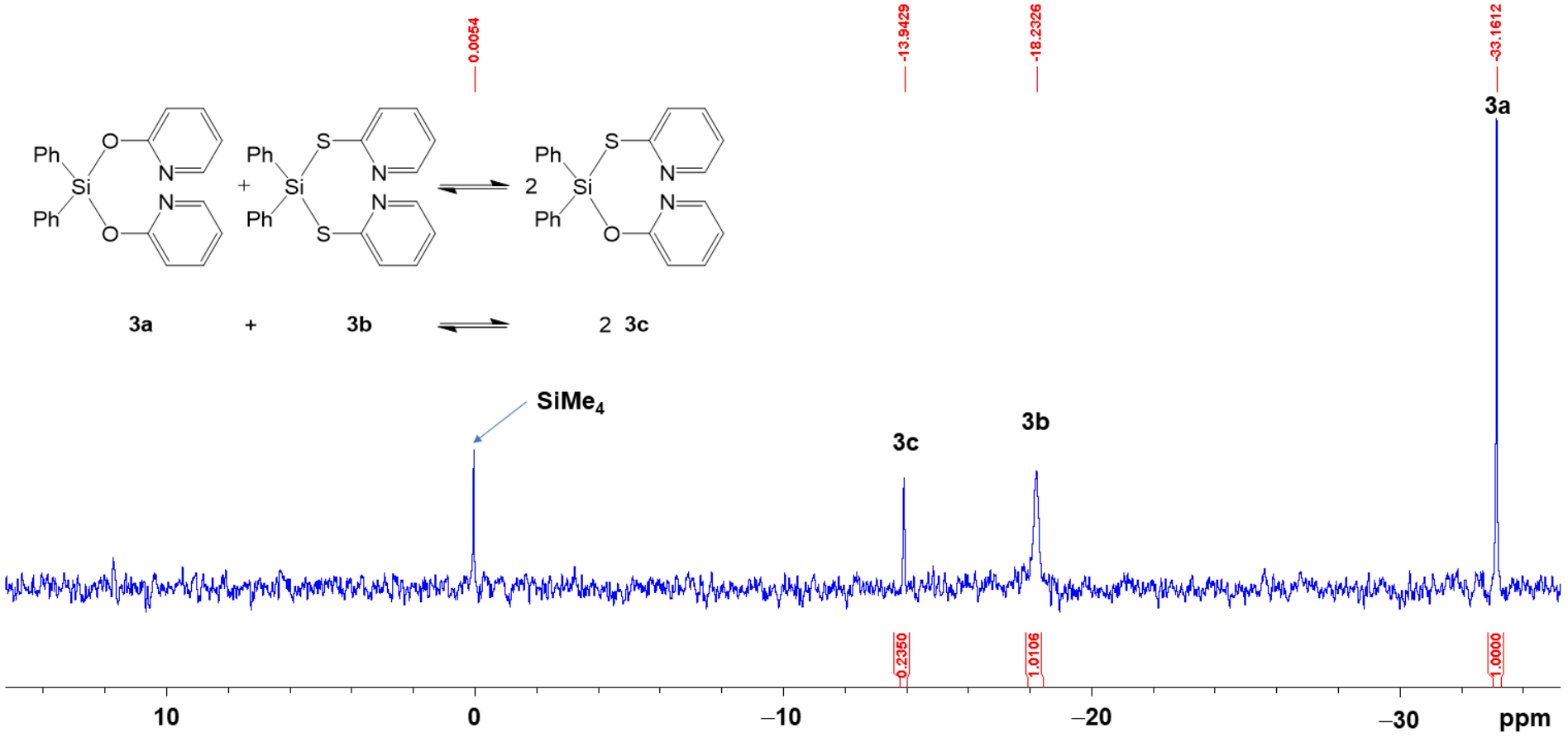

Figure S16. $^{29}Si\{^{1}H\}$ NMR spectrum of an equimolar mixture of **3a** and **3b** in $CDCl_3$ (with integrals of the signal intensities of **3a**, **3b** and **3c**).

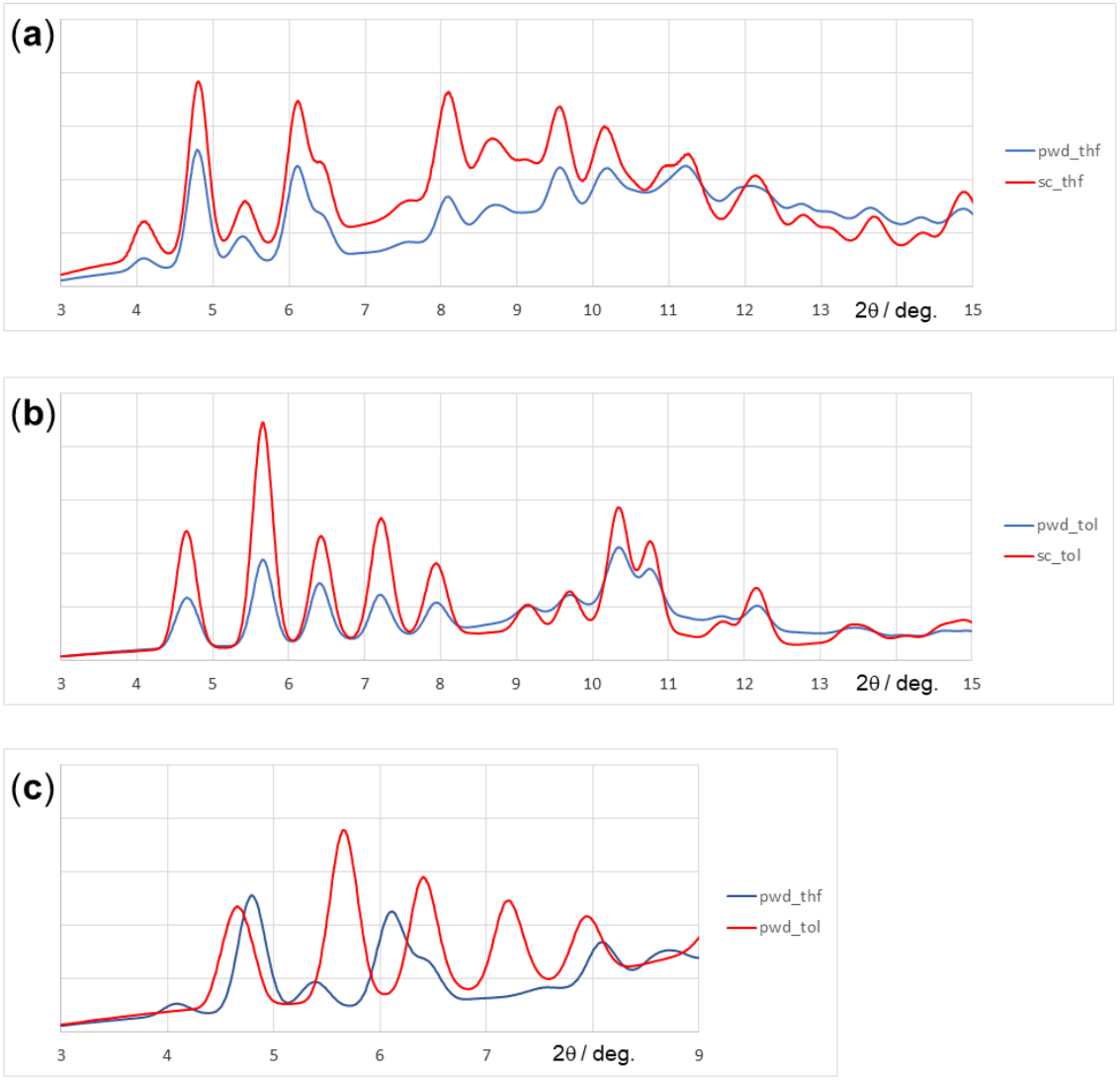

Figure S17. X-ray powder diffraction patterns of compounds **3b**^{1} and **3b**^{2} (modification 1) recorded with Mo Kα radiation using Gandolfi scans. (**a**) Diffraction pattern recorded from a powdered bulk sample (blue trace) and from a single crystal (red trace) of compound **3b**^{1}. (**b**) Diffraction pattern recorded from a powdered bulk sample (blue trace) and from a single crystal (red trace) of modification 1 of compound **3b**^{2}. (**c**) Superposition (low-angle fraction) of the diffraction patterns recorded from powdered bulk samples of compound **3b**^{1} (blue trace) and of modification 1 of compound **3b**^{2} (red trace).

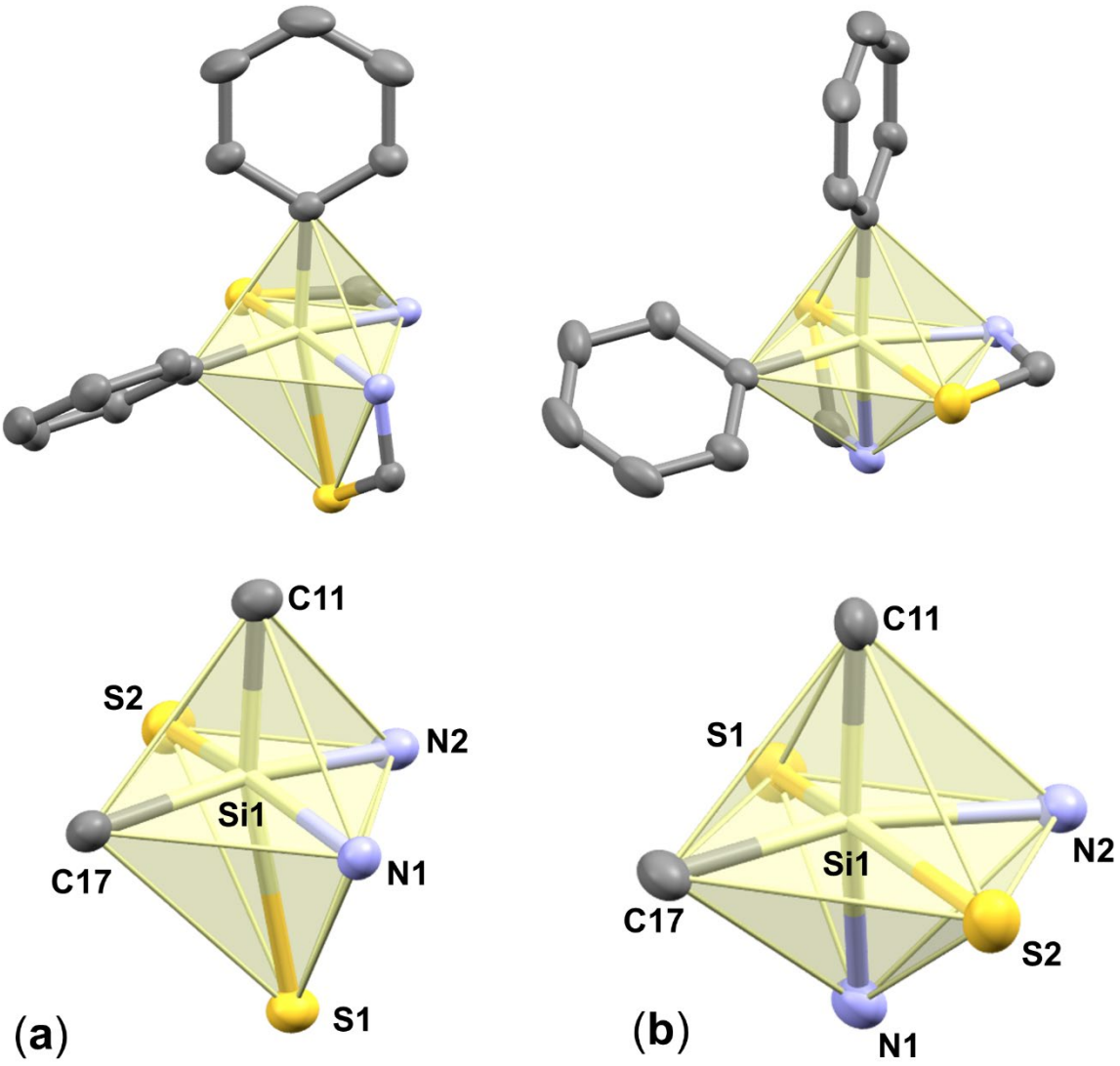

Figure S18. Graphical representations of the Si coordination polyhedra of compounds **3b**[1] (**a**) and **3b**[2] (modification 1) (**b**) with atom labels (bottom) and with some additional atoms attached for a better image of the polyhedron within the molecule (top). Thermal displacement ellipsoids are shown at the 50% probability level.

Atomic coordinates and total energies:

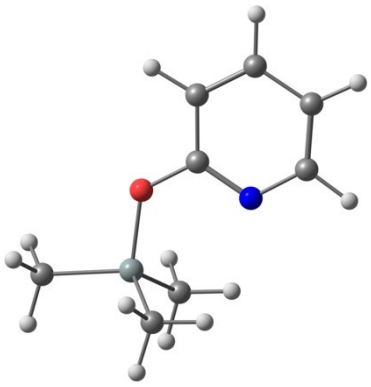

Figure S19. Optimized molecular structure of **1a^{O0}**.

PBE0:
final single point energy: -733.115769572522 a.u.
final Gibbs free energy: -732.95891063 a.u.
B2T-PLYP:
final single point energy: -733.182559307509 a.u.

Table S1. Atomic coordinates for optimized structure of **1a^{O0}**.

Si	1.64226471121404	11.63269310574833	9.49661201628772
O	1.58421658680012	9.95543507091513	9.25036189387188
N	3.72162905143113	9.56589041958931	9.95647235918383
C	2.57855190888991	9.09647613604556	9.48195373332088
C	2.36439650042564	7.74172956039284	9.21055577732996
H	1.40687258648760	7.41659178704202	8.82627009997140
C	3.39909098465388	6.86231954057217	9.44542336980121
H	3.26792759712726	5.80530965742259	9.24587326650475
C	4.60860233054710	7.34426277758359	9.93807054293026
H	5.44447530109052	6.68557443359806	10.13193038850608
C	4.71287688997745	8.70034428215870	10.17561321078449
H	5.63505033517565	9.12380672723781	10.56160924692602
C	2.96517778476654	12.40711061654416	8.44216630863426
H	3.96137818200530	12.13976984515202	8.79410531297085
H	2.86607620753795	13.49569005210375	8.46950298591259
H	2.86658692233509	12.08813268935693	7.40182030417734
C	1.86378833281038	12.01457916002057	11.30432335880757
H	1.11965366815576	11.48737732102761	11.90583332809422
H	1.73281919626403	13.08691781500667	11.47296307439932
H	2.85688875062564	11.72911283332268	11.65180130951820
C	-0.04489244496929	12.16127755802551	8.91632640742531
H	-0.19467786170256	11.90755670763437	7.86463355664270
H	-0.16006611727093	13.24270001411969	9.02331441368990
H	-0.83093940437827	11.67769388937980	9.50047973430907

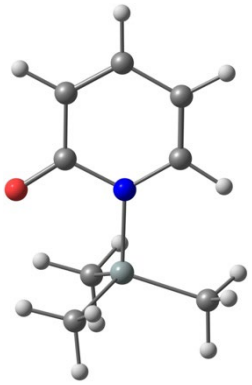

Figure S20. Optimized molecular structure of **1a**^{N}.

PBE0:

final single point energy: -733.106672500659 a.u.

final Gibbs free energy: -732.9491742 a.u.

B2T-PLYP:

final single point energy: -733.169954670087 a.u.

Table S2. Atomic coordinates for optimized structure of **1a**^{N}.

