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Phosphatetrasilatricyclo[2.1.0.0^{2,5}]pentane

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Contents of the Supporting Information:

1. Experimental Section.

General procedures. All experimental manipulations were performed using high-vacuum line techniques, or in an argon atmosphere of MBRAUN MB 150B-G glove box. All solvents were predried by conventional methods and finally dried and degassed over a potassium mirror in vacuum immediately prior to use. NMR spectra were recorded on Bruker AV-400FT (^{1}H NMR at 400.1 MHz; ^{13}C NMR at 100.6 MHz; ^{29}Si NMR at 79.5 MHz; ^{31}P NMR at 161.9 MHz) NMR spectrometer. Starting dipotassium salt of the tetrasilacyclobutadiene dianion **3^{2-}•[K^{+}(thf)$_2$]$_2$** was synthesized by the reduction of tetrabromocyclotetrasilane *cyclo*-[Si$_4$Br$_4$(SiMe^{t}Bu$_2$)$_4$][S1] with potassium graphite KC_8, according to a previously reported procedure[S2].

(a) Experimental procedure, spectroscopic and crystallographic data for 1-phospha-2,3,4,5-tetrasilatricyclo[2.1.0.0^{2,5}]pentane 4.

The dipotassium salt of the tetrasilacyclobutadiene dianion [prepared by the reduction of (^{t}Bu$_2$MeSi)$_4$Si$_4$Br$_4$ (80 mg, 0.076 mmol) with KC$_8$ (72 mg, 0.53 mmol), and used freshly without isolation] was placed in the glass reaction tube, into which dry degassed hexane (2 mL) was introduced by the vacuum transfer. Then a PCl$_3$/hexane solution (0.7 mL of 1% solution, 0.080 mmol) was added to the reaction mixture. Solution color quickly changed from dark green to pale-yellow. After inorganic salts were filtered off, hexane solution was concentrated and cooled to –30 °C to give almost colorless crystals of **4a** (25 mg, 41%). mp 151–153 °C. ^{1}H NMR (C$_6$D$_6$, δ, ppm) 0.18 (s, 6 H, 2 Me), 0.37 (s, 3 H, Me), 0.41 (s, 3 H, Me), 1.17 (s, 18 H, 2 ^{t}Bu), 1.24 (s, 18 H, 2 ^{t}Bu), 1.27 (s, 36 H, 4 ^{t}Bu); ^{13}C NMR (C$_6$D$_6$, δ, ppm) –6.83 (CH$_3$), –6.42 (CH$_3$), –6.39 (CH$_3$), 20.7 [(CH$_3$)$_3$*C*], 21.5 [(CH$_3$)$_3$*C*], 21.7 [(CH$_3$)$_3$*C*], 22.6 [(CH$_3$)$_3$*C*], 29.3 [(*C*H$_3$)$_3$C], 29.6 [(*C*H$_3$)$_3$C], 29.8 [(*C*H$_3$)$_3$C], 30.1 [(*C*H$_3$)$_3$C]; ^{29}Si (C$_6$D$_6$, δ, ppm) –198.2 (d, $^1J_{Si\text{-}P}$ = 59.6 Hz, bridgehead Si), –93.1 (d, $^1J_{Si\text{-}P}$ = 60.6 Hz, two bridging Si), 8.49, 21.5, 32.3 (Si substituents), 64.4; ^{31}P NMR (C$_6$D$_6$, δ, ppm) –380.0. Anal. Calcd. for C$_{36}$H$_{84}$ClPSi$_8$: C, 53.50; H, 10.48. Found: C, 54.02; H, 10.67.

Single crystals of **4** for X-ray diffraction analysis were grown from a saturated hexane solution. Diffraction data were collected at 150 K on a Bruker AXS APEX II CCD X-ray diffractometer (Mo-Kα radiation, λ = 0.71073 Å, 50 kV/30 mA). The structure was solved by the direct method with the SHELXS-97 program[S3,S4] and refined by the full-matrix least-squares method with the SHELXL-2014 program[S5]. Crystal data for **4**: MF = C$_{36}$H$_{84}$ClPSi$_8$, MW = 808.17, monoclinic, $P2_1/c$, a = 15.624(3), b = 17.873(3), c = 17.796(3) Å, β = 93.931(2)°, V = 4975.8(15) Å^3, Z = 4, D_{calcd} = 1.083 g cm^{-3}. The final R factor was 0.0848 for 6489 reflections with $I_o > 2\sigma(I_o)$ (R_w = 0.2360 for all data), GOF = 1.196.

The X-ray crystallographic data for **4** have been deposited at the Cambridge Crystallographic Data Centre (CCDC) under deposition no. CCDC 2094603. These data can be obtained free of charge from the CCDC (www.ccdc.cam.ac.uk/data_request/cif).

b) X-ray crystallography of 4.

Table S1. Crystallographic data for **4**.

Identification code	PSi4_0bis
Empirical formula	$C_{36}H_{84}ClPSi_8$
Formula weight	808.17
Temperature	150(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a = 15.624(3) Å
	b = 17.873(3) Å β = 93.931(2)°
	c = 17.796(3) Å
Volume	4957.8(15) $Å^{-3}$
Z	4
Density (calculated)	1.083 g/cm^3
Absorption coefficient	0.326 mm^{-1}
F(000)	1776
Crystal size	0.150 x 0.117 x 0.085 mm
Theta range for data collection	5.108 to 23.255°
Index ranges	–17<=h<=17, –19<=k<=19, –19<=l<=19
Reflections collected	68725
Independent reflections	7020 [R(int) = 0.0717]
Completeness to theta = 23.255°	98.4 %
Absorption correction	empirical
Max. and min. transmission	0.9729 and 0.9528
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7020 / 248 / 527
Goodness-of-fit on F^2	1.196
Final R indices [I>2sigma(I)]	R1 = 0.0848, wR2 = 0.2342
R indices (all data)	R1 = 0.0883, wR2 = 0.2360
Highest difference peak/deepest hole	1.026 and –0.555 e•$Å^{-3}$

