Supplementary Materials: Hexacoordinate Silicon Compounds with a Dianionic Tetradentate (N,N′,N′,N)-Chelating Ligand

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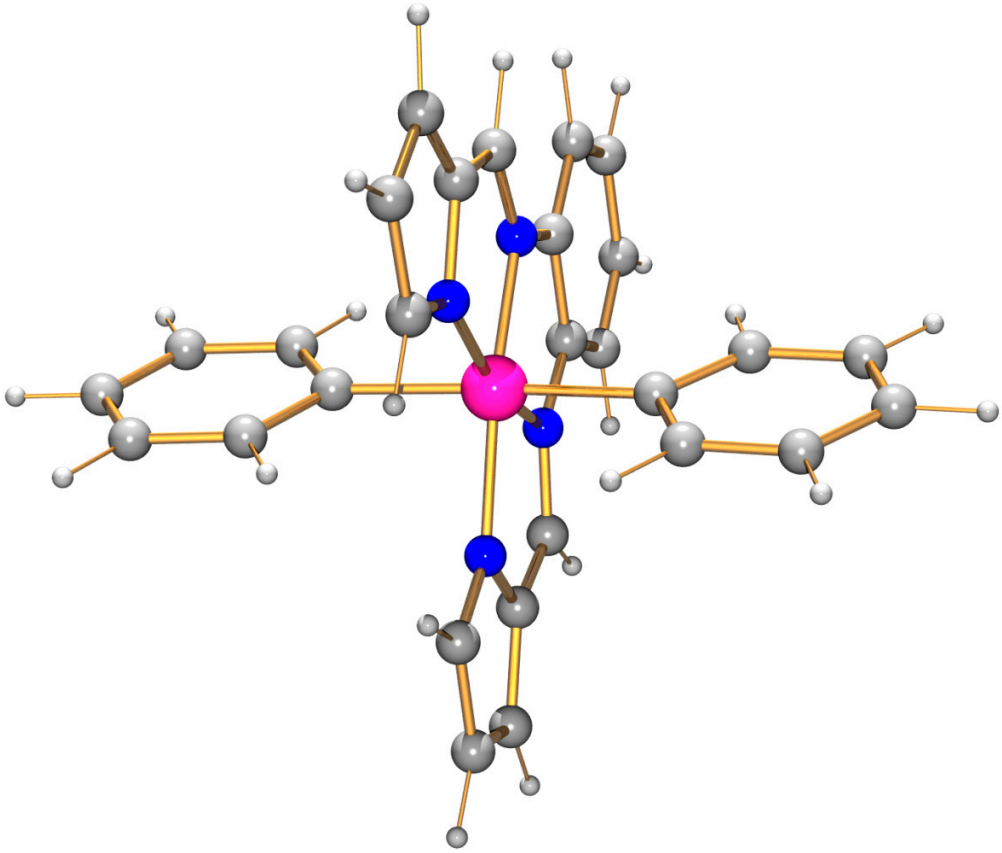

Figure S1. Molecular structure of **LSiPh$_2$** optimized at the MPW1PW91/6–311G(d,p) level.

Table S1. Cartesian coordinates of the optimized (MPW1PW91/6–311G(d,p)) molecular structure of **LSiPh$_2$** (55 atoms), E = −1558.77069689 Hartree.

H	5.875948	−0.732293	−0.000262
H	4.456530	−2.770199	−0.000031
C	4.795192	−0.647800	−0.000189
C	3.998915	−1.786774	−0.000054
H	4.789699	1.498807	−0.000314
C	4.185486	0.597806	−0.000220
C	2.616060	−1.667769	0.000046
H	2.030586	−2.581309	0.000173
C	2.797031	0.699256	−0.000132
C	1.966805	−0.427261	−0.000004
H	2.369282	1.695531	−0.000161
H	0.010652	−3.626476	−4.062236
H	0.010099	−3.521990	−1.367061
C	0.008014	−2.732367	−3.458822
H	0.010731	−3.626609	4.062189
C	0.007791	−2.688649	−2.053500

H	0.010069	−3.522059	1.367025
C	0.008117	−2.732483	3.458800
H	0.003368	−1.066631	−4.921716
C	0.004301	−1.418520	−3.901740
C	0.007794	−2.688729	2.053480
H	0.003571	−1.066780	4.921732
C	0.004428	−1.418647	3.901748
N	0.004089	−1.426563	−1.621576
N	0.004133	−1.426633	1.621581
C	0.001862	−0.616876	−2.748277
C	0.001985	−0.616974	2.748307
Si	0.000997	−0.347403	0.000015
C	−0.002012	0.761197	2.515082
C	−0.002120	0.761287	−2.515004
H	−0.003982	1.480460	3.328023
H	−0.004157	1.480579	−3.327919
N	−0.003200	1.122439	1.256043
N	−0.003230	1.122485	−1.255951
C	−0.007007	2.396609	0.708258
H	−0.010693	3.613192	2.482811
C	−0.007020	2.396637	−0.708118
C	−0.010636	3.604313	1.400012
C	−0.010654	3.604365	−1.399832
H	−0.010716	3.613282	−2.482630
C	−0.014207	4.799656	0.696493
H	−0.017032	5.737989	1.236972
C	−0.014214	4.799682	−0.696269
H	−2.015929	−2.592861	0.000109
H	−0.017047	5.738035	−1.236712
C	−1.964308	−0.438452	0.000007
C	−2.606536	−1.682628	0.000053
H	−2.378801	1.682010	−0.000098
C	−2.800906	0.683334	−0.000068
C	−3.988694	−1.809471	0.000010
H	−4.440720	−2.795477	0.000047
C	−4.188760	0.574013	−0.000100
C	−4.791407	−0.675022	−0.000062
H	−4.798072	1.471575	−0.000155
H	−5.871669	−0.765626	−0.000092