Si	3.06495509912255	11.18865502097981	8.95652280554664
O	1.51895111814178	9.40461257538295	7.41654987734985
N	2.68586317315991	9.45333202238622	9.35545179696170
C	1.88709543203838	8.79246992885387	8.42381328027453
C	1.55630013027601	7.42960827642696	8.72660604440754
H	0.93432201249191	6.90803236011042	8.01136420580282
C	2.00711355617696	6.83253600009054	9.86138318160422
H	1.74366529441023	5.80156369284731	10.07004688687909
C	2.81717610115456	7.54503102746666	10.77290747315198
H	3.18739065280841	7.09034127874271	11.68022427592883
C	3.12548245499655	8.83538356258612	10.48270342653188
H	3.73931331932488	9.43257020797432	11.14273908143729
C	4.03210640294363	11.26457399651166	7.37127769502850
H	4.90095616285982	10.60415582118015	7.42119088545945
H	4.39550673468980	12.28453375308252	7.21974604861647
H	3.42155500615978	10.97632815228424	6.51753003518082
C	4.14622870091864	11.78567712332376	10.35688896080022
H	3.64101562875853	11.75322691619138	11.32453922856078
H	4.40382128666819	12.82918871531347	10.15593201011065
H	5.08098856309126	11.22574249132984	10.43128618366594
C	1.48108359738076	12.16114326512790	8.94578424538081
H	0.83881491763027	11.86689618983452	8.11731100378915
H	1.70921719744193	13.22648039635110	8.85599582541736
H	0.93786626835522	12.01236174862139	9.88193838211330

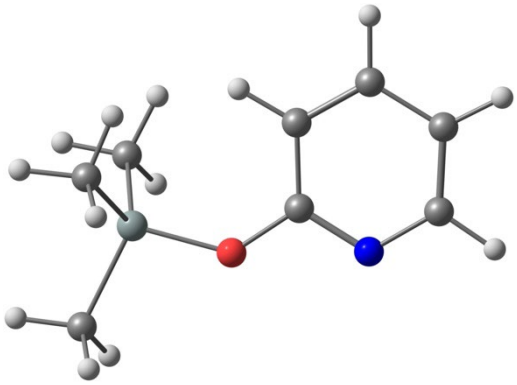

Figure S21. Optimized molecular structure of **1a**^{O180}.

PBE0:

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final Gibbs free energy: -732.95426769 a.u.

B2T-PLYP:

final single point energy: -733.177586030146 a.u.

Table S3. Atomic coordinates for optimized structure of **1a** ^{O180}.

Si	-0.36229981055877	9.77907772110308	8.83538435279658
O	1.31796104688907	9.86865671819777	8.82906123688020
N	3.50761112090744	9.38895201277160	8.83895118152150
C	2.26914030721977	8.94021329270512	8.69437547758556
C	1.98151302944634	7.59974309399788	8.41766830232536
H	0.96031316829266	7.26381033623869	8.30197425723522
C	3.03353491477278	6.71476630308153	8.29348230480768
H	2.83744878210907	5.67060711767835	8.07992253918464
C	4.33450236554300	7.17607523929180	8.44334920234419
H	5.18635503286474	6.51557394679751	8.35279593772077
C	4.50904316743832	8.52098959261506	8.71443474260440
H	5.50716328018521	8.92999167772427	8.83967071633193
C	-0.87071075952651	11.54167601427691	9.11868312947662
H	-0.49298449062698	11.90759561584730	10.07566809875439
H	-1.95991324894210	11.62779344410965	9.12590883297577
H	-0.48337072289563	12.18750010712919	8.32786092494361
C	-0.92214444314118	8.67996838882514	10.23063036398813
H	-0.61350983443825	7.64177744985527	10.09664346341673
H	-2.01323229032948	8.69834594512804	10.29658967555981
H	-0.52090233910743	9.03529935140675	11.18241635401218
C	-0.98325909774809	9.17008648046828	7.18740281304459
H	-0.56060327126370	9.76397554863762	6.37383392835303
H	-2.07081235747991	9.27706754300549	7.15150912712862
H	-0.74662269761035	8.12091362310752	7.00392391600834

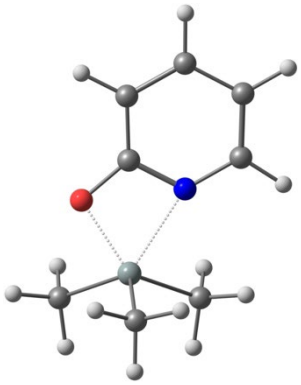

Figure S22. Optimized molecular structure of **1a**^{TS}.

PBE0:

final single point energy: -733.085804038855 a.u.
final Gibbs free energy: -732.92717431 a.u.

Table S4. Atomic coordinates for optimized structure of **1a**^{TS}.

Si	-0.597454000	1.112969000	-0.147809000
O	-1.045757000	-0.449697000	-1.176030000
N	0.579671000	-0.670695000	0.247405000
C	-0.164390000	-1.289527000	-0.695035000
C	0.042335000	-2.648349000	-1.008505000
H	-0.547429000	-3.140469000	-1.779821000
C	1.002741000	-3.324997000	-0.265221000
H	1.172318000	-4.385681000	-0.453185000
C	1.745337000	-2.673197000	0.736976000
H	2.483298000	-3.206113000	1.331589000
C	1.502398000	-1.324818000	0.962241000
H	2.027626000	-0.744662000	1.722954000
C	0.516879000	2.033673000	-1.355501000
H	1.578153000	1.812943000	-1.177236000
H	0.371701000	3.114676000	-1.211734000
H	0.278426000	1.790347000	-2.398662000
C	-0.115850000	1.673594000	1.614218000
H	-0.623977000	1.079179000	2.387638000
H	-0.411596000	2.724416000	1.755524000
H	0.968072000	1.594308000	1.783802000
C	-2.410447000	1.655160000	-0.222959000
H	-2.839640000	1.542448000	-1.226593000
H	-2.513934000	2.697277000	0.110565000
H	-2.998480000	1.027212000	0.465378000

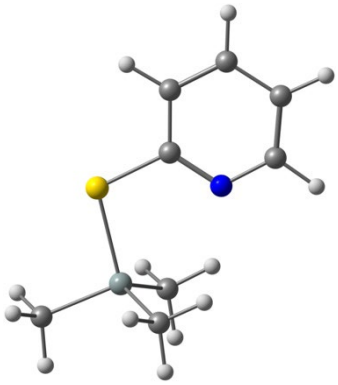

Figure S23. Optimized molecular structure of **1b**^{S0}.

PBE0:

final single point energy: -1057.6378331962 a.u.

final Gibbs free energy: -1057.48480527 a.u.

B2T-PLYP:

final single point energy: -1057.66436563872 a.u.

Table S5. Atomic coordinates for optimized structure of **1b**^{S0}.

Si	1.51395315432863	11.74017915482680	9.45953345807495
S	1.03429633916081	9.66625529171296	8.99734743136695
N	3.54672024082379	9.44388597705147	9.89036306392399
C	2.50373602108898	8.78315673620272	9.40245732231337
C	2.51447757906052	7.40193502970686	9.19200080656339
H	1.64092057707917	6.90530920384770	8.78982232957921
C	3.65904342258437	6.69873718146588	9.50834109761625
H	3.69718219921448	5.62654340747605	9.35633118479833
C	4.75508469765323	7.38206863753093	10.02039562708109
H	5.67123588908599	6.86889807568345	10.28104181118605
C	4.64378555785960	8.75000027346710	10.18957865345544
H	5.47452829216600	9.32588374066332	10.58588188187890
C	2.91480005077170	12.36445837231293	8.40110626356178
H	3.84417731843091	11.84871621608500	8.63985995415529
H	3.05253331435077	13.43524005460189	8.57694550381028
H	2.69237891901759	12.21803666430859	7.34245222734806
C	1.83547553355389	11.97073376034966	11.28032330093722
H	0.97996443673578	11.63232303056497	11.86788704131676
H	1.99595361994962	13.03240931733265	11.48889449155886
H	2.71944950035947	11.41597618687931	11.59268075802773
C	-0.08597287802489	12.57652913638722	8.97390630579332
H	-0.29878497100180	12.44407593662989	7.91131024795995
H	-0.00709506514583	13.64891300069544	9.17253208510447
H	-0.93009574910285	12.18808761421701	9.54702315258815

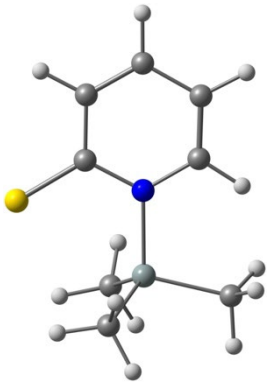

Figure S24. Optimized molecular structure of **1b^{N}**.

PBE0:

final single point energy: -1057.63464573041 a.u.

final Gibbs free energy: -1057.47967314 a.u.

B2T-PLYP:

final single point energy: -1057.66064039419 a.u.

Table S6. Atomic coordinates for optimized structure of **1b^{N}**.

Si	3.02513466414811	11.18533125376102	8.90884220445865
S	1.24881334834660	9.42128777269851	7.06275906145684
N	2.63876229193046	9.42881526664140	9.32446695715012
C	1.84655847009911	8.70530012214406	8.46366323133692
C	1.57150477662990	7.35947808818922	8.81382871849555
H	0.94794294940605	6.79134201469152	8.13789029448923
C	2.07418857524850	6.80395882410166	9.95418279398747
H	1.85086691678506	5.77230873461662	10.19942354775942
C	2.88103214375256	7.57522818827850	10.80723166679380
H	3.29809410171797	7.17323657973671	11.71926580841627
C	3.13259048100938	8.86600973045888	10.45711686244146
H	3.74420510650807	9.50543002371096	11.07503605961599
C	4.06560555468147	11.27043053428686	7.36749048941298
H	4.66925844171928	10.36541391868073	7.26803301782810
H	4.74773871892130	12.12114299384075	7.45002718621665
H	3.46269417240018	11.37759440854767	6.46881709509865
C	4.10177340803854	11.75219975205719	10.33132379422212
H	3.59189816844576	11.72626825405449	11.29684887600680
H	4.35903304014705	12.79565914943504	10.12730257745979
H	5.03856726188765	11.19657049202351	10.41125213949725
C	1.47555416589160	12.21659413310411	8.94551726513824
H	1.00887974597158	12.29251471135593	7.96616327729438
H	1.72751378001697	13.21771107710881	9.30614396330237
H	0.74857852729673	11.78461849947554	9.63710595212054

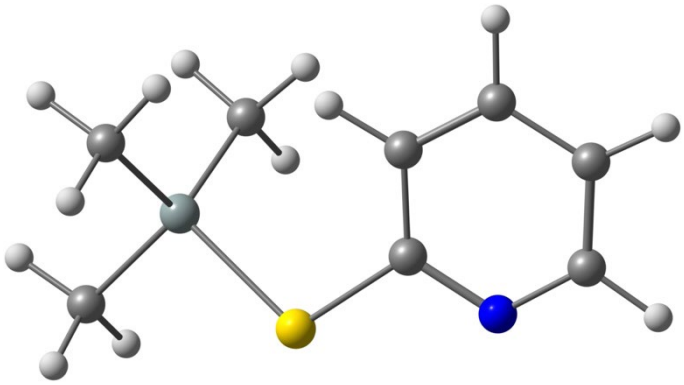

Figure S25. Optimized molecular structure of **1b**[S180].

PBE0:

final single point energy: -1057.63345192101 a.u.

final Gibbs free energy: -1057.48067333 a.u.

B2T-PLYP:

final single point energy: -1057.65973921804 a.u.

Table S7. Atomic coordinates for optimized structure of **1b**[180].

Si	-0.45999718559208	9.90884652357587	8.78070742571387
S	1.61899263612028	10.50118572848793	8.57445777778445
N	3.86951971285975	9.24260924918210	8.92577762895009
C	2.60503319287443	9.03322554162746	8.57087174087432
C	2.12916863059291	7.77619263760287	8.19940395279630
H	1.10463250218136	7.63735344728307	7.88700498721646
C	3.00387697365245	6.70636395573826	8.22450005427220
H	2.65765808421046	5.71840459417446	7.94477906316013
C	4.32277970703316	6.91613664751765	8.59891197831689
H	5.04023412342581	6.10676731345063	8.62829486377421
C	4.70197667492830	8.20536769106248	8.93107756555633
H	5.72576174875890	8.42092175397007	9.22108524820632
C	-1.25738344145474	11.55640368029029	9.13909116177961
H	-0.89697510210060	11.97293500538142	10.08115825813847
H	-2.34095426518539	11.43055620192017	9.20974234112766
H	-1.05190428341933	12.27437880507326	8.34247337451749
C	-0.65935457997961	8.72950012306971	10.21103015297129
H	-0.13543947380935	7.78708847479409	10.04624265989948
H	-1.72097400816117	8.50624931121298	10.34897275123819
H	-0.27899734908479	9.17867182913729	11.13008182067954
C	-1.16210696968637	9.20507105847725	7.19905567667362
H	-0.99842196669779	9.89814371729626	6.37148856638812
H	-2.24050729148398	9.06730548188410	7.31999603521795
H	-0.73239721798266	8.24077779178992	6.92593579374674

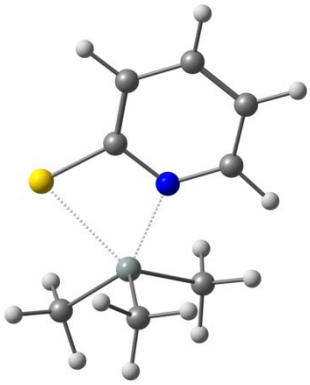

Figure S26. Optimized molecular structure of **1b**^{TS}.

PBE0:

final single point energy: -1057.617930513610 a.u.
final Gibbs free energy: -1057.46268293 a.u.

Table S8. Atomic coordinates for optimized structure of **1b**^{TS}.

Si	-0.64281450138202	1.04267078855865	-0.05287585149029
S	-1.73992242965822	-0.76161065247304	-1.43386654134499
N	0.25988690274388	-0.72289086791610	0.08352043371108
C	-0.39607453143061	-1.55436338779400	-0.75076098147692
C	0.07138595085885	-2.85825484736934	-0.94729390197316
H	-0.45870268426796	-3.52135940713769	-1.61648726697844
C	1.20433376490611	-3.26121504345935	-0.27654440744008
H	1.58123433984281	-4.26786732865170	-0.41387882846298
C	1.87093109723912	-2.37912063619418	0.57713335009818
H	2.76334517864890	-2.67419718308217	1.11052904332113
C	1.36380444288867	-1.11084494610022	0.72920317311127
H	1.83173139054810	-0.37760601363492	1.37154546828349
C	0.59319980232127	1.81752205540543	-1.22815234101800
H	1.61844728919665	1.63862593423798	-0.89836290171677
H	0.42736717083018	2.89709648723971	-1.26534860892032
H	0.48309777409425	1.42417827916155	-2.23974601676052
C	-0.22498702322008	1.46553420945910	1.74400815597095
H	-0.83845670873348	0.87025530309895	2.42734761608744
H	-0.46658925792991	2.51545822321996	1.92510712003358
H	0.81994079253892	1.31214346763319	2.01805812562455
C	-2.28181539199323	1.98190202000387	-0.19900581206625
H	-2.63639026811740	1.99785851486547	-1.23137080715722
H	-2.14825098217766	3.01069791699870	0.15060776778489
H	-3.05470211774714	1.51538611393018	0.41663201277937

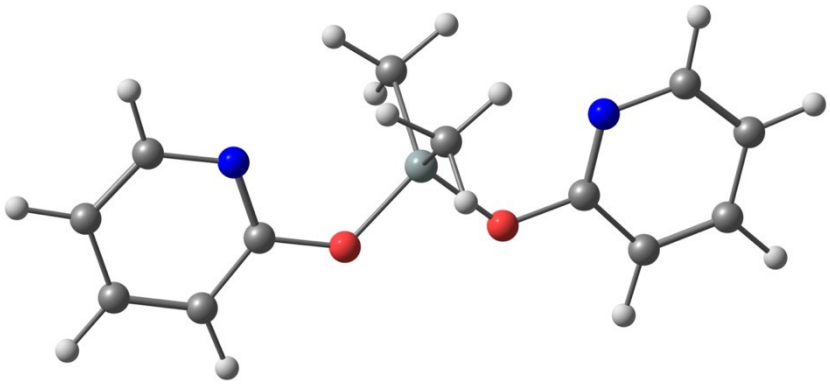

Figure S27. Optimized molecular structure of **2a**^{OO}.

PBE0:

final single point energy: -1016.20537541228 a.u.
final Gibbs free energy: -1016.00584693 a.u.

B2T-PLYP:

final single point energy: -1016.34079108298 a.u.

Table S9. Atomic coordinates for optimized structure of **2a**^{OO}.

