

proportional to the above estimated time (t_{tw} and t_0). With the measured $v_{\{111\}}$ and $v_{\{422\}}$ values, the EM-induced void growth rate for the twin-modified Cu grain ($l = 5$ nm) is calculated to be approximately one order of magnitude lower than that for the twin-free Cu grain. The effect of twin boundaries on slowing down the EM-induced voiding is expected to decrease with an increase of the twin-lamella width (that is, a decrease in the twin density). The twin boundary-induced atomic-migration delay may also decrease with rising temperature because the EM-induced atomic diffusion is a thermally activated process. However, typical integrated circuit devices usually operate at temperatures $\sim 100^\circ\text{C}$.

We have observed the atomic-scale EM process in twin-modified Cu grains near room temperature with the use of ultrahigh-vacuum and high-resolution TEM technique. The EM-induced atomic migration along a twin-modified grain boundary was observed, and the presence of the triple point of a coherent twin boundary meeting a grain bound-

ary was found to retard the EM-induced atomic transport.

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A Stable Silicon(0) Compound with a Si=Si Double Bond

Yuzhong Wang, Yaoming Xie, Pingrong Wei, R. Bruce King, Henry F. Schaefer III, Paul von R. Schleyer,* Gregory H. Robinson*

Dative, or nonoxidative, ligand coordination is common in transition metal complexes; however, this bonding motif is rare in compounds of main group elements in the formal oxidation state of zero. Here, we report that the potassium graphite reduction of the neutral hypervalent silicon-carbene complex $\text{L}:\text{SiCl}_4$ {where L is $:\text{C}[\text{N}(2,6\text{-Pr}^i_2\text{C}_6\text{H}_3)\text{CH}]_2$ and Pr^i is isopropyl} produces $\text{L}:(\text{Cl})\text{Si}-\text{Si}(\text{Cl})\text{L}$, a carbene-stabilized bis-silylene, and $\text{L}:\text{Si}=\text{Si}:\text{L}$, a carbene-stabilized diatomic silicon molecule with the Si atoms in the formal oxidation state of zero. The Si-Si bond distance of 2.2294 ± 0.0011 (standard deviation) angstroms in $\text{L}:\text{Si}=\text{Si}:\text{L}$ is consistent with a Si=Si double bond. Complementary computational studies confirm the nature of the bonding in $\text{L}:(\text{Cl})\text{Si}-\text{Si}(\text{Cl})\text{L}$ and $\text{L}:\text{Si}=\text{Si}:\text{L}$.

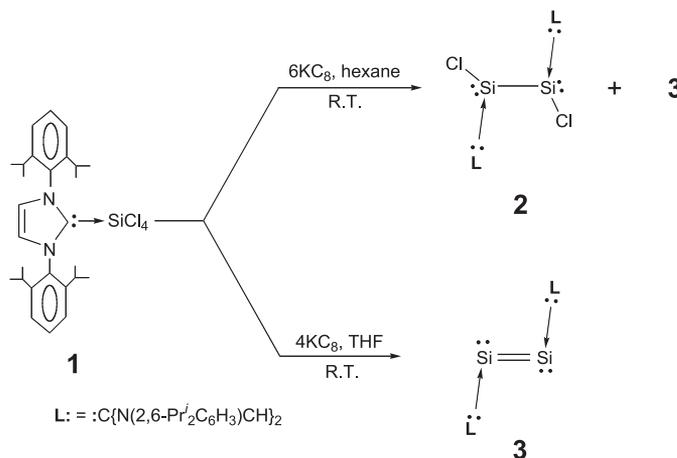
Although silicon is predominantly associated with semiconductors, integrated circuits, and advanced electronic devices, its structures and bonding motifs intrigue chemists because they are often substantially different from those of silicon's lighter congener carbon. For example, the chemical and physical properties of CO_2 are totally unlike those of SiO_2 , and hypervalent species such as $[\text{SiF}_5]^-$ are unknown for carbon (1). Even though molecules containing C-C multiple bonds are ubiquitous and have been studied for more than two centuries, it was not until 1981 that a disilene, a compound containing a Si-Si double bond ($\text{R}_2\text{Si}=\text{SiR}_2$, where R is $\text{Me}_3\text{C}_6\text{H}_2$) was prepared by West *et al.* (2); a disilyne ($\text{RSi}=\text{SiR}$, where R is an extremely bulky ligand), a compound