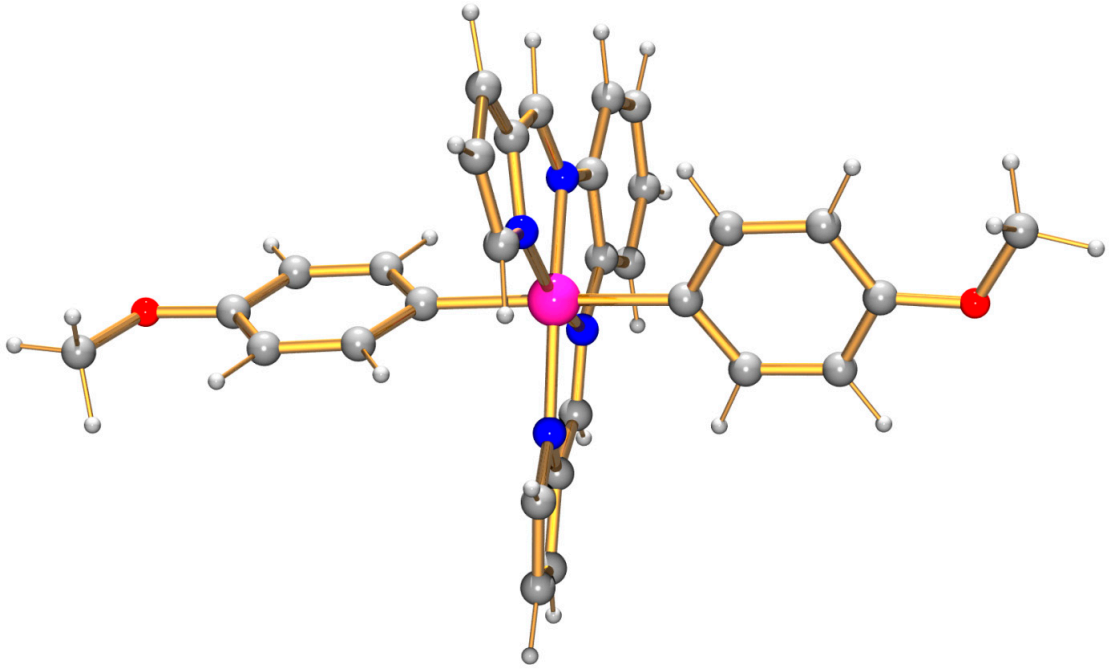

Figure S2. Molecular structure of **LSi(Anis)$_2$** optimized at the MPW1PW91/6–311G(d,p) level.

Table S2. Cartesian coordinates of the optimized (MPW1PW91/6–311G(d,p)) molecular structure of **LSi(Anis)$_2$** (63 atoms), E = −1817.81859329 Hartree.

H	−1.007894	5.626559	−1.587800
H	−0.902531	5.811870	0.876859
C	−0.809233	4.747372	−0.987646
C	−0.749683	4.851739	0.399979
H	−0.687330	3.444996	−2.686963
C	−0.626008	3.521137	−1.608416
H	−6.824163	−0.347680	−1.406024
C	−0.507054	3.730945	1.179510
H	−7.929167	−1.226117	−0.323289
H	−0.477665	3.817460	2.258600
C	−0.373389	2.388770	−0.839685
C	−6.901467	−1.160850	−0.675787
H	−0.007862	1.346546	−3.387967
C	−0.313754	2.494575	0.570273
H	−6.628314	−2.104485	−1.160853
H	−4.657774	−1.077504	−1.846004
O	−6.112598	−0.914420	0.463209
C	−0.006484	0.676290	−2.533754
N	−0.162312	1.099964	−1.306683
C	−4.112964	−0.889040	−0.930008
C	−4.770458	−0.792396	0.290911
H	−2.264594	−0.846685	−1.955607
C	−2.726892	−0.750511	−0.979988
H	2.137888	2.002901	−0.219900
N	−0.059823	1.287956	1.205129
C	−4.019567	−0.559010	1.441396
H	−4.536716	−0.492146	2.391209
C	−1.938163	−0.512911	0.148691
H	0.332186	−1.306501	−4.804821

C	0.156126	−0.709047	−2.674085
C	−2.644950	−0.425358	1.360064
H	0.281753	1.843510	3.203550
H	4.576894	2.066274	−0.322409
C	2.673735	1.061500	−0.160314
C	0.206257	1.052039	2.464177
H	−2.111423	−0.258974	2.288647
C	0.275227	−1.586153	−3.764155
Si	0.006368	−0.276014	0.055402
C	4.057001	1.120984	−0.220444
N	0.103178	−1.440048	−1.498231
C	1.971492	−0.144994	−0.028823
C	0.378738	−0.297928	2.797946
C	0.285696	−2.867474	−3.229491
N	0.222198	−1.196979	1.754535
C	0.173019	−2.728570	−1.834964
C	4.811492	−0.047343	−0.150717
H	0.361403	−3.799529	−3.767300
C	2.763128	−1.291862	0.038191
O	6.161147	0.102279	−0.217732
C	0.587859	−1.003120	3.994393
H	0.136168	−3.508953	−1.089803
H	0.732371	−0.570923	4.972511
C	4.153423	−1.266788	−0.019889
H	2.293561	−2.265243	0.140973
C	0.316010	−2.420567	2.275674
H	0.211910	−3.303923	1.663656
C	0.547360	−2.349794	3.661020
C	6.953832	−1.058606	−0.152670
H	4.704633	−2.196409	0.037960
H	7.987037	−0.723649	−0.223481
H	6.740605	−1.741215	−0.982705
H	6.813921	−1.591840	0.794152
H	0.662871	−3.191443	4.325783