Si	9.29694643154187	10.38389441586424	8.20882699481765
O	8.21502932647646	11.20984087633818	7.22137006050122
O	10.50713455590216	11.54717716845065	8.09767128304447
N	6.55581091256024	9.66245451637609	7.46550185483932
N	11.93721860163477	10.40253606279914	9.45746743427239
C	6.95775063595121	10.82685560672297	6.98206263049361
C	6.13307086500475	11.67291350922289	6.23734576621897
H	6.51959961563661	12.61383623361121	5.86970702710158
C	4.83661376724099	11.26760566372483	6.00313502556866
H	4.16640053894799	11.89889237729180	5.43184398347608
C	4.39906443510436	10.04631731550145	6.50759807194541
H	3.38866474744325	9.69597597207352	6.34476010524183
C	5.29749923372797	9.28645970845468	7.22988344843455
H	5.00313811829139	8.32749466669806	7.64460921174049
C	11.67650119101457	11.48378675556413	8.74040315181637
C	12.56108241339403	12.55809547096044	8.62482680029877
H	12.28912512387512	13.41638271845965	8.02544459197422
C	13.76366960668319	12.47801956568148	9.29371525478879
H	14.47516414242732	13.29264753958292	9.22822853692923
C	14.05193886463581	11.34664558815316	10.05163058698362
H	14.98460406092966	11.24856242147373	10.59067038097994
C	13.10544707886278	10.34258783222944	10.09912985378913
H	13.28339750760724	9.44146917317580	10.67751855470658
C	8.65597196229019	10.27387790782956	9.93780426404397
H	7.80046709202479	9.59952536854903	9.98213773403501
H	8.33910094119768	11.25935653381449	10.28652062490644
H	9.43626954361794	9.90462078835139	10.60393953091645
C	9.82154920110016	8.80096587211417	7.41680073962406
H	10.59378902370660	8.31506738761619	8.01372388130314
H	10.22264696854051	8.99195393530323	6.41909027173580
H	8.96607449262766	8.13055304801051	7.32499434347148

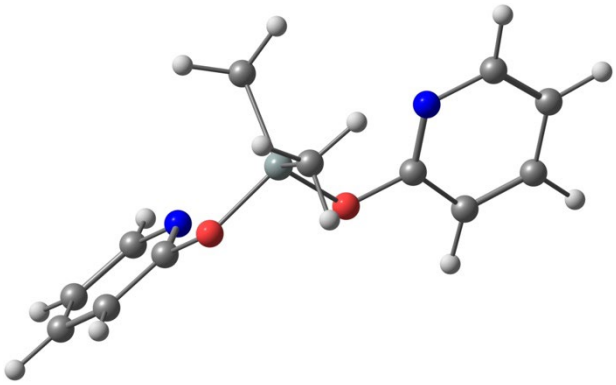

Figure S28. Optimized molecular structure of **2a**^{OC}.

PBE0:

final single point energy: -1016.20489226343 a.u.

final Gibbs free energy: -1016.0045722 a.u.

B2T-PLYP:

final single point energy: -1016.34062391185 a.u.

Table S10. Atomic coordinates for optimized structure of **2a**^{OC}.

Si	-1.97585532387687	3.19901263466484	2.16303097792054
O	-1.15346365385241	2.38336128743815	0.95195382866852
O	-0.73216938027425	3.99898999050924	2.96391553661992
N	-0.48671725277913	4.24012209932066	-0.20292981724849
N	-2.17098568352051	4.86850249314498	4.49864934671661
C	-0.54664814975182	2.92306327755570	-0.11272358482815
C	-0.00783546076919	2.06265242058170	-1.07137211946679
H	-0.08877503836723	0.99213099733797	-0.93949386737634
C	0.61638872982848	2.62453139723057	-2.16466449105584
H	1.04620668462321	1.98877646013461	-2.92964267927994
C	0.68676164687804	4.00988446007853	-2.27406226450841
H	1.16817873211651	4.48777296754973	-3.11668440725780
C	0.12033784145111	4.76663962498338	-1.26730625853283
H	0.15087813706477	5.85098101727963	-1.30774175573440
C	-0.93431240353223	4.76612856557233	4.03913290468785
C	0.15616390807920	5.41412450794267	4.62157211190377
H	1.14385225245826	5.29270815196323	4.19801970818787
C	-0.07901874075546	6.19570915755867	5.73273668666586
H	0.74194122206218	6.71470535314199	6.21309215213059
C	-1.37450965133344	6.31164040897121	6.22858651510450
H	-1.59570415515370	6.91590839187048	7.09807009283160
C	-2.38062648514500	5.62913640623890	5.57408180255799
H	-3.40717096039523	5.68806123783653	5.92171501776281
C	-2.65402861771893	1.82259717122400	3.19116109211784
H	-3.34158485238175	1.21669817097917	2.59629805741811
H	-3.19525822683455	2.21820207431031	4.05074970403735
H	-1.85103279298799	1.17596799451812	3.55021792303446
C	-3.25294240385624	4.34234396241884	1.47008993628510
H	-2.81048376423555	5.29701425427403	1.18756362508057
H	-4.03696180614664	4.51903806779469	2.20721205852716
H	-3.70369998589360	3.89710881157499	0.57979795002986

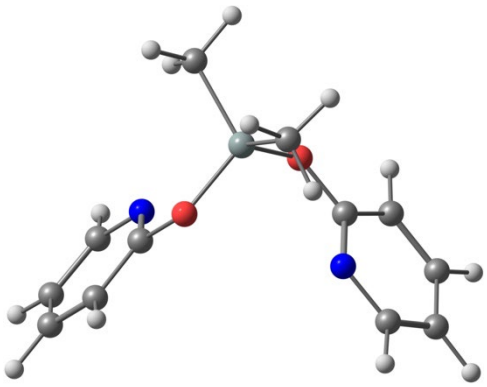

Figure S29. Optimized molecular structure of **2a**^{CC}.

PBE0:

final single point energy: -1016.20461047664 a.u.

final Gibbs free energy: -1016.00526258 a.u.

B2T-PLYP:

final single point energy: -1016.34057880634 a.u.

Table S11. Atomic coordinates for optimized structure of **2a**^{CC}.

Si	-1.53879749523286	2.50364295835553	2.37438775097594
O	-1.20593404148877	1.71359340440571	0.93913897824916
O	-0.19272875506531	3.28561634100759	2.98404832476902
N	-0.41353584863319	3.54086141332346	-0.18138468586610
N	1.17327732633901	1.45427884047241	3.01964847446699
C	-0.71174339586182	2.25323463550163	-0.18193340278732
C	-0.53458573604262	1.42468281447384	-1.29134679027271
H	-0.79731930193183	0.37741743225041	-1.22769395453914
C	-0.02120598853680	1.98676038884063	-2.44078405704761
H	0.13034794182232	1.37521490158033	-3.32234278193316
C	0.29830990775458	3.34090492509673	-2.45552816206995
H	0.70357652644515	3.81767280735372	-3.33792218241349
C	0.08194498206451	4.06816022685675	-1.30169582791572
H	0.31495148171018	5.12770059189925	-1.26425757825315
C	0.99535714858859	2.73944036298265	3.27133703310409
C	1.98481669618171	3.55898936743167	3.81726812765409
H	1.77755177778013	4.60506314417509	3.99773452182552
C	3.20662987938099	2.98967330524157	4.10726062846363
H	3.99932444108037	3.59415262826197	4.53185595020218
C	3.40913807725235	1.63750387431600	3.84874172182979
H	4.35383224805180	1.15533993906946	4.06156299886654
C	2.36150419376668	0.92016475491088	3.30546311290973
H	2.47145482830415	-0.13694652840800	3.08471607414183
C	-2.12347046401705	1.16542529870905	3.50447661857281
H	-3.06561380825401	0.75149629034651	3.13744602246844
H	-2.29730783550457	1.56600515035855	4.50564318233512
H	-1.39117790436452	0.36139295930147	3.57285263013718
C	-2.78197666185321	3.84954525786568	2.14598356421636
H	-2.37600068031662	4.65820807268477	1.53921768039301
H	-3.07850864862536	4.25209228411133	3.11736044782570
H	-3.67545889079395	3.45747715722324	1.65489457969115

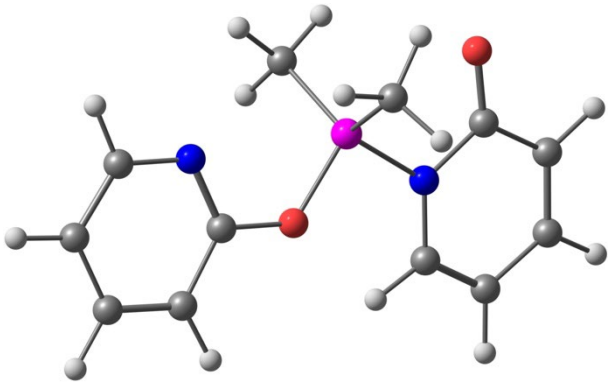

Figure S30. Optimized molecular structure of **2a´^{NO}**.

PBE0:

final single point energy: -1016.19657375118 a.u.

final Gibbs free energy: -1015.99686015 a.u.

B2T-PLYP:

final single point energy: -1016.32858889964 a.u.

Table S12. Atomic coordinates for optimized structure of **2a´^{NO}**.

Si	9.47611596790838	11.75412777698802	8.91747534702957
O	8.76023359366890	10.60463612513671	7.90899959494763
O	11.62520097786807	13.11659016767037	9.78494436856974
N	6.68217398701167	10.88091882421570	8.80579667656959
N	11.10955454804291	11.67646953816507	8.14176223941426
C	7.46042551899846	10.28981238880736	7.91496720760962
C	6.99320143795304	9.35929181069264	6.98516928877227
H	7.67988046529511	8.90825398960536	6.28148192423612
C	5.64936999442182	9.05119163176287	7.00170910620041
H	5.24879294168534	8.33527534391990	6.29381873416560
C	4.81721780386980	9.66703744877713	7.93162670668233
H	3.75811435202136	9.45105409129554	7.97342963058492
C	5.38434030772478	10.57102871370344	8.80808042743987
H	4.77670870037720	11.07678218157288	9.55168806980190
C	12.02430626335585	12.49142703696541	8.79267781420261
C	13.34633171334432	12.52995912136853	8.24665318691330
H	14.07022784536812	13.16118884503788	8.74431602316036
C	13.66019148500163	11.79648069009694	7.14411714041986
H	14.66579126792575	11.83535276401760	6.74040999496894
C	12.69036523430638	10.98411594639349	6.51629275353927
H	12.92474297156982	10.39746809464538	5.64001520577879
C	11.43778145555223	10.95238198465971	7.04133765117864
H	10.64158756070634	10.35653795657532	6.61854144273972
C	8.73201761157544	13.41730433294846	8.61237927646564
H	7.79073730085058	13.51054597231323	9.15458496489160
H	8.52797342088514	13.54347227083853	7.54682987943368
H	9.41283895410111	14.20209634160897	8.93965796097558
C	9.51263003049308	11.09219237721550	10.64045707707590
H	9.84475039667330	11.85637630166602	11.34111275219759
H	10.19422416986534	10.24148478950889	10.70505831564816
H	8.51163838557793	10.75773863882624	10.91701126638593

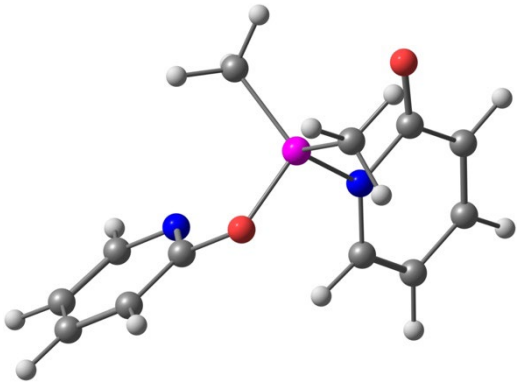

Figure S31. Optimized molecular structure of **2a´**^{OC}.

PBE0:

final single point energy: -1016.19669796871 a.u.

final Gibbs free energy: -1015.99590271 a.u.

B2T-PLYP:

final single point energy: -1016.32856724497 a.u.

Table S13. Atomic coordinates for optimized structure of **2a´**^{OC}.

Si	-1.85399480704273	3.29820659596385	2.29078223965830
O	-1.54101668172443	1.70236868977645	1.84413464159247
O	-2.18755925189027	5.42109751887506	3.84291114759701
N	0.67342952351815	1.71741906478311	2.40008936100191
N	-1.70034048205676	3.25156477410033	4.08846849437513
C	-0.32915547234065	1.13356429130204	1.76634847059599
C	-0.19245631656394	-0.04712163321858	1.03520639869681
H	-1.05262376106119	-0.47608249096892	0.53915045957572
C	1.05825687985714	-0.62482602668460	0.97271171777232
H	1.20469325243871	-1.54149982936433	0.41385881389486
C	2.12498526996872	-0.01876985958119	1.62941114453678
H	3.12013413337721	-0.44191540014995	1.60140508532747
C	1.87748068696904	1.14750215146378	2.32627936269459
H	2.67642990831421	1.65584377939848	2.85657223251103
C	-1.92382822747112	4.50406492116856	4.63475134374255
C	-1.82879828704508	4.60564758756921	6.05758736813466
H	-1.98912501344416	5.57929359163636	6.50073322545206
C	-1.55475075532262	3.50266144694851	6.80736266764906
H	-1.49004188718743	3.59026779345032	7.88617570434287
C	-1.35614656819414	2.24250723381174	6.20068652820939
H	-1.14400838878661	1.35981963195008	6.78601663989178
C	-1.43568119290158	2.16022553249100	4.84685811981613
H	-1.29464727288488	1.23130519866123	4.31275395969926
C	-3.62927413301764	3.48648841856390	1.81801255459941
H	-3.72899998421330	3.39201206944342	0.73408658941474
H	-4.00890526702069	4.46055729653102	2.12288603342202
H	-4.23432383727092	2.70675559917656	2.28458125463060
C	-0.64769116797780	4.43450131895428	1.47188649453082
H	0.19700885325783	4.64600422227270	2.12639548426625
H	-1.13945274753933	5.37419117403461	1.22105549662453
H	-0.26646646674364	3.97406226564073	0.55761351374323

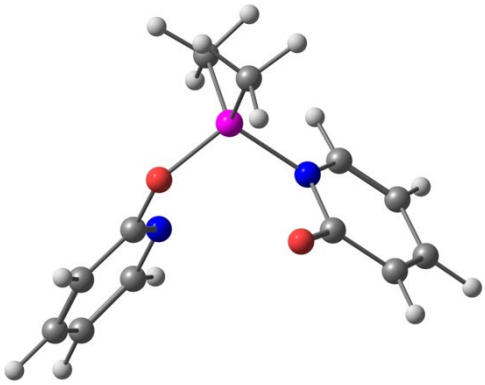

Figure S32. Optimized molecular structure of **2a´^{CC}**.

PBE0:

final single point energy: -1016.19386752798 a.u.

final Gibbs free energy: -1015.99330533 a.u.

B2T-PLYP:

final single point energy: -1016.32593329201 a.u.

Table S14. Atomic coordinates for optimized structure of **2a´^{CC}**.

Si	-2.09426704298407	3.58834625985772	2.17310026376958
O	-1.15413174179676	4.82456448313900	1.56718872043194
O	0.38868352426739	3.06655806253974	3.46175497712767
N	-1.91420071209493	6.41870176179590	3.01503246075555
N	-1.80095231978160	3.40865509563373	3.94004421143573
C	-1.06708523455741	6.06638843978955	2.06371847737074
C	-0.08777577881508	6.91760371927383	1.55146815882452
H	0.58052125630444	6.56539395479806	0.77746797566651
C	-0.00791106872713	8.19221601129624	2.07111173516574
H	0.74134868479802	8.88214050163085	1.70145735657208
C	-0.89232217441902	8.57929336072189	3.07328533539153
H	-0.85857482040157	9.56978734321515	3.50681094349290
C	-1.82100329736798	7.65470074181899	3.50850246005291
H	-2.52953083281919	7.90795394630107	4.29076934169543
C	-0.48361322224764	3.15389085597047	4.32782635384044
C	-0.25886910828414	3.01899334269133	5.73978187248177
H	0.75662401885144	2.81565067752614	6.05258340521609
C	-1.27497249174598	3.15329394531380	6.63044953332082
H	-1.07863924027059	3.05422668330138	7.69224496133959
C	-2.58929714908549	3.42552272590416	6.18551395506592
H	-3.41110085892884	3.53928277932590	6.87726276667209
C	-2.80205098684955	3.54594114217816	4.85223267089577
H	-3.78223842095459	3.76080358910321	4.45054872764855
C	-1.59910035502822	2.06670208409608	1.25610224169656
H	-1.86891656988494	2.17197119446003	0.20256690385441
H	-2.13310708202312	1.20133613715554	1.65545005173640
H	-0.52874398524333	1.88757696459933	1.33550309832117
C	-3.89368656224463	3.95859233150533	1.93678038413149
H	-4.20956678436318	4.85124468653562	2.47557430795779
H	-4.52055957992191	3.11492661092989	2.23401468233733
H	-4.05617945138026	4.13092222959166	0.86955294373078

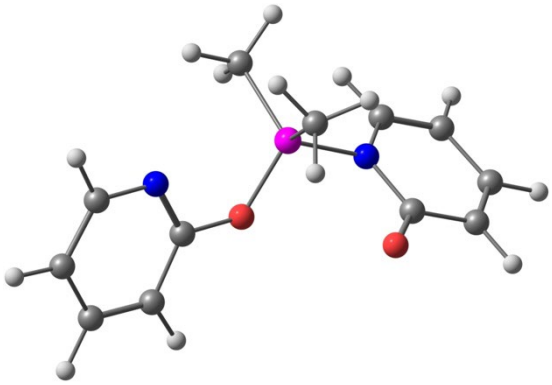

Figure S33. Optimized molecular structure of **2a´**^{NC}.