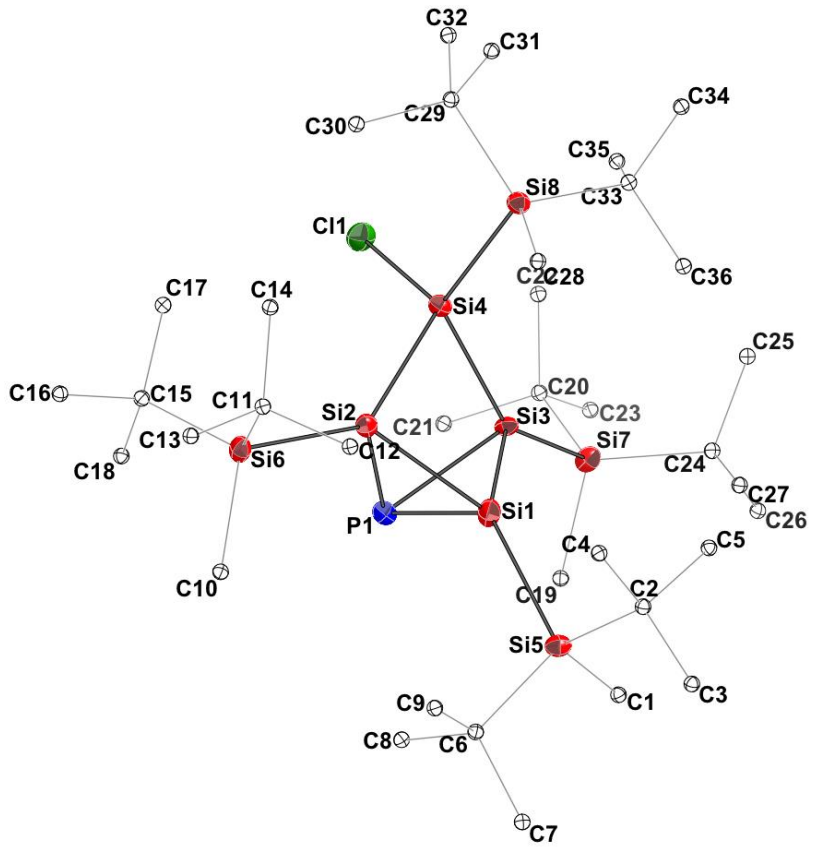


Figure S1. Crystal structure of the 1-phospha-2,3,4,5-tetrasilatricyclo[2.1.0.0^{2,5}]pentane **4** (ORTEP view with the thermal ellipsoids given at 40% probability, hydrogen atoms are not shown). The Si5-substituent is positionally disordered, and only major configuration (74%) is shown here.

Table S2. Atomic coordinates and equivalent isotropic atomic displacement parameters ($Å^2$) for **4**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Cl(1)	2258(1)	549(1)	358(1)	23(1)
P(1)	2330(1)	2898(1)	-9(1)	19(1)
Si(1)	2429(1)	3280(1)	1236(1)	20(1)
Si(2)	3314(1)	2362(1)	825(1)	16(1)
Si(3)	1437(1)	2394(1)	822(1)	13(1)
Si(4)	2384(1)	1413(1)	1169(1)	14(1)
Si(5)	2311(2)	4572(2)	1573(2)	16(1)
C(1)	1218(7)	4913(7)	1216(7)	27(3)
C(2)	2361(8)	4556(7)	2656(6)	23(2)
C(3)	2326(9)	5345(7)	2976(7)	36(3)
C(4)	3182(8)	4169(7)	2982(6)	34(3)
C(5)	1596(8)	4118(7)	2901(6)	35(3)
C(6)	3129(6)	5189(6)	1120(6)	20(2)
C(7)	2873(9)	6020(6)	1201(7)	33(3)
C(8)	3129(10)	4998(9)	277(8)	29(3)
C(9)	4035(7)	5074(7)	1477(7)	33(3)
Si(5')	2772(7)	4437(4)	1824(5)	16(2)
C(1')	3974(12)	4521(16)	1941(18)	27(6)
C(2')	2378(14)	5163(11)	1079(11)	21(4)
C(3')	2940(30)	5130(20)	413(19)	28(7)
C(4')	2380(20)	5962(13)	1403(18)	31(6)
C(5')	1461(16)	4980(17)	790(20)	31(6)
C(6')	2334(17)	4499(15)	2792(12)	25(4)
C(7')	2450(20)	3723(13)	3175(14)	24(5)
C(8')	1371(15)	4698(18)	2747(16)	29(6)
C(9')	2820(20)	5076(16)	3290(15)	30(6)
Si(6)	4784(1)	2478(1)	579(1)	18(1)
Si(7)	-35(1)	2586(1)	425(1)	17(1)

Si(8)	2499(1)	872(1)	2392(1)	14(1)
C(10)	4945(5)	3449(4)	190(5)	30(2)
C(11)	5471(5)	2375(5)	1507(5)	32(2)
C(12)	5120(6)	2915(6)	2087(5)	43(3)
C(13)	6403(5)	2592(6)	1406(5)	39(2)
C(14)	5431(7)	1580(6)	1804(6)	53(3)
C(15)	5008(5)	1780(4)	-202(5)	25(2)
C(16)	5975(6)	1696(6)	-298(6)	43(3)
C(17)	4628(6)	1001(5)	-47(5)	37(2)
C(18)	4576(6)	2075(6)	-930(5)	38(2)
C(19)	4(5)	3471(4)	-143(5)	24(2)
C(20)	-396(5)	1789(4)	-249(4)	23(2)
C(21)	141(6)	1842(5)	-944(5)	38(2)
C(22)	-247(6)	1017(5)	109(5)	34(2)
C(23)	-1348(6)	1873(5)	-515(6)	36(2)
C(24)	-764(5)	2765(4)	1222(4)	20(2)
C(25)	-1066(6)	2043(5)	1598(5)	33(2)
C(26)	-1566(5)	3216(5)	915(5)	28(2)
C(27)	-294(5)	3253(5)	1831(5)	28(2)
C(28)	3137(5)	1568(4)	2992(4)	24(2)
C(29)	3121(5)	-53(4)	2415(4)	21(2)
C(30)	3923(5)	18(5)	1968(5)	32(2)
C(31)	3427(6)	-235(5)	3242(5)	29(2)
C(32)	2578(5)	-716(4)	2096(5)	25(2)
C(33)	1358(5)	807(4)	2724(4)	23(2)
C(34)	1330(5)	362(5)	3473(5)	26(2)
C(35)	749(5)	446(5)	2139(5)	30(2)
C(36)	1062(5)	1605(4)	2877(5)	25(2)

Table S3. Bond lengths [Å] for **4**.

Cl(1)-Si(4)	2.114(3)
P(1)-Si(2)	2.274(3)
P(1)-Si(3)	2.286(3)
P(1)-Si(1)	2.313(3)
Si(1)-Si(2)	2.297(3)
Si(1)-Si(3)	2.301(3)
Si(1)-Si(5')	2.363(8)
Si(1)-Si(5)	2.396(4)
Si(2)-Si(4)	2.343(3)
Si(2)-Si(6)	2.376(3)
Si(3)-Si(4)	2.349(3)
Si(3)-Si(7)	2.384(3)
Si(4)-Si(8)	2.377(3)
Si(5)-C(1)	1.882(11)
Si(5)-C(6)	1.908(10)
Si(5)-C(2)	1.924(11)
C(1)-H(1A)	0.9800
C(1)-H(1B)	0.9800
C(1)-H(1C)	0.9800
C(2)-C(5)	1.519(16)
C(2)-C(3)	1.523(16)
C(2)-C(4)	1.536(17)
C(3)-H(3A)	0.9800
C(3)-H(3B)	0.9800
C(3)-H(3C)	0.9800
C(4)-H(4A)	0.9800
C(4)-H(4B)	0.9800
C(4)-H(4C)	0.9800
C(5)-H(5A)	0.9800
C(5)-H(5B)	0.9800
C(5)-H(5C)	0.9800