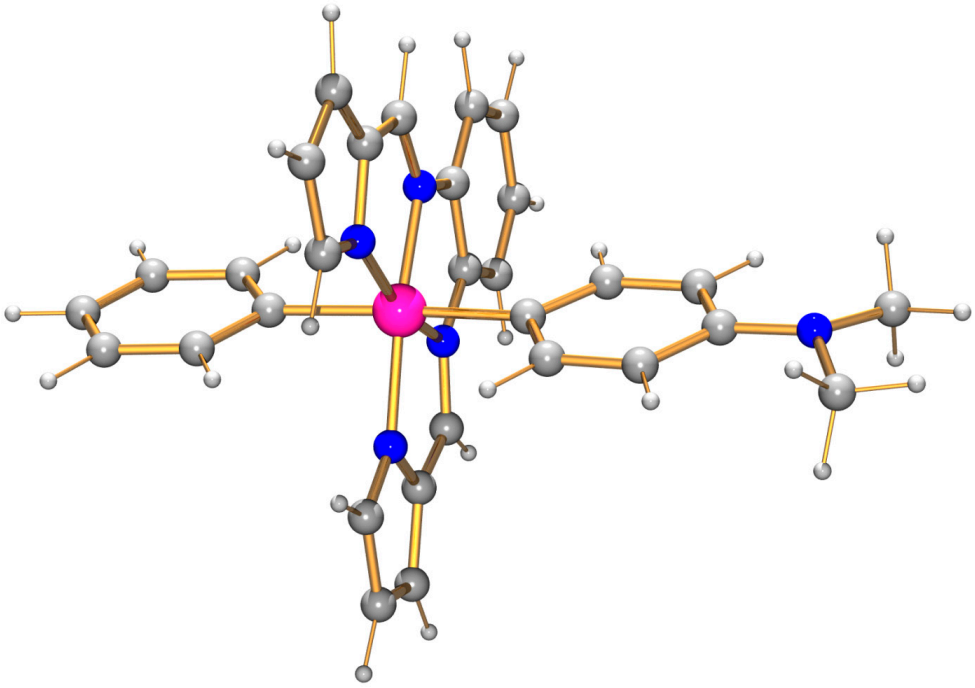

Figure S3. Molecular structure of **LSiPh(*p*-Me$_2$N-C$_6$H$_4$)** optimized at the MPW1PW91/6–311G(d,p) level.

Table S3. Cartesian coordinates of the optimized (MPW1PW91/6–311G(d,p)) molecular structure of **LSiPh(*p*-Me$_2$N-C$_6$H$_4$)** (63 atoms), E = −1722.73875481 Hartree.

H	−1.295483	5.707855	1.224860
H	−1.260546	5.705799	−1.248852
C	−1.185268	4.774708	0.686545
C	−1.165555	4.773570	−0.706064
H	−1.080080	3.596732	2.475354
C	−1.064551	3.586884	1.392636
H	5.963248	1.952208	0.654327
C	−1.024882	3.584531	−1.406389
H	−1.009980	3.592453	−2.489141
H	7.352470	1.062102	0.049119
H	3.921391	2.037546	0.071679
C	6.279016	1.201031	−0.074132
H	6.096840	1.607005	−1.080501
C	−0.922575	2.385400	0.704260
H	1.535321	1.946642	0.033183
C	−0.902409	2.384299	−0.712186
C	3.450173	1.063680	0.071350
H	−0.871520	1.477543	3.325989
C	2.062914	0.998996	0.046519
N	5.612333	−0.056312	0.159669
N	−0.789718	1.120140	1.255486
C	−0.774412	0.762132	2.515328
C	4.228793	−0.103041	0.095358
H	7.426062	−1.051002	0.045564
N	−0.754501	1.118055	−1.257494
H	−3.188329	1.406879	−0.040399
H	−0.776091	1.472878	−3.329834
C	6.365240	−1.262633	−0.083726

C	1.351489	−0.204027	0.032231
C	−0.702623	0.758440	−2.515828
H	6.099981	−2.040786	0.636409
C	−0.621999	−0.606586	2.754007
H	6.215537	−1.670549	−1.094592
C	3.533545	−1.324170	0.063140
H	−5.569789	0.928429	−0.072537
C	−3.497253	0.367582	−0.041122
Si	−0.595717	−0.342964	0.002666
H	−0.610966	−1.046277	4.929842
C	2.149409	−1.353091	0.037764
C	−0.551055	−1.399202	3.911954
C	−4.864389	0.104279	−0.059564
H	4.073342	−2.261593	0.056705
C	−2.540588	−0.653517	−0.023666
N	−0.506882	−1.414274	1.631780
C	−0.544273	−0.610780	−2.748078
H	1.682524	−2.333014	0.016225
N	−0.462061	−1.416639	−1.621779
H	−0.474811	−1.054432	−4.922030
C	−5.324176	−1.204032	−0.061236
C	−0.390292	−2.705307	3.476170
C	−0.443417	−1.405612	−3.902253
C	−0.368346	−2.665979	2.070359
C	−3.040564	−1.961409	−0.025552
H	−6.387560	−1.414449	−0.075565
H	−0.298261	−3.591654	4.084115
C	−0.315374	−2.669663	−2.054183
C	−4.399864	−2.241654	−0.043969
H	−2.352770	−2.800584	−0.011758
H	−0.258024	−3.495778	1.388495
C	−0.298079	−2.711408	−3.459917
H	−0.227485	−3.498584	−1.368012
H	−4.738966	−3.272034	−0.044592
H	−0.192022	−3.599148	−4.063534

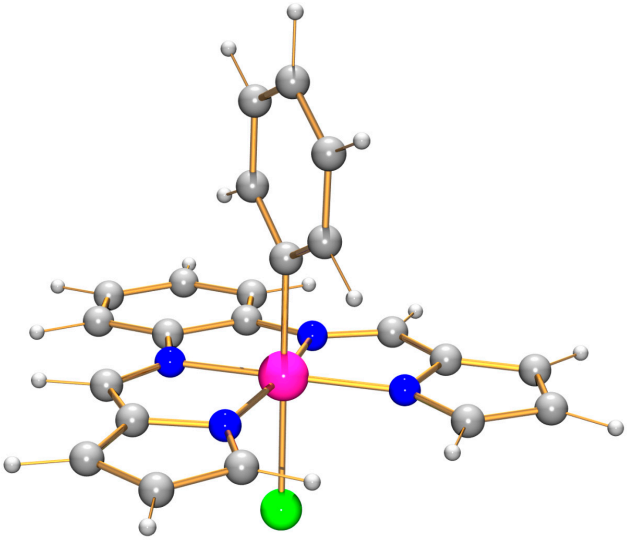

Figure S4. Molecular structure of **LSiPhCl** optimized at the MPW1PW91/6–311G(d,p) level.

