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Valence isomerization of 2-phospha-4-silabicyclo[1.1.0]butane: a high-level ab initio study

Abstract The rearrangements for 2-phospha-4-silabicyclo[1.1.0]butane, analogous to the valence isomerization of the hydrocarbons bicyclobutane, 1,3-butadiene, and cyclobutene, were studied at the (U)QCISD(T)/6-311 + G**//(U)QCISD/6-31G* level of theory. The monocyclic 1,2-dihydro-1,2-phosphasiletes are shown to be the thermodynamically preferred product, in contrast to the isomerization of the hydrocarbons, which favors the 1,3-butadiene structure. Furthermore, an unprecedented direct isomerization pathway to the 1,2-dihydro-1,2-phosphasiletes was identified. This pathway is competitive with the isomerization via the open-chain butadienes and becomes favorable when electron-donating substituents are present on silicon.

Keywords Heterobicyclobutanes · Valence isomerization · Ab initio theory

Introduction

Bicyclo[1.1.0]butane with its strain energy of over 60 kcal mol^{-1} is a fascinating compound that has attracted the interest of both experimental and theoretical chemists [1]. It is now well established that bicyclo[1.1.0]butane (**1**) opens to the more stable valence isomer *gauche*-butadiene (**2**) by a pericyclic rearrangement,

Dedicated to Professor Dr. Paul von Ragué Schleyer on the occasion of his 75th birthday.

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which is characterized by a concerted, asynchronous conrotatory ring opening where the central C–C bond remains intact [2, 3]. This is an allowed [$\sigma 2s + \sigma 2a$] conrotatory rearrangement according to the Woodward–Hoffmann (W–H) orbital-symmetry rules [4–6], affording kinetic intermediate **2** that can easily rotate to *s-trans*-1,3-butadiene (**3**). The activation barrier of 41.5 kcal mol^{-1} calculated at the multiconfiguration self-consistent field level of theory [2] agrees closely with the experimental value of 40.6 kcal mol^{-1} [7, 8]. The disrotatory, W–H forbidden, thermal ring opening of **1** is less favorable, and was calculated to be about 15 kcal mol^{-1} higher in energy [2]. Another rearrangement is also feasible; stretching of the central C–C bond leads to a planar singlet diradical transition structure for inversion, which is also a higher energy process with a barrier of 47.4 kcal mol^{-1} [9].


1 **2** **3** **4**
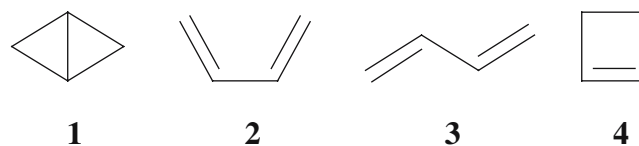
Valence isomer cyclobutene (**4**) is of intermediate stability between **1** and **3** and converts thermally to *gauche*-butadiene **2** by an electrocyclic ring opening [10, 11]. This pericyclic rearrangement follows a W–H allowed concerted, conrotatory pathway. The calculated activation barrier at the MP2/6-311G** level of theory of 33.7 kcal mol^{-1} [12–14] for this process is in agreement with the experimental value of 32.9 ± 0.5 kcal mol^{-1} [10, 11]. Usually for the ring opening of cyclobutenes, steric effects dominate the preference for inward versus outward rotation [15]. However, electronic effects can also dictate this rearrangement, as was reported very recently for the sterically hindered substrate **5**, which prefers to react via the more crowded inward rotatory pathway, leading mainly to butadiene **6** (Scheme 1) [16, 17].
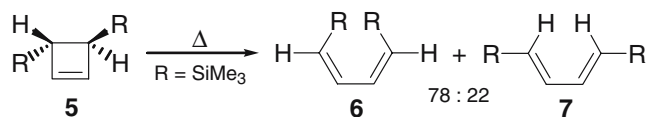
Scheme 1 Ring opening of cyclobutene 5

Bicyclo[1.1.0]butanes with main-group hetero-elements in the ring have also received considerable attention [18]. However, little is known about the phosphorus-containing analogues [19–22]. In our ongoing research on small strained organophosphorus ring systems, we became interested in the yet unknown 2-phospha-4-silabicyclo[1.1.0]butanes, whose occurrence we reported as a reactive intermediate recently [23, 24]. Valence isomerization of the 2-phospha-4-silabicyclo[1.1.0]butane 9 to the 1,2-dihydro-1,2-phosphasiletes 10a,b was indicated by reacting 1H-phosphirene 8 with silylene $Si[(NCH_2^tBu)_2C_6H_4-1,2]$ $[\equiv Si(NN)]$ (Scheme 2).
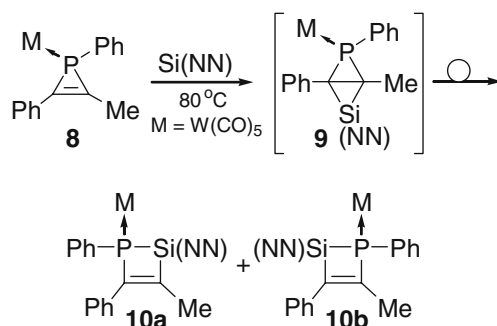
Scheme 2 Isomerization of bicyclo[1.1.0]butane 9

