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A bis(phosphasilene) featuring non-conjugated Si═P double bonds

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The synthesis and isolation of multiply-bonded main-group compounds have attracted considerable research interest owing to their unusual bonding and reactivity. Herein, we report the synthesis of a novel bis(phosphasilene), Ph–P═Si(L)–P(Ph)–Si(L)═P–Ph [L = PhC(ᵗBuN)$_2$] (1), featuring two non-conjugated Si═P units separated by two Si–P single bonds. Density functional theory (DFT) calculations reveal highly polarized, non-delocalized Si═P double bonds.

The study of multiply bonded main-group compounds has been a cornerstone of inorganic chemistry following the groundbreaking 1973 report of a distannene by Michael F. Lappert.[1–4] This was followed by Brook's synthesis of the first silene in 1981 and West's subsequent report of the first disilene.[5,6] These seminal discoveries demonstrate the crucial role of sterically demanding substituents in kinetic stabilization of heavier main-group multiple bonds. Since then, bulky substituents have enabled the isolation of stable homo- and heteronuclear multiple bonds involving heavier main-group elements across nearly the entire p-block.[2–4,7] Unlike their lighter carbon-based analogues, heavier main-group multiply bonded compounds often exhibit poor orbital overlap because of their larger and more diffuse orbitals, resulting in weaker bonds. Consequently, these compounds often display high reactivity and can activate strong bonds such as C–H, N–H, O–H, and S–H, as well as small molecules including CO_2, CO, N_2O, and H_2.[2–4]

Significant progress has been made in stabilizing multiply bonded systems involving heavier main-group elements in recent decades.[4,8,9] For example, phosphasilenes (RP═SiR_2), which are heavier analogues of imines, have attracted significant interest due to their unique reactivity with main-group compounds and transition metals. Various acyclic and cyclic phosphasilenes have been synthesized, and their reactivity has been investigated extensively.[8–23] Notable cyclic phosphasilenes include a four-membered zwitterionic Si_2P_2 ring,[13,24] a stable cationic CSi_3P five-membered ring,[25] and a three-membered cyclic phosphasilene.[22] Scheer and co-workers synthesized the first phosphorus–silicon congeners of benzene.[26]

Among acyclic phosphasilenes, Roesky and co-workers in 2011 reported an unusual acyclic P_4 chain compound, LSi═P–P═P–P═SiL (**I**) (L = PhC(N^{t}Bu)$_2$), obtained by reacting PhC(N^{t}Bu)$_2$SiN(SiMe$_3$)$_2$ with P_4.[14] Recently, P. W. Roesky and co-workers synthesized the longest silaphospha-chain compound **II**.[27] Roesky and co-workers also synthesized the first example of an acyclic 4π-electron motif, specifically a 1,4-diphospha-2,3-disilabutadiene derivative **III** featuring an alternating Si═P bond.[28] Schulz and co-workers utilized [2+1+1] fragmentation of P_4 by metallasilylene to synthesize **IV**.[29] However, these elegant examples feature alternating Si═P bonds or Si═P bonds alternating with P═P bonds, and they also benefit from extensive steric stabilization. Despite substantial progress in phosphasilene chemistry, acyclic systems containing two non-conjugated Si═P units separated by two single bonds remain unknown. These compounds might offer opportunities for exploring new coordination modes and reactivity in both transition-metal and main-group chemistry (Fig. 1).

However, the design and synthesis of non-conjugated multiply bonded main-group systems are challenging due to their intrinsic instability, arising from weak orbital overlap and high susceptibility to polarization. These factors often lead to rapid oligomerization or polymerization, hindering their isolation.[2,3] A thorough literature survey reveals that non-conjugated multiply bonded homo- or heteronuclear main-group compounds have only scarcely been documented.[28,29]

We hypothesized that preserving the amidinate-supported silylene framework while employing a less-bulky phosphorus precursor would enable the synthesis of a non-conjugated,