Table S4. Cartesian coordinates of the optimized (MPW1PW91/6–311G(d,p)) molecular structure of **LSiPhCl** (45 atoms), E = −1817.41785613 Hartree.

H	−1.763719	−0.000368	5.230641
H	−3.514710	−0.000744	3.472106
C	−1.486813	−0.000324	4.182591
C	−2.465759	−0.000488	3.196660
H	0.625979	0.000013	4.565246
C	−0.150769	−0.000072	3.808253
C	−2.102389	−0.000323	1.856529
H	−2.894981	−0.000429	1.114915
H	−3.608707	3.840478	−1.395033
H	−3.609435	−3.839667	−1.395359
C	0.197637	0.000041	2.461269
H	−3.378125	1.156266	−1.314413
C	−2.717550	3.284524	−1.150821
C	−0.764678	−0.000056	1.445256
H	−3.378684	−1.155567	−1.313726
C	−2.612340	1.886377	−1.106555
C	−2.718165	−3.283910	−1.151113
H	1.253364	0.000204	2.212449
C	−2.612822	−1.885772	−1.106457
H	−1.173364	−4.833365	−0.785880
C	−1.465301	3.796805	−0.837789
H	−1.172646	4.833744	−0.785016
C	−1.465948	−3.796388	−0.838342
N	−1.369223	1.526330	−0.775366
N	−1.369548	−1.525904	−0.775712
C	−0.635395	−2.690801	−0.611099
C	−0.635018	2.691091	−0.610225
Si	−0.324450	0.000063	−0.453297
C	0.723118	−2.503823	−0.332418
H	1.416416	−3.330552	−0.223909
C	0.723512	2.503824	−0.331647
N	1.096418	−1.252977	−0.241030
N	1.096693	1.252920	−0.240999
H	1.416908	3.330441	−0.222802
C	2.360127	−0.707114	−0.072811
C	2.360264	0.706783	−0.072721
H	3.563628	−2.483644	0.079220
C	3.555011	−1.400921	0.084028
C	3.555309	1.400331	0.084070
H	3.564132	2.483055	0.079264
C	4.738938	−0.696920	0.242983
C	4.739089	0.696083	0.242993
H	5.669509	−1.236996	0.364294
H	5.669778	1.235951	0.364296
Cl	0.173896	0.000237	−2.692010

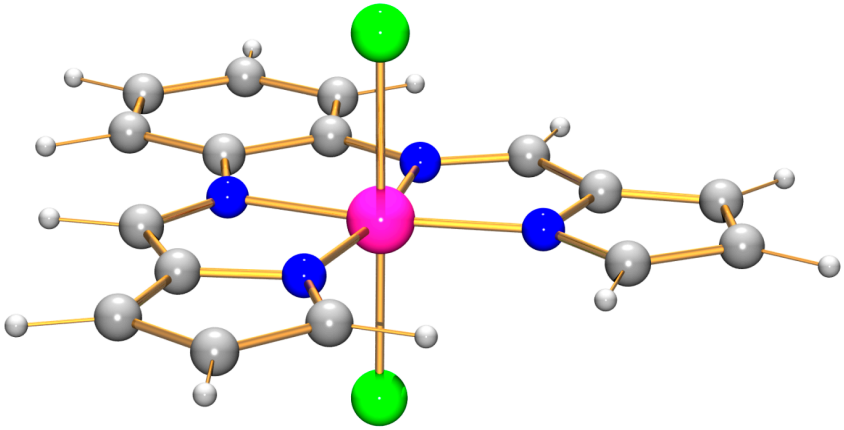

Figure S5. Molecular structure of **LSiCl$_2$** optimized at the MPW1PW91/6–311G(d,p) level.

Table S5. Cartesian coordinates of the optimized (MPW1PW91/6–311G(d,p)) molecular structure of **LSiCl$_2$** (35 atoms), E = −2046.05922426 Hartree.

H	−3.932354	3.766252	−0.000159
H	−3.932459	−3.766200	−0.001395
H	−3.642843	1.089550	−0.001347
C	−2.998858	3.226773	−0.000176
H	−3.643013	−1.089535	−0.000128
C	−2.862849	1.832709	−0.000456
C	−2.998969	−3.226715	−0.000400
C	−2.862986	−1.832668	−0.000199
H	−1.438683	−4.804931	0.000457
C	−1.716278	3.762734	0.000408
H	−1.438624	4.805017	0.001117
C	−1.716376	−3.762657	0.000409
N	−1.568238	1.497667	−0.000724
N	−1.568384	−1.497561	0.001663
C	−0.836666	−2.674427	0.001993
C	−0.836540	2.674508	−0.000096
Si	−0.479632	−0.000011	−0.000454
C	0.551780	−2.500423	0.001459
H	1.250612	−3.328604	0.002096
C	0.551900	2.500448	−0.000202
N	0.938934	−1.251210	0.000119
N	0.938987	1.251206	−0.000569
H	1.250792	3.328579	0.000244
C	2.214133	−0.705769	0.000067
C	2.214157	0.705727	−0.000477
H	3.425036	−2.483559	0.000636
C	3.417506	−1.400976	0.000128
C	3.417581	1.400855	−0.000949
H	3.425191	2.483433	−0.001373
C	4.611411	−0.696633	−0.000291
C	4.611444	0.696441	−0.000851
H	5.549898	−1.236385	−0.000238
H	5.549964	1.236153	−0.001317
Cl	−0.455451	−0.001419	−2.227585
Cl	−0.453966	0.001425	2.227711