SCS-MP2/6-311 + G** calculations on B3LYP/6-31G* model structures show that the intermediate 2-phospha-4-silabicyclo[1.1.0]butane isomerizes directly, via an unprecedented W–H allowed [σ2s + σ2a] process, to the thermodynamically preferred 1,2-dihydro-1,2-phosphasilete [23, 24]. This pathway is favored over the concerted, asynchronous conrotatory ring opening leading to s-trans-1-phospha-4-sila-1,3-butadiene [25].

Here, we report on the isomerization of 2-phospha-4-silabicyclo[1.1.0]butane A to its valence isomers 1-phospha-4-sila-1,3-butadiene B and 1,2-dihydro-1,2-phosphasilete C (only one other synthesis of 1,2-dihydro-1,2-phosphasiletes was reported: [26–28]), using high-level ab initio calculations at the (U)QCISD(T)/6-311 + G**//(U)QCISD/6-31G* level of theory. We will compare the differences between a direct A → C pathway versus the isomerization via butadiene B. In addition, the influence of substituents on silicon on the rearrangements will also be discussed.
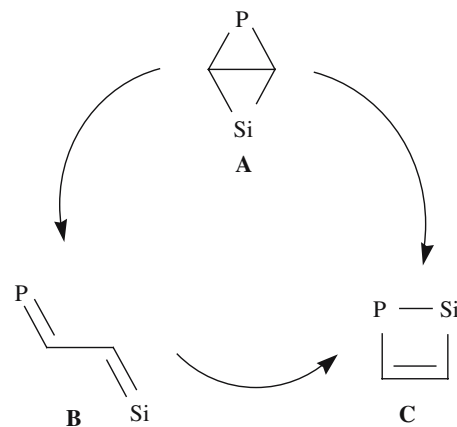
Computational details

All calculations were performed using the GAUSSIAN 98 [29] suite of programs. Geometries were optimized using the standard 6-31G* basis set at the (U)MP2 and (U)QCISD [30, 31] level of theory, while single-point calculations were preformed at the (U)QCISD(T)/6-311 + G** level using the (U)QCISD/6-31G* geometries. First and second order energy derivatives were computed to confirm that minima or transition structures had been located at the (U)MP2/6-31G* level. Intrinsic reaction coordinate driving calculations were performed at the (U)MP2/6-31G* level to establish the connections between transition structures and minima. The total energies calculated at the (U)MP2, (U)QCISD, and (U)QCISD(T) levels were corrected for the (U)MP2/6-31G* level zero-point energies scaled by a factor of 0.967 [32].

Results and discussion

First, we investigated the rearrangements of bicyclo[1.1.0]butane (1) and cyclobutene (4) into the more stable s-trans-1,3-butadiene (3) at the (U)QCISD(T)/6-311 + G**//(U)QCISD/6-31G* level of theory (this method gives similar energies when compared to the CASSCF(10,10)/6-31G* level of theory as was reported for the isomerization of 2-oxabicyclo[1.1.0]butane: [33]), since no complete study of the valence isomerizations of all C_4H_6 isomers at the same level of theory were reported to date. Subsequently, we investigated the rearrangements of the 2-phospha-4-silabicyclo[1.1.0]butanes, where the effects of heteroatom substitution on the characteristics of the rearrangements become apparent.

Bicyclo[1.1.0]butane (1) leads to gauche-butadiene 2 via a concerted, asynchronous conrotatory ring opening [2, 3], which has a barrier of 39.2 kcal mol^{-1}, and is exothermic by 26.0 kcal mol^{-1} (Fig. 1). This closed-shell rearrangement is favored over the corresponding