PBE0:

final single point energy: -1016.19294839839 a.u.

final Gibbs free energy: -1015.99222467 a.u.

B2T-PLYP:

final single point energy: -1016.32518572426 a.u.

Table S15. Atomic coordinates for optimized structure of **2a´**^{NC}.

Si	-0.88189682575781	2.76313098544533	2.81005801672528
O	-0.16035656743046	4.24450946168505	2.50219728579562
O	-2.74498082739418	4.52636412698025	3.96768476631146
N	1.77995080307418	3.56409441745997	3.47392417259166
N	-2.56101525313282	3.08320073875989	2.23244280567931
C	1.07137040027761	4.54124893467565	2.93278113263012
C	1.54230897866208	5.84671919303732	2.79194342881326
H	0.91091840664238	6.60261640644990	2.34523443944067
C	2.81523449890253	6.12087801724648	3.24610745403489
H	3.21743992146056	7.12305428444740	3.15730926828342
C	3.57236618032241	5.10440493652015	3.82144125908977
H	4.57298154236633	5.28465781275687	4.19072902378663
C	3.00793827278004	3.84742541251111	3.91120800614531
H	3.55826241335807	3.02257237148358	4.35231794620832
C	-3.29224884009373	3.99068943907020	3.00243160696670
C	-4.64826434077361	4.21856918708560	2.59033507326718
H	-5.22693884368013	4.91369593400752	3.18386894622273
C	-5.16822306180559	3.58810340993158	1.50556275360512
H	-6.19497441237098	3.77684062525648	1.21250158327314
C	-4.38154167010299	2.68710829350560	0.75177816680369
H	-4.77491639178988	2.17900378818976	-0.11647933167994
C	-3.10234014063878	2.46789117258529	1.14602730128293
H	-2.45218593702098	1.78954329198883	0.61130578218096
C	-0.90113400863660	2.22966942643892	4.57889261791894
H	-0.09471399524759	1.51819977751682	4.76081221944341
H	-1.85507829094900	1.75098170454880	4.81084471108956
H	-0.78066605096791	3.08325481528071	5.24367985214866
C	-0.18153480653547	1.47174489780513	1.68097258332348
H	-0.15358949998907	1.79698871096669	0.63939861333529
H	-0.74497436830167	0.53783846676669	1.74326343555349
H	0.84214035877311	1.27015187959616	2.00077859072867

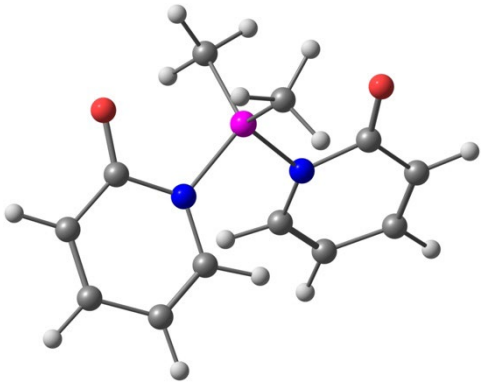

Figure S34. Optimized molecular structure of **2a´´^{NN}**.

PBE0:

final single point energy: -1016.17722689273 a.u.

final Gibbs free energy: -1015.97658705 a.u.

B2T-PLYP:

final single point energy: -1016.30548514771 a.u.

Table S16. Atomic coordinates for optimized structure of **2a´´^{NN}**.

Si	9.57433241237193	11.50746956685402	8.51082418644479
O	7.59443175108664	9.80143969809789	9.44836991891977
O	12.08866503376629	12.54482528862138	8.08677449372070
N	7.87168423549381	11.39761514392089	7.87791066875316
N	9.94142129783863	13.22731262774095	8.04550270092592
C	7.08913832753927	10.44446808517984	8.52430864715952
C	5.74984978910897	10.28435658913450	8.03512845450007
H	5.11214595753428	9.59425459385460	8.57110347773929
C	5.33455004317069	10.93449256436435	6.91695761208189
H	4.32862476824374	10.77870917969031	6.54369121136478
C	6.21055522093172	11.80007499958244	6.22253653555006
H	5.91276897285099	12.29797374457634	5.31133856621979
C	7.45286217347038	11.99818914041534	6.72914097842295
H	8.16755548176020	12.64427810087359	6.23720820151729
C	11.30291946315027	13.48017607550034	7.90749385688558
C	11.66978144990777	14.82801690720103	7.58295383012512
H	12.71940802214738	15.02250441601572	7.40805114195327
C	10.73612199663305	15.81469543212988	7.55577297944803
H	11.03421965814418	16.83431585766878	7.33903269229493
C	9.37884378083788	15.52758602235000	7.82797742104946
H	8.62742156127173	16.30332026647301	7.84831822789163
C	9.02981598025726	14.23878455095721	8.06611583493903
H	8.00790365371294	13.96029120578770	8.28564558183226
C	9.74451803277400	11.52533701016609	10.34784290007122
H	9.75644330395714	10.51757237845010	10.75640802978381
H	8.91547495409221	12.07337413975000	10.79957548449670
H	10.67749766653443	12.03574165903806	10.59804874554008
C	10.46148080572280	10.21234333984703	7.54099658771260
H	11.43927006256581	9.99723737478963	7.96575975241805
H	10.59704592058758	10.54000379970043	6.50836805827836
H	9.85149119653545	9.30593482026767	7.54118895495937

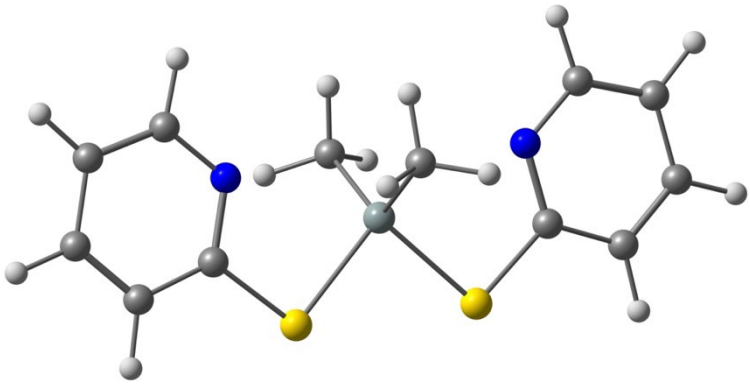

Figure S35. Optimized molecular structure of **2b**^{SS}.

PBE0:

final single point energy: -1665.24690848091 a.u.

final Gibbs free energy: -1665.05356639 a.u.

B2T-PLYP:

final single point energy: -1665.30079264606 a.u.

Table S17. Atomic coordinates for optimized structure of **2b**^{SS}.

Si	9.30390502839405	11.09662443302652	7.88902382175970
S	7.92942001881526	12.24911917428762	6.63177122101662
S	10.86912544321070	12.61789871251863	7.70073405190595
N	6.81952812746695	10.01155116730602	7.45598916274852
N	11.70555026733710	10.62964714910991	9.21507983415413
C	6.59761765537694	11.11035902535675	6.74127055799389
C	5.38062184944695	11.36608691997191	6.10864384418943
H	5.24097123387449	12.27342299886609	5.53572886819119
C	4.37127982481148	10.43279884975703	6.24011502422519
H	3.41272792060731	10.60049536068885	5.76352841138823
C	4.59626037137931	9.28240408608682	6.98726838619625
H	3.82852357781862	8.53045300773628	7.11208831060068
C	5.83791719781304	9.12048793287512	7.57383829558952
H	6.06257263707128	8.23971065740668	8.16695668666379
C	12.05270106297374	11.81209960808448	8.71631665767256
C	13.28852563471021	12.40758757947217	8.97335288640670
H	13.52959895015895	13.37270138307445	8.54736452439203
C	14.18058661949792	11.73203325478456	9.78211066417393
H	15.14831263007300	12.16638107196513	10.00342799386590
C	13.82454883980959	10.49504473620680	10.30722479035730
H	14.49720484427127	9.93713859095270	10.94492047272544
C	12.57602387911760	9.99015099497209	9.99330353733808
H	12.25198202077895	9.02935178737015	10.38051784789850
C	8.68144079511317	11.03300199828668	9.64572103167963
H	8.65060588247869	9.99671124413278	9.98481533745055
H	7.67573170967294	11.44882100057134	9.70235404599640
H	9.34339667789555	11.59782629960650	10.30138868799384
C	9.82002207040550	9.52440009012321	7.02866015485688
H	9.67490068581580	8.67669523453922	7.69966280464382
H	10.87242497760989	9.57520362871803	6.75079882668143
H	9.21671256619350	9.37016402214503	6.13438525924353

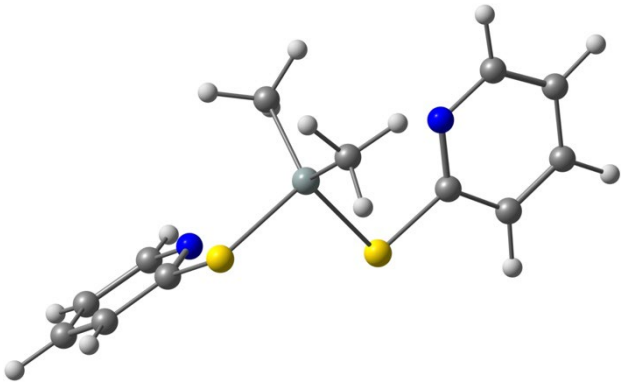

Figure S36. Optimized molecular structure of **2b**^{SC}.

PBE0:

final single point energy: -1665.24605991582 a.u.

final Gibbs free energy: -1665.05372524 a.u.

B2T-PLYP:

final single point energy: -1665.30081142176 a.u.

Table S18. Atomic coordinates for optimized structure of **2b**^{SC}.

Si	-1.87035557416757	3.04164329214161	2.28278457245907
S	-1.17270529856306	1.59637777385906	0.81865364685736
S	0.00767232019607	3.74520830109170	3.10543890267737
N	-0.45785986590877	3.89726467521028	-0.33748391804613
N	-1.94528921059982	4.91383547312479	4.45564344910439
C	-0.50449120136237	2.58009250304773	-0.48303631983076
C	-0.04367752715379	1.92538127968351	-1.62705345363188
H	-0.10302655339022	0.84722567867412	-1.70128657633386
C	0.48373309643064	2.68909000721197	-2.64904143102653
H	0.85039784382473	2.21179425064871	-3.55003426223365
C	0.53632176769670	4.06994412324732	-2.50632231842112
H	0.94208579035226	4.70421307804345	-3.28330201631576
C	0.05226643684517	4.61953903548726	-1.33295368111085
H	0.07316760420557	5.69361069206243	-1.17617632426593
C	-0.62448560837286	4.82251801807031	4.34318217466017
C	0.25575368909774	5.53919510850306	5.15497962815955
H	1.32537788006142	5.43454340211230	5.02805140920396
C	-0.27806857248330	6.37774573962262	6.11347501300044
H	0.37734374302790	6.94834898292318	6.76071559066481
C	-1.65849859672852	6.48159525206967	6.23598339279799
H	-2.11395356484504	7.12881167465921	6.97366673534092
C	-2.44454131044425	5.72840279554539	5.38291367517054
H	-3.52751689232008	5.77560911852981	5.44056943581597
C	-2.75423835879798	1.89946548944724	3.45793628210709
H	-3.64109610472462	1.49016166619939	2.96737540382867
H	-3.06594182241870	2.45023914449231	4.34483488889427
H	-2.11165477555894	1.07175186470416	3.76130015086893
C	-2.96681365780212	4.34133811157749	1.52991131066730
H	-2.40555671445812	5.24886271811399	1.31623121198381
H	-3.77232115304745	4.57261606622876	2.22755057794715
H	-3.39110344359055	3.96708849966699	0.59651863200663

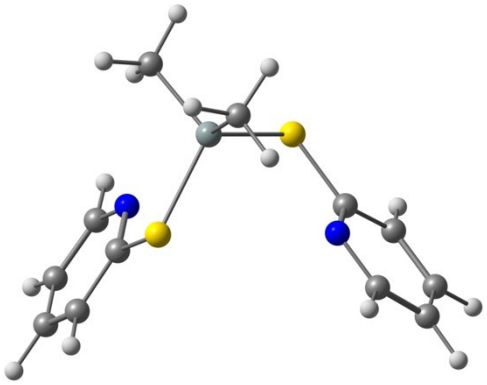

Figure S37. Optimized molecular structure of **2b**^{CC}.

PBE0:

final single point energy: -1665.24463070467 a.u.

final Gibbs free energy: -1665.05251403 a.u.

B2T-PLYP:

final single point energy: -1665.29950463299 a.u.

Table S19. Atomic coordinates for optimized structure of **2b**^{CC}.

Si	-1.62310312288637	2.49682397557066	2.46102914792733
S	-0.92485238338964	1.15149050325388	0.92505106105043
S	-0.11611446338402	3.87975889128979	3.15153417258249
N	-0.67893151965557	3.49227495989826	-0.35671429896015
N	1.07757222886179	1.54307705501198	3.68164962543325
C	-0.56825653970739	2.17639027742359	-0.46651584787846
C	-0.16653507382459	1.54328019143189	-1.64488175256860
H	-0.09007398117713	0.46443446260043	-1.68745736410467
C	0.12555414172960	2.32883144148229	-2.74202045056434
H	0.43849662730649	1.86841553153981	-3.67161036436289
C	0.01241832419614	3.70934053506750	-2.63709480620656
H	0.23226970020264	4.36057128378526	-3.47271992597189
C	-0.39298455273657	4.23571886324873	-1.42397116532803
H	-0.49539536186783	5.30874682726603	-1.29429024382900
C	1.26199991028377	2.84860319141713	3.54268271697180
C	2.50826802965211	3.46002834953422	3.68959797489917
H	2.61124318913232	4.52931448328025	3.55819678979244
C	3.59525467632147	2.66415431678038	3.99334550081304
H	4.57681617938349	3.10723714768020	4.11260116092225
C	3.41405746201418	1.29429427674967	4.13249749394861
H	4.23982881792905	0.63460906828285	4.36414896279363
C	2.13753886081213	0.78833840130567	3.96422380280485
H	1.94850889653797	-0.27628749419050	4.06126180174267
C	-2.21289593556401	1.32547471492679	3.77917693143244
H	-3.08606872406634	0.77688738221285	3.41809154272040
H	-2.50359132337581	1.89714372044468	4.66341305369950
H	-1.43094986039429	0.62228678844517	4.05943500432540
C	-2.99489666905106	3.62604418321324	1.91491915228458
H	-2.64823106482179	4.34077579201587	1.17171975531041
H	-3.38501722737205	4.16399529919453	2.78280223989207
H	-3.80527724108871	3.03271057983679	1.48604732842779

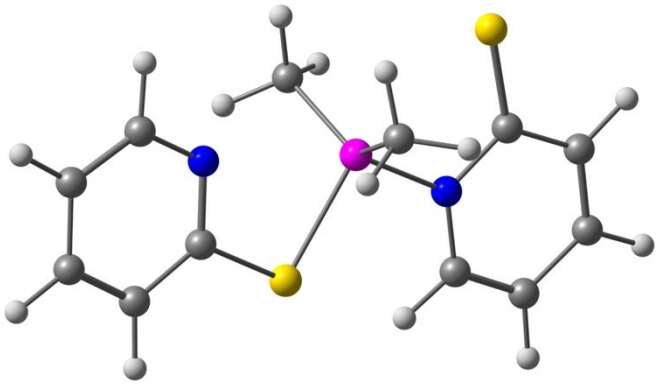

Figure S38. Optimized molecular structure of **2b´**^{NS}.

PBE0:

final single point energy: -1665.24480081193 a.u.

final Gibbs free energy: -1665.04945783 a.u.

B2T-PLYP:

final single point energy: -1665.29773202014 a.u.

Table S20. Atomic coordinates for optimized structure of **2b´**^{NS}.