C(6)-C(9)	1.525(14)
C(6)-C(8)	1.539(16)
C(6)-C(7)	1.548(15)
C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800
C(7)-H(7C)	0.9800
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
Si(5')-C(1')	1.881(18)
Si(5')-C(6')	1.902(19)
Si(5')-C(2')	1.925(18)
C(1')-H(1'1)	0.9800
C(1')-H(1'2)	0.9800
C(1')-H(1'3)	0.9800
C(2')-C(5')	1.52(2)
C(2')-C(3')	1.52(2)
C(2')-C(4')	1.54(2)
C(3')-H(3'1)	0.9800
C(3')-H(3'2)	0.9800
C(3')-H(3'3)	0.9800
C(4')-H(4'1)	0.9800
C(4')-H(4'2)	0.9800
C(4')-H(4'3)	0.9800
C(5')-H(5'1)	0.9800
C(5')-H(5'2)	0.9800
C(5')-H(5'3)	0.9800
C(6')-C(9')	1.52(2)
C(6')-C(8')	1.54(2)
C(6')-C(7')	1.55(2)

C(7')-H(7'1)	0.9800
C(7')-H(7'2)	0.9800
C(7')-H(7'3)	0.9800
C(8')-H(8'1)	0.9800
C(8')-H(8'2)	0.9800
C(8')-H(8'3)	0.9800
C(9')-H(9'1)	0.9800
C(9')-H(9'2)	0.9800
C(9')-H(9'3)	0.9800
Si(6)-C(10)	1.891(8)
Si(6)-C(11)	1.916(8)
Si(6)-C(15)	1.918(8)
Si(7)-C(19)	1.882(8)
Si(7)-C(24)	1.907(7)
Si(7)-C(20)	1.921(8)
Si(8)-C(28)	1.880(8)
Si(8)-C(29)	1.916(8)
Si(8)-C(33)	1.920(8)
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-C(14)	1.519(13)
C(11)-C(13)	1.529(12)
C(11)-C(12)	1.541(13)
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800

C(15)-C(18)	1.515(12)
C(15)-C(16)	1.540(12)
C(15)-C(17)	1.544(12)
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-C(22)	1.530(11)
C(20)-C(23)	1.537(11)
C(20)-C(21)	1.544(12)
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
C(24)-C(27)	1.537(11)
C(24)-C(25)	1.542(11)
C(24)-C(26)	1.557(11)
C(25)-H(25A)	0.9800
C(25)-H(25B)	0.9800
C(25)-H(25C)	0.9800

C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800
C(29)-C(30)	1.536(11)
C(29)-C(32)	1.543(11)
C(29)-C(31)	1.550(11)
C(30)-H(30A)	0.9800
C(30)-H(30B)	0.9800
C(30)-H(30C)	0.9800
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800
C(31)-H(31C)	0.9800
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(33)-C(35)	1.506(12)
C(33)-C(36)	1.530(11)
C(33)-C(34)	1.556(11)
C(34)-H(34A)	0.9800
C(34)-H(34B)	0.9800
C(34)-H(34C)	0.9800
C(35)-H(35A)	0.9800
C(35)-H(35B)	0.9800
C(35)-H(35C)	0.9800
C(36)-H(36A)	0.9800
C(36)-H(36B)	0.9800
C(36)-H(36C)	0.9800

Table S4. Bond angles [°] for **4**.

Si(2)-P(1)-Si(3)	80.05(9)
Si(2)-P(1)-Si(1)	60.09(9)
Si(3)-P(1)-Si(1)	60.04(9)
Si(2)-Si(1)-Si(3)	79.26(10)
Si(2)-Si(1)-P(1)	59.12(9)
Si(3)-Si(1)-P(1)	59.39(9)
Si(2)-Si(1)-Si(5')	130.0(3)
Si(3)-Si(1)-Si(5')	150.6(3)
P(1)-Si(1)-Si(5')	132.9(2)
Si(2)-Si(1)-Si(5)	145.71(13)
Si(3)-Si(1)-Si(5)	132.99(14)
P(1)-Si(1)-Si(5)	121.56(13)
P(1)-Si(2)-Si(1)	60.79(9)
P(1)-Si(2)-Si(4)	94.12(10)
Si(1)-Si(2)-Si(4)	92.06(10)
P(1)-Si(2)-Si(6)	117.51(11)
Si(1)-Si(2)-Si(6)	127.37(11)
Si(4)-Si(2)-Si(6)	137.40(11)
P(1)-Si(3)-Si(1)	60.57(9)
P(1)-Si(3)-Si(4)	93.66(10)
Si(1)-Si(3)-Si(4)	91.81(10)
P(1)-Si(3)-Si(7)	111.77(11)
Si(1)-Si(3)-Si(7)	127.66(11)
Si(4)-Si(3)-Si(7)	139.64(11)
Cl(1)-Si(4)-Si(2)	112.34(11)
Cl(1)-Si(4)-Si(3)	109.75(11)
Si(2)-Si(4)-Si(3)	77.35(9)
Cl(1)-Si(4)-Si(8)	109.03(11)
Si(2)-Si(4)-Si(8)	121.64(11)
Si(3)-Si(4)-Si(8)	123.50(11)
C(1)-Si(5)-C(6)	106.8(5)

C(1)-Si(5)-C(2)	108.5(6)
C(6)-Si(5)-C(2)	116.7(5)
C(1)-Si(5)-Si(1)	108.1(4)
C(6)-Si(5)-Si(1)	112.7(3)
C(2)-Si(5)-Si(1)	103.8(4)
Si(5)-C(1)-H(1A)	109.5
Si(5)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
Si(5)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
C(5)-C(2)-C(3)	108.7(10)
C(5)-C(2)-C(4)	108.3(10)
C(3)-C(2)-C(4)	109.1(11)
C(5)-C(2)-Si(5)	108.5(8)
C(3)-C(2)-Si(5)	111.1(8)
C(4)-C(2)-Si(5)	111.1(8)
C(2)-C(3)-H(3A)	109.5
C(2)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	109.5
C(2)-C(3)-H(3C)	109.5
H(3A)-C(3)-H(3C)	109.5
H(3B)-C(3)-H(3C)	109.5
C(2)-C(4)-H(4A)	109.5
C(2)-C(4)-H(4B)	109.5
H(4A)-C(4)-H(4B)	109.5
C(2)-C(4)-H(4C)	109.5
H(4A)-C(4)-H(4C)	109.5
H(4B)-C(4)-H(4C)	109.5
C(2)-C(5)-H(5A)	109.5
C(2)-C(5)-H(5B)	109.5
H(5A)-C(5)-H(5B)	109.5
C(2)-C(5)-H(5C)	109.5