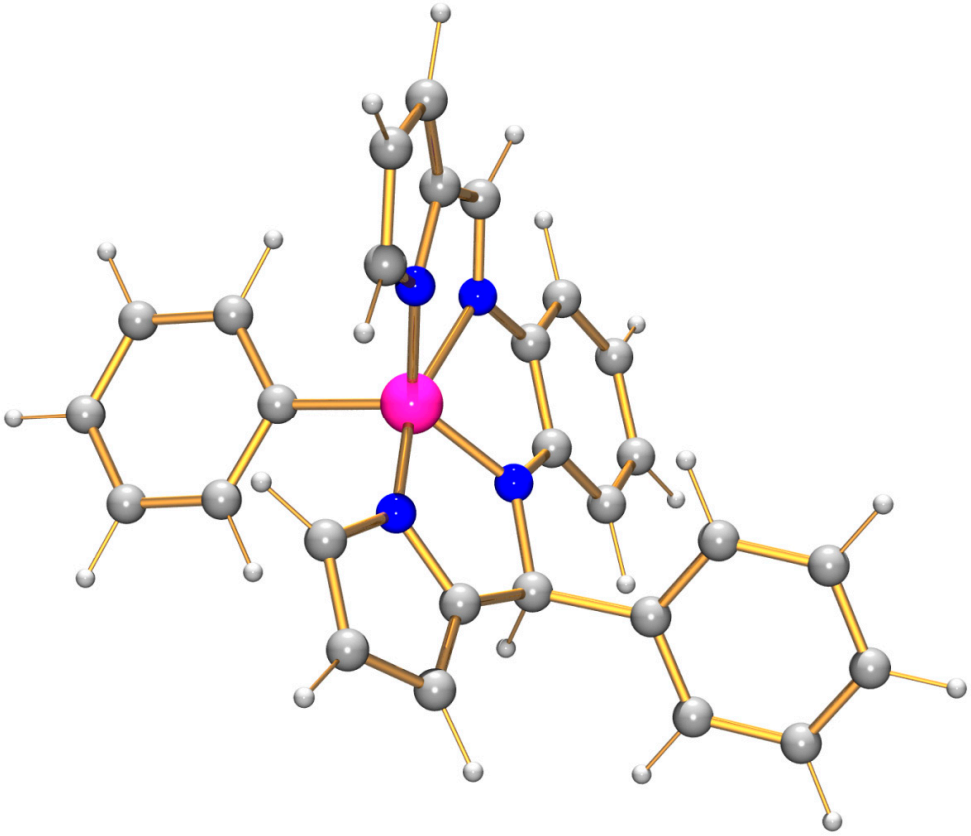

Figure S6. Molecular structure of **L^{Ph}SiPh** optimized at the MPW1PW91/6–311G(d,p) level.

Table S6. Cartesian coordinates of the optimized (MPW1PW91/6–311G(d,p)) molecular structure of **L^{Ph}SiPh** (55 atoms), E = −1588.82501610 Hartree.

H	0.711733	5.622790	−0.283202
H	2.488513	4.451290	−1.538010
C	0.738636	4.540938	−0.303837
C	1.733616	3.876902	−1.014089
H	−1.015440	4.307750	0.927556
C	−0.226585	3.807947	0.377200
C	1.786156	2.488023	−1.071311
H	2.580586	1.994880	−1.614990
C	−0.178652	2.425561	0.325636
C	0.820250	1.737918	−0.403093
H	−1.775635	2.504415	2.641311
N	−1.006822	1.507391	0.962004
C	−1.634424	1.576802	2.094394
N	0.713798	0.364548	−0.342939
H	−3.559583	1.121050	0.200321
H	1.788823	−0.264636	−2.029879
C	1.680681	−0.520865	−0.965580
C	−2.022881	0.311310	2.591128
H	−5.364173	1.307069	−1.442809
C	−3.449078	0.623606	−0.756802
Si	−0.859537	−0.300955	0.178331
H	−3.119900	0.404825	4.503396
C	−2.659077	−0.181691	3.723697
C	−4.476639	0.733438	−1.684605

C	−2.294902	−0.117196	−1.032320
N	−1.547500	−0.744562	1.832025
C	1.057895	−1.885731	−0.852379
N	−0.187792	−1.921004	−0.274900
H	2.340609	−3.429804	−1.733387
C	−4.365142	0.111559	−2.921901
C	−2.567868	−1.578436	3.649354
C	1.413426	−3.147138	−1.259914
C	−1.879006	−1.884079	2.482091
C	−2.208738	−0.745177	−2.281190
H	−5.163280	0.200167	−3.649979
H	−2.937056	−2.293136	4.367517
C	−0.640989	−3.216624	−0.340501
C	−3.227259	−0.627030	−3.218862
H	−1.337825	−1.345005	−2.521445
H	−1.580829	−2.846670	2.100229
C	0.323427	−3.995788	−0.932507
H	−1.630694	−3.481722	−0.005867
H	−3.134003	−1.119433	−4.180018
H	0.253519	−5.056997	−1.116362
C	3.064061	−0.460353	−0.337440
C	4.195770	−0.543820	−1.142854
C	3.223473	−0.360889	1.042398
C	5.468168	−0.536930	−0.581870
H	4.080901	−0.614721	−2.220061
C	4.491545	−0.346730	1.604264
H	2.345333	−0.290934	1.673601
C	5.618828	−0.436770	0.794165
H	6.340470	−0.603531	−1.221712
H	4.602797	−0.265769	2.679387
H	6.608705	−0.425672	1.234828