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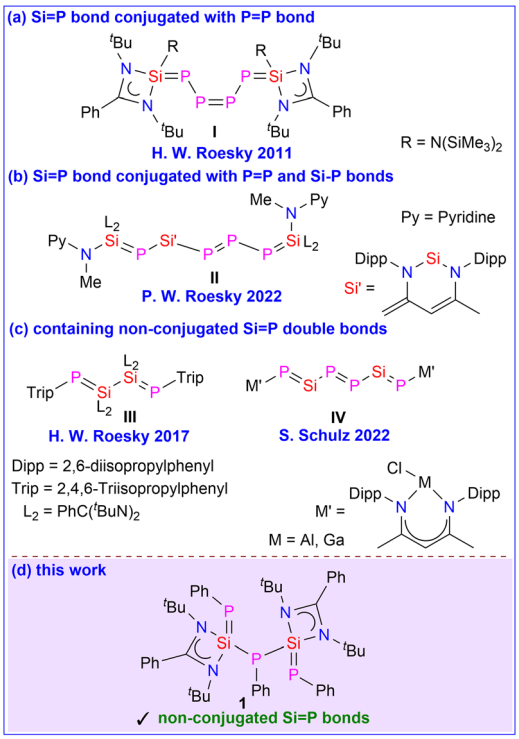
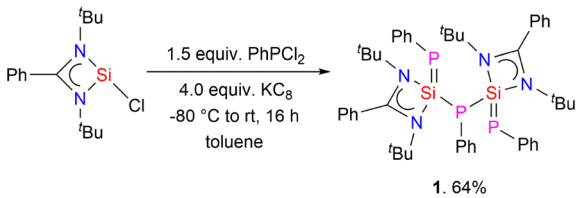


Fig. 1 Notable examples of earlier reported acyclic phosphasilenes. (a) Acyclic phosphasilenes containing conjugated double bonds. (b) Si=P conjugated with P=P and Si–P bonds (c) Containing non-conjugated Si=P double bonds. (d) This work.

multiply-bonded compound. Interestingly, the reaction of $[PhC(^tBuN)_2SiCl]$[30,31] with dichlorophenylphosphine in a 1 : 1.5 molar ratio in toluene at −80 °C, followed by reduction with KC_8, afforded $[PhP\{PhC(^tBuN)_2Si{=}PPh\}_2]$ (**1**) as orange-red crystals in 64% isolated yield after crystallization from toluene at −35 °C (Scheme 1). Structural analysis reveals that the Si=P double bonds are oriented in a *trans*-disposition, with the PPh group bridging the two distinct Si=P units.

Compound **1** is stable under an inert atmosphere for months at room temperature. However, upon exposure to air, it decomposes rapidly. It was fully characterized by NMR spectroscopy (^{1}H, ^{13}C, ^{31}P, ^{29}Si), LIFDI mass spectrometry and the molecular structure was established using a single-crystal X-ray diffraction study (SC-XRD).[32–36] The ^{1}H NMR spectrum shows a singlet resonance at 1.32 ppm, assigned to the N^{t}Bu groups, while the aromatic protons appear as multiplets in the range of 6.90 to 8.35 ppm. The ^{29}Si{^{1}H} NMR spectrum of **1** displayed a doublet of doublets centered at 35.25 ppm ($^1J_{PSi}$ = 196.0 and 66.2 Hz),



Scheme 1 Synthesis of **1**.

indicating the presence of two magnetically non-equivalent phosphorus sites. The $^1J_{PSi}$ coupling constant of 196 Hz is smaller than the 241.37 Hz reported for $(Mes^*P(SiMe_3)Si(PhC(N^tBu)_2))$ (Mes* = 2,4,6-tri-*tert*-butyl-phenyl),[23] supporting a more polarised Si=P bond.

The reduced $^1J_{PSi}$ value relative to phosphasilenes reported in the literature suggests increased polarization and reduced classical double-bond character. As expected, the $^{31}P\{^1H\}$ NMR spectrum of **1** showed a triplet centered at −118.56 ppm with a coupling constant of J = 40.8 Hz, along with silicon satellites ($^1J_{PSi}$ = 148.89 Hz), and a doublet centered at −122.64 ppm with J = 40.8 Hz, accompanied by silicon satellites ($^1J_{PSi}$ = 239.68 Hz, and $^3J_{PSi}$ = 157.14 Hz). These results further confirm the presence of two distinct types of phosphorus atoms in the molecule. Further, compound formation was confirmed using LIFDI mass spectrometry and HRMS data, which showed peaks at m/z 841.3 and 765.5 for the $[M]^+$ and $[M-Ph]^+$ ions, respectively. The UV/vis spectrum of **1** displays an absorption maximum at *ca.* 302 nm, consistent with the TD-DFT calculations (Fig. S13, see SI). VT-NMR studies revealed that **1** is thermally stable in C_6D_6 up to 120 °C, with no detectable decomposition even after 16 h of heating. Reactivity studies with P_4 and CO_2 showed no reaction at room temperature; however, heating to 60 °C led to the decomposition of **1**. No reaction was observed under UV irradiation at room temperature or upon heating to 60 °C.

