

Stable Aromatic Carbocyclic Silylene

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Stable divalent silicon compounds, silylenes, eluded isolation until the first N-Heterocyclic Silylene (NHSi) was discovered in 1994.^[1] More recently Kira and coworkers reported the first isolable carbocyclic silylene, which is stabilized by hyperconjugation with the four adjacent trimethylsilyl groups.^[2] Unfortunately, in solution, it slowly undergoes 1,2 silyl migration to yield a stable silene.

Herein we report the synthesis of a new type of carbocyclic silylene that is indefinitely stable in solution. In this species the low valent silicon center is stabilized by two carbanionic substituents situated in a 10 electron conjugated π -system. The carbanions are additionally stabilized as part of phosphorus ylides thereby maintaining electro-neutrality of the species. The stability of this new silylene can be attributed to the decreased electronegativity of carbon (as compared to the nitrogens of NHSi's) and the superior π -donor/aromaticity of the system (as compared to the carbocyclic system of Kira). Density Functional Theory (DFT) calculations have been performed to investigate the electronics of this new silylene, including the singlet-triplet energy difference and the Nucleus Independent Chemical Shift (NICS).

The dibromosilane precursor is most effectively reduced to the silylene using the β -diketiminato Mg(I) dimer reported by one of us.^[3] This once again demonstrates the unique strong but gentle reducing properties of this Mg(I) species.

Literature:

[1] M. Denk, R. Lennon, R. Hayashi, R. West, A. V. Belyakov, H. P. Verne, A. Haaland, M. Wagner, N. Metzler, *J. Am. Chem. Soc.* **1994**, *116*, 2691-2692. [2] S. Tsutsui, K. Sakamoto, M. Kira, *J. Am. Chem. Soc.* **1998**, *120*, 9955-9956. [3] S. P. Green, C. Jones, A. Stasch, *Science* **2007**, *318*, 1754-1757.