H(5A)-C(5)-H(5C)	109.5
H(5B)-C(5)-H(5C)	109.5
C(9)-C(6)-C(8)	108.3(10)
C(9)-C(6)-C(7)	109.2(9)
C(8)-C(6)-C(7)	108.8(10)
C(9)-C(6)-Si(5)	112.1(7)
C(8)-C(6)-Si(5)	109.2(8)
C(7)-C(6)-Si(5)	109.3(8)
C(6)-C(7)-H(7A)	109.5
C(6)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(6)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
C(6)-C(8)-H(8A)	109.5
C(6)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(6)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(6)-C(9)-H(9A)	109.5
C(6)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(6)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(1')-Si(5')-C(6')	108.3(12)
C(1')-Si(5')-C(2')	107.0(11)
C(6')-Si(5')-C(2')	117.8(11)
C(1')-Si(5')-Si(1)	108.3(10)
C(6')-Si(5')-Si(1)	111.5(9)
C(2')-Si(5')-Si(1)	103.5(8)
Si(5')-C(1')-H(1'1)	109.5

Si(5')-C(1')-H(1'2)	109.5
H(1'1)-C(1')-H(1'2)	109.5
Si(5')-C(1')-H(1'3)	109.5
H(1'1)-C(1')-H(1'3)	109.5
H(1'2)-C(1')-H(1'3)	109.5
C(5')-C(2')-C(3')	108(2)
C(5')-C(2')-C(4')	107.9(19)
C(3')-C(2')-C(4')	109(2)
C(5')-C(2')-Si(5')	109.5(16)
C(3')-C(2')-Si(5')	109.7(18)
C(4')-C(2')-Si(5')	111.9(16)
C(2')-C(3')-H(3'1)	109.5
C(2')-C(3')-H(3'2)	109.5
H(3'1)-C(3')-H(3'2)	109.5
C(2')-C(3')-H(3'3)	109.5
H(3'1)-C(3')-H(3'3)	109.5
H(3'2)-C(3')-H(3'3)	109.5
C(2')-C(4')-H(4'1)	109.5
C(2')-C(4')-H(4'2)	109.5
H(4'1)-C(4')-H(4'2)	109.5
C(2')-C(4')-H(4'3)	109.5
H(4'1)-C(4')-H(4'3)	109.5
H(4'2)-C(4')-H(4'3)	109.5
C(2')-C(5')-H(5'1)	109.5
C(2')-C(5')-H(5'2)	109.5
H(5'1)-C(5')-H(5'2)	109.5
C(2')-C(5')-H(5'3)	109.5
H(5'1)-C(5')-H(5'3)	109.5
H(5'2)-C(5')-H(5'3)	109.5
C(9')-C(6')-C(8')	108(2)
C(9')-C(6')-C(7')	108.2(19)
C(8')-C(6')-C(7')	108(2)
C(9')-C(6')-Si(5')	111.8(16)

C(8')-C(6')-Si(5')	112.1(17)
C(7')-C(6')-Si(5')	108.0(16)
C(6')-C(7')-H(7'1)	109.5
C(6')-C(7')-H(7'2)	109.5
H(7'1)-C(7')-H(7'2)	109.5
C(6')-C(7')-H(7'3)	109.5
H(7'1)-C(7')-H(7'3)	109.5
H(7'2)-C(7')-H(7'3)	109.5
C(6')-C(8')-H(8'1)	109.5
C(6')-C(8')-H(8'2)	109.5
H(8'1)-C(8')-H(8'2)	109.5
C(6')-C(8')-H(8'3)	109.5
H(8'1)-C(8')-H(8'3)	109.5
H(8'2)-C(8')-H(8'3)	109.5
C(6')-C(9')-H(9'1)	109.5
C(6')-C(9')-H(9'2)	109.5
H(9'1)-C(9')-H(9'2)	109.5
C(6')-C(9')-H(9'3)	109.5
H(9'1)-C(9')-H(9'3)	109.5
H(9'2)-C(9')-H(9'3)	109.5
C(10)-Si(6)-C(11)	108.8(4)
C(10)-Si(6)-C(15)	107.3(4)
C(11)-Si(6)-C(15)	116.2(4)
C(10)-Si(6)-Si(2)	107.6(3)
C(11)-Si(6)-Si(2)	108.9(3)
C(15)-Si(6)-Si(2)	107.7(3)
C(19)-Si(7)-C(24)	107.5(4)
C(19)-Si(7)-C(20)	107.9(4)
C(24)-Si(7)-C(20)	115.1(3)
C(19)-Si(7)-Si(3)	102.3(3)
C(24)-Si(7)-Si(3)	114.6(3)
C(20)-Si(7)-Si(3)	108.3(3)
C(28)-Si(8)-C(29)	108.1(4)

C(28)-Si(8)-C(33)	109.4(4)
C(29)-Si(8)-C(33)	114.9(3)
C(28)-Si(8)-Si(4)	104.8(3)
C(29)-Si(8)-Si(4)	112.2(2)
C(33)-Si(8)-Si(4)	107.0(3)
Si(6)-C(10)-H(10A)	109.5
Si(6)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
Si(6)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(14)-C(11)-C(13)	109.9(8)
C(14)-C(11)-C(12)	109.2(8)
C(13)-C(11)-C(12)	107.8(7)
C(14)-C(11)-Si(6)	110.9(6)
C(13)-C(11)-Si(6)	110.8(6)
C(12)-C(11)-Si(6)	108.2(6)
C(11)-C(12)-H(12A)	109.5
C(11)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(11)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(11)-C(13)-H(13A)	109.5
C(11)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(11)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(11)-C(14)-H(14A)	109.5
C(11)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(11)-C(14)-H(14C)	109.5

H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(18)-C(15)-C(16)	108.8(7)
C(18)-C(15)-C(17)	108.2(7)
C(16)-C(15)-C(17)	108.9(7)
C(18)-C(15)-Si(6)	107.5(6)
C(16)-C(15)-Si(6)	111.9(6)
C(17)-C(15)-Si(6)	111.4(6)
C(15)-C(16)-H(16A)	109.5
C(15)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(15)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(15)-C(17)-H(17A)	109.5
C(15)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(15)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(15)-C(18)-H(18A)	109.5
C(15)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(15)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
Si(7)-C(19)-H(19A)	109.5
Si(7)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
Si(7)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(22)-C(20)-C(23)	109.4(7)

C(22)-C(20)-C(21)	108.3(7)
C(23)-C(20)-C(21)	108.3(7)
C(22)-C(20)-Si(7)	112.2(6)
C(23)-C(20)-Si(7)	110.9(5)
C(21)-C(20)-Si(7)	107.5(6)
C(20)-C(21)-H(21A)	109.5
C(20)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(20)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(20)-C(22)-H(22A)	109.5
C(20)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(20)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(20)-C(23)-H(23A)	109.5
C(20)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(20)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(27)-C(24)-C(25)	108.3(7)
C(27)-C(24)-C(26)	106.8(6)
C(25)-C(24)-C(26)	108.8(6)
C(27)-C(24)-Si(7)	109.8(5)
C(25)-C(24)-Si(7)	113.4(5)
C(26)-C(24)-Si(7)	109.4(5)
C(24)-C(25)-H(25A)	109.5
C(24)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
C(24)-C(25)-H(25C)	109.5

