Supporting Information for

Synthesis and Structural Characterisation of Neutral Pentacoordinate Silicon(IV) Complexes with a Tridentate Dianionic *N*,*N*,*S* Chelate Ligand

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Table S1. Cartesian coordinates [Å] and ADF total energies [kcal mol^{-1}] of species **7**, **7a** und **7b** solvated in dichloromethane, computed at COSMO-BP86/TZ2P.

Species 7: (–4441.09 kcal mol^{-1}, 0 imaginary frequencies)

C	-0.277606	-3.880588	-2.085325
C	-1.126680	-2.811911	-1.829051
C	1.045126	-3.829391	-1.629057
C	-0.628472	-1.715279	-1.125845
C	2.601903	0.354256	-0.923600
C	1.470756	-2.710343	-0.935981
C	-1.425057	-0.505830	-0.769351
C	-2.536447	1.901935	0.221770
C	-1.179712	1.593855	0.418748
C	-3.076817	3.086984	0.734312
C	-0.371863	2.504991	1.141019
C	-2.275931	3.977850	1.450619
C	-0.923785	3.681950	1.653591
H	-0.638594	-4.749770	-2.632462
H	-2.162935	-2.814992	-2.162107
H	1.736461	-4.649391	-1.807328
H	-1.838348	-0.053940	-1.686480
H	2.249419	0.995374	-1.746282
H	3.026802	-0.557906	-1.359123
H	2.481178	-2.620768	-0.546995
H	3.391902	0.902746	-0.394642
H	-3.180791	1.225493	-0.335504
H	-2.285804	-0.810125	-0.149854
H	-4.130909	3.306512	0.567770
H	-2.695205	4.900309	1.850317
H	-0.287042	4.369921	2.209512
N	0.641032	-1.670513	-0.696845
N	-0.567164	0.427642	-0.059263
Si	1.151438	0.058670	0.244585
S	1.321523	2.062936	1.331231
Cl	1.812062	-1.130577	1.928782

Species 7a: (–4432.77 kcal mol^{-1}, 0 imaginary frequencies)

Si	-2.602385	-0.481858	0.399956
S	-3.156813	1.463001	-0.326805
N	-1.015682	-0.496724	-0.316740
C	-2.683333	-0.750489	2.235449
Cl	-3.786093	-2.015952	-0.446453
C	-0.730834	0.526174	-1.227278
C	-1.694214	1.557462	-1.355399
C	-1.502669	2.610646	-2.248170
C	-0.340847	2.664195	-3.025926
C	0.616478	1.654703	-2.906254
C	0.427692	0.592251	-2.018149
C	-0.077255	-1.597991	-0.105897
C	1.153402	-1.244567	0.718601
C	2.410100	-1.736331	0.348472
C	3.512979	-1.447808	1.150899
C	3.323059	-0.673574	2.294483
C	2.032381	-0.227424	2.583332
N	0.960700	-0.503416	1.822856
H	-2.362643	-1.771488	2.484449
H	-2.025204	-0.035757	2.745216
H	-3.715949	-0.620849	2.586038
H	-2.259960	3.389388	-2.331525
H	-0.190521	3.491102	-3.718108
H	1.524188	1.687722	-3.507783
H	1.188087	-0.181875	-1.937342
H	-0.615195	-2.399822	0.420125
H	0.235308	-2.026154	-1.069015
H	4.502862	-1.815553	0.883166
H	4.153796	-0.416458	2.950181
H	1.847544	0.380161	3.471549
H	2.520402	-2.333698	-0.556988

Species 7b: (–4257.16 kcal mol^{-1}, 0 imaginary frequencies)

Si	-1.222967	-0.326265	0.402316
S	-1.816050	1.708134	0.154767
N	-0.306334	-0.473347	-1.064697
C	-2.580299	-1.438342	0.991884
C	-0.355603	0.635706	-1.931514
C	-1.046957	1.777735	-1.467933
C	-1.140844	2.922684	-2.258809
C	-0.535540	2.942225	-3.518664
C	0.159518	1.821133	-3.978632
C	0.247312	0.668884	-3.194157
C	0.911070	-1.274021	-0.938145
C	1.226622	-1.406097	0.534345
C	2.372106	-1.989874	1.060016
C	2.533765	-2.037290	2.441968
C	1.537887	-1.523947	3.280107
C	0.403571	-0.976878	2.713504
N	0.267532	-0.915747	1.364436
H	-1.678989	3.794731	-1.890515
H	-0.610197	3.835727	-4.136222
H	0.629653	1.835093	-4.960818
H	0.771467	-0.210259	-3.566324
H	0.804285	-2.278182	-1.375578
H	1.748169	-0.780769	-1.449320
H	3.434124	-2.474881	2.868659
H	1.636616	-1.553746	4.361859
H	-0.416132	-0.578416	3.305192
H	3.127255	-2.390206	0.387242
H	-3.446495	-1.347917	0.323778
H	-2.896245	-1.142307	2.002949
H	-2.244889	-2.483811	1.022558

Cl^- (–157.69 kcal mol^{-1})

Cl	0.000000	0.000000	0.000000

$Si(CH_3)_4$

Si	0.014222	-0.000031	0.000017
C	1.910408	-0.000080	0.000051
C	-0.617825	1.787693	-0.000087
C	-0.617881	-0.893626	1.548346
C	-0.617481	-0.893926	-1.548336
H	2.306769	-1.027390	-0.003224
H	2.306724	0.516294	-0.888053
H	2.306726	0.510781	0.891336
H	-1.718540	-0.907529	1.576321
H	-0.267375	-1.937118	1.574741
H	-0.264101	-0.396380	2.464887
H	-1.718501	1.818870	0.002596
H	-0.263572	2.333335	0.888296
H	-0.267724	2.331707	-0.891110
H	-1.718136	-0.911216	-1.574845
H	-0.266596	-0.394789	-2.464958
H	-0.263678	-1.936279	-1.576134