Electronic Supplementary Material (ESI) for Chemical Communications

ELECTRONIC SUPPLEMENTARY INFORMATION

Hydrolytically Stable Octahedral Silicon Complexes as Bioactive Scaffolds: Application to the Design of DNA Intercalators

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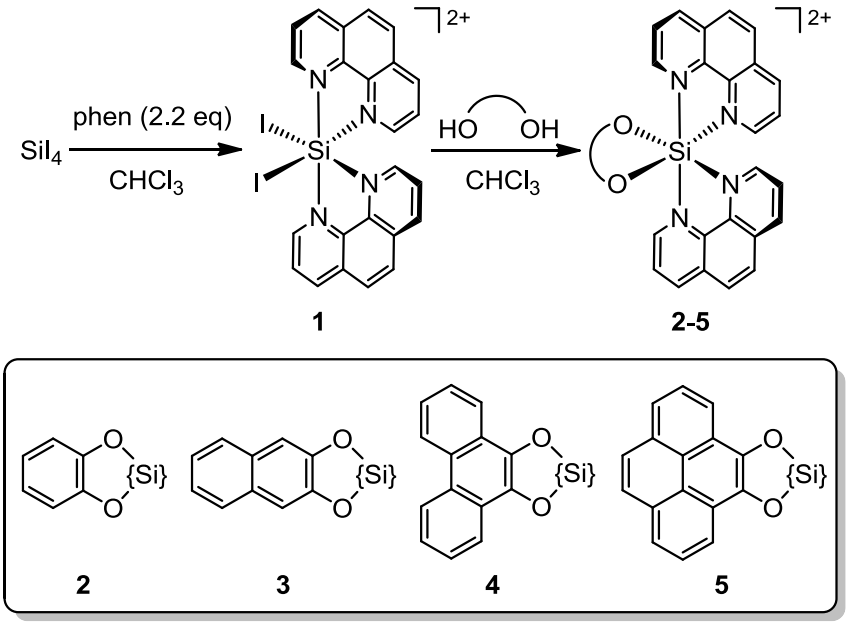
Content:

I.) Synthesis of Octahedral Silicon Complexes

General Methods:

All reactions were carried out under a nitrogen atmosphere. Chloroform was distilled under nitrogen from calcium hydride. Phenanthrene-9,10-diol[1] and pyrene-4,5-diol[2] were prepared according to published procedures. 1,10-Phenanthroline was sublimated before use. SiI_4 was purchase from Strem and Alfa. All other reagents were purchased from Acros, Aldrich, Strem or Alfa and used without further purification. Column chromatography was performed with silica gel (230-400 mesh). ^{1}H- and ^{13}C-NMR spectra were recorded on a Bruker Advance (300 MHz) at ambient temperature. NMR standards are used as follows: (^{1}H-NMR) CD_3CN = 1.94 ppm, $CDCl_3$ = 7.26 ppm. (^{13}C-NMR) CD_3CN = 1.32 ppm, $CDCl_3$ = 77.16 ppm. ^{1}H-NMR data are reported as follows: chemical shift in ppm downfield from tetramethylsilane (δ-scale), multiplicity (s =singlet, d = doublet, t = triplet, q = quartet, m = multiplet, and br = broad), coupling constant (Hz) and integration. ^{13}C-NMR chemical shifts are reported in ppm downfield from tetramethylsilane (δ-scale). IR spectra were obtained on a Bruker Alpha-P series FT-IR spectrometer. CD spectra were recorded on a JASCO J-810 CD spectropolarimeter. High-resolution mass spectra were recorded on a Micromass AutoSpec instrument using ESI technique.



Scheme S1. Synthesis of octahedral silicon compounds as racemates. As counterions served iodides (**1**) or hexafluorophosphates (**2-5**).

Synthesis of Silicon Complex 1:

This complex was synthesized by a modified literature procedures.[3] Accordingly, a suspension of silicon(IV) iodide (1.83 g, 3.42 mmol) and 1,10-phenanthroline (1.35 g, 7.53 mmol) in dry $CHCl_3$ (40 mL) was purged with N_2 for 15 min and was then heated to 55 °C for 24 hours under N_2. The resulting brownish red suspension was cooled to room temperature and filtered to remove the solvent. The solid was washed with dry $CHCl_3$, MeOH, and Et_2O successively and was then dried in vaccum to afford the brownish red solid (2.58 g, 84%). The complex was used directly for the next step without further purification.

General Procedure for the Synthesis of Silicon Complexes 2-5:

A suspension of $[Si(phen)_2I_2]I_2$ (**1**) (352 mg, 0.4 mmol) and 4 equivalents of arenediol (1.6 mmol) in dry $CHCl_3$ (20 mL) was purged with N_2 for 15 min and then heated to reflux for 12 hours. The resulting dark-brown suspension was cooled to room temperature and the solvent was removed in vacuum. The crude material was subjected to silica gel chromatography with

acetonitrile:water:saturated aqueous KNO_3 50:3:1. The product eluents were concentrated to dryness and the resulting material was dissolved in minimal amounts of water. The product was precipitated by the addition of excess solid NH_4PF_6. The precipitate was centrifuged, washed twice with water and dried under high vacuum to afford the pure diolate complexes **2**-**5**.

Complex 2: Yield = 147 mg of a yellow solid (47%).

^{1}H-NMR (300 MHz, CD_3CN): δ (ppm) 9.46 (dd, J = 5.4, 1.1 Hz, 2H), 9.38 (dd, J = 8.3, 1.1 Hz, 2H), 9.09 (dd, J = 8.3, 1.0 Hz, 2H), 8.60 (d, J = 9.1 Hz, 2H), 8.51 (d, 9.1 Hz, 2H), 8.49 (dd, J = 8.3, 5.5 Hz, 2H), 7.92 (dd, J = 8.3, 5.5 Hz, 2H), 7.73 (dd, J = 5.5, 1.0 Hz, 2H), 6.81 (m, 4H).