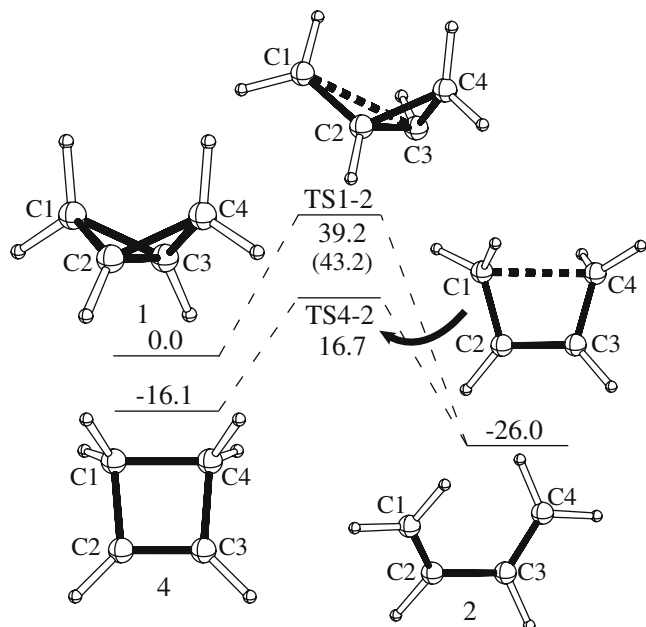**Fig. 1** Relative QCISD(T)/6-311 + G**//QCISD/6-31G* (UQ-CISD(T)/6-311 + G**//UQCISD/6-31G* in parenthesis) energies (ZPE corrected, in kcal mol^{-1}) for the rearrangements of **1** and **4** into **2**. Selected bond lengths [Å], angles and torsion angles [°] of **1** (C_{2v}): C1–C2 1.498, C2–C3 1.494, C2–C1–C3 59.8, C1–C2–C3–C4 121.9; **2** (C_2): C1–C2 1.342, C2–C3 1.479, C3–C4 1.342, C1–C2–C3–C4 37.9; **4** (C_{2v}): C1–C2 1.520, C1–C4 1.570, C2–C3 1.346, C1–C2–C3 94.2; **TS1–2** (closed-shell): C1–C2 1.403, C1–C3 2.344, C2–C3 1.542, C2–C4 1.569, C2–C1–C3 39.4; **TS4–2** (C_2): C1–C2 1.430, C1–C4 2.150, C2–C3 1.379, C1–C2–C3–C4 21.7

Fig. 2 Relative QCISD(T)/6-311 + G**//QCISD/6-31G* energies (ZPE corrected, in kcal mol^{-1}) for the rearrangements of **2**. Selected bond lengths [Å], angles and torsion angles [°] of **3** (C_{2h}): C1–C2 1.343, C2–C3 1.467, C1–C2–C3 123.8; **TS2–3** (C_2): C1–C2 1.340, C2–C3 1.490, C1–C2–C3–C4 101.9; **TS2–2'** (C_{2v}): C1–C2 1.430, C2–C3 1.379, C1–C2–C3–C4 0.0

diradical open-shell pathway ($\Delta E^{\ddagger} = 43.2$ kcal mol^{-1}, $<S^2> = 0.85$). In addition, cyclobutene (**4**) also gives **2** via a synchronous (C_s symmetry) conrotatory ring opening [12–14] that requires 32.8 kcal mol^{-1}, and is exothermic by 9.9 kcal mol^{-1}. Both calculated reaction barriers are in excellent agreement with the experimental values of 40.6 kcal mol^{-1} [7, 8] and 32.9 kcal mol^{-1} [10, 11], respectively.

The kinetic *gauche*-butadiene **2** can easily transform into its enantiomer **2'** via the planar *s-cis*-1,3-butadiene (**TS2-2'**) [2, 34] with a barrier of only 0.7 kcal mol^{-1}, or can rotate to the more stable *trans*-butadiene **3** ($\Delta E^{\ddagger} = 2.5$ kcal mol^{-1}) with an exothermicity of 2.6 kcal mol^{-1} (Fig. 2) [12–14]. The geometrical parameters of the optimized structures **1**, **3**, and **4** at the QCISD/6-31G* level of theory are in excellent agreement with the experimental estimates (experimental structures—**1**, **3**, and **4**: [35–37]).