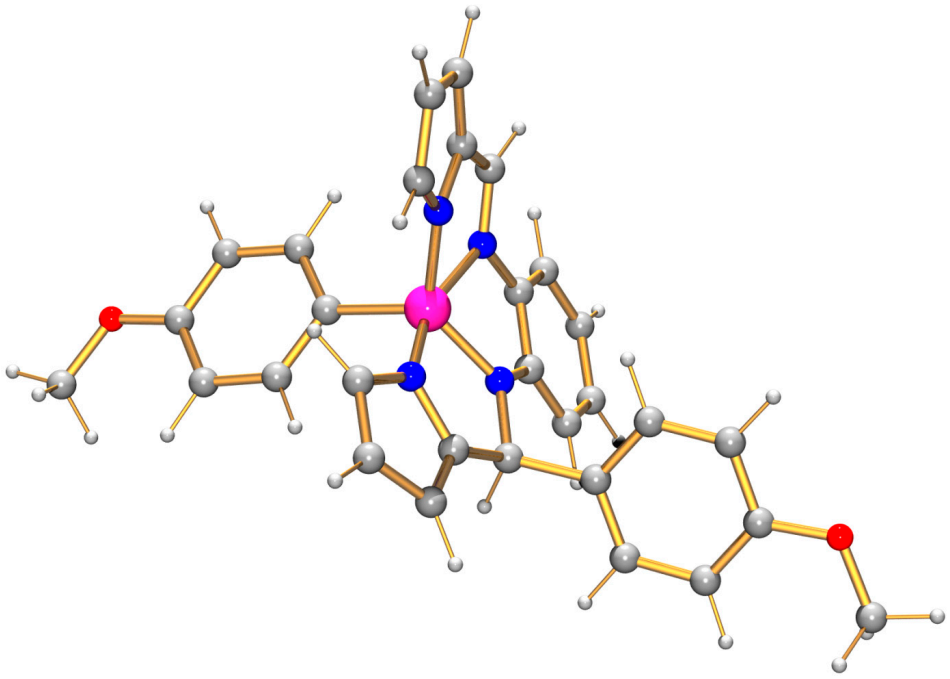

Figure S7. Molecular structure of **L^{Anis}Si(Anis)** optimized at the MPW1PW91/6–311G(d,p) level.

Table S7. Cartesian coordinates of the optimized (MPW1PW91/6–311G(d,p)) molecular structure of **L^{Anis}Si(Anis)** (63 atoms), E = −1817.87393570 Hartree.

H	0.443770	5.337356	−1.892493
H	1.889341	3.750271	−3.115638
C	0.485296	4.298265	−1.592211
C	1.293217	3.399625	−2.281279
H	−0.919947	4.536081	0.025392
C	−0.275459	3.853650	−0.516801
C	1.357186	2.055831	−1.927800
H	2.006970	1.381202	−2.468190
C	−0.215277	2.517828	−0.159336
C	0.594905	1.590799	−0.857213
H	−1.216245	3.362921	2.332369
N	−0.854352	1.876131	0.895904
C	−1.195025	2.309351	2.069324
N	0.532012	0.305983	−0.363255
H	−3.487208	1.504400	0.786943
H	1.189270	−0.852465	−1.984629
C	1.340114	−0.777540	−0.897386
C	−1.432752	1.268664	2.996755
H	−5.624814	1.286635	−0.401216
C	−3.602390	0.704688	0.064070
Si	−0.869991	−0.088024	0.673338
H	−2.046447	1.979465	4.993632
C	−1.773977	1.165535	4.339727
C	−4.811866	0.597783	−0.594834
C	−2.545925	−0.187346	−0.172987
N	−1.133087	0.012372	2.498538
C	0.779293	−2.010635	−0.243209
N	−0.296631	−1.806195	0.584779
H	1.847762	−3.812866	−0.887801
C	−5.007708	−0.411649	−1.539442
C	−1.680052	−0.194427	4.665828
C	1.050842	−3.353854	−0.323815
C	−1.282516	−0.866245	3.516204
C	−2.773002	−1.194275	−1.114427
H	−1.856724	−0.645703	5.629173
C	−0.731045	−3.036594	1.015974
C	−3.978156	−1.312373	−1.799060
H	−1.994657	−1.920555	−1.320755
H	−1.068455	−1.913524	3.379781
C	0.081469	−4.007501	0.481384
H	−1.610574	−3.136976	1.630967
H	−4.100705	−2.109483	−2.520015
H	−0.011387	−5.070223	0.645868
C	2.829181	−0.608579	−0.654113
C	3.743849	−0.876758	−1.660663
C	3.317701	−0.220869	0.595645
C	5.117463	−0.771032	−1.447888
H	3.387167	−1.177737	−2.641019
C	4.673323	−0.104014	0.823403
H	2.618997	−0.006663	1.395967

C	5.586784	−0.381134	−0.198126
H	5.799349	−0.988244	−2.258857
H	5.059619	0.198717	1.788677
O	−6.220045	−0.433595	−2.140713
O	6.895755	−0.238839	0.125208
C	7.854818	−0.514007	−0.868938
H	8.825112	−0.345623	−0.406332
H	7.794866	−1.553159	−1.210058
H	7.746396	0.154895	−1.729567
C	−6.464635	−1.433847	−3.103943
H	−6.396403	−2.436359	−2.668957
H	−7.479352	−1.266597	−3.458998
H	−5.771025	−1.358036	−3.947766