containing a Si-Si triple bond (albeit with a decidedly nonlinear, transbent geometry), was ultimately achieved by Sekiguchi *et al.* in 2004 (3). In addition to disilenes and disilynes, a number of other interesting stable low-coordinate Si

compounds have been reported (4–7). Regarding the oxidation state of Si in low-coordinate compounds, the central Si atoms in disilenes and disilynes are in the formal oxidation states of two (+2) and one (+1), respectively. It is well known for transition metals to assume the formal oxidation state of zero in organometallic compounds [for example, $\text{Ni}(\text{CO})_4$, $(\text{C}_6\text{H}_6)_2\text{Cr}$, etc.]; however, the formal oxidation state of zero is rare for main group elements in their compounds (apart from those in Zintl phases) (8, 9).

The study of highly reactive Si(0) intermediates may prove critical in the development of new synthetic strategies in Si chemistry. Such experimental studies, however, require sophisticated instruments and elaborate techniques (10). For example, the diatomic Si_2 molecule, having a triplet ground state ($X^3\Sigma_g^-$), has been studied only in the gas phase and in argon matrices (11). Recently, the CO complex of the Si_2 molecule, $\text{OC}:\text{Si}=\text{Si}:\text{CO}$, was examined with argon matrix isolation absorption infrared spectroscopy and computed to have an unusual transbent structure

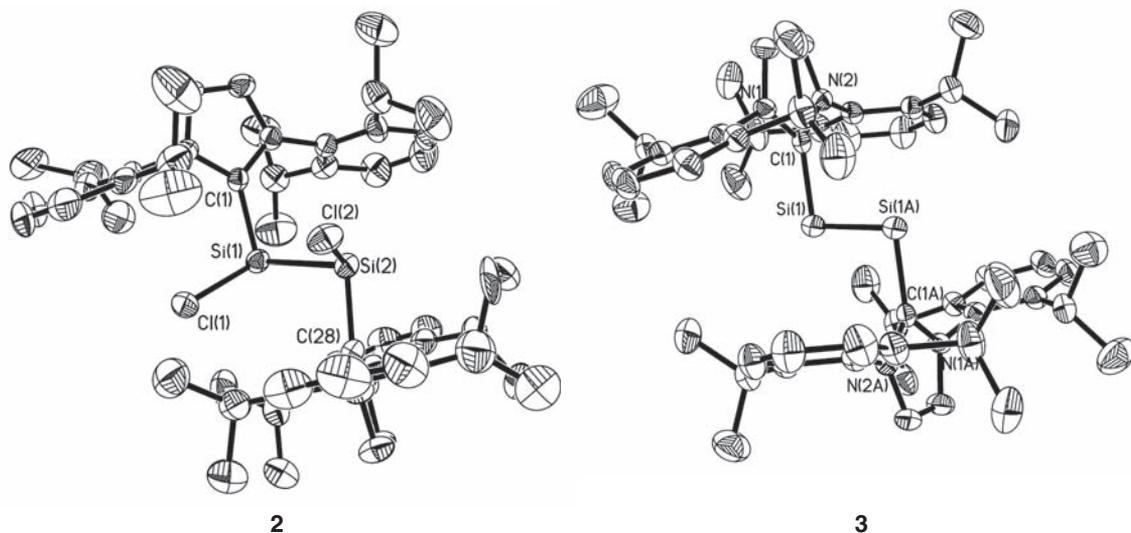
Fig. 1. Synthetic scheme for compounds 2 and 3.