Si	9.53200321439334	11.61264395954216	8.61136005379728
S	8.92979733299729	10.15627403421036	7.05902675146935
S	11.25493540191066	13.35426681894973	10.16059290313195
N	6.89809768321431	10.81759772330770	8.60216114403384
N	11.30863364649139	11.73811668021835	8.09363270239786
C	7.25620107139789	10.05276525312035	7.57630953180790
C	6.36715580069810	9.19906907229446	6.92237776975442
H	6.70158498086262	8.59217591277135	6.09120631975283
C	5.06130984924499	9.15601930975398	7.36877447321237
H	4.34418019244280	8.50425242483949	6.88402403084685
C	4.67912154723500	9.95395465462203	8.44104461557924
H	3.66491120273284	9.94688902437138	8.81752662376723
C	5.63608734417145	10.76511659838955	9.02249802527448
H	5.38748963588646	11.40475077732246	9.86314503179579
C	12.04374240231521	12.57913152786947	8.88903413243909
C	13.41499608789080	12.74162909584834	8.58766139313239
H	13.99090355405057	13.40350075891389	9.21931448345901
C	13.98235828763405	12.08366915103741	7.53389167772304
H	15.03477662386012	12.21744128568397	7.31346236062697
C	13.19725783711999	11.23569251107438	6.73614036531542
H	13.61056030047859	10.70181214349602	5.89272535689517
C	11.87900807233479	11.09268693265764	7.04798953869088
H	11.23391632567775	10.45322647082154	6.46288253028319
C	8.69275174637981	13.21837929768750	8.19443141764302
H	8.20988895742413	13.62598692452679	9.08223182106413
H	7.93985381307130	13.05389573791357	7.42342062887279
H	9.42888611891879	13.94160008411555	7.84232717256095
C	9.44367713897551	10.70009462787663	10.23120020220626
H	8.93713612867422	11.31257868556930	10.97651430778890
H	10.45083501326026	10.48788264519698	10.59180970846443
H	8.89740935225473	9.76549337299742	10.10368495421282

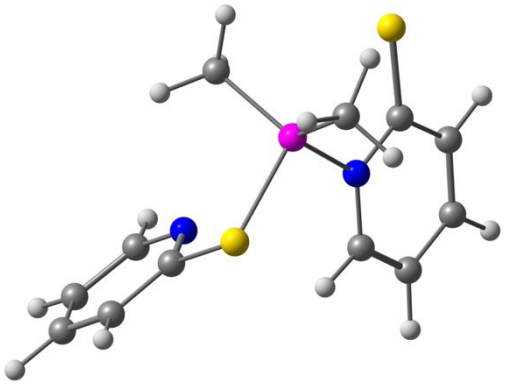

Figure S39. Optimized molecular structure of **2b´**^{SC}.

PBE0:

final single point energy: -1665.24724112912 a.u.

final Gibbs free energy: -1665.05203345 a.u.

B2T-PLYP:

final single point energy: -1665.3000924499 a.u.

Table S21. Atomic coordinates for optimized structure of **2b´**^{SC}.

Si	-2.07607311719392	3.44307057061319	2.26096521136884
S	-2.08745895640587	1.35191201628880	1.58932660691129
S	-2.04021422332656	5.88064290471620	3.81595687636466
N	0.42356786757824	1.64949989361061	2.42607879001250
N	-1.79113817119596	3.28987401868000	4.07082627652236
C	-0.38861741220691	0.89554503142118	1.69450184285906
C	0.04118194466686	-0.24814798265636	1.01944079698314
H	-0.65697855836700	-0.82998685196029	0.43191415159576
C	1.37174785860781	-0.60377512999709	1.11793677464332
H	1.73801348386226	-1.48510929951184	0.60503830542404
C	2.23050875976471	0.18407259175771	1.87431430733513
H	3.28028154829217	-0.05835249607664	1.97325367324523
C	1.70561426638298	1.29741146499328	2.50451578165873
H	2.33825181030254	1.94240458487480	3.10609793513861
C	-1.75783362371484	4.49130149044613	4.72740727769290
C	-1.49785965530114	4.47411325322976	6.11487565716667
H	-1.45882876196194	5.42287338084743	6.63156960175123
C	-1.31185545814915	3.29030241409495	6.77254514430724
H	-1.11737864927093	3.28879843166601	7.83865201669121
C	-1.37709562228207	2.07774511635743	6.06793775916346
H	-1.24130813866970	1.12547923651858	6.55979736257813
C	-1.61290608804632	2.12024124730918	4.72667657804623
H	-1.67654118463308	1.22955551523855	4.11910281101123
C	-3.85698412192426	3.81660716073674	1.87046859833046
H	-4.08833825429355	3.43696148430960	0.87233041116969
H	-4.05752218099872	4.88468605535654	1.90523016823428
H	-4.51270551633855	3.31358756270535	2.58426270184266
C	-0.72849015222629	4.30361056162910	1.31495869773028
H	0.09338519402574	4.57139021432327	1.97658635567572
H	-1.13261634360049	5.21789828159778	0.87937724351006
H	-0.35067800537598	3.65350420487991	0.52482683303573

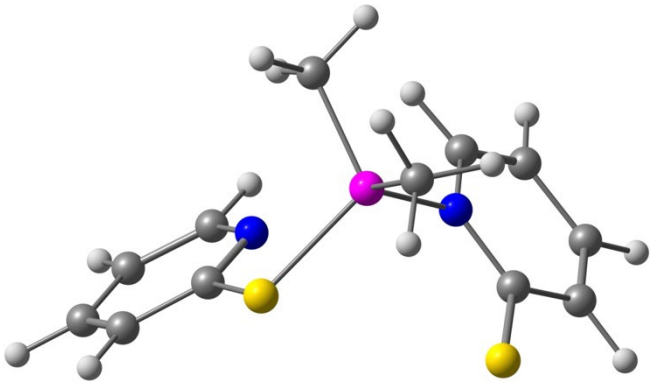

Figure S40. Optimized molecular structure of **2b′^{CC}**.

PBE0:

final single point energy: -1665.24229063867 a.u.

final Gibbs free energy: -1665.0474898 a.u.

B2T-PLYP:

final single point energy: -1665.29616506502 a.u.

Table S22. Atomic coordinates for optimized structure of **2b′^{CC}**.

Si	-1.87237413540471	3.40357483346653	2.16287351418725
S	-0.38023152999477	4.68088154754175	1.29018084058596
S	0.62634172976853	2.03565593766643	3.46311487669520
N	-1.54240415530808	6.30471748108903	3.06339603824964
N	-1.67343449738672	3.26383105140748	3.97005191374111
C	-0.75223890511118	6.25183552552264	1.99918392498806
C	-0.15944375400229	7.38257819713603	1.43529984724458
H	0.47719098928506	7.29025417792032	0.56493996542002
C	-0.40877062729754	8.60860968466218	2.01930312957195
H	0.03787018689500	9.50606453380646	1.60827459101076
C	-1.23803461787381	8.67538624736036	3.13194073549103
H	-1.45780309706780	9.61682922485754	3.61757404453718
C	-1.77998477119300	7.49585229578182	3.60896405700267
H	-2.43427608685041	7.49761167755715	4.47537318011364
C	-0.54914662062618	2.65982520161069	4.48697474846658
C	-0.44271547336717	2.60515102510252	5.90060529577026
H	0.43650590866192	2.12677986368372	6.30875305752712
C	-1.40403372414666	3.13619060824452	6.70821003992978
H	-1.29777401222401	3.08258949261406	7.78529955432858
C	-2.53005407946573	3.75775258647524	6.13863358401155
H	-3.31009653322522	4.19494740491346	6.74500613202917
C	-2.62025665552874	3.80274998896258	4.78404100281629
H	-3.45302879041510	4.27714338406010	4.28890923287232
C	-1.80025874470615	1.75916575339373	1.30043740277916
H	-2.57287646771902	1.73486113044308	0.52758857951411
H	-1.99639555641893	0.95859803197717	2.01642068892402
H	-0.82788596162642	1.57062213849620	0.85124925319797
C	-3.57024345743046	4.10971911050558	1.87571174273682
H	-3.71567963888652	5.10775981388487	2.28319086426267
H	-4.33649676016087	3.43799222839736	2.27211822292268
H	-3.70318954917296	4.15765148345931	0.79208121707179

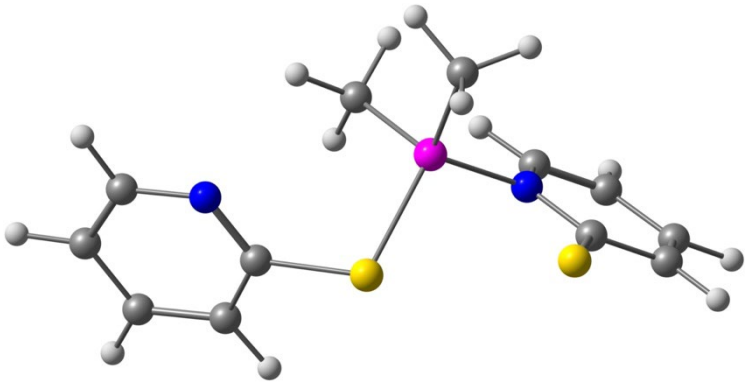

Figure S41. Optimized molecular structure of **2b´^{NC}**.

PBE0:

final single point energy: -1665.24162347115 a.u.

final Gibbs free energy: -1665.04672803 a.u.

B2T-PLYP:

final single point energy: -1665.29586316274 a.u.

Table S23. Atomic coordinates for optimized structure of **2b´^{NC}**.

Si	-1.18702227640727	2.82330854353010	3.53150806227135
S	-0.47994629811277	4.71650497245610	4.25335490797735
S	-3.53550169041051	4.06574904825134	4.82045403628031
N	2.06964207898258	3.88770328592139	4.13263360778758
N	-2.68793097337662	3.14589097434281	2.51947457474303
C	1.19045574698878	4.74331658716697	3.62187289394397
C	1.52999194908962	5.70018095819697	2.66967124154544
H	0.77494067518977	6.37245370171312	2.28468996576736
C	2.84224093006160	5.76221834207053	2.23363276190914
H	3.13830398037314	6.49611467949940	1.49353856936929
C	3.76366647687745	4.86748222995287	2.75430120502988
H	4.79980940027855	4.87706394012063	2.44185479574256
C	3.32501385434171	3.95094412657682	3.69672803506646
H	4.01587428551303	3.23370655305154	4.12885363055987
C	-3.74036697622160	3.71682754052895	3.18719240491029
C	-4.91714758437306	3.97941200050222	2.44988904008017
H	-5.74948383968395	4.42692653743324	2.97481816118919
C	-4.98770828684104	3.68225228694820	1.11824939823035
H	-5.89491050817208	3.89273424110352	0.56431331263876
C	-3.88388394435943	3.10702158630578	0.46666898188409
H	-3.90705906340506	2.86237242919667	-0.58537776880526
C	-2.76239312443979	2.85720597021055	1.19760318869542
H	-1.88075327727550	2.41714855483658	0.75611985788251
C	-1.49511284026311	1.49737432485048	4.79784659470461
H	-0.68735628417131	0.76326123049353	4.74462462276204
H	-2.44181100816437	0.99115793164104	4.59900806258124
H	-1.53799534195712	1.91482635884800	5.80155459564470
C	0.03271078557189	2.16347710764389	2.28380069624983
H	0.27051010043285	2.86812132625625	1.48557324259162
H	-0.34465531457700	1.23596159058943	1.84506254842121
H	0.95721601251066	1.92643295976091	2.81183828334551

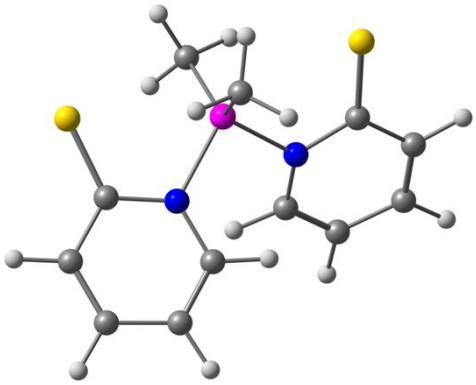

Figure S42. Optimized molecular structure of **2b´´^{NN}**.

PBE0:

final single point energy: -1665.23376168991 a.u.

final Gibbs free energy: -1665.0372234 a.u.

B2T-PLYP:

final single point energy: -1665.28641176546 a.u.

Table S24. Atomic coordinates for optimized structure of **2b´´^{NN}**.

Si	9.63477445202229	11.43329063080587	8.56184646212070
S	7.63823337994136	9.46519573674433	9.68772092442686
S	12.46330198159912	12.37263972897466	8.12373124151869
N	7.90053465751839	11.37978882075119	7.89651671977613
N	9.96153483565432	13.19244734799991	8.05581909445967
C	7.04986114357456	10.47308561352528	8.47754193439605
C	5.72997662500005	10.39841829969106	7.96779948782245
H	5.03931715266329	9.73771531028223	8.47295371580643
C	5.36963507892185	11.08978364813205	6.84809723699158
H	4.36429827635046	11.00119030881791	6.45392814459590
C	6.31887135971333	11.89028739933807	6.18806924056481
H	6.08870029974234	12.40946783068643	5.26898381277796
C	7.55545471396510	12.00812319711390	6.74110362528183
H	8.32256601220982	12.61034864147727	6.27588701698159
C	11.27591008392890	13.53364253460630	7.86032916930703
C	11.55506143453504	14.87695655094072	7.50727220762945
H	12.58230366258576	15.12840025711923	7.28275663332485
C	10.57184406906243	15.82275001713662	7.51134066637389
H	10.80632138965346	16.85187976757237	7.26666268013601
C	9.26026438929530	15.46250190399780	7.86839098527382
H	8.46518355611033	16.19098233106822	7.93501523347574
C	9.00157757553201	14.15270714646069	8.12667675108872
H	8.01130099132826	13.82134479964490	8.40464114081756
C	9.84255448984000	11.62580624933759	10.39211585526561
H	10.12275575643355	10.68248364589068	10.85525880782946
H	8.90497687120861	11.95791041494278	10.84129108152764
H	10.61746324168406	12.37276133799060	10.57541581147747
C	10.37399002248227	10.08362881036658	7.53111251169760
H	11.23928111178704	9.64587664224803	8.02363264122294
H	10.69716980465628	10.48411630533186	6.56882913141142
H	9.61322455500003	9.31716335000437	7.36960576761977

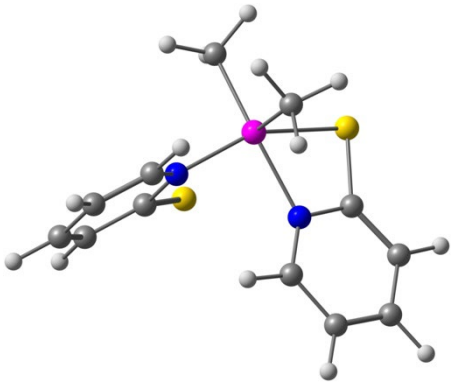

Figure S43. Optimized molecular structure of **2b´´^{SSiScis}**.

PBE0:

final single point energy: -1665.24731238844 a.u.

final Gibbs free energy: -1665.05085854 a.u.

B2T-PLYP:

final single point energy: -1665.29594621735 a.u.

Table S25. Atomic coordinates for optimized structure of **2b´´^{SSiScis}**.