Incorporating heteroatoms into the bicyclo[1.1.0]butane framework has a profound impact. We found that 2-phospha-4-silabicyclo[1.1.0]butane (**11**) opens with a modest exothermicity (0.4 kcal mol^{-1}) directly to valence isomer *s*-1-phospha-4-sila-1,3-butadiene (**12**) in its *trans* configuration via a concerted, asynchronous conrotatory ring opening. In this process, the P–C2 bond becomes elongated well before that of the Si–C1 bond (Fig. 3). The activation barrier of 38.8 kcal mol^{-1} is very similar to the calculated activation barrier of
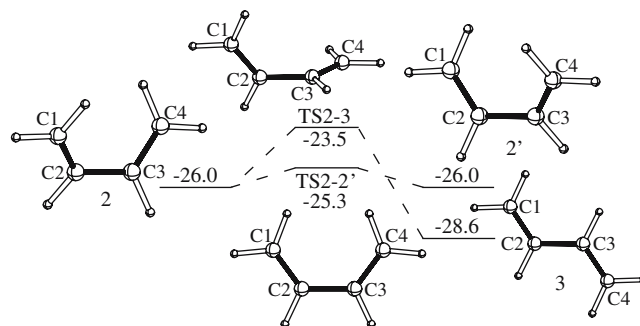
39.2 kcal mol^{-1} for the [$\sigma 2s + \sigma 2a$] process in bicyclo[1.1.0]butane (**1**). The closed-shell rearrangement **11** → **12** is favored over the corresponding diradical open-shell pathway ($\Delta E^{\ddagger} = 41.3$ kcal mol^{-1}, $<S^2> = 0.97$).

s-Trans-butadiene **12** can transform into the slightly less stable *gauche*-butadiene **13** ($\Delta E = 2.6$ kcal mol^{-1}) with an energy barrier of 7.5 kcal mol^{-1}. Subsequently, butadiene **13** can isomerize via a conrotatory electrocyclic ring closure to the much more stable 1,2-dihydro-1,2-phosphasilete (**14**) ($\Delta E = -23.9$ kcal mol^{-1}), with a rearrangement barrier of only 3.2 kcal mol^{-1}. Clearly, if a 1-phospha-4-sila-butadiene is to be formed from **11**, it will rearrange to the four-membered ring structure **14**. We conclude that in contrast to the hydrocarbons, where butadiene **3** is the favored product, the P,Si-derivatives **12** and **13** are not likely candidates to be observed on rearranging bicyclic compound **11**.

As **14** is thermodynamically the preferred valence isomer, we also explored whether it could be formed directly from bicyclic **11**. Indeed, forcing an asynchronous conrotatory ring opening with an initial SiH$_2$-group rotation resulted in a transition structure **TS11–14** for the direct rearrangement of **11** into **14** (Fig. 4). The barrier of 39.0 kcal mol^{-1} for this closed-shell process is similar to the conversion via the P,Si-butadienes ($\Delta E^{\ddagger} = 38.8$ kcal mol^{-1}, Fig. 3)[1]. The rearrangement via **TS11–14** obeys the orbital symmetry rules and can be described as a [$\sigma 2s + \sigma 2a$] process. Such a pathway is unprecedented for the isomerization of the carbon analogue bicyclo[1.1.0]butane (**1**) [2], for which *s-trans*-1,3-butadiene is the favored product.

Due to the similarities in activation energy for the conversions **11** → **12** and **11** → **14** at the QCISD(T)/6-311 + G**//QCISD/6-31G* level of theory, we have also incorporated in our computational model the cyclic diamine HN-C=C-NH as substituent on silicon to investigate the effect of donating N atoms, which are also present in our experimental system [23, 24] on the rearrangements.

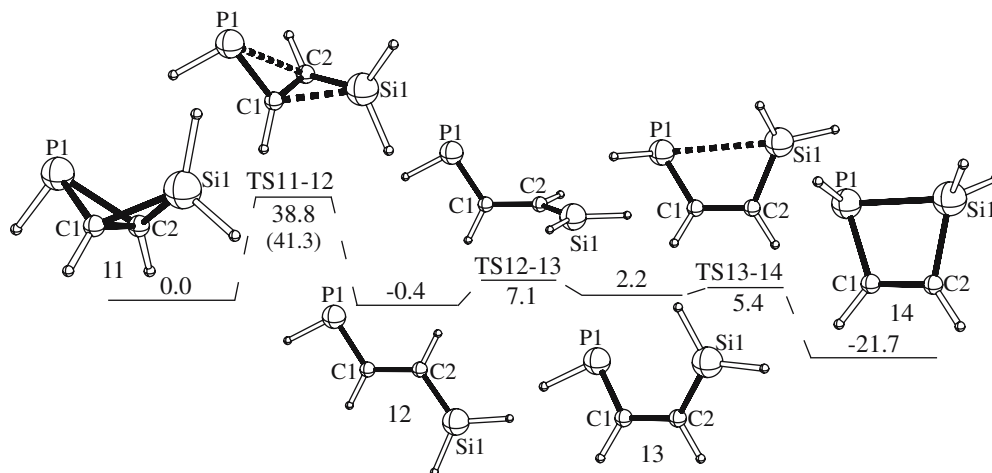[1] No competitive open-shell rearrangement is present for **TS11–14**.