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Fig. 2. Molecular structures of $L:(Cl)Si-Si(Cl):L$, (**2**), and $L:Si=Si:L$, (**3**). L is $:C\{N(2,6-Pr^i_2C_6H_3)CH\}_2$. Thermal ellipsoids represent 30% probability. Hydrogen atoms were omitted for clarity. Selected bond distances (Å) and angles (deg) for (**2**) are Si(1)–Si(2), 2.393(3); Si(1)–C(1), 1.939(6); Si(1)–Cl(1), 2.161(3); Si(2)–C(28), 1.929(7); Si(2)–Cl(2), 2.168(3); C(1)–Si(1)–Si(2), 98.76(19); Cl(1)–Si(1)–Si(2), 108.75(11); C(1)–Si(1)–Cl(1), 101.2(2); C(28)–Si(2)–Si(1), 98.7(2); Cl(2)–Si(2)–Si(1), 107.96(11); and C(28)–Si(2)–Cl(2), 100.7(2). Selected bond distances (Å) and angles (deg) for (**3**) are Si(1)–Si(1A), 2.2294(11); Si(1)–C(1), 1.9271(15); and C(1)–Si(1)–Si(1A), 93.37(5).



with Si-Si-C angles approaching 90° (*12*). How might the fleeting diatomic Si_2 molecule be sufficiently stabilized for routine laboratory inquiry? We recently produced neutral diborenes, $L:(H)B=B(H):L$, by employing N-heterocyclic carbene ligands, L ;, to complex the highly reactive and electron-deficient diborene(2) parent $H-B=B-H$ (*13*, *14*). Extending this strategy, we now report the syntheses (Fig. 1) (*15*), molecular structures (Fig. 2) (*15*), and computational analyses (*16*) of $L:SiCl_4$, **1**; $L:(Cl)Si-Si(Cl):L$, **2**, a carbene-stabilized bis-silylene; and $L:Si=Si:L$, **3**, a carbene-stabilized $:Si=Si:$ compound {where L is $:C\{N(2,6-Pr^i_2C_6H_3)CH\}_2$ and Pr^i is isopropyl}. Both Si atoms in compound **3** are in the formal oxidation state of zero.

Kuhn *et al.* synthesized hypervalent $L':SiCl_4$ {where L' is $:C[N(R)C(CH_3)]_2$ and R is alkyl} complexes (*17*), which are neutral equivalents of $[SiCl_5]^-$. Consistently, we found that room-temperature reaction of a sterically demanding N-heterocyclic carbene ligand, L ;, with $SiCl_4$ in hexane, gives $L:SiCl_4$, **1**, in an essentially quantitative yield. The potassium graphite reduction of **1** (in a $1:KC_8$ ratio of 1:6) in hexane produced air-sensitive, orange-red, sheetlike crystals of **2** (6.1% yield) and air-sensitive, dark red, block crystals of **3** (as a minor product) (Fig. 1). However, when the potassium graphite reduction of **1** is performed (with a $1:KC_8$ ratio of 1:4) in tetrahydrofuran (THF) (Fig. 1), compound **3** can be exclusively isolated and in higher yield (23.2%). In the 1H nuclear magnetic resonance (NMR) spectra, the imidazole resonances (in C_6D_6) of compounds **1**, **2**, and **3** appear at 6.40, 6.31, and 6.58 parts per million (ppm), respectively. The 1H -decoupled ^{29}Si NMR spectra of compounds **1** to **3** were also determined. The ^{29}Si NMR chemical shift of **1** (in CD_2Cl_2), -108.9 ppm, is comparable to reported values (-104.7 to -105.9 ppm) of hypervalent Si compounds $L':SiCl_4$ {where L' is $:C[N(R)C(CH_3)]_2$ and R

is alkyl} (*17*). The ^{29}Si NMR resonance of **2** (in C_6D_6), 38.4 ppm, compares with 78.3 ppm of $[C(H)N(tBu)]_2Si$: (*18*) and 14.6 ppm of $[PhC(NiBu)_2]SiCl$ (*19*), but is at a considerably lower field than the -48.6 - to -57.4 -ppm range of silylene-isocyanide complexes (*20*). The ^{29}Si chemical shift of **3** (in C_6D_6), 224.5 ppm, resides at an even lower field than typical disilene resonances (50 to 155 ppm) (*5*).