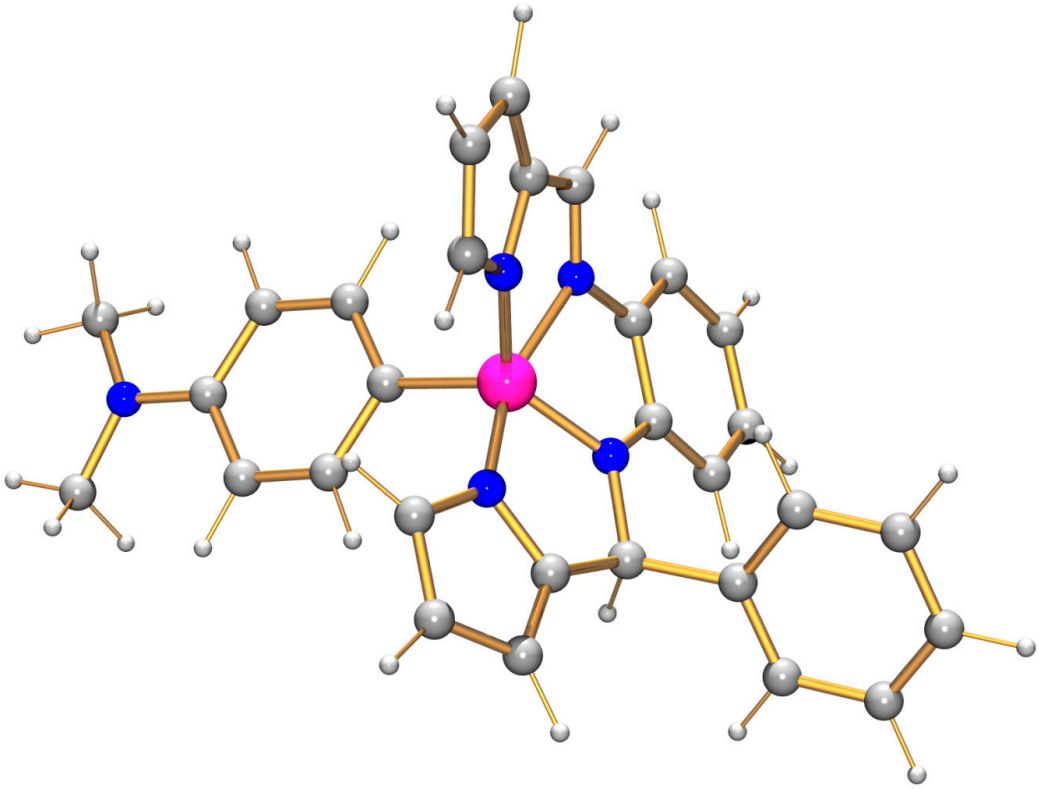

Figure S8. Molecular structure of **L^{Ph}Si(*p*-NMe$_2$-C$_6$H$_4$)** optimized at the MPW1PW91/6–311G(d,p) level.

Table S8. Cartesian coordinates of the optimized (MPW1PW91/6–311G(d,p)) molecular structure of **L^{Ph}Si(*p*-NMe$_2$-C$_6$H$_4$)** (63 atoms), E = −1722.79548056 Hartree.

H	1.026131	5.638204	−0.175701
H	2.307202	4.554514	−1.989593
C	1.082492	4.558642	−0.230807
C	1.797686	3.943845	−1.253430
H	−0.136135	4.238247	1.518801
C	0.434358	3.778157	0.720024
C	1.877379	2.559002	−1.358373
H	2.454309	2.106171	−2.153392
C	0.510461	2.399755	0.621785
C	1.225699	1.760939	−0.419311
H	−0.185042	2.380982	3.348638

N	−0.018959	1.441680	1.479197
C	−0.213635	1.468123	2.760599
N	1.194936	0.385034	−0.358674
H	−2.629173	1.158720	1.479100
H	1.656054	−0.176691	−2.326447
C	1.921190	−0.452323	−1.294911
C	−0.357984	0.180265	3.326200
H	−4.853911	1.291488	0.582057
C	−2.849872	0.579602	0.589196
Si	−0.097662	−0.348324	0.639616
H	−0.724579	0.200521	5.502442
C	−0.541957	−0.354884	4.595499
C	−4.133709	0.660834	0.079213
C	−1.854147	−0.209546	0.002799
N	−0.135634	−0.842784	2.421261
C	1.418066	−1.842551	−1.015673
N	0.441609	−1.935655	−0.055745
H	2.385096	−3.322385	−2.313118
C	−4.499666	−0.056028	−1.075548
C	−0.429262	−1.744806	4.455843
C	1.661180	−3.083799	−1.549616
C	−0.177835	−2.003653	3.113398
C	−2.227863	−0.912279	−1.150796
H	−0.498326	−2.484696	5.237350
C	0.040094	−3.248068	0.004602
C	−3.501600	−0.837352	−1.686412
H	−1.502489	−1.545182	−1.650106
H	0.004241	−2.946676	2.624546
C	0.776188	−3.980702	−0.895525
H	−0.769267	−3.556907	0.646080
H	−3.719121	−1.398902	−2.584507
H	0.687180	−5.042180	−1.069847
C	3.432773	−0.347239	−1.167611
C	4.229263	−0.360501	−2.308545
C	4.044766	−0.274680	0.081490
C	5.615247	−0.309389	−2.207776
H	3.760593	−0.410493	−3.286538
C	5.426603	−0.217130	0.184923
H	3.428486	−0.258650	0.972797
C	6.217392	−0.236205	−0.959489
H	6.222640	−0.320631	−3.105438
H	5.890910	−0.157283	1.162554
N	−5.778630	−0.000844	−1.580618
C	−6.066297	−0.600955	−2.861380
H	−5.849202	−1.672965	−2.853410
H	−7.126757	−0.484461	−3.078203
H	−5.496210	−0.145030	−3.682393
C	−6.724836	0.938816	−1.029696
H	−7.685765	0.806972	−1.524112
H	−6.879818	0.762897	0.038759
H	−6.412992	1.984373	−1.160337
H	7.296901	−0.190786	−0.876575