H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
C(24)-C(26)-H(26A)	109.5
C(24)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(24)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
C(24)-C(27)-H(27A)	109.5
C(24)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(24)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
Si(8)-C(28)-H(28A)	109.5
Si(8)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
Si(8)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(30)-C(29)-C(32)	108.7(7)
C(30)-C(29)-C(31)	107.4(7)
C(32)-C(29)-C(31)	108.4(6)
C(30)-C(29)-Si(8)	110.4(5)
C(32)-C(29)-Si(8)	112.9(5)
C(31)-C(29)-Si(8)	108.9(5)
C(29)-C(30)-H(30A)	109.5
C(29)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
C(29)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5
C(29)-C(31)-H(31A)	109.5

C(29)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(29)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(29)-C(32)-H(32A)	109.5
C(29)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(29)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(35)-C(33)-C(36)	109.7(7)
C(35)-C(33)-C(34)	108.7(7)
C(36)-C(33)-C(34)	107.3(6)
C(35)-C(33)-Si(8)	111.7(5)
C(36)-C(33)-Si(8)	107.3(5)
C(34)-C(33)-Si(8)	112.1(5)
C(33)-C(34)-H(34A)	109.5
C(33)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
C(33)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
C(33)-C(35)-H(35A)	109.5
C(33)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5
C(33)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5
C(33)-C(36)-H(36A)	109.5
C(33)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36B)	109.5
C(33)-C(36)-H(36C)	109.5

H(36A)-C(36)-H(36C)	109.5
H(36B)-C(36)-H(36C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S5. Anisotropic atomic displacement parameters ($Å^2$) for **4**. The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cl(1)	30(1)	21(1)	19(1)	-5(1)	0(1)	0(1)
P(1)	20(1)	19(1)	20(1)	4(1)	5(1)	1(1)
Si(1)	18(1)	18(1)	26(1)	-8(1)	7(1)	-5(1)
Si(2)	16(1)	14(1)	16(1)	-4(1)	4(1)	-4(1)
Si(3)	13(1)	9(1)	17(1)	0(1)	-1(1)	-1(1)
Si(4)	15(1)	14(1)	13(1)	0(1)	0(1)	-2(1)
Si(5)	19(2)	13(2)	16(2)	0(1)	-2(1)	-1(1)
C(1)	26(5)	20(6)	34(6)	3(5)	0(5)	6(5)
C(2)	36(5)	19(5)	15(4)	-5(4)	3(4)	2(4)
C(3)	53(8)	28(5)	26(6)	-6(5)	3(6)	4(5)
C(4)	51(6)	33(6)	18(5)	0(5)	-8(5)	6(5)
C(5)	52(6)	35(6)	20(5)	1(5)	7(5)	-8(5)
C(6)	23(4)	16(4)	20(5)	1(4)	-3(4)	-5(4)
C(7)	40(7)	19(5)	41(7)	2(5)	4(6)	-3(5)
C(8)	27(7)	36(8)	24(6)	0(5)	7(5)	-9(6)
C(9)	22(5)	38(7)	37(6)	-1(6)	0(5)	-5(5)
Si(5')	19(5)	10(4)	18(4)	2(3)	-2(4)	-2(3)
C(1')	19(8)	12(13)	50(17)	3(13)	-3(9)	5(11)
C(2')	26(8)	12(7)	24(8)	6(6)	-4(7)	-2(7)
C(3')	48(15)	9(15)	30(12)	9(10)	9(12)	-8(14)
C(4')	38(16)	14(8)	40(16)	1(9)	0(13)	-3(11)
C(5')	27(10)	17(13)	48(17)	-3(14)	-14(10)	9(11)

C(6')	37(8)	21(9)	17(8)	-4(7)	1(8)	-3(9)
C(7')	41(14)	21(9)	7(10)	-5(8)	-2(11)	-8(10)
C(8')	37(9)	28(13)	24(13)	-8(12)	9(9)	-2(10)
C(9')	44(13)	25(11)	21(11)	-8(10)	10(11)	-12(12)
Si(6)	12(1)	18(1)	24(1)	-4(1)	5(1)	-1(1)
Si(7)	14(1)	16(1)	21(1)	-4(1)	-2(1)	-1(1)
Si(8)	16(1)	14(1)	13(1)	1(1)	1(1)	0(1)
C(10)	25(4)	22(4)	43(5)	-3(4)	11(4)	-4(4)
C(11)	19(4)	47(6)	28(5)	-2(4)	-5(4)	-5(4)
C(12)	25(5)	79(8)	26(5)	-17(5)	4(4)	-22(5)
C(13)	20(5)	54(6)	42(5)	-10(5)	-1(4)	-8(4)
C(14)	49(6)	53(7)	55(7)	28(5)	-19(5)	-6(5)
C(15)	25(4)	21(4)	29(5)	-4(4)	4(4)	3(3)
C(16)	30(5)	51(6)	51(6)	-26(5)	12(4)	0(5)
C(17)	44(6)	25(5)	42(5)	-12(4)	7(4)	2(4)
C(18)	47(6)	49(6)	19(4)	-7(4)	5(4)	1(5)
C(19)	23(4)	21(4)	27(4)	2(3)	-6(3)	-4(3)
C(20)	23(4)	19(4)	26(4)	1(3)	1(3)	3(3)
C(21)	47(6)	40(6)	27(5)	-14(4)	1(4)	-3(5)
C(22)	36(5)	19(4)	45(6)	-2(4)	-6(4)	-4(4)
C(23)	32(5)	25(5)	48(6)	-10(4)	-13(4)	-5(4)
C(24)	11(4)	24(4)	26(4)	0(3)	7(3)	2(3)
C(25)	29(5)	37(5)	36(5)	2(4)	17(4)	2(4)
C(26)	21(4)	32(5)	33(5)	-2(4)	5(4)	4(4)
C(27)	21(4)	36(5)	29(5)	-5(4)	2(4)	1(4)
C(28)	32(5)	22(4)	17(4)	-2(3)	0(3)	-1(4)
C(29)	26(4)	17(4)	18(4)	2(3)	-1(3)	0(3)
C(30)	29(5)	36(5)	31(5)	4(4)	8(4)	7(4)
C(31)	35(5)	29(5)	24(4)	7(4)	-4(4)	8(4)
C(32)	34(5)	16(4)	26(4)	0(3)	0(4)	1(4)
C(33)	24(4)	19(4)	26(4)	2(3)	4(3)	3(3)
C(34)	24(4)	27(5)	27(4)	8(4)	7(4)	-2(4)
C(35)	21(4)	44(5)	25(5)	12(4)	3(4)	4(4)

C(36)	27(4)	24(4)	24(4)	3(3)	6(3)	4(4)

Table S6. Hydrogen atomic coordinates and isotropic atomic displacement parameters (Å^2) for **4**.