Fig. 3 Relative QCISD(T)/6-311 + G**//QCISD/6-31G* (UQ-CISD(T)/6-311 + G**//UQCISD/6-31G* in parenthesis) energies (ZPE corrected, in kcal mol^{-1}) for the rearrangements of **11** into **14**. Selected bond lengths [Å], angles and torsion angles [°] of **11** (C$_s$): P1–C1 1.852, Si1–C1 1.840, C1–C2 1.548, C1–P1–C2 49.4, C1–Si1–C2 49.7, P1–C1–C2–Si1 119.0; **TS11–12**: P1–C1 1.782,

P1–C2 2.664, Si1–C1 1.982, Si1–C2 1.785; **12** (C$_s$): P1–C1 1.708, Si1–C2 1.741, C1–C2 1.443; **TS12–13**: P1–C1–C2–Si1 103.3; **13**: P1–C1–C2–Si1 36.3; **TS13–14**: P1–C1 1.736, P1–Si1 3.001, Si1–C2 1.774, C1–C2 1.414, P1–C1–C2–Si1 34.1; **14**: P1–C1 1.869, P1–Si1 2.290, Si1–C2 1.872, C1–C2 1.354.
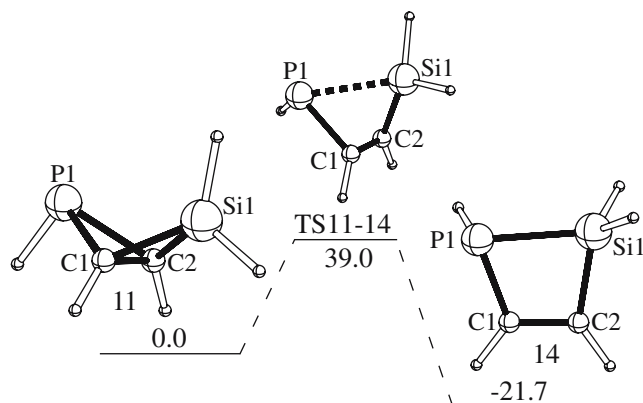

Fig. 4 Relative QCISD(T)/6-311 + G**//QCISD/6-31G* energies (ZPE corrected, in kcal mol^{-1}) for the direct rearrangement of **11** into **14**. Selected bond lengths [Å] and torsion angles [°] of **TS11–14**: P1–C1 1.834, P1–Si1 2.431, Si1–C2 1.800, C1–C2 1.422, P1–C1–C2–Si1 76.0

Substituted 2-phospha-4-silabicyclo[1.1.0]butane **15** leads to its valence isomer *s-trans*-1-phospha-4-sila-1,3-butadiene **16** via a concerted, asynchronous conrotatory ring opening ($\Delta E^{\ddagger} = 39.0$ kcal mol^{-1}), with a modest endothermicity of 1.5 kcal mol^{-1} (Fig. 5). The associated transition structure **TS15–16** shows features similar to the parent analogue **TS11–12**, and the closed-shell rearrangement **15 → 16** is favored over the corresponding diradical open-shell pathway ($\Delta E^{\ddagger} = 46.1$ kcal mol^{-1}, $<S^2> = 0.97)^2$. In addition, *s-trans*-butadiene **16** can transform into the slightly more stable planar *cis*-butadiene **17** ($\Delta E = -1.5$ kcal mol^{-1}), which is now an energy minimum, with an energy barrier of only 8.2 kcal mol^{-1}.

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[2]Open-shell **TS15–16** was calculated at the UQCISD(T)/6-311 + G**//UMP2/6-31G* level of theory.

Subsequently, **17** can isomerize via a conrotatory electrocyclic ring closure to the much more stable 1,2-dihydro-1,2-phosphasilete **18** ($\Delta E = -25.6$ kcal mol^{-1}) with a minute barrier of only 1.3 kcal mol^{-1}. The geometrical parameters of the optimized **18** are in good agreement with the single-crystal X-ray analysis of **10a** [23, 24].

Interestingly, the direct valence isomerization now becomes favorable, and 2-phospha-4-silabicyclo[1.1.0] butane **15** gives cyclobutene derivative **18** ($\Delta E^{\ddagger} = 27.7$ kcal mol^{-1}) via a W–H allowed [$\sigma 2s + \sigma 2a$] process, with an exothermicity of 25.6 kcal mol^{-1} (Fig. 6).