Si	9.83791517599673	11.55627434593158	8.45060887894532
S	9.55018297793415	11.25570024065686	5.79851860164985
S	12.18628793465957	11.74420475970541	8.24194118269591
N	8.14434436208677	10.86648118354229	7.90920596146077
N	10.62452696447264	9.78295392834877	8.19242572470204
C	8.10578824777060	10.78859123282846	6.55386882925016
C	6.92159955792964	10.34577339911674	5.93780976371533
H	6.88881380849697	10.27878359377359	4.85916075820140
C	5.83959692736939	10.01181124878696	6.71274627911327
H	4.92511856429509	9.67045568765514	6.24199607462216
C	5.91159661725372	10.11038616202421	8.10837722938498
H	5.07196427853313	9.85492458188821	8.73879780470753
C	7.08487839609557	10.54325030658014	8.66706442539977
H	7.21387383262841	10.64281833253513	9.73609435408960
C	11.94308340418258	10.05232142919713	8.14903386189335
C	12.86624857484992	9.01219327717762	8.03417988221999
H	13.92416263883308	9.23171374253733	7.99753962479951
C	12.39035723816343	7.72049231456990	7.96704248901890
H	13.08707605600633	6.89615214618990	7.87278937796563
C	11.01767497728581	7.46754175529185	8.02154888025131
H	10.62777422025295	6.46078853342020	7.97207473868192
C	10.15889755137550	8.53455771483241	8.13875485186160
H	9.08400576743714	8.41513406792476	8.18381927290591
C	9.48252913048315	13.39920615390007	8.21573670579266
H	9.94040499925412	13.92659169658983	9.05848027266705
H	8.40779650273030	13.59766383702276	8.23516903454748
H	9.89547664712035	13.79536489458788	7.29066726817884
C	9.65123637826122	11.33533162001454	10.32300517457331
H	8.85930916601205	11.98815720275054	10.70097483051998
H	10.57532261534241	11.62419749153192	10.82566525343239
H	9.41932097588649	10.30909525008704	10.61615309275141

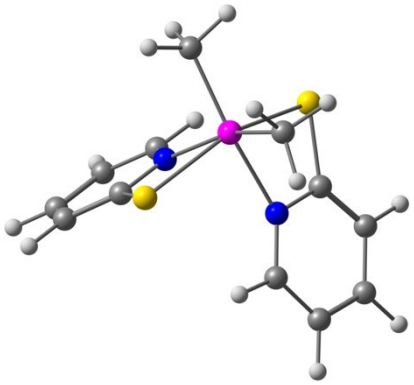

Figure S44. Optimized molecular structure of **2b´´^{SSiStrans}**.

PBE0:

final single point energy: -1665.24680539603 a.u.

final Gibbs free energy: -1665.05072335 a.u.

B2T-PLYP:

final single point energy: -1665.29487879155 a.u.

Table S26. Atomic coordinates for optimized structure of **2b´´^{SSiStrans}**.

Si	9.78637541480845	11.59583350066301	8.37755652779148
S	11.01909438615789	9.58947089397710	8.52928019251180
S	9.22540037236085	13.70214716901477	7.47333658699564
N	10.13397051543578	10.83953078236385	6.52799999414474
N	11.46341193086424	12.63718527669925	7.92350135178808
C	10.79179693202304	9.70688477899152	6.82846635869934
C	11.17990294959487	8.82603302680316	5.81914852325927
H	11.70806181290078	7.91597945422412	6.06812681354487
C	10.86877806639852	9.15099021308497	4.51494169753710
H	11.16011615657823	8.48475239734364	3.71157071464945
C	10.17812106630075	10.32784627746937	4.22702726782799
H	9.92278381785795	10.59705158020372	3.21172077443282
C	9.82193484423992	11.15212590554662	5.27200224389599
H	9.28558058703133	12.08309716246579	5.13486102123288
C	10.94304169617853	13.79225360547682	7.47560428372309
C	11.77836362193495	14.84384284597657	7.09878713926886
H	11.35340299567399	15.77111852165099	6.74008053229147
C	13.14235495624244	14.66158764966173	7.19852688101578
H	13.81354638921580	15.46167840396680	6.90961972821702
C	13.65977459073742	13.45625124705155	7.67217978089979
H	14.72517416828744	13.29596899298203	7.75984832521275
C	12.77840766974644	12.46055579152215	8.03228311948609
H	13.09717270502965	11.49666435460190	8.40938179818967
C	8.01282061923457	10.90650907381434	8.34761118211198
H	7.40088743753662	11.51423490953416	9.02048302485729
H	7.97847205181972	9.87483416692246	8.70379946424779
H	7.56386009705977	10.94382577735873	7.35360314032837
C	9.96099470682629	12.05222321141323	10.21672656680866
H	9.50191781577559	11.25460621198301	10.80806462430750
H	9.43805934390662	12.98263081389902	10.44803637961830
H	11.00096192524117	12.15326422033320	10.53128095210387

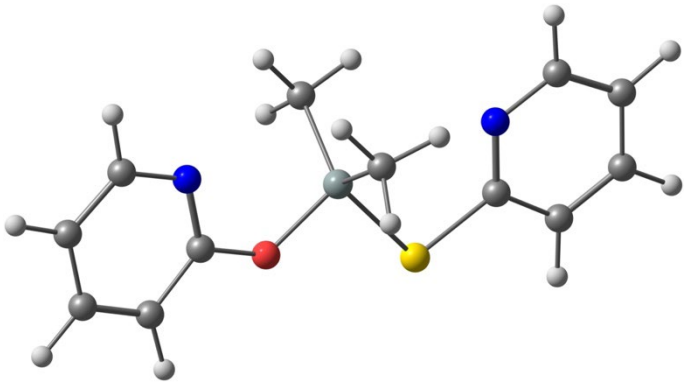

Figure S45. Optimized molecular structure of **2c**^{SO}.

PBE0:

final single point energy: -1340.72427964441 a.u.

final Gibbs free energy: -1340.53014313 a.u.

B2T-PLYP:

final single point energy: -1340.81962797691 a.u.

Table S27. Atomic coordinates for optimized structure of **2c**^{SO}.

Si	9.14289709666646	10.71519305281524	8.18102648078064
O	7.90767118550110	11.45112297134044	7.28850391874845
S	10.53446566423314	12.34778319700809	7.83212231012403
N	6.47991170622731	9.70357917721572	7.60158637069778
N	11.88977008200485	10.61265603495619	9.33226572893372
C	6.73888462597212	10.86119184141136	7.01643641309164
C	5.85697382610087	11.48926059756735	6.13474433110898
H	6.12701534964639	12.43584630952931	5.68636182893403
C	4.66039972407942	10.85980665775670	5.86451803944041
H	3.95132438659918	11.31442181360831	5.18282027341069
C	4.37541086182433	9.63944477675365	6.47027163647562
H	3.44784289212647	9.11626101163096	6.28050239611043
C	5.31777440652331	9.10822733876929	7.32840078534497
H	5.14151491491997	8.15950531771603	7.82538590103961
C	11.94235134335181	11.79683915168875	8.73352570645663
C	13.06662986928401	12.62280668113856	8.78735127694694
H	13.06456546715258	13.58049590234870	8.28318381889106
C	14.16668795576390	12.18499660153600	9.49716203976336
H	15.05427043705580	12.80340152332999	9.55861181962616
C	14.11971060883512	10.94798120486953	10.12870324999109
H	14.96005668623549	10.56934127064406	10.69524228345696
C	12.95916132680915	10.20493621598570	10.01368719606882
H	12.87548368928141	9.23260499275087	10.48908105636012
C	8.66430349295419	10.58793493220390	9.96461210195839
H	7.98112931959459	9.74895132059187	10.10462238673959
H	8.16154888736503	11.50465874025702	10.27867577625145
H	9.54775034056127	10.43908380753927	10.58413020053912
C	9.69333284194667	9.15607194727559	7.34696296182453
H	10.67455017257394	8.86224792115428	7.71791963580238
H	9.75770366169650	9.31520503950888	6.26875181689971
H	8.97964817711267	8.35451464909725	7.54119225818170

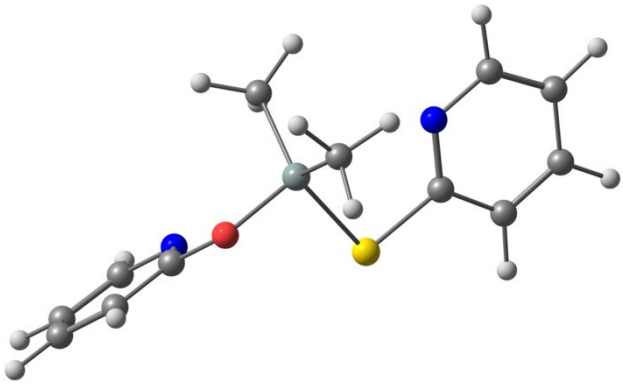

Figure S46. Optimized molecular structure of **2c**^{OC}.

PBE0:

final single point energy: -1340.72398273724 a.u.

final Gibbs free energy: -1340.52768963 a.u.

B2T-PLYP:

final single point energy: -1340.81903271733 a.u.

Table S28. Atomic coordinates for optimized structure of **2c**^{OC}.

Si	-1.73170800811380	3.29756119087068	2.11587247290658
O	-1.12543525384895	2.37993601126400	0.83383062066165
S	0.10452881482097	4.13994895083278	2.93040554040990
N	-0.46531108452302	4.14327154446354	-0.46051401058256
N	-1.92125475322972	4.90061200136427	4.44458063612342
C	-0.60205155314354	2.83752899134484	-0.30859013112082
C	-0.22502381720856	1.90837599577354	-1.28102039493414
H	-0.36056094231940	0.85134289023681	-1.09562536018668
C	0.31399493308607	2.38679742872878	-2.45598408161146
H	0.61826402776716	1.69627520781133	-3.23364627404115
C	0.46299874204586	3.75945800235733	-2.63062030412531
H	0.88267551329945	4.17240133739122	-3.53809462600664
C	0.05861101144611	4.58906845157701	-1.60336699492763
H	0.15672194434009	5.66653182942058	-1.69169180234301
C	-0.59960752631952	4.95781467881982	4.31526018139191
C	0.21908475917497	5.63695857470477	5.21871504158316
H	1.29158423917217	5.65866836511954	5.07620565524335
C	-0.37930401089606	6.27367928635542	6.28805038009331
H	0.22724939930822	6.81002748520069	7.00812554768893
C	-1.76078184405070	6.21903204034167	6.42957259285942
H	-2.26470877865732	6.70585864663063	7.25390786663492
C	-2.48327036978103	5.51921082096810	5.48062464901175
H	-3.56435379540037	5.44756081491949	5.54775831755677
C	-2.42816552820099	1.96305515617557	3.19734993384639
H	-3.25640484814191	1.47532551620204	2.67594834381879
H	-2.79663824641552	2.36903502289872	4.13753706107538
H	-1.66551357588807	1.21141647770251	3.40716145080402
C	-2.97310156846530	4.52818113312381	1.49570665672654
H	-2.50233401220577	5.48240015421159	1.26360774393241
H	-3.74660649072765	4.68512540943215	2.24714141347471
H	-3.43265301192378	4.14105439975656	0.58281765703594

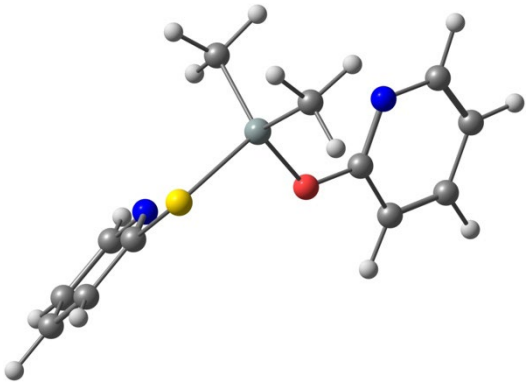

Figure S47. Optimized molecular structure of **2c**^{SC}.

PBE0:

final single point energy: -1340.7228854534 a.u.

final Gibbs free energy: -1340.52687392 a.u.

B2T-PLYP:

final single point energy: -1340.81852096013 a.u.

Table S29. Atomic coordinates for optimized structure of **2c**^{SC}.

Si	-2.28045766879936	2.94739850821653	2.27888694072664
S	-1.43313743956675	1.62903368398765	0.78963873091878
O	-0.92842170274777	3.68437985867195	2.95115135535222
N	-0.69779093832928	4.03175751161075	-0.12910211220975
N	-2.14462599190965	4.85821854308127	4.48125099329943
C	-0.53732083859609	2.72278319411443	-0.26971359776760
C	0.31702795558880	2.16091013791019	-1.22014144847282
H	0.41936647358974	1.08621009686543	-1.29668577025703
C	1.02786830089131	3.01080382364998	-2.04471339866490
H	1.70159768582028	2.60616282749405	-2.79070074448360
C	0.87178650452006	4.38315912335475	-1.90029779311179
H	1.41298768396321	5.08326073446189	-2.52299105039567
C	-0.00259945738393	4.83756054675418	-0.92922396420599
H	-0.15747173110356	5.90172330705285	-0.78022160290442
C	-0.97705250733090	4.61513046658441	3.90981217498445
C	0.20238555968713	5.27438581904883	4.26120019902192
H	1.12611941039635	5.03113976865115	3.75380746671912
C	0.13507228775867	6.22605445853878	5.25635513772961
H	1.02895043429983	6.75977060391471	5.55677354964774
C	-1.08680113024602	6.49389138943127	5.86689467588210
H	-1.17754447077146	7.23358260475550	6.65089821492182
C	-2.19181579025677	5.78370122013719	5.44114390238655
H	-3.16650881655668	5.95738955282668	5.88595622206335
C	-3.04117672606978	1.73202808749572	3.45741686607893
H	-3.78345078769818	1.11813113164884	2.94199766019010
H	-3.53641551527340	2.26668394796768	4.26913798903442
H	-2.28352791756274	1.07209808369063	3.88339918887175
C	-3.50308540557301	4.15076971921603	1.58154243439099
H	-2.99705528425470	4.94363572707050	1.03328505902310
H	-4.09399682130793	4.58524385144096	2.38882476521297
H	-4.17198099017738	3.62651548635481	0.89544373901741

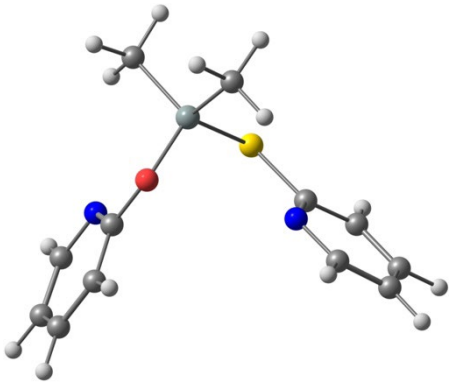

Figure S48. Optimized molecular structure of **2c**^{CC}.

PBE0:

final single point energy: -1340.72349256371 a.u.

final Gibbs free energy: -1340.52770266 a.u.

B2T-PLYP:

final single point energy: -1340.81895132914 a.u.

Table S30. Atomic coordinates for optimized structure of **2c**^{CC}.

Si	-1.67836602428964	2.63114978460606	2.32834775922336
O	-1.24058429609468	1.80727120771344	0.93894880213447
S	-0.14764836580274	3.98719555048623	3.02157094458258
N	-0.87324221668383	3.62688971423884	-0.39625696455891
N	1.15632099168154	1.65159426051506	3.02282722676736
C	-0.75896054051809	2.32553168828543	-0.19821039993705
C	-0.16472215586471	1.45778699306276	-1.11596611097788
H	-0.10031422100759	0.40149857048931	-0.89229259015413
C	0.32936470968744	1.99526529194349	-2.28565148023165
H	0.79915914797450	1.35332070155436	-3.02135592897579
C	0.22146600278181	3.36469544382333	-2.50661553527065
H	0.59910941916147	3.82390101362604	-3.41035725040245
C	-0.38676173441248	4.13060363177809	-1.53132684803881
H	-0.49436164994949	5.20324643080309	-1.65867769362004
C	1.23410032741234	2.93668532015888	3.34155918415201
C	2.37257163197703	3.51071464682446	3.91023461826396
H	2.39047403509921	4.56532333768465	4.15278876068755
C	3.46357496315487	2.69895233069929	4.15035533887569
H	4.36298102143558	3.11354290278660	4.58994391540476
C	3.39084240110697	1.35082977679782	3.82366668649280
H	4.22273950049502	0.68074898256464	3.99576084795800
C	2.21554345325861	0.88162882168266	3.26543661943011
H	2.11200571098397	-0.16462186852797	2.99493339967251
C	-2.06696663277715	1.29694859937952	3.54984839461606
H	-2.89818747182721	0.69244797599648	3.17795038463778
H	-2.36588121767368	1.74334792694621	4.50025125672586
H	-1.20503944149786	0.65340572337711	3.71536274649400
C	-3.12936945770491	3.75427983323355	2.05337177750399
H	-2.86749036659872	4.60220265144557	1.42163832138665
H	-3.50311807593317	4.12324738429968	3.01124509600177
H	-3.93258744757438	3.19513037172515	1.56681772115601

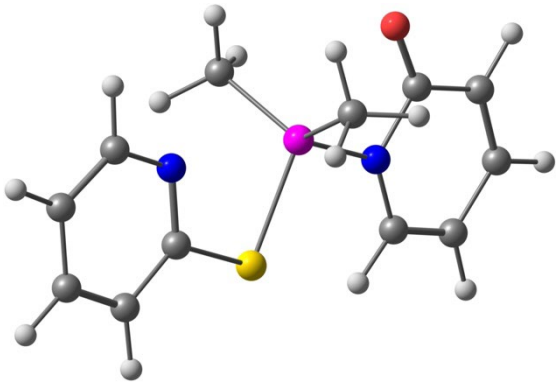

Figure S49. Optimized molecular structure of **2c´**^{NS}.