The x-ray structural analysis of **2** (Fig. 2) reveals that the $(Cl)Si-Si(Cl)$ core is sterically well-shielded by the two L ligands. The central Si-Si bond distance, 2.393(3) Å, is only about 0.05 Å longer than the sum of Si covalent radii (2.34 Å) (*21*) and about 0.03 Å longer than the Si-Si single-bond distance in α -silicon (2.36 Å) (*22*). Each Si atom in **2**, in the formal +1 oxidation state, is three-coordinate in a trigonal pyramidal geometry. The sum of the bond angles of the Si atoms in **2**, 308.0° (mean), compares very well with that in $(tBu)_2MeSi)_2Si(F)Li\cdot(THF)_3$ (307.6°) (*23*) as well as with the computed value for $Ph_2Si:CNPh$ (306.8°) (*20*). The pyramidal geometry at each Si atom in **2** results from substantial lone electron-pair character on both Si atoms. The two $L:(Cl)Si$ moieties of **2** adopt a gauche conformation [the $Cl(1)-Si(1)-Si(2)-Cl(2)$ torsion angle is -46.5°]. These structural features of **2** are akin to those of its isolobal equivalent H_2P-PH_2 , which also favors a gauche conformation (*24*). Although a Lewis base-stabilized silylene was reported a decade ago (*20*), **2** is noteworthy as a Lewis base-stabilized bis-silylene—namely, two silylene units bridged by a Si-Si bond. The Si-C bond distances [1.934(6) Å, mean] of **2** are comparable to that of **1** [1.928(2) Å] (fig. S1) whereas the mean Si-Cl bond distance [2.164(3) Å] of **2** matches the sum of the Si and Cl covalent radii (2.16 Å) (*21*). The visible absorption maximum of **2** ($\lambda_{max} = 510$ nm, in hexane) is similar to that of an intramolecularly base-stabilized three-coordinate silylene ($\lambda_{max} = 478$ nm) (*25*).

The nature of the bonding in **2** was delineated by density functional theory (DFT) computations at the B3LYP/6-311+G** level on the simplified $L:(Cl)Si-Si(Cl):L$ [where L is $:C(NHCH)_2$] model, **2-H**. The computed Si-Si (2.405 Å) and Si-C (1.926 Å) bond distances of **2-H** compare well with the experimental values [2.393(3) and 1.934(6) (mean) Å, respectively] of **2**. The computed Si-Cl bond distance of 2.238 Å in **2-H** is about 0.07 Å longer than that in **2** [2.164(3) Å, mean]. The fact that the sum of the bond angles around the Si atoms in **2-H** (298.2°) is smaller than that of **2** (308.0°) may be attributed to the substantially lower steric crowding of the model ligands used in **2-H**. The theoretical analysis of **2-H** included both localized molecular orbitals (LMOs) (fig. S2) and canonical molecular orbitals (fig. S3). The LMOs reveal a Si-Si σ bonding orbital and two nonbonding lone-pair orbitals, one at each Si atom. Natural bonding orbital (NBO) analysis shows that the Si-Si σ single bond [Wiberg bond index (WBI) = 0.94] has 12.1% s-, 87.4% p-, and 0.5% d-character, whereas the nonbonding Si lone-pair orbitals have 68.3% s-, 31.6% p-, and 0.1% d-character. The Si-Cl bond has 8.5% s-, 89.9% p-, and 1.6% d-character.