The lower barrier for the direct conversion **15 → 18** compared to that of the parent **11 → 14** can be ascribed to the presence of the donating amino groups on silicon. Generally, π-donor (e.g., NH$_2$) and σ-acceptor (e.g., F) substituents destabilize three-membered rings, making them more reactive, as indicated by their increased ring strain [38, 39]. This is also evident for the **15 → 18** conversion by an increased exothermicity ($\Delta E_{11 \to 14} = 21.7$ kcal mol^{-1}; $\Delta E_{15 \to 18} = 25.6$ kcal mol^{-1}). Additionally, the analogous rearrangement for the fluoro-substituted 2-phospha-4-silabicyclo[1.1.0]butane **19** confirms this trend ($\Delta E_{19 \to 20} = 28.1$ kcal mol^{-1}, Fig. 7). Furthermore, the associated transition state of this novel pathway is stabilized by the electron-donating *N*-heterocyclic substituent on silicon ($\Delta E^{\ddagger}_{11 \to 14} = 39.0$ kcal mol^{-1}; $\Delta E^{\ddagger}_{15 \to 18} = 27.7$ kcal mol^{-1}; $\Delta E^{\ddagger}_{19 \to 20} = 35.0$ kcal mol^{-1}).

Conclusions

Hetero substitution changes the stability of the valence isomers of bicyclo[1.1.0]butane (**1**). 2-Phospha-4-silabicyclo[1.1.0]butane (**11**) is the least stable isomer and 1,2-dihydro-1,2-phosphasilete (**14**) the most stable one at the
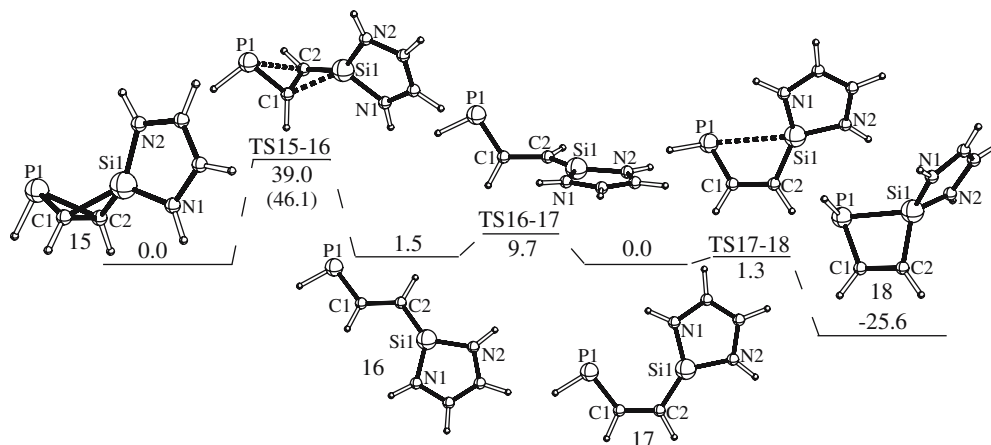
Fig. 5 Relative QCISD(T)/6-311 + G**//QCISD/6-31G* (UQ-CISD(T)/6-311 + G**//UMP2/6-31G* in parenthesis) energies (ZPE corrected, in kcal mol^{-1}) for the rearrangements of **15** into **18**. Selected bond lengths [Å], angles and torsion angles [°] of **15** (C_s): P1–C1 1.852, Si1–C1 1.823, Si1–N1 1.730, C1–C2 1.613, C1–P1–C2 51.6, C1–Si1–C2 52.5, P1–C1–C2–Si1 122.1; **TS15–16**: P1–C1 1.768, P1–C2 2.590, Si1–C1 1.977, Si1–C2 1.748, Si1–N1 1.726;