The molecular structure of **1** was conclusively established through single-crystal X-ray diffraction analysis (Fig. 2). Compound **1** crystallized in the monoclinic space group *C*2/*c* with one molecule of **1** in the asymmetric unit. Within the P2–Si1–P1–Si2–P3 framework, the Si=P units adopt a *trans* arrangement.

The Si=P bond distances, Si1–P2 (2.1236(7) Å) and Si2–P3 (2.1155(7) Å), are shorter than the Si–P single bond distance reported for the $LSiP(^iPr)_2$ derivative (2.307(8) Å)[37] as well as

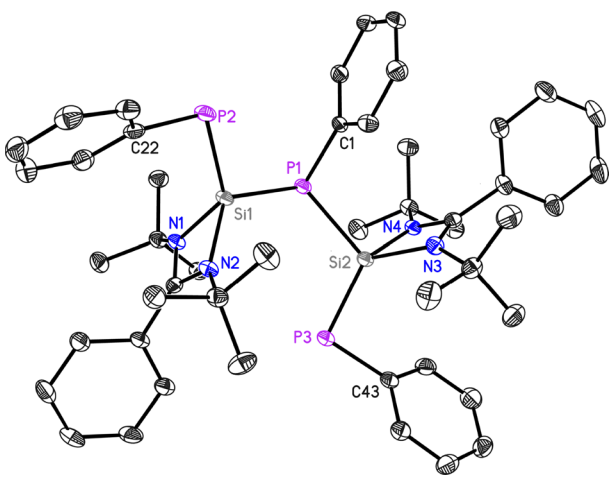


Fig. 2 The molecular structure of **1**. Anisotropic displacement parameters are drawn at the 50% probability level, and all the hydrogen atoms have been removed for clarity. Selected bond lengths [Å] and bond angles [°]: Si1–P1 2.2493(6), Si2–P1 2.2616(7), Si1–P2 2.1236(7), Si2–P3 2.1155(7), Si1–N1 1.8522(14), Si1–N2 1.8296(14), Si2–N3 1.8362(15), Si2–N4 1.8581(14), Si1–P1–Si2 115.71(3), Si1–P1–C1 101.96(5), Si2–P1–C1 106.96(6), P1–Si2–P3 113.02(3), P1–Si1–P2 107.41(2).

those observed in **1** (Si1–P1: 2.2493(6) Å, Si2–P1: 2.2616(7) Å). However, the Si═P bond distances in **1** are slightly longer than those in LSi(SiMe$_3$)═PSiMe$_3$ (2.095(3) Å)[13] and comparable to those in phosphasilenes with three-coordinate silicon atoms.[18,21,22] The bond angles around the central phosphorus atom (P1) are Si1–P1–Si2 = 115.71(3)°, Si1–P1–C1 = 101.96(5)°, and Si2–P1–C1 = 106.96(6)°, indicating a pyramidal geometry for the P1 atom. The differences between the Si═P double bond distances and Si–P single bond distances in **1** and the pyramidal geometry around the central phosphorus atoms suggest that the Si═P units are best described as localised double bonds rather than a part of a delocalised bonding framework.

The quantum chemical calculations were carried out to explore the nature of the bonding in compound **1** at the M06/def2-TZVPP//BP86-D3(BJ)/def2-SVP level of theory. The calculated bond lengths and bond angles of **1** (Fig. S15, see SI) match well with the experimentally observed values from a single-crystal X-ray diffraction study. One tricoordinated phosphorous atom (P1) and two dicoordinated phosphorus atoms (P2 and P3) exist in **1**. The Si–P1 bond distances (2.260 and 2.272 Å) are longer than the Si–P2 and Si–P3 bond distances (2.135 and 2.131 Å). The Si–P2 and Si–P3 bond distances are comparable to the same in phosphasilenes (2.11–2.13 Å) isolated before.[28,38] The bridging phosphorus atom P1 is significantly pyramidized (the pyramidalization at the P1 atom is 42.1°), suggesting the presence of a sp^n lone pair. Therefore, **1** can be recognised as a bis(phosphasilene) where the two LSi═P–Ph fragments are linked through a tricoordinated phosphorous atom P1.