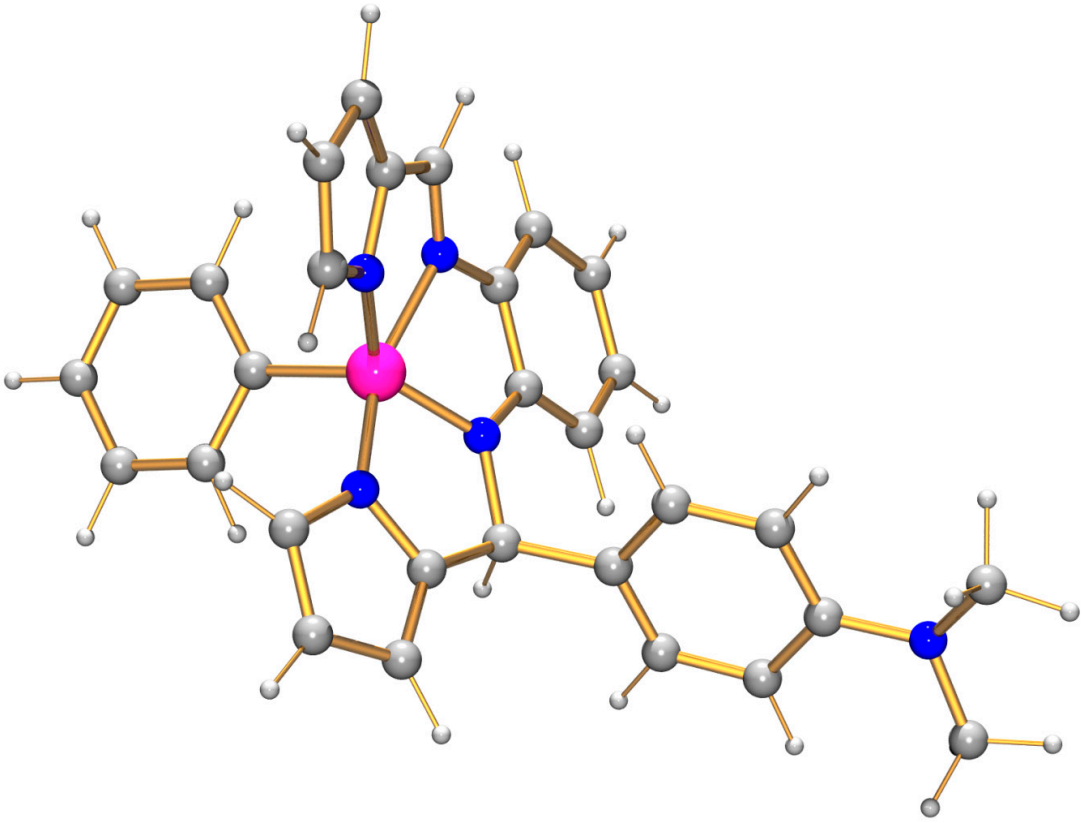

Figure S9. Molecular structure of **L**$^{4\text{-NMe2-C6H4}}$**SiPh** optimized at the MPW1PW91/6–311G(d,p) level.

Table S9. Cartesian coordinates of the optimized (MPW1PW91/6–311G(d,p)) molecular structure of **L**$^{4\text{-NMe2-C6H4}}$**SiPh** (63 atoms), E = −1722.79349632 Hartree.

H	−0.276941	5.676743	−0.095582
H	1.411380	4.653432	−1.581527
C	−0.206888	4.599675	−0.177276
C	0.738158	4.018711	−1.017283
H	−1.816973	4.222539	1.205577
C	−1.066933	3.788822	0.554074
C	0.843007	2.638844	−1.155361
H	1.598179	2.211068	−1.800213
C	−0.966212	2.414319	0.422984
C	−0.017199	1.810274	−0.435868
H	−2.347266	2.308485	2.874611
N	−1.688585	1.429135	1.086262
C	−2.215106	1.415480	2.270743
N	−0.059403	0.433259	−0.440954
H	−4.272592	1.010588	0.514587
H	0.837917	−0.065933	−2.269248
C	0.870787	−0.375814	−1.213874
C	−2.501867	0.110454	2.734293
H	−6.223027	1.192629	−0.952910
C	−4.236464	0.544673	−0.463870
Si	−1.542095	−0.328986	0.197141
H	−3.420748	0.061196	4.739811
C	−3.008292	−0.465102	3.892937

C	−5.346458	0.652202	−1.291864
C	−3.092740	−0.153688	−0.865129
N	−2.052182	−0.884003	1.882697
C	0.319059	−1.771378	−1.103321
N	−0.854148	−1.894175	−0.399711
H	1.563159	−3.207468	−2.194973
C	−5.331417	0.071337	−2.553730
C	−2.861693	−1.850889	3.739869
C	0.680728	−2.993580	−1.612457
C	−2.270514	−2.067422	2.501302
C	−3.103856	−0.740658	−2.136921
H	−6.194301	0.158615	−3.204006
H	−3.130653	−2.615521	4.451131
C	−1.257226	−3.205692	−0.485228
C	−4.205854	−0.624371	−2.975115
H	−2.242382	−1.306658	−2.473861
H	−1.965544	−2.995150	2.045929
C	−0.330633	−3.908212	−1.217107
H	−2.192996	−3.533875	−0.062945
H	−4.186655	−1.084772	−3.956305
H	−0.375264	−4.961652	−1.448134
C	2.312481	−0.268632	−0.755132
C	3.345070	−0.176078	−1.679964
C	2.657640	−0.312934	0.592619
C	4.675365	−0.127993	−1.289525
H	3.111350	−0.146852	−2.740274
C	3.976901	−0.258393	1.003482
H	1.874821	−0.394002	1.338474
C	5.026913	−0.153724	0.070422
H	5.438855	−0.065807	−2.052350
H	4.191543	−0.300722	2.062218
N	6.344915	−0.067330	0.476897
C	7.392421	−0.193896	−0.507124
H	8.357104	−0.071518	−0.017128
H	7.386789	−1.167533	−1.018296
H	7.312781	0.587636	−1.267717
C	6.677453	−0.332737	1.855915
H	6.164502	0.363592	2.524739
H	6.424874	−1.355599	2.170518
H	7.747455	−0.187429	1.996600