16 (C_s): P1–C1 1.718, Si1–C2 1.724, Si1–N1 1.717, C1–C2 1.434; **TS16–17**: P1–C1–C2–Si1 98.2; **17** (C_s): P1–C1 1.727, Si1–C2 1.732, Si1–N1 1.710, Si1–N2 1.717; **TS17–18**: P1–C1 1.743, P1–Si1 3.103, Si1–C2 1.765, Si1–N1 1.719, C1–C2 1.406, P1–C1–C2–Si1 24.8; **18**: P1–C1 1.867, P1–Si1 2.309, Si1–C2 1.867, Si1–N1 1.741, C1–C2 1.356
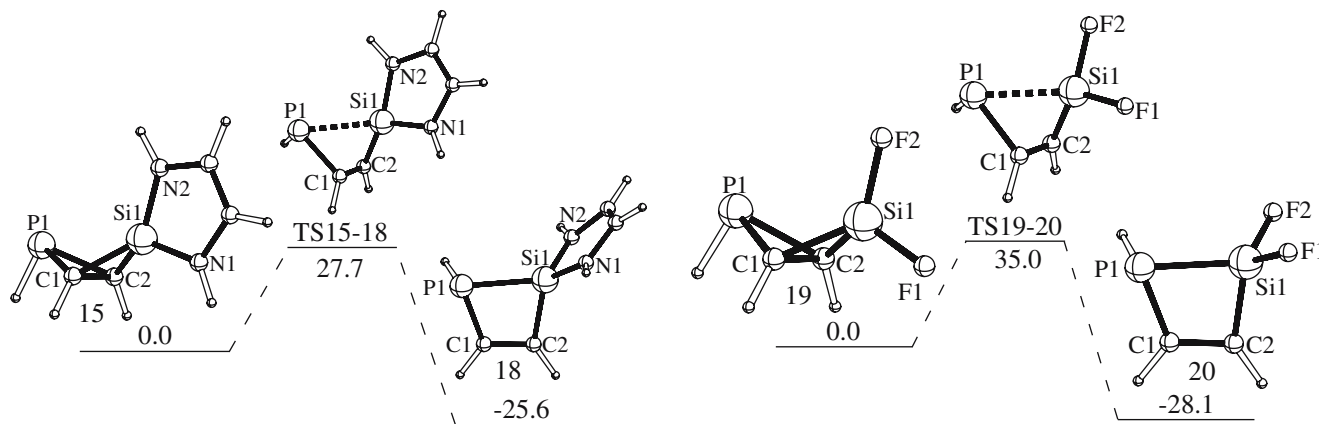

Fig. 6 Relative QCISD(T)/6-311 + G**//QCISD/6-31G* energies (ZPE corrected, in kcal mol^{-1}) for the direct rearrangement of **15** into **18**. Selected bond lengths [Å] and torsion angles [°] of **TS15–18**: P1–C1 1.841, P1–Si1 2.458, Si1–C2 1.777, Si1–N1 1.742, Si1–N2 1.736, C1–C2 1.444, P1–C1–C2–Si1 78.0

Fig. 7 Relative QCISD(T)/6-311 + G**//QCISD/6-31G* energies (ZPE corrected, in kcal mol^{-1}) for the direct rearrangement of **19** into **20**. Selected bond lengths [Å] and torsion angles [°] of **19** (C_s): P1–C1 1.852, Si1–C1 1.797, Si1–F1 1.600, C1–C2 1.631, C1–P1–C2 52.2, C1–Si1–C2 54.0, P1–C1–C2–Si1 122.0; **TS19–20**: P1–C1 1.834, P1–Si1 2.383, Si1–C2 1.758, Si1–F1 1.613, Si1–F2 1.610, C1–C2 1.457, P1–C1–C2–Si1 77.5; **20**: P1–C1 1.879, P1–Si1 2.252, Si1–C2 1.841, Si1–F1 1.607, C1–C2 1.357

Cartesian coordinates and energies of all stationary points are available in the electronic supplementary material.

QCISD(T)/6-311 + G**//QCISD/6-31G* level of theory [40]. Two reaction pathways for the thermal isomerization of 2-phospha-4-silabicyclo[1.1.0]butane (**11**) have been found: (a) a three-step process starting with a barrier of 38.8 kcal mol^{-1} for the concerted, asynchronous conrotatory ring opening of **11** to s-trans-1-phospha-4-sila-1,3-butadiene (**12**), followed by a conformational change to the gauche isomer **13** and a subsequent conrotatory electrocyclic ring closure to **14**, and (b) a direct transformation of **11** into **14** via a [σ2s + σ2a] process with a barrier of 39.0 kcal mol^{-1} which becomes favorable when electron-donating substituents are present on silicon. This latter path is unprecedented for the analogous isomerization of bicyclo[1.1.0]butane.

References

1. Hoz S (1987) Bicyclo[1.1.0]butane. In: Rappoport Z (ed) The chemistry of the cyclopropyl group, Part 2, chapter 19. Wiley, Chichester
2. Nguyen KA, Gordon MS (1995) J Am Chem Soc 117:3835–3847