We analysed the frontier molecular orbitals of **1**. The HOMO and HOMO−1 are π-type lone pair orbitals on P2 and P3 atoms with significant polarization towards the tetracoordinate silicon atom (Fig. 3a). Accordingly, these molecular orbitals can be considered as pseudo-π-MOs. The HOMO−2 and HOMO−3 are σ-type lone pair orbitals on the dicoordinated phosphorus atoms, and the HOMO−4 is the lone pair-type orbital on the tricoordinated phosphorus atom.

The numerical data from natural population analysis are well corroborated by the above-discussed geometrical and molecular orbital picture. The P2 and P3 atoms have slightly more negative charges (−0.24*e* and −0.30*e*, Table S4, see SI) than the P1 atom (−0.11*e*), indicating a dual lone pair character at the P2 and P3 atoms. The Wiberg bond indices (Table S3, see SI) for the Si═P double bonds (1.41 and 1.45) are significantly higher than those for the Si–P single bonds (0.92 and 0.93). The π-type lone pair at P2 and P3 atoms has the lowest orbital occupancy (1.55*e* and 1.57*e*, Table S8, see SI), followed by the lone pair at P1 atom (1.85*e*). Hence, the lone pairs at the P2 and P3 atoms are significantly delocalized towards the silicon atom by hyperconjugative interaction as compared to the lone pair at the P1 atom. The estimated value of hyperconjugative stabilization energy from the π-type lone pair at the dicoordinated phosphorous atom to the Si–N σ* orbital is 34.0 kcal mol^{-1} from P2 and 33.7 kcal mol^{-1} from P3 (Table S5, see SI). The corresponding values from the σ-type lone pairs are much less (9.5 kcal mol^{-1} and 8.5 kcal mol^{-1}). The hyperconjugative stabilization energy for the lone pair orbital of the tri-coordinated phosphorus atom P1 towards the silicon atoms (10.3 kcal mol^{-1} and 12.6 kcal mol^{-1}) is close to that of the hyperconjugative stabilization energy of the σ-type lone pair at the di-coordinated phosphorus atoms P2 and P3.

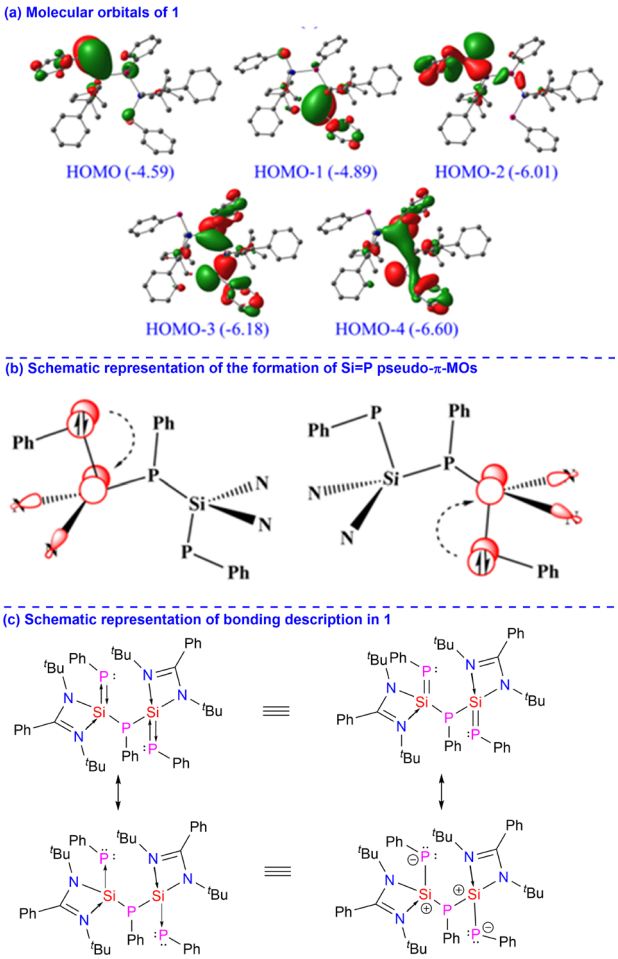


Fig. 3 (a) Molecular orbitals corresponding to the Si–P pseudo-π-MOs (HOMO and HOMO−1), and the σ-type lone pair on the phosphorous centers (HOMO−2–HOMO−4) of **1** calculated at M06/def2-TZVPP//BP86-D3(BJ)/def2-SVP level. The energy values are in eV. (b) Schematic representation of the formation of Si–P pseudo-π-MOs. (c) Schematic representation of bonding description in **1**.