We also examined the structure of the uncomplexed Si_2Cl_2 parent molecule. Unlike acetylenes and Sekiguchi's disilyne (**3**), a doubly-bridged (C_{2v}) $Si(\mu-Cl)_2Si$ geometry with a 102.1° dihedral angle between the two Si_2Cl rings is preferred in the B3LYP/6-311+G* (*16*) optimization, which compares with the doubly-bridged (C_{2v}) global minimum of Si_2H_2 (*26*). The Si-Si bond distance, 2.361 Å, corresponds to a single Si-Si bond. The symmetrical Cl-bridged bonding elongates the Cl-Si distance (2.387 Å) and involves Cl lone pairs. However, in **2** these Cl-bridging interactions are replaced by the complexation of two-electron donor carbene ligands to the Si atoms.

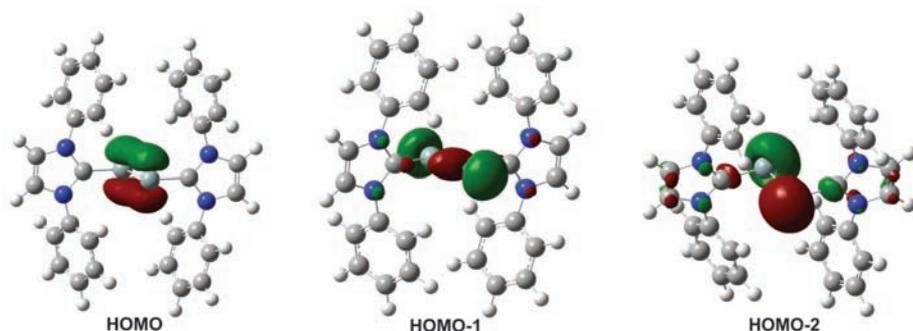


Fig. 3. The HOMO (π), HOMO-1 (σ), and HOMO-2 (lone pair) of **3-Ph**.

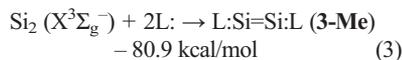
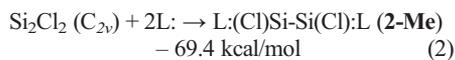
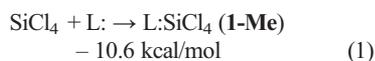
One structural feature of **3**, of C_i symmetry, is the $:\text{Si}=\text{Si}$: core (Fig. 2). The $\text{Si}=\text{Si}$ bond distance in **3**, 2.2294(11) Å, is within the reported range of disilene bond distances (2.14 to 2.29 Å) (5) and compares well with the computed [2.249 Å, B3LYP (27); 2.281 Å, B3LYP (16)] and experimental (2.246 Å) (28) bond distances of Si_2 . Both $\text{OC}:\text{Si}=\text{Si}:\text{CO}$ (2.310 Å, B3LYP) (12) and singlet $\text{Si}_2\text{H}_2^{2-}$ (2.288 Å, B3LYP) (29) suggest further comparisons. The $\text{Si}=\text{Si}$ double-bond character of **3** is further supported by the $\pi_{\text{Si}=\text{Si}}-\pi_{\text{Si}=\text{Si}}$ absorption ($\lambda_{\text{max}} = 466$ nm, in THF), which is comparable to the reported ultraviolet/visible absorption maxima (390 to 480 nm) of stable disilenes (5). However, in contrast to previously reported disilenes, in which three-coordinate Si atoms (in the +2 formal oxidation state) reside in trigonal planar environments, the Si atoms in **3**—in the formal oxidation state of zero—are only two-coordinate and have transbent geometries with C–Si–Si angles of 93.37(5)°. The two parallel carbene ligands are bound almost perpendicularly to the central $\text{Si}=\text{Si}$ double bond. Generally, Si does not hybridize extensively. The almost-90° transbent skeletal conformation is consistent with the predominantly 3p-character of the $\text{Si}=\text{Si}$ bonding orbitals in **3** and the predominantly 3s-character of the Si lone-pair molecular orbitals (see the NBO analysis below). Indeed, the nearly orthogonal transbent conformation of **3** is shared by the $\text{OC}:\text{Si}=\text{Si}:\text{CO}$ complex, the dianionic $\text{Si}_2\text{H}_2^{2-}$, and the simple valence isoelectronic $\text{HP}=\text{PH}$ model of the dipnictene family, $\text{R}\ddot{\text{E}}=\ddot{\text{E}}\text{R}$ ($\text{E} = \text{P}, \text{As}, \text{Sb}, \text{Bi}$) (30), all of which possess an electron lone pair on the central core (E) atoms. The Si–C bonds [1.9271(15) Å] of **3** are only marginally shorter than those of **1** and **2**. The fact that no ^{29}Si - ^1H coupling was observed in the ^1H -coupled ^{29}Si NMR spectrum further supports the formulation of **3**.

