Supporting Information for

[1]Ferrocenophane Bridged by a 9-Silafluorenylidene Moiety

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Contents

1. NMR spectra of sila[1]ferrocenophane 1.

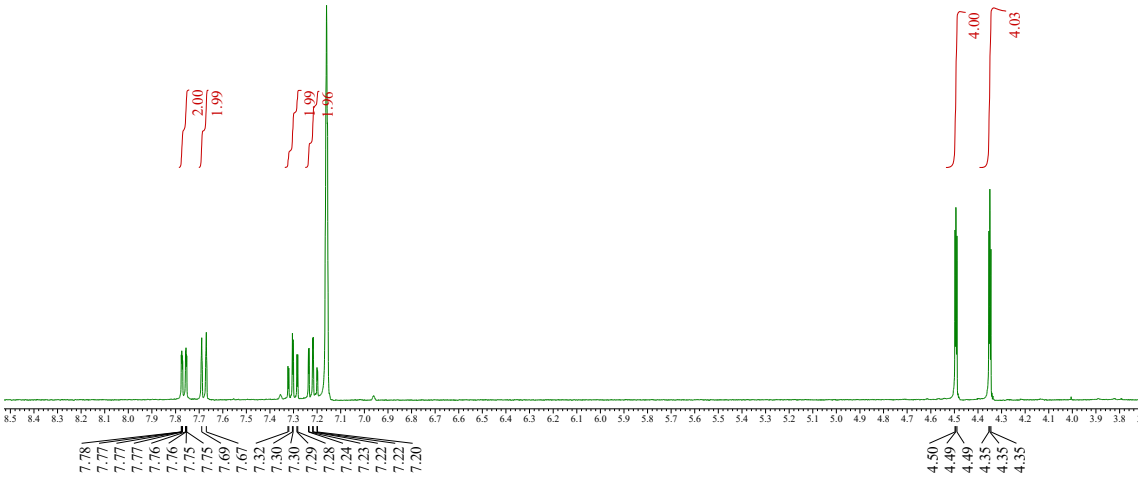

Figure S1. ^{1}H NMR spectrum of **1** in C_6D_6.

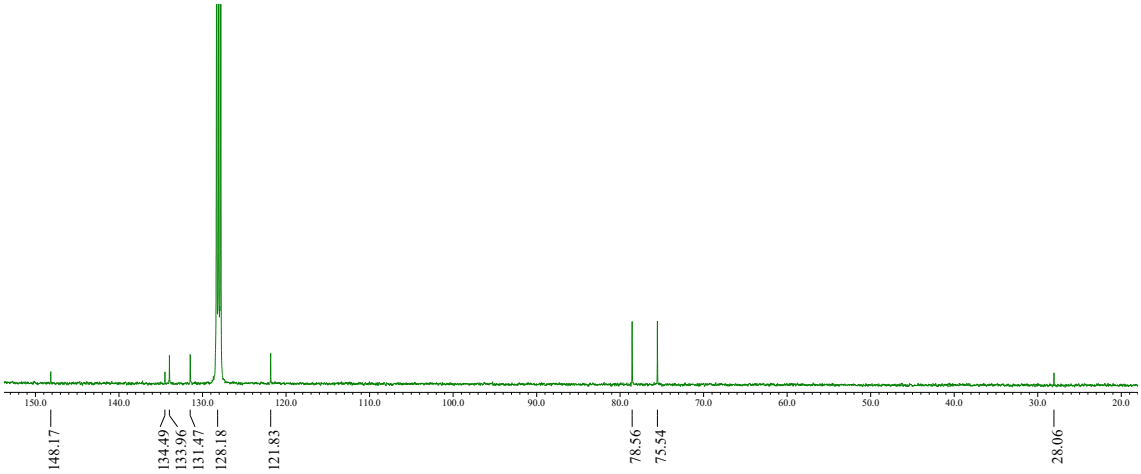

Figure S2. $^{13}C\{^{1}H\}$ NMR spectrum of **1** in C_6D_6.

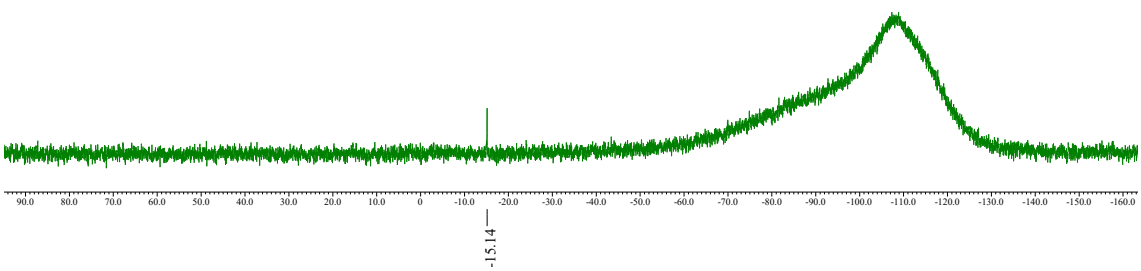

Figure S3. $^{29}Si\{^{1}H\}$ NMR spectrum of **1** in C_6D_6.