PBE0:

final single point energy: -1340.7149414208 a.u.

final Gibbs free energy: -1340.51808668 a.u.

B2T-PLYP:

final single point energy: -1340.80593360056 a.u.

Table S31. Atomic coordinates for optimized structure of **2c´**^{NS}.

Si	9.54344977433427	11.54816491164375	8.57419931853674
S	8.90640359655701	10.09538472525058	7.06107501210195
O	11.26808553883559	13.05532750545648	9.79245212013013
N	6.88870260914256	10.78092404203572	8.61318319360310
N	11.28901429628087	11.66430312087651	8.04177032394935
C	7.22952907302290	10.02290469612178	7.57656882926774
C	6.32248485715674	9.20076635113119	6.90798731628769
H	6.64396515616575	8.59911482333917	6.06793865317487
C	5.01455805787181	9.18308750264714	7.35061919398779
H	4.28287094296862	8.55676575083361	6.85424190635609
C	4.64932576693640	9.97445853083453	8.43329073847624
H	3.63410476017157	9.98726336443161	8.80687013730811
C	5.62448254502699	10.75316514863605	9.02916885693266
H	5.38896631061645	11.38662880208103	9.87816715085965
C	11.94522070229975	12.54585476135656	8.88557014565911
C	13.33034204152482	12.77964662658021	8.62509375158869
H	13.85274245028288	13.46481689569893	9.27909353935404
C	13.94870566708023	12.15459290194242	7.58539559089747
H	14.99979386227695	12.33979123849670	7.39448967628065
C	13.23661776609331	11.26759744913399	6.74981968816833
H	13.71262991225695	10.76566116576973	5.92016089500434
C	11.91981694156348	11.05227281658849	7.01084970541087
H	11.32374210693304	10.38428458302556	6.40323237761435
C	8.74278080512934	13.19048544714106	8.23862345245955
H	8.34898226136712	13.60527612818275	9.16698877637739
H	7.92420099334592	13.07984591463213	7.52874626080823
H	9.47984507406511	13.88649087430999	7.83652446582353
C	9.49483238494116	10.75078212439048	10.25153813796106
H	9.06505334510584	11.44479934427331	10.97447025162510
H	10.50708870901109	10.50358991513342	10.57364548610412
H	8.89112835563495	9.84454603502463	10.23062707589075

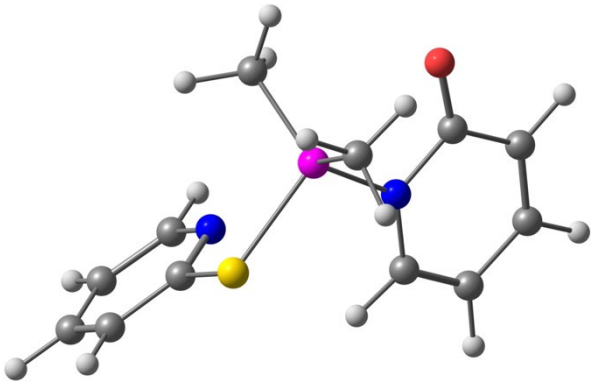

Figure S50. Optimized molecular structure of **2c´**^{SC}.

PBE0:

final single point energy: -1340.71745156175 a.u.

final Gibbs free energy: -1340.52065924 a.u.

B2T-PLYP:

final single point energy: -1340.80853232971 a.u.

Table S32. Atomic coordinates for optimized structure of **2c´**^{SC}.

Si	-1.03900587077222	1.21346600888744	2.44059102948141
S	-0.80625553199348	-0.24993105651197	0.85174672411791
O	-0.49879036356705	2.90782679718423	4.41536097412010
N	0.22454622994826	1.96224202616429	-0.20958310476244
N	0.64104982557857	1.63044430332933	2.96674712844980
C	-0.21741624664366	0.74125727289986	-0.48396834293854
C	-0.21856315598338	0.20575679636309	-1.77233961326960
H	-0.59218115272208	-0.79424873309428	-1.94993683613019
C	0.26495085277586	0.98755478083067	-2.80344405005025
H	0.27999097649481	0.60255430777011	-3.81613659556881
C	0.72394538159273	2.26903570172526	-2.52702383327965
H	1.10706821313164	2.91304722616394	-3.30746546188170
C	0.67825454303700	2.70695677839153	-1.21578155563421
H	1.02434340300117	3.70120322915985	-0.95148541389443
C	0.61466906370602	2.54644982911992	4.00811788495662
C	1.88286870849643	2.98092837649694	4.50575524548458
H	1.87979551949546	3.70060838341485	5.31332939623423
C	3.03644591827313	2.49173441723498	3.97391966827816
H	3.99157384517182	2.82714668283650	4.36246291984062
C	3.00693044646776	1.55026558288768	2.92189852868787
H	3.91476521503578	1.15213326152201	2.49293214960164
C	1.79741818584857	1.15119818423458	2.44880599909826
H	1.69159625655796	0.43550463451648	1.64491616940390
C	-1.85031104181023	0.16232590392947	3.73764731143835
H	-2.84544526448887	-0.13473017021352	3.39916600060269
H	-1.94746296936556	0.72489809855269	4.66540753359560
H	-1.27019728735150	-0.74228856594441	3.92961950895525
C	-2.01008368073779	2.68085810714631	1.85616164473959
H	-1.35477244579542	3.53669153061874	1.70326384872669
H	-2.75023528392934	2.93827511730854	2.61468808014575
H	-2.51633254545241	2.45489530307469	0.91696187145067

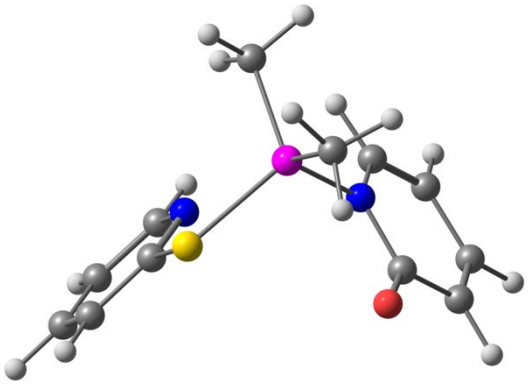

Figure S51. Optimized molecular structure of **2c´**^{CC}.

PBE0:

final single point energy: -1340.71405391523 a.u.

final Gibbs free energy: -1340.51695493 a.u.

B2T-PLYP:

final single point energy: -1340.80536507018 a.u.

Table S33. Atomic coordinates for optimized structure of **2c´**^{CC}.

Si	-1.49569823605878	1.65565261088814	1.98436848356215
S	-0.59027740120447	-0.21034472497056	1.40810270246980
O	-2.54530037309505	0.12612450323995	4.16324854896820
N	1.45245388440859	1.14492371741160	2.47044134292845
N	-1.27352205923343	1.95752424754596	3.74635896745056
C	1.07645851041448	-0.01664970979193	1.95272735192846
C	1.93615031711552	-1.10964092070436	1.83379876288421
H	1.58221106625135	-2.04094238475604	1.41102863509241
C	3.23620479658495	-0.96736402324056	2.27655545808258
H	3.92895521515725	-1.79698476635769	2.20062351378595
C	3.63932702219020	0.24477591941965	2.82295154813335
H	4.64781280071313	0.39443415982502	3.18490743326631
C	2.70806446453503	1.26437564245687	2.89736383293590
H	2.97470960647488	2.22773404206911	3.32103041229715
C	-1.88169838245298	1.05593968492910	4.62312650506780
C	-1.66815423721853	1.29866270583420	6.02244523512109
H	-2.14100101310079	0.61103164411016	6.71085315384815
C	-0.90068144906473	2.33417580494758	6.44910634648753
H	-0.74935273859068	2.49270305766663	7.51106753190857
C	-0.29220638140172	3.20746177564771	5.51809594298707
H	0.32590549949296	4.03462242334014	5.83532978339782
C	-0.49788141486670	2.98158078847775	4.19749273720670
H	-0.04955232941391	3.60477155308545	3.43749389598633
C	-3.28651425578110	1.47842192039397	1.53703321121727
H	-3.39660191091849	1.56625887016854	0.45367713567106
H	-3.85677430189513	2.28684919169821	2.00159059326215
H	-3.69834329682236	0.52906694817218	1.87097286986996
C	-0.77208083177688	3.10457169367750	1.07507292687826
H	0.29864501665762	3.21336166311556	1.23629874262620
H	-1.27989392600690	4.03004881986836	1.35883705939082
H	-0.94617914809332	2.94042303583167	0.00915308528743

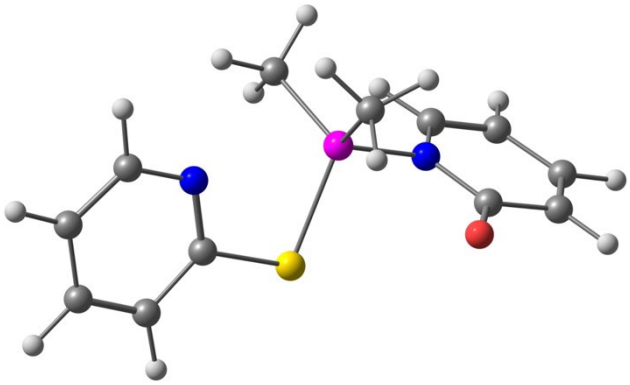

Figure S52. Optimized molecular structure of **2c´^{NC}**.

PBE0:

final single point energy: -1340.71327924328 a.u.

final Gibbs free energy: -1340.51621768 a.u.

B2T-PLYP:

final single point energy: -1340.80479595093 a.u.

Table S34. Atomic coordinates for optimized structure of **2c´^{NC}**.

Si	-1.01305737904486	3.01397626959379	2.83688800574957
S	-0.48107533075571	5.10022260729568	2.60849866675370
O	-3.18532770092051	4.19997866929820	4.21667607977276
N	1.64757146038759	3.77804726141564	3.44460127324306
N	-2.74783900075666	3.09155918213666	2.29235465542112
C	1.21942602504606	4.96469146092412	3.02868939995446
C	2.05291919040886	6.07901794808116	2.92879025314377
H	1.66057752787230	7.02812758841169	2.58782320545297
C	3.38141097315726	5.92928371678722	3.27450662849854
H	4.05709477597617	6.77364928032522	3.20753768838972
C	3.83927548785829	4.68996141171193	3.70577444298620
H	4.87323195433661	4.53479271210100	3.98349185248563
C	2.93127644369703	3.64918864843979	3.77313450296329
H	3.24015919819448	2.66334611896571	4.10604943405403
C	-3.63113542398217	3.71615411669273	3.17441968841359
C	-5.01059429367803	3.74189877184117	2.77869758887626
H	-5.70431879469600	4.20956246791071	3.46452882515939
C	-5.41160523441770	3.21536211454330	1.59272428869917
H	-6.45784462523748	3.25356825570777	1.31049439289397
C	-4.47325970933537	2.61850378523468	0.72048580178842
H	-4.76839287670166	2.19786838985039	-0.22974028192042
C	-3.17307321105447	2.57839295749485	1.10567890034238
H	-2.41343192001021	2.13093412189578	0.48085949697098
C	-0.93154950502517	2.28272964064681	4.53791860652967
H	-0.04731003419141	1.64956813261356	4.61573433483726
H	-1.82477468697461	1.68138463828184	4.72028708133152
H	-0.88543665494005	3.06136033735827	5.29658453214256
C	-0.17440487599379	1.94756399668418	1.56439614875966
H	-0.18861022226190	2.38947668757875	0.56735225278692
H	-0.65414991105375	0.96579738470827	1.52298051815511
H	0.86358599809692	1.80918324546885	1.86313524636455

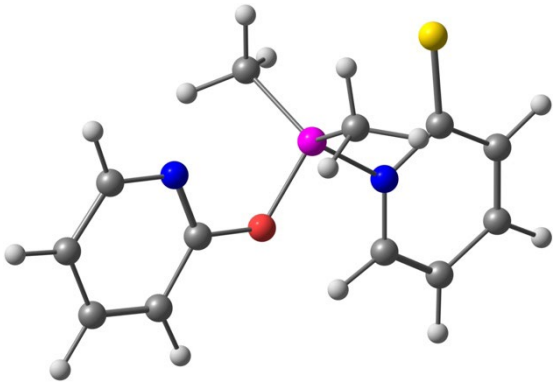

Figure S53. Optimized molecular structure of **2c´´^{NO}**.

PBE0:

final single point energy: -1340.72761155381 a.u.

final Gibbs free energy: -1340.52895022 a.u.

B2T-PLYP:

final single point energy: -1340.82125903126 a.u.

Table S35. Atomic coordinates for optimized structure of **2c´´^{NO}**.

Si	9.46400681686763	11.80371266047544	8.90829885493087
O	8.79341908411183	10.68013291215710	7.80927950165954
S	11.52116308331665	13.40552558598649	10.09220778305425
N	6.76000109738731	10.90116529195832	8.80308639224172
N	11.13614458297558	11.69921075078219	8.15450129737659
C	7.50424753677465	10.34139181899195	7.86119460748952
C	7.00255487445406	9.42542270283829	6.93393959402365
H	7.65863044008067	9.00122588997107	6.18567312804301
C	5.66634166302286	9.09502857776606	7.01256977724840
H	5.24083868896521	8.38842181319466	6.30983175439409
C	4.87316825589802	9.67513503676510	7.99843723345532
H	3.82150976604437	9.43910693254780	8.08989221948162
C	5.46936600972930	10.56977708688106	8.86495496169115
H	4.89275813107311	11.04902911962062	9.64973460077017
C	12.05647345569627	12.50137488380094	8.77231967332851
C	13.37101055526645	12.51046190393630	8.25817971711832
H	14.09973968940565	13.14353971641182	8.74489311994763
C	13.69793314869394	11.73907214958219	7.17743262966574
H	14.70953217394090	11.75331357514005	6.78909662288769
C	12.72464629178516	10.92991749035624	6.56955700931909
H	12.95368988185668	10.31121616488501	5.71393403665842
C	11.46251516729518	10.93669880612617	7.08420989253753
H	10.65962893609791	10.34387131487191	6.67298603136233
C	8.67755379280700	13.43875821243406	8.52388373595140
H	8.35664553399581	13.93116648895625	9.44179010539428
H	7.80891886096829	13.29025529805685	7.88062538324681
H	9.39125503550707	14.09485328753739	8.02461020886053
C	9.41620128997403	10.98841443745243	10.57360953665089
H	9.04449245915558	11.68650374275571	11.32368454702172
H	10.41669850252742	10.67634047213153	10.87460061954446
H	8.75838185832491	10.11854937262839	10.54338745264441

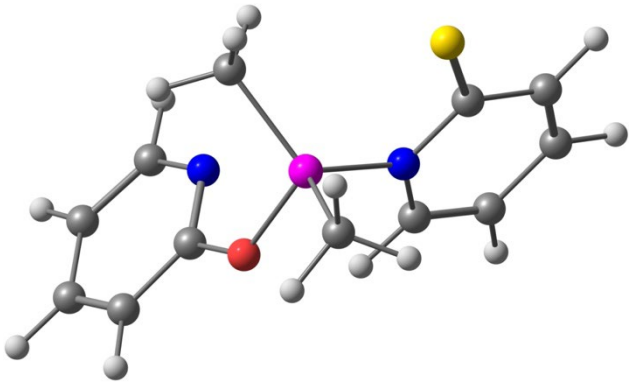

Figure S54. Optimized molecular structure of **2c´´^{OC}**.

PBE0:

final single point energy: -1340.72704167786 a.u.

final Gibbs free energy: -1340.52825279 a.u.

B2T-PLYP:

final single point energy: -1340.82063906332 a.u.

Table S36. Atomic coordinates for optimized structure of **2c´´^{OC}**.