DFT computations at the B3LYP/6-311+G** level on the simplified $\text{L}:\text{Si}=\text{Si}:\text{L}$ {where L: is $:\text{C}[\text{N}(\text{C}_6\text{H}_5)\text{CH}]_2$ } model, **3-Ph**, support the bonding analysis. The computed $\text{Si}=\text{Si}$ bond distance (2.2407 Å), the $\text{Si}=\text{Si}-\text{C}$ bond angle (99.2°), and the C–Si–Si–C torsion angle (180.0°) are very close to the experimental values of **3** [$d_{\text{Si}=\text{Si}} = 2.2294(11)$ Å; $\text{Si}=\text{Si}-\text{C}$ bond angle = 93.37(5)°, C–Si–Si–C torsion angle = 180.0°]. The highest

occupied molecular orbital (HOMO) corresponds to the $\text{Si}=\text{Si}$ π bond, whereas the HOMO-1 is dominated by the $\text{Si}=\text{Si}$ σ bond. The HOMO-2 is one of the two nonbonding lone-pair molecular orbitals (Fig. 3).

The molecular orbital (MO) profile of **3-Ph** differs from that of the triplet ($X^3\Sigma_g^-$) ground state of the isolated Si_2 species, in which each of the two degenerate $1\pi_u$ MOs are occupied by one electron with the same spin (31). Complexation of Si_2 by two carbene ligands (as electron-pair donors) results in the occupancy of all valence orbitals of Si. Indeed, the WBI, 1.73, is supportive of a $\text{Si}=\text{Si}$ double bond in **3-Ph**. NBO analysis characterizes the occupancies of the $\text{Si}=\text{Si}$ σ bond as 17.3% s, 82.2% p, and 0.5% d, the $\text{Si}=\text{Si}$ π bond as 0.0% s, 99.6% p, and 0.4% d, and the Si lone-pair nonbonding orbitals as 72.8% s, 27.2% p, and 0.0% d.

The B3LYP/6-311+G** computed (16) binding energies [zero point energy-corrected based on data in the supporting online material (SOM)] of the carbene ligand models {where L: is $:\text{C}[\text{N}(\text{Me})\text{CH}]_2$ } to the Si-based cores are particularly noteworthy (Eqs. 1 to 3)



The very large binding energies of **2-Me** and **3-Me** reflect the coordinatively unsaturated character of $\text{Si}_2 (X^3\Sigma_g^-)$ and of $\text{Si}_2\text{Cl}_2 (C_{2v})$, respectively, as well as the remarkable complexation proclivity of the carbene ligand (32). Bulky N-heterocyclic carbene ligands are further demonstrated to be effective lone-pair donors capable of stabilizing—both thermodynamically and kinetically—unusual molecules.

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- Computations: The structures of **2-H** and **3-Ph** were optimized at the B3LYP/6-311+G** DFT level with the Gaussian 94 program (33) and Gaussian 03 program (34). Computational details can be found in the SOM.
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- We thank NSF for support of this work through grants CHE-0608142 (G.H.R.) and CHE-0716718 (P.v.R.S. and R.B.K.). Coordinates and other crystallographic information for compounds **1**, **2**, and **3** have been deposited in the Cambridge Crystallographic Database Center with deposition numbers 686707, 686708, and 687305, respectively.

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Tables S1 to S3

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A Stable Silicon(0) Compound with a Si=Si Double Bond

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