3. Shevlin PB, McKee ML (1988) J Am Chem Soc 110:1666–1671
4. Woodward RB, Hoffmann R (1969) Angew Chem 81:797–870
5. Woodward RB, Hoffmann R (1969) Angew Chem Int Ed 8:781–853
6. Woodward RB, Hoffmann R (1970) The conservation of orbital symmetry. Academic, New York
7. Frey HM, Stevens IDR (1965) Trans Faraday Soc 61:90–94
8. Srinivasan R, Levi AA, Haller I (1965) J Phys Chem 69:1775–1777
9. Nguyen KA, Gordon MS, Boatz JA (1994) J Am Chem Soc 116:9241–9249
10. Cooper W, Walters WD (1958) J Am Chem Soc 80:4220–4224
11. Carr RW Jr, Walters WD (1965) J Phys Chem 69:1073–1075
12. Deng L, Ziegler T (1995) J Phys Chem 99:612–618
13. Wiest O, Houk KN, Black KA, Thomas BE IV (1995) J Am Chem Soc 117:8594–8599
14. Spellmeyer DC, Houk KN (1988) J Am Chem Soc 110:3412–3416
15. Niwayama S, Kallel EA, Spellmeyer DC, Sheu C, Houk KN (1996) J Org Chem 61:2813–2825
16. Murakami M, Hasegawa M (2004) Angew Chem 116:4981–4984
17. Murakami M, Hasegawa M (2004) Angew Chem Int Ed 43:4873–4876
18. Iwamoto T, Yin D, Kabuto C, Kira M (2001) J Am Chem Soc and references therein 123:12730–12731
19. Tebby JC (2001) Bicyclic and polycyclic systems with a ring junction phosphorus atom. In: Mathey F (ed) Phosphorus-carbon heterocyclic chemistry: the rise of a new domain. Pergamon, Amsterdam, pp 683
20. Niecke E, Fuchs A, Nieger M (1999) Angew Chem 111:3213–3216
21. Niecke E, Fuchs A, Nieger M (1999) Angew Chem Int Ed 38:3028–3031
22. Jones C, Platts JA, Richards AF (2001) Chem Commun 663–664
23. Slootweg JC, de Kanter FJJ, Schakel M, Ehlers AW, Gehrhus B, Lutz M, Mills AM, Spek AL, Lammertsma K (2004) Angew Chem 116:3556–3559
24. Slootweg JC, de Kanter FJJ, Schakel M, Ehlers AW, Gehrhus B, Lutz M, Mills AM, Spek AL, Lammertsma K (2004) Angew Chem Int Ed 43:3474–3477
25. Slootweg JC, Ehlers AW, Lammertsma K (2004) Phosphorus, sulfur and silicon 179:803–807
26. Haber S, Boese R, Regitz M (1990) Angew Chem 102:1523–1525
27. Haber S, Boese R, Regitz M (1990) Angew Chem Int Ed 29:1436–1438
28. Haber S, Schmitz M, Bergsträßer U, Hoffmann J, Regitz M (1999) Chem Eur J 5:1581–1589
29. Frisch MJ, Trucks GW, Schlegel HB, Scuseria GE, Robb MA, Cheeseman JR, Zakrzewski VG, Montgomery JA Jr, Stratmann RE, Burant JC, Dapprich S, Millam JM, Daniels AD, Kudin KN, Strain MC, Farkas O, Tomasi J, Barone V, Cossi M, Cammi R, Mennucci B, Pomelli C, Adamo C, Clifford S, Ochterski J, Petersson GA, Ayala PY, Cui Q, Morokuma K, Rega N, Salvador P, Dannenberg JJ, Malick DK, Rabuck AD, Raghavachari K, Foresman JB, Cioslowski J, Ortiz JV, Baboul AG, Stefanov BB, Liu G, Liashenko A, Piskorz P, Komaromi I, Gomperts R, Martin RL, Fox DJ, Keith T, Al-Laham MA, Peng CY, Nanayakkara A, Challacombe M, Gill PMW, Johnson B, Chen W, Wong MW, Andres JL, Gonzalez C, Head-Gordon M, Replogle ES, Pople JA (2002) Gaussian 98 (Revision A.11.4). Gaussian Inc., Pittsburgh
30. Gauss J, Cremer C (1988) Chem Phys Lett 150:280–286
31. Lee TJ, Rendell AP, Taylor PR (1990) J Phys Chem 94:5463–5468
32. Scott AP, Radom L (1996) J Phys Chem 100:16502–16513
33. Okovytyy S, Gorb L, Leszczynski J (2001) Tetrahedron 57:1509–1513
34. Breulet J, Lee TJ, Schaefer HF III (1984) J Am Chem Soc 106:6250–6253
35. Bock CW, Panchenko YN (1989) J Mol Struct 187:69–82
36. Kuchitsu K, Fukuyama T, Morino Y (1968) J Mol Struct 1:463–479
37. Bak B, Led JJ, Nygaard L, Rastrup-Andersen J, Sørensen GO (1969) J Mol Struct 3:369–378
38. Bach RD, Dmitrenko O (2002) J Org Chem 67:2588–2599
39. Cremer D, Kraka E (1985) J Am Chem Soc 107:3811–3819
40. Driess M, Pritzkow H, Rell S, Janoschek R (1997) For $P_2Si_2H_4$ the diphospha-disilabicyclo[1.1.0]butane isomers are the most stable ones. Inorg Chem 36:5212–5217