	x	y	z	U(eq)
H(1A)	1161	5444	1337	40
H(1B)	776	4626	1456	40
H(1C)	1147	4845	669	40
H(3A)	2214	5320	3510	54
H(3B)	1867	5627	2701	54
H(3C)	2876	5596	2921	54
H(4A)	3667	4517	2972	52
H(4B)	3296	3726	2679	52
H(4C)	3109	4017	3503	52
H(5A)	1643	4060	3450	53
H(5B)	1584	3623	2664	53
H(5C)	1066	4388	2748	53
H(7A)	3337	6341	1046	50
H(7B)	2769	6125	1728	50
H(7C)	2349	6121	882	50
H(8A)	3592	5272	54	43
H(8B)	2577	5141	23	43
H(8C)	3219	4459	217	43
H(9A)	4159	4538	1515	49
H(9B)	4080	5297	1982	49
H(9C)	4448	5315	1165	49
H(1'1)	4129	5003	2176	41
H(1'2)	4212	4491	1446	41
H(1'3)	4207	4114	2261	41
H(3'1)	2660	5405	-14	43

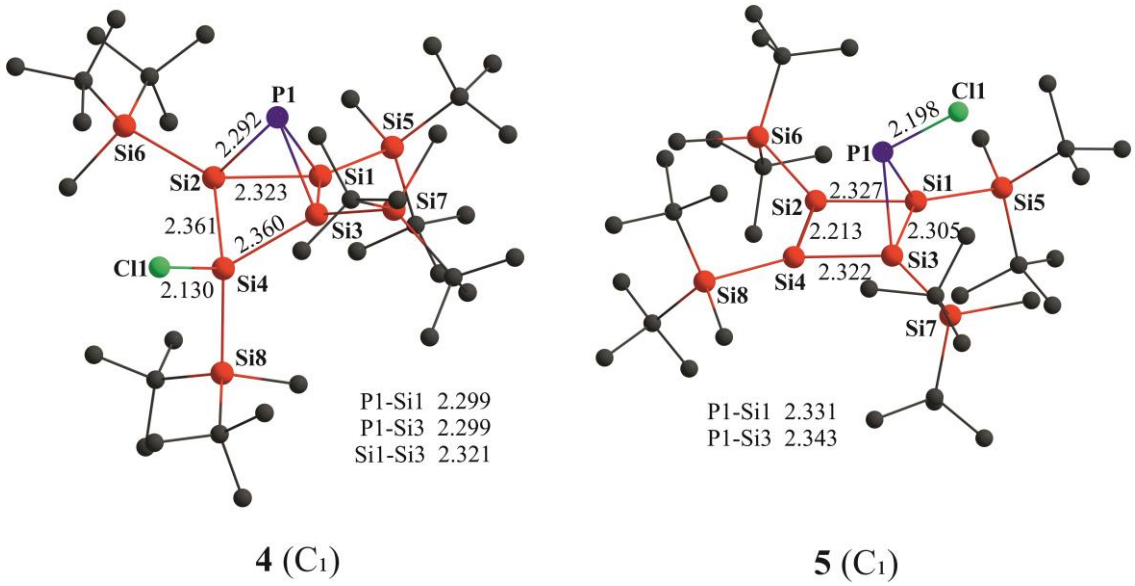
H(3'2)	3029	4611	270	43
H(3'3)	3497	5365	556	43
H(4'1)	2415	6324	993	46
H(4'2)	2885	6024	1761	46
H(4'3)	1859	6046	1662	46
H(5'1)	1416	4983	242	47
H(5'2)	1070	5355	982	47
H(5'3)	1306	4484	976	47
H(7'1)	2055	3681	3580	35
H(7'2)	3040	3668	3385	35
H(7'3)	2317	3329	2802	35
H(8'1)	1063	4340	3048	44
H(8'2)	1141	4676	2222	44
H(8'3)	1297	5204	2944	44
H(9'1)	2912	5527	2995	44
H(9'2)	3370	4868	3479	44
H(9'3)	2477	5202	3716	44
H(10A)	4982	3811	605	44
H(10B)	4459	3577	-164	44
H(10C)	5476	3462	-71	44
H(12A)	4538	2763	2193	65
H(12B)	5107	3425	1883	65
H(12C)	5492	2901	2553	65
H(13A)	6722	2611	1899	59
H(13B)	6420	3084	1165	59
H(13C)	6664	2219	1089	59
H(14A)	5688	1238	1453	80
H(14B)	4831	1439	1853	80
H(14C)	5748	1549	2298	80
H(16A)	6060	1443	-776	65
H(16B)	6239	1399	119	65
H(16C)	6242	2192	-298	65
H(17A)	4023	1054	55	55

H(17B)	4944	776	391	55
H(17C)	4678	680	-488	55
H(18A)	4613	1698	-1327	57
H(18B)	4864	2534	-1076	57
H(18C)	3972	2182	-859	57
H(19A)	498	3454	-454	36
H(19B)	60	3902	197	36
H(19C)	-525	3519	-469	36
H(21A)	752	1810	-782	57
H(21B)	24	2321	-1200	57
H(21C)	-14	1430	-1290	57
H(22A)	-560	982	567	51
H(22B)	367	946	238	51
H(22C)	-454	629	-248	51
H(23A)	-1502	1495	-899	54
H(23B)	-1448	2373	-729	54
H(23C)	-1702	1804	-86	54
H(25A)	-1389	2173	2032	50
H(25B)	-566	1740	1766	50
H(25C)	-1434	1757	1234	50
H(26A)	-1925	3332	1329	42
H(26B)	-1896	2917	535	42
H(26C)	-1381	3682	685	42
H(27A)	-93	3713	1601	43
H(27B)	197	2977	2063	43
H(27C)	-688	3380	2217	43
H(28A)	3068	1462	3525	35
H(28B)	2931	2074	2872	35
H(28C)	3745	1529	2893	35
H(30A)	4279	432	2172	48
H(30B)	3751	116	1437	48
H(30C)	4253	-448	2009	48
H(31A)	3750	-705	3259	44

H(31B)	2928	-284	3544	44
H(31C)	3796	170	3447	44
H(32A)	2926	-1172	2120	38
H(32B)	2384	-613	1570	38
H(32C)	2079	-784	2393	38
H(34A)	1729	588	3857	39
H(34B)	1497	-159	3391	39
H(34C)	747	376	3644	39
H(35A)	171	438	2318	45
H(35B)	937	-67	2048	45
H(35C)	745	733	1669	45
H(36A)	1103	1910	2423	37
H(36B)	1427	1821	3291	37
H(36C)	465	1596	3014	37