The topological parameters of electron density calculated at the Si–P bond critical points (BCPs) support the covalent nature of these bonds, where the corresponding BCPs have a negative sign for $\nabla^2\rho(r)$ (Table S6, see SI). The ellipticity of the Si–P2 and Si–P3 bonds is large (0.42 and 0.45), suggesting non-cylindrical polar Si–P bonding. We have earlier reported similar bonding description in pseudo-silapnictenes, which unequivocally established the occurrence of two lone pairs (one with σ- and the second with π-local symmetry) at the dicoordinated pnictogen center and the presence of strong hyperconjugative stabilization.[39,40] The geometrical and bonding analysis suggests that the π-type lone pairs on the di-coordinated phosphorus atoms P2 and P3 are stabilized by hyperconjugative donation to low-lying Si–N σ* orbitals, resulting in pseudo-Si–P π-bonds. The extent of hyper-conjugative stabilization of σ-type lone pair on dicoordinated and tricoordinated phosphorous

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atoms is much less. Accordingly, the Si═P π-bonds are considered non-conjugated and strongly polarized (Fig. 3b).

While the ellipticity values are relatively large, this parameter alone cannot be taken as definitive evidence for π-bonding in such highly polarized heteronuclear bonds.[41] Previous charge density studies have demonstrated that significant ellipticity may arise from polarization effects and lone-pair density accumulation rather than genuine π-character.[42–44] Therefore, the observed ellipticity in the present system is more appropriately attributed to anisotropic electron density distribution resulting from donor–acceptor interactions between phosphorus and silicon. In this context, the Si═P bond is best described as a strongly polarized multiple bond with contributions from both phosphasilene and silylene–phosphinidene resonance forms (Fig. 3c), rather than a classical double bond.

Given the localized phosphorus lone pairs, proton affinity calculations were performed to assess the reactivity of the chemically distinct phosphorus centres. Both di-coordinated and tri-coordinated phosphorus lone pairs exhibit very high proton affinity. The highest first proton affinity was observed at the di-coordinated phosphorus atoms (268.3 kcal mol^{-1} for P2 and 260.2 kcal mol^{-1} for P3), and the next highest proton affinity was observed at the tri-coordinated phosphorus atom (245.1 kcal mol^{-1}). The first protonation occurs at the highly polarized Si═P bond, showing very high reactivity. The addition of a second proton at the P3 center occurs at the σ-type lone pair, resulting in a tetra-coordinated phosphorus atom (Fig. S16, see SI). The corresponding second proton affinity value is 164.5 kcal mol^{-1}. On the other hand, the second proton addition at the P2 atom enhances the Lewis acidic character of the silicon atom (Si1), leading to the coordination of the σ-type lone pair on the other di-coordinated phosphorous atom, resulting in pentacoordination at Si1 (Fig. S16, see SI). Since the hyperconjugative stabilization of lone pairs is a second-order interaction, these lone pairs exhibit high reactivity in the presence of external stimuli such as protons.

In conclusion, we have synthesized and structurally characterized a rare bis(phosphasilene) featuring two electronically isolated, non-conjugated Si═P units separated by Si–P single bonds. Spectroscopic and crystallographic analyses, supported by DFT calculations, reveal highly polarized Si═P π-bonds with minimal delocalization and substantial hyperconjugative stabilization. Computational studies further suggest pronounced reactivity associated with phosphorus lone pairs, highlighting the potential of this motif as a versatile platform for developing new low-valent compounds and ligand systems.

Conflicts of interest

There are no conflicts to declare.

Data availability

The NMR, mass and DFT calculation data that support the findings of this work have been included in the supplementary information (SI). See DOI: https://doi.org/10.1039/d6cc03111k.

CCDC 2444828 (**1**) contains the supplementary crystallographic data for this paper.[45]

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