2. Coordinates of theoretically optimized structures

Theoretical calculations: All calculations were carried out using the density functional theory (DFT) method with a B3PW91-D3(BJ) functional,[S1,S2] and geometry optimizations and vibrational frequencies were calculated in the gas phase using the 6-311G(3d) basis sets, as implemented in the Gaussian 16 program package.[S3] Computational time was generously provided by the Supercomputer Laboratory at the Institute for Chemical Research (Kyoto University). The coordinates of the optimized structures are shown below.

Optimized structures: .xyz file format.

· Compound **1**

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Compound_1,9-Sifluorenylidene[1]ferrocenophane
Fe          2.43864        -0.00042         0.00005
Si         -0.22958        -0.00067        -0.00017
C           1.87333         1.14752         1.56464
H           1.56345         2.17833         1.45958
C           1.87383        -1.14762         1.56535
H           1.56440        -2.17865         1.46114
C           1.87346         1.14680        -1.56504
H           1.56333         2.17760        -1.46068
C           3.20825        -0.71063         1.78514
H           4.07032        -1.34754         1.92541
C           1.01416        -0.00109        -1.40699
C          -2.78825         0.74136        -0.00004
C           1.87424        -1.14836        -1.56485
H           1.56497        -2.17940        -1.46018
C           3.20816         0.71063        -1.78467
H           4.07000         1.34795        -1.92451
C          -1.51243        -1.34508         0.00007
C          -2.78895        -0.74027         0.00006
C           3.20865        -0.71128        -1.78456
H           4.07084        -1.34811        -1.92440
C           1.01392        -0.00028         1.40684
C          -2.54748         3.52333        -0.00029
H          -2.46101         4.60539        -0.00039
C          -1.51119         1.34496        -0.00036
C           3.20794         0.71127         1.78467
H           4.06976         1.34860         1.92455
C          -3.92829        -1.54032         0.00009
H          -4.91751        -1.09357         0.00006
C          -1.40543         2.72937        -0.00046
H          -0.42815         3.20409        -0.00070
C          -3.92689         1.54243         0.00017
H          -4.91650         1.09656         0.00044
C          -3.80247         2.92597         0.00003
```

H	-4.69469	3.54466	0.00019
C	-1.40792	-2.72957	0.00009
H	-0.43107	-3.20518	0.00005
C	-3.80514	-2.92399	0.00009
H	-4.69794	-3.54183	0.00008
C	-2.55072	-3.52250	0.00008
H	-2.46521	-4.60463	0.00006

· Compound **I**

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Compound_I, Ph2Si-[1]ferrocenophane

Fe	-2.14318	-0.00001	-0.00000
Si	0.48689	0.00000	-0.00000
C	-1.59622	1.14850	-1.57306
H	-1.28229	2.17712	-1.45822
C	-1.59641	-1.14836	-1.57321
H	-1.28267	-2.17706	-1.45860
C	-1.59638	1.14833	1.57322
H	-1.28258	2.17701	1.45861
C	-2.93251	-0.71116	-1.77600
H	-3.79791	-1.34745	-1.89797
C	-0.73401	-0.00005	1.42663
C	1.87080	2.17181	-1.20058
C	-1.59624	-1.14853	1.57308
H	-1.28231	-2.17715	1.45825
C	-2.93247	0.71116	1.77604
H	-3.79786	1.34746	1.89803
C	1.48538	-1.56881	0.00003
C	1.87092	-2.17174	1.20056
C	-2.93238	-0.71155	1.77594
H	-3.79769	-1.34799	1.89779
C	-0.73402	-0.00001	-1.42663
C	2.62150	3.34002	1.20331
H	2.91146	3.79790	2.14425
C	1.48530	1.56886	-0.00004
C	-2.93239	0.71155	-1.77589
H	-3.79768	1.34802	-1.89773
C	2.62221	-3.33953	1.20342
H	2.91272	-3.79705	2.14437
C	1.87020	2.17223	1.20049
H	1.57067	1.72528	2.14497
C	2.62212	3.33958	-1.20344
H	2.91259	3.79712	-2.14439
C	2.99867	3.92426	-0.00007
H	3.58390	4.83887	-0.00009
C	1.87019	-2.17223	-1.20050
H	1.57061	-1.72530	-2.14497
C	2.99868	-3.92425	0.00005
H	3.58389	-4.83888	0.00006
C	2.62146	-3.34004	-1.20333
H	2.91135	-3.79796	-2.14428
H	1.57168	1.72455	-2.14504
H	1.57186	-1.72445	2.14503

3. References

[S1] Tao, J.; Perdew, J. P.; Staroverov, V. N.; Scuseria, G. E. *Phys. Rev. Lett.* **2003,** *91*, 146401.

[S2] Grimme, S.; Ehrlich, S.; Goerigk, L. *J. Comp. Chem.* **2011,** *32*, 1456-1465.

[S3] Gaussian 16, Revision C.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A. V.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Ortiz, J. V.; Izmaylov, A. F.; Sonnenberg, J. L.; Williams-Young, D.; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M. J.; Heyd, J. J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.; Keith, T. A.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A. P.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Millam, J. M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Farkas, O.; Foresman, J. B.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2016.