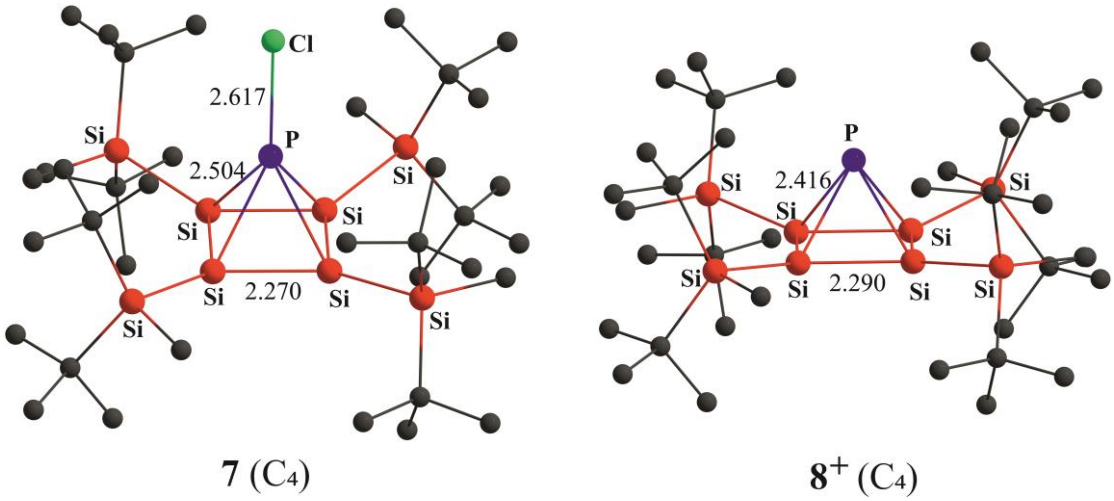
2. Computations.

Geometry optimization, frequency analysis, wave function stability and all related calculations were performed using the Gaussian 16 program[S6] at the TPSSh/Def2TZVP level of theory. The views of the optimized geometries were generated using Chemcraft 1.8 program.[S7]



4 (C_1) **5** (C_1)

Figure S2. Optimized geometries (bond lengths, in Å) of **4** and **5**. Hydrogens atoms are omitted.



7 (C_4) **8**$^+$ (C_4)

Figure S3. Optimized geometries (bond lengths, in Å) of **7** and **8**$^+$. Hydrogens atoms are omitted.

Cartesian coordinates: NI – number of imaginary frequencies, ω_1 – lowest harmonic frequency (cm^{-1}), E – total electronic energy (a.u.)

Compound 4: NI = 0, ω_1 = 15, E = –4541.0356898

C,0,1.1232572363,0.1630886296,11.9722138821
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C,0,3.1772693168,1.1320876085,14.0552611798
C,0,4.4411560511,1.9587365783,14.3408164305
H,0,5.3497521247,1.4490836482,14.0143215258
H,0,4.4072820521,2.9320760147,13.8447989114
H,0,4.530372089,2.1367940709,15.4198011092
C,0,1.9647878299,1.886290432,14.6374914634
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H,0,1.798177837,2.8429443614,14.1319751182
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H,0,5.7782004848,2.6913792073,8.3079064214
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C,0,6.4622377444,7.3221820287,8.8232340431
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H,0,7.0872405002,7.6647154694,9.650698295
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C,0,5.9210543039,5.5410225374,7.1668246681
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H,0,6.183393255,4.5734905884,6.7310442401
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Compound 5: NI = 0, ω_1 = 12, E = – 4540.9657445

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Si,0,1.4385779613,3.7339181336,-0.0938362442

Si,0,3.6877290599,-1.4750479087,0.3271008502
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C,0,-2.3796367622,-4.035127452,1.3321913068
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C,0,-4.9562659777,-0.0231441519,-0.2536407539
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C,0,2.1974648297,3.7270864843,-1.8750478825
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C,0,-5.5918325026,2.6711598336,-1.9859705018
H,0,-6.0213978227,3.2591343163,-1.1722832031
H,0,-5.7711508931,3.2195593723,-2.9194003752
H,0,-6.1418226341,1.7289781397,-2.0499477866
C,0,-3.3665239288,3.8029902745,-1.814607886
H,0,-3.720199251,4.4562412483,-1.0130849854
H,0,-2.2861666479,3.6847049952,-1.7045823706
H,0,-3.5486960248,4.3190139329,-2.7658311088
C,0,-3.5782169598,1.6400560254,-3.0291945208
H,0,-2.4937535447,1.4950572151,-3.0043885625
H,0,-4.0460267201,0.653298882,-3.0931993873
H,0,-3.8228803507,2.1803442546,-3.9524811894
Cl,0,1.6721899744,0.8765550965,3.736159326

Compound 7: NI = 2, $\omega_1 = i55$, E = – 4540.9509354

Si,0,0.8411824925,1.3672822784,0.469447583
Si,0,1.3672822784,-0.8411824925,0.469447583
Si,0,-0.8411824925,-1.3672822784,0.469447583
Si,0,-1.3672822784,0.8411824925,0.469447583
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Si,0,-3.3641115066,2.138558493,0.0901662402
Si,0,-2.138558493,-3.3641115066,0.0901662402
Si,0,3.3641115066,-2.138558493,0.0901662402
P,0,0.,0.,-1.4518227307
C,0,3.9621545832,2.8856307896,0.1834385023
C,0,1.806996813,4.4912466566,1.6292952708
C,0,1.8069568888,4.1090398926,-1.654896124
C,0,-4.1090398926,1.8069568888,-1.654896124
C,0,-4.4912466566,1.806996813,1.6292952708
C,0,-2.8856307896,3.9621545832,0.1834385023
C,0,-3.9621545832,-2.8856307896,0.1834385023
C,0,-1.806996813,-4.4912466566,1.6292952708
C,0,-1.8069568888,-4.1090398926,-1.654896124
C,0,4.1090398926,-1.8069568888,-1.654896124
C,0,4.4912466566,-1.806996813,1.6292952708
C,0,2.8856307896,-3.9621545832,0.1834385023
H,0,-3.7332524092,4.5737372867,-0.143025544

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H,0,3.7332524092,-4.5737372867,-0.143025544
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H,0,-4.2622529402,-2.6378924222,1.2039092942
H,0,2.6378924222,-4.2622529402,1.2039092942
H,0,4.2622529402,2.6378924222,1.2039092942
C,0,0.3133845969,4.2741089262,-1.9669253271
H,0,-0.2147311479,3.3194928556,-1.9039210598
H,0,-0.1683225709,4.9912559819,-1.2979139105
H,0,0.1908626364,4.6431002838,-2.9919742187
C,0,2.4941888069,5.4830130058,-1.7846400271
H,0,3.5640641079,5.4386075079,-1.5608257313
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C,0,2.409585997,3.1597293503,-2.7093634996
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H,0,1.9254366289,2.1796392039,-2.7098253132
C,0,2.9299983062,5.5398467908,1.7669992717
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H,0,2.7448309328,6.1502439751,2.6596612847
H,0,3.911539934,5.0747937269,1.8869128891
C,0,1.824579732,3.6162221166,2.897900411
H,0,0.9996805104,2.8968494685,2.9092204807
H,0,2.7593098563,3.0576386333,3.0027480429
H,0,1.7213683626,4.2535113127,3.7851646303
C,0,0.4566075843,5.217302357,1.5646661234
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H,0,4.2535113127,-1.7213683626,3.7851646303
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H,0,0.1683225709,-4.9912559819,-1.2979139105
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H,0,-0.4052675649,-5.9176424389,0.7274233792
H,0,0.373568133,-4.5143049671,1.470272043
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C,0,-2.9299983062,-5.5398467908,1.7669992717
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C,0,-1.824579732,-3.6162221166,2.897900411
H,0,-2.7593098563,-3.0576386333,3.0027480429
H,0,-1.7213683626,-4.2535113127,3.7851646303
H,0,-0.9996805104,-2.8968494685,2.9092204807
C,0,-4.2741089262,0.3133845969,-1.9669253271
H,0,-3.3194928556,-0.2147311479,-1.9039210598
H,0,-4.9912559819,-0.1683225709,-1.2979139105
H,0,-4.6431002838,0.1908626364,-2.9919742187
C,0,-3.1597293503,2.409585997,-2.7093634996
H,0,-3.5882883938,2.2536013492,-3.7061977652
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H,0,-2.1796392039,1.9254366289,-2.7098253132
C,0,-5.4830130058,2.4941888069,-1.7846400271
H,0,-5.83821575,2.3918764554,-2.8171542179
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C,0,-5.5398467908,2.9299983062,1.7669992717
H,0,-6.2160367699,2.9774841038,0.911002594
H,0,-6.1502439751,2.7448309328,2.6596612847
H,0,-5.0747937269,3.911539934,1.8869128891
C,0,-5.217302357,0.4566075843,1.5646661234