Si	-1.00048654478701	1.38341460354550	2.35014674422960
O	-0.60551047963404	0.50437297106082	0.94664344604980
S	-0.79165122683669	2.85118393118183	4.79067610930509
N	0.28985750903092	2.24808816202727	-0.22775468339860
N	0.69142827227379	1.73444579140810	2.96865928680239
C	-0.20893344978038	1.02223349693287	-0.22188051175898
C	-0.32264807610111	0.23742551071627	-1.37132996780796
H	-0.73939412495362	-0.75846353134084	-1.30252968746031
C	0.10668421856566	0.77437770000105	-2.56646224220984
H	0.03340702381571	0.19450315363079	-3.47888128022511
C	0.62971016843892	2.06384679983401	-2.58776451195822
H	0.97584954174790	2.51933055603737	-3.50584732416059
C	0.69603981029773	2.75401596933824	-1.39346386390489
H	1.09580162075662	3.76259136480380	-1.35906409190466
C	0.70839696000119	2.44795892281014	4.13424965996635
C	1.96429073758372	2.77058747299002	4.69003260503861
H	1.98189224911980	3.34855084418719	5.60344306704104
C	3.11567043748098	2.34641929416485	4.08581070776012
H	4.07652143128215	2.59320690820267	4.52189331440616
C	3.05580767134916	1.58611024826962	2.90684103718683
H	3.94873702363183	1.22773890882751	2.41567180241041
C	1.83033003545623	1.30460399261493	2.38053460702693
H	1.70907191163160	0.72425628767140	1.47920209305193
C	-1.81002556310847	0.05230562849913	3.35502890278111
H	-2.13139303648912	-0.75915016809944	2.69885299510877
H	-2.67315990383257	0.44830813880487	3.88853747331721
H	-1.11737262008229	-0.35102529391614	4.09551153247750
C	-2.01003615305128	2.83608013575535	1.79228241583538
H	-1.42873630375510	3.75685959592978	1.81333425006908
H	-2.86400643270856	2.95699686643201	2.45854138186932
H	-2.36298296334368	2.67288585367891	0.77141954305545

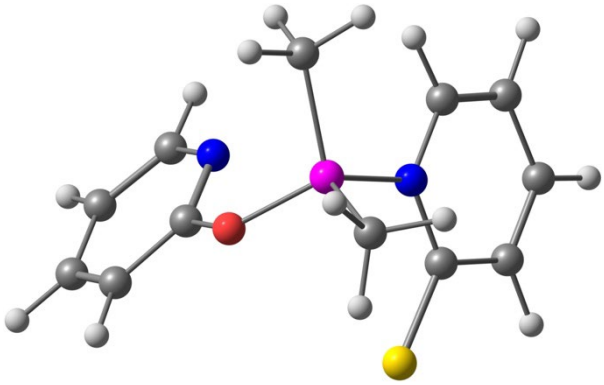

Figure S55. Optimized molecular structure of **2c´´^{CC}**.

PBE0:

final single point energy: -1340.72178856295 a.u.

final Gibbs free energy: -1340.52291949 a.u.

B2T-PLYP:

final single point energy: -1340.81671688475 a.u.

Table S37. Atomic coordinates for optimized structure of **2c´´^{CC}**.

Si	-1.29451567000339	1.65210922871861	1.99912315048144
O	-0.27133666845681	0.42127158774118	1.54972487422115
S	-1.91014056970020	-0.53840677482651	4.19352535949101
N	1.57870065863044	1.23848484375341	2.60674401726506
N	-1.17876875378471	1.99133368012386	3.78769624026787
C	0.99086133509045	0.24460241573574	1.96417246917548
C	1.61128552202916	-0.97552056691746	1.69736015084896
H	1.06972772046571	-1.75181509187381	1.17430329607422
C	2.90930755279320	-1.14401618622794	2.13094599096448
H	3.42541397763601	-2.07869364900197	1.94651547897741
C	3.54308214327162	-0.10834763099994	2.81087175478130
H	4.55920659940106	-0.20536439158835	3.16900139655550
C	2.83319191362728	1.05680193433012	3.02309587350898
H	3.28387467496130	1.89132438962999	3.55077183604353
C	-1.47313489653408	1.00272765720097	4.70141770752431
C	-1.37648598614460	1.35074627477673	6.07359697629894
H	-1.61554387802753	0.57955978648164	6.79227349308685
C	-0.99025506197531	2.59645411738807	6.46987593792220
H	-0.92015189038169	2.83301211379036	7.52500044348652
C	-0.67935153342313	3.57062530945420	5.50436163977857
H	-0.36288827766549	4.56699689507582	5.77676094786088
C	-0.78452344744389	3.22821463141114	4.19420296880260
H	-0.55274983369915	3.93150611948165	3.40927080419604
C	-3.00701670631418	1.19476727875673	1.48270093792472
H	-3.13654758503929	1.44735558335601	0.42715062009268
H	-3.73525484857157	1.77063986247456	2.05871614946943
H	-3.21005058629518	0.13759491601383	1.63195627580229
C	-0.77820892402161	3.20582764795415	1.12769461633480
H	0.23521200843203	3.51948502805789	1.37692660494169
H	-1.46947548326212	4.03199863531147	1.30779801848850
H	-0.80827899259432	2.98229424841779	0.05759771933240

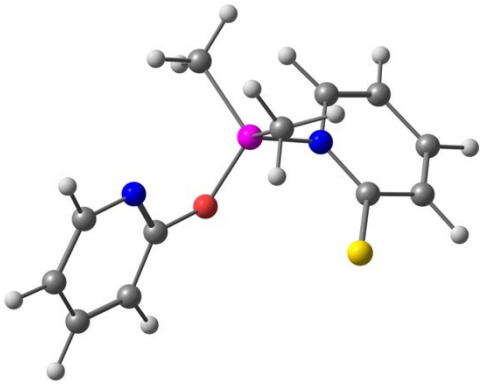

Figure S56. Optimized molecular structure of **2c´´^{NC}**.

PBE0:

final single point energy: -1340.72085275713 a.u.

final Gibbs free energy: -1340.5222748 a.u.

B2T-PLYP:

final single point energy: -1340.8158785842 a.u.

Table S38. Atomic coordinates for optimized structure of **2c´´^{NC}**.

Si	-0.87841903778852	2.76127009773598	2.80963659871287
O	-0.13238253899478	4.21448133545557	2.45215436046184
S	-2.68575493973867	4.84424127626413	4.29495827900146
N	1.78937430159614	3.56212997936716	3.47626625653880
N	-2.58569749714905	3.11756295733931	2.26923870300675
C	1.08349413493493	4.52925223657492	2.91405050122133
C	1.54017578892408	5.84002842504127	2.78084183843109
H	0.90948666709820	6.58634453502588	2.31748646306884
C	2.79844866691143	6.13124126248607	3.26481438324926
H	3.19028812084003	7.13807754735082	3.18291179350398
C	3.55311338828892	5.12608873444539	3.86247695292319
H	4.54181067139583	5.32006054900348	4.25609384936155
C	3.00209785346025	3.86237234493450	3.94365194847396
H	3.55098083874453	3.04629583320771	4.40240678072344
C	-3.33653975077812	4.03511034096069	2.97439596375812
C	-4.66652589375127	4.25118742106089	2.52962245400066
H	-5.25730731178979	4.96878264465073	3.08147972067416
C	-5.17755318513888	3.58604505042920	1.45499335278624
H	-6.19684804189359	3.77108745787390	1.13719098322484
C	-4.37725722647924	2.66136845405702	0.76049487412302
H	-4.74478229883275	2.11614837295445	-0.09669091274637
C	-3.10551195837992	2.46254959909266	1.19596835321687
H	-2.44398203634812	1.76659696846613	0.70275367170749
C	-0.84442088365833	2.13166018038276	4.54814685535364
H	-0.17458880880090	1.27050548259941	4.60076452184493
H	-1.84649214133296	1.82463095217568	4.85393596149869
H	-0.50029431793543	2.89511014059610	5.24169426321570
C	-0.22648319676996	1.48171410416796	1.63538002438241
H	-0.22408898573608	1.81428183554159	0.59601648366749
H	-0.77283835202149	0.53868052276805	1.70855704045474
H	0.80783561512361	1.29024527799033	1.92966119115880

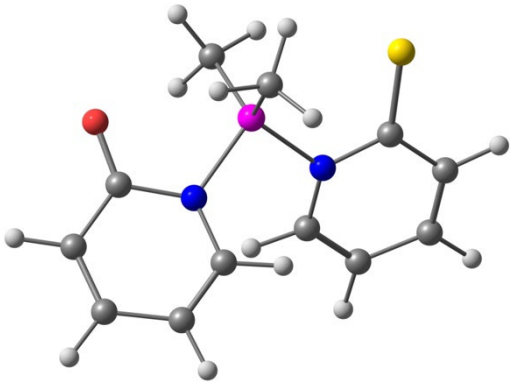

Figure S57. Optimized molecular structure of **2c´´´^{NN}**.

PBE0:

final single point energy: -1340.70537980238 a.u.

final Gibbs free energy: -1340.50697315 a.u.

B2T-PLYP:

final single point energy: -1340.7958833235 a.u.

Table S39. Atomic coordinates for optimized structure of **2c´´´^{NN}**.

Si	9.66296971365667	11.47247816417032	8.50524055167029
O	7.51383660217403	9.93147846212268	9.56179612743024
S	12.47943992720650	12.41868698212381	8.14155159505477
N	7.93588088157426	11.40560155367669	7.89624419790889
N	9.98052131034076	13.23180881283817	8.05188704737762
C	7.07965493165298	10.55307255067228	8.58930494671266
C	5.73819885236467	10.45659658009524	8.08449604228436
H	5.04413529192674	9.85808962259609	8.65937387262601
C	5.38742961210833	11.04038415721386	6.90983057213311
H	4.37891280013228	10.92668162654311	6.52845183163282
C	6.33645957860990	11.78243235617678	6.16930381141215
H	6.09372326868698	12.22370199797493	5.21367978902660
C	7.57821598239221	11.93451680906719	6.69238719238435
H	8.34351222337274	12.49299950544275	6.16854389027664
C	11.29673538999954	13.58822891409177	7.89657873449331
C	11.57297583600483	14.94151864643776	7.58638372534712
H	12.60475203590068	15.21145485031660	7.40973200131817
C	10.57599543911799	15.87306740325810	7.56072183264313
H	10.80690487212224	16.90932083127263	7.34425802624867
C	9.25321508694139	15.48929566689158	7.84304774558813
H	8.44482816387297	16.20538912809217	7.87261424446312
C	9.00052281561209	14.17387242719354	8.07767131320702
H	8.00424137450271	13.82095425171978	8.30046708208990
C	9.81023726365379	11.49173054885904	10.34500481106448
H	9.87711671813198	10.47898722425873	10.73783264174007
H	8.93455853426410	11.97189919039856	10.78432819610346
H	10.70531504215175	12.05115761113223	10.62108165451993
C	10.38729244530677	10.09437726770000	7.50319170065978
H	11.31562747116339	9.72900473381075	7.93427892229138
H	10.58755341062105	10.42455612795327	6.48216126312556
H	9.64748009843295	9.28935057489868	7.46890037016569

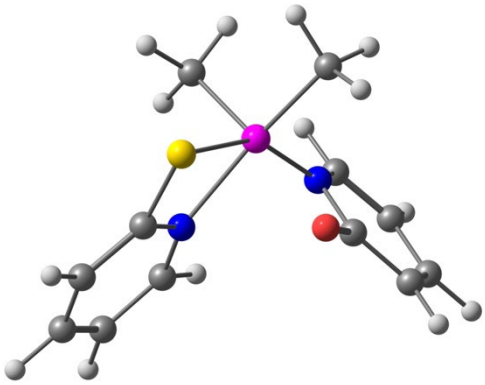

Figure S58. Optimized molecular structure of **2c´´´^{OSiCtrans}**.

PBE0:

final single point energy: -1340.71270724651 a.u.

final Gibbs free energy: -1340.51380467 a.u.

B2T-PLYP:

final single point energy: -1340.80019328328 a.u.

Table S40. Atomic coordinates for optimized structure of **2c´´´^{OSiCtrans}**.

Si	9.80173860902315	11.57865650154364	8.42484701823001
O	9.37744267002106	11.26944316274191	6.47369596663783
S	12.08769749304626	11.72394894771672	7.93706239541880
N	8.04293219412635	10.85593735201525	8.11176674274255
N	10.56942522390982	9.73961258888908	8.21059028128964
C	8.20430876586424	10.85294537432982	6.77148514201680
C	7.15600784903585	10.42620150611489	5.93956714277940
H	7.28295422445058	10.41966795819800	4.86592377897963
C	5.98900273775426	10.02822578519718	6.54783784522585
H	5.16004162398555	9.69154902216589	5.93596005846617
C	5.84694887004427	10.04732279681387	7.94425916775258
H	4.92736733825922	9.73488255154348	8.41776403099344
C	6.90847514003778	10.47401142991862	8.70269829366576
H	6.88173994292530	10.51878616916210	9.78458669403214
C	11.86384763096072	10.02189714456591	7.98257047403694
C	12.79291114127779	8.99185547143932	7.82833008080091
H	13.83263155611894	9.22434150989525	7.64421863484080
C	12.34536932414311	7.69037308535440	7.91682444127415
H	13.04623202034952	6.87255421556408	7.79830245031012
C	10.99787370148913	7.42161388574100	8.16042225710531
H	10.62942152606748	6.40817635603893	8.23477082150542
C	10.13490631915291	8.48496002504799	8.30484529232233
H	9.07699769828975	8.35198546143523	8.49549601988330
C	9.41231707860152	13.42311249300998	8.23219087822929
H	10.02519705071170	13.98358320386665	8.94379107818956
H	8.36409295426496	13.63084834896664	8.46470187511139
H	9.62410764248666	13.79412198587047	7.22933929898250
C	9.81638003010658	11.40447926929324	10.31766146222455
H	9.06833252631119	12.08027393474197	10.74314709571492
H	10.78548992930244	11.68325033634629	10.73526297085672
H	9.58497367688080	10.39029425747100	10.65133079038026

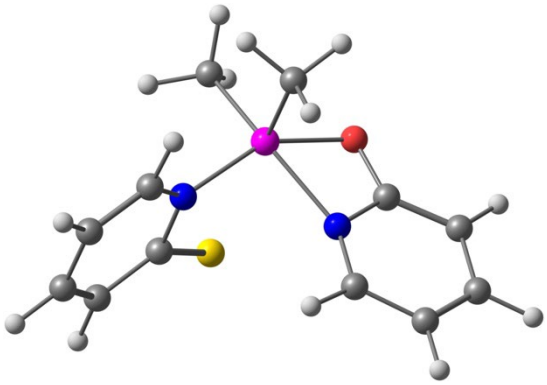

Figure S59. Optimized molecular structure of **2c´´´^{SSiCtrans}**.

PBE0:

final single point energy: -1340.71599711703 a.u.

final Gibbs free energy: -1340.51647176 a.u.

B2T-PLYP:

final single point energy: -1340.80420306491 a.u.

Table S41. Atomic coordinates for optimized structure of **2c´´´^{SSiCtrans}**.

Si	9.81915379953407	11.45686862978887	8.42660195634980
S	9.49182158386666	11.17717771330595	5.81557990507035
O	11.64499786326572	11.36086945596342	8.24533446376237
N	8.07013416795097	10.89717450109855	7.92207680829199
N	10.47141171166357	9.56706181564543	8.19236384545991
C	8.01531776866593	10.81399040105631	6.56922146120132
C	6.80060025433533	10.45220145183043	5.96259804692469
H	6.75205990029269	10.38951975440422	4.88427263041489
C	5.70752496252068	10.18464511507366	6.74923262198820
H	4.76805944429685	9.90386748127429	6.28769731315071
C	5.80114070047301	10.27129279156150	8.14378314820835
H	4.95451709361817	10.06374034950093	8.78249564646996
C	7.00445430054447	10.63296095864775	8.69141686950540
H	7.15088584653039	10.72301873669943	9.75907221101116
C	11.71319542799673	10.06051936951462	8.17022831358734
C	12.82558916987383	9.22680615823411	8.07594599410488
H	13.82542741154575	9.63693214830182	8.05990926707895
C	12.57609317141405	7.87111138088043	8.00023294314356
H	13.40879761044253	7.18235443875011	7.92046580461774
C	11.27061583893533	7.37039929315748	8.02521880751950
H	11.07758596156893	6.30878424555309	7.96409598820387
C	10.22620493215903	8.26239888855845	8.12679952346870
H	9.18738283676781	7.95473035201970	8.14805745306868
C	9.66081344945868	13.31543403561916	8.14642099432883
H	9.78532342382752	13.83946241051932	9.09901489396410
H	8.68260510967002	13.57819102561921	7.74006764491813
H	10.42152671031919	13.67383416444559	7.45374543901185
C	9.64827184044608	11.27208770083227	10.30102411950285
H	8.88548710760024	11.95607531035486	10.68338769487909
H	10.59237366109789	11.55327092452008	10.77350757129456
H	9.39779142831670	10.26213112826769	10.63138109949723