H,0,-5.9176424389,0.4052675649,0.7274233792
H,0,-4.5143049671,-0.373568133,1.470272043
H,0,-5.7931619035,0.3002845723,2.485571178
C,0,-3.6162221166,1.824579732,2.897900411
H,0,-2.8968494685,0.9996805104,2.9092204807
H,0,-3.0576386333,2.7593098563,3.0027480429
H,0,-4.2535113127,1.7213683626,3.7851646303
Cl,0,0.,0.,-4.0683263818

Compound 8^+: NI = 0, ω_1 = 14, E = – 4080.5520128

Si,0,-0.6033116595,-1.5023709668,-0.5478033567
Si,0,1.5023709668,-0.6033116595,-0.5478033567
Si,0,0.6033116595,1.5023709668,-0.5478033567
Si,0,-1.5023709668,0.6033116595,-0.5478033567
Si,0,-1.4662386871,-3.751545258,-0.2047409169
Si,0,-3.751545258,1.4662386871,-0.2047409169
Si,0,1.4662386871,3.751545258,-0.2047409169
Si,0,3.751545258,-1.4662386871,-0.2047409169
P,0,0.,0.,1.2460527216
C,0,-0.0022595781,-4.9333849208,-0.2796218416
C,0,-2.5282022644,-4.0691949699,-1.7814061446
C,0,-2.2910383847,-3.9090399123,1.5239129532
C,0,-3.9090399123,2.2910383847,1.5239129532
C,0,-4.0691949699,2.5282022644,-1.7814061446
C,0,-4.9333849208,0.0022595781,-0.2796218416
C,0,0.0022595781,4.9333849208,-0.2796218416
C,0,2.5282022644,4.0691949699,-1.7814061446
C,0,2.2910383847,3.9090399123,1.5239129532
C,0,3.9090399123,-2.2910383847,1.5239129532
C,0,4.0691949699,-2.5282022644,-1.7814061446
C,0,4.9333849208,-0.0022595781,-0.2796218416
H,0,-5.9300792115,0.3417159907,0.021019644
H,0,0.3417159907,5.9300792115,0.021019644
H,0,5.9300792115,-0.3417159907,0.021019644
H,0,-0.3417159907,-5.9300792115,0.021019644
H,0,-4.6469066614,-0.8087956107,0.3882338561
H,0,-0.8087956107,4.6469066614,0.3882338561
H,0,4.6469066614,0.8087956107,0.3882338561
H,0,0.8087956107,-4.6469066614,0.3882338561
H,0,-5.0180610242,-0.3993266273,-1.2911681741
H,0,-0.3993266273,5.0180610242,-1.2911681741
H,0,5.0180610242,0.3993266273,-1.2911681741
H,0,0.3993266273,-5.0180610242,-1.2911681741
C,0,-3.3084267428,-2.7977236439,1.8146551825
H,0,-2.8488929752,-1.8066988084,1.7539041973
H,0,-4.1573861487,-2.8311064097,1.1290267599
H,0,-3.7015917693,-2.9143308034,2.8311568381

C,0,-3.0010227354,-5.2742004982,1.6361604459
H,0,-2.3309292464,-6.1125348721,1.4275078991
H,0,-3.37362484,-5.4023239297,2.6589303857
H,0,-3.8596058897,-5.3459928385,0.9644964285
C,0,-1.1845808208,-3.8423331096,2.5945071353
H,0,-1.6378202233,-3.9318307738,3.5883047466
H,0,-0.4585296351,-4.6517365547,2.4901614625
H,0,-0.6462662791,-2.8900663475,2.5640374134
C,0,-2.7182799885,-5.5890954198,-1.9732439592
H,0,-3.2622293422,-6.0490332137,-1.1457006039
H,0,-3.2994412258,-5.7640269064,-2.8859540619
H,0,-1.7659310473,-6.1119069828,-2.0874624746
C,0,-1.7634307477,-3.5269654028,-3.0053231135
H,0,-1.6708540622,-2.4350123561,-2.9803743885
H,0,-0.7590215203,-3.9514985439,-3.0911947788
H,0,-2.3061605967,-3.7845422757,-3.9221998255
C,0,-3.9068110427,-3.3968122859,-1.7318447638
H,0,-4.5324603233,-3.7984003028,-0.9313718847
H,0,-3.8244627175,-2.316782473,-1.5905489172
H,0,-4.4350421013,-3.5674387287,-2.6771496738
C,0,3.8423331096,-1.1845808208,2.5945071353
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C,0,2.7977236439,-3.3084267428,1.8146551825
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C,0,3.5269654028,-1.7634307477,-3.0053231135
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H,0,3.7845422757,-2.3061605967,-3.9221998255
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C,0,3.3084267428,2.7977236439,1.8146551825
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H,0,4.1573861487,2.8311064097,1.1290267599
H,0,3.7015917693,2.9143308034,2.8311568381
C,0,1.1845808208,3.8423331096,2.5945071353
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H,0,2.3309292464,6.1125348721,1.4275078991
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H,0,4.5324603233,3.7984003028,-0.9313718847
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H,0,4.4350421013,3.5674387287,-2.6771496738
C,0,2.7182799885,5.5890954198,-1.9732439592
H,0,3.2622293422,6.0490332137,-1.1457006039
H,0,3.2994412258,5.7640269064,-2.8859540619
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H,0,-3.9318307738,1.6378202233,3.5883047466
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H,0,-2.8900663475,0.6462662791,2.5640374134
C,0,-5.2742004982,3.0010227354,1.6361604459
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H,0,-3.5674387287,4.4350421013,-2.6771496738
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H,0,-2.4350123561,1.6708540622,-2.9803743885
H,0,-3.9514985439,0.7590215203,-3.0911947788
H,0,-3.7845422757,2.3061605967,-3.9221998255

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