^{13}C-NMR (75 MHz, CD_3CN): δ (ppm) 149.5, 147.5, 147.3, 147.0, 146.4, 135.8, 134.8, 131.4, 131.0, 129.7, 129.6, 129.3, 128.9, 123.0, 114.6.

IR (neat): $\tilde{\nu}$ (cm^{-1}) 3075, 1629, 1585, 1528, 1482, 1437, 1335, 1244, 1154, 1115, 1019, 884, 826, 759, 738, 714, 666, 620, 582, 554, 521, 484, 456, 416.

HRMS calcd for $C_{30}H_{20}F_6N_4O_2PSi$ $(M\text{-}PF_6)^+$ 641.1003, found: 641.0978.

Complex 3: Yield = 117 mg of a yellow solid (35%).

^{1}H-NMR (300 MHz, CD_3CN): δ (ppm) 9.51 (dd, J = 5.4, 1.0 Hz, 2H), 9.37 (dd, J = 8.4, 1.0 Hz, 2H), 9.11 (dd, J = 8.3, 0.8 Hz, 2H), 8.61 (d, J = 9.1 Hz, 2H), 8.52 (d, 9.1 Hz, 2H), 8.45 (dd, J = 8.3, 5.4 Hz, 2H), 7.94 (dd, J = 8.3, 5.6 Hz, 2H), 7.75 (dd, J = 5.5, 0.8 Hz, 2H), 7.66 (m, 2H), 7.30 (m, 2H), 7.15 (s, 2H).^{13}C-NMR (75 MHz, CD_3CN): δ (ppm) 149.6, 147.6, 147.5, 147.1, 146.5, 135.8, 134.9, 131.6, 131.4, 131.1, 129.79, 129.75, 129.4, 128.9, 127.7, 125.3, 109.9.

IR (neat): $\tilde{\nu}$ (cm^{-1}) 3112, 1625, 1586, 1530, 1464, 1436, 1323, 1249, 1221, 1161, 880, 833, 757, 741, 715, 667, 621, 579, 556, 520, 508, 486, 463, 411, 385.

HRMS calcd for $C_{34}H_{22}F_6N_4O_2PSi$ $(M\text{-}PF_6)^+$ 691.1159, found: 691.1143.

Complex 4: Yield = 60 mg of a brown-red solid (17%).

^{1}H-NMR (300 MHz, CD_3CN): δ (ppm) 9.41(dd, J = 5.4, 1.2 Hz, 2H), 9.31 (dd, J = 8.4, 1.2 Hz, 2H), 9.13 (dd, J = 8.3, 1.1 Hz, 2H), 8.70 (m, 2H), 8.59 (d, 9.2 Hz, 2H), 8.53 (d, J = 9.2 Hz, 2H), 8.35 (dd, J = 8.3, 5.4 Hz, 2H), 7.98 (dd, J = 8.3, 5.6 Hz, 2H), 7.82 (dd, J = 5.6, 1.1 Hz, 2H), 7.80 (m, 2H), 7.53 (m, 4H).

^{13}C-NMR (75 MHz, CD_3CN): δ (ppm) 149.9, 147.6, 146.8, 146.3, 137.4, 135.9, 134.8, 131.4, 131.1, 129.7, 129.7, 129.3, 128.9, 128.0, 127.8, 125.9, 125.2, 124.1, 121.6.

IR (neat): $\tilde{\nu}$ (cm^{-1}) 1626, 1586, 1530, 1436, 1367, 1341, 1115, 1054, 1030, 886, 833, 802, 757, 738, 715, 686, 669, 650, 581, 556, 546, 523, 508, 483, 468, 443, 414, 394, 382.

HRMS calcd for $C_{38}H_{24}F_6N_4O_2PSi$ $(M\text{-}PF_6)^+$ 741.1316, found: 741.1285.

Complex 5: Yield = 62 mg of a brown-red solid (17%).

^{1}H-NMR (300 MHz, CD_3CN): δ (ppm) 9.49 (dd, J = 5.4, 1.1 Hz, 2H), 9.29 (dd, J = 8.4, 1.1 Hz, 2H), 9.16 (dd, J = 8.3, 1.0 Hz, 2H), 8.59 (d, J = 9.1 Hz, 2H), 8.54 (d, J = 9.1 Hz, 2H), 8.31 (dd, J = 8.4, 5.4 Hz, 2H), 8.15-7.93 (m, 10H), 7.87 (dd, J = 5.5, 1.0 Hz, 2H).

^{13}C-NMR (75 MHz, CD_3CN): δ (ppm) 150.0, 147.7, 146.8, 146.4, 138.3, 135.9, 134.8, 132.3, 131.4, 131.1, 129.8, 129.7, 129.3, 129.0, 128.6, 127.1, 124.7, 124.4, 122.0, 118.8.

IR (neat): $\tilde{\nu}$ (cm^{-1}) 3110, 1625, 1600, 1585, 1529, 1435, 1399, 1363, 1312, 1215, 1154, 1117, 1097, 1037, 903, 886, 827, 797, 757, 738, 715, 668, 622, 587, 555, 524, 508, 481, 449, 429, 386.

HRMS calcd for $C_{40}H_{24}F_6N_4O_2PSi$ $(M\text{-}PF_6)^+$ 765.1305, found: 765.1296.

II.) Evaluation of Hydrolytic Stabilities

The hydrolytic stability of the complexes **2-5** were evaluated by ^{1}H-NMR in CD_3CN/D_2O 5:1. No signs of decomposition were observed after 7 days at room temperature. See Figures S1 and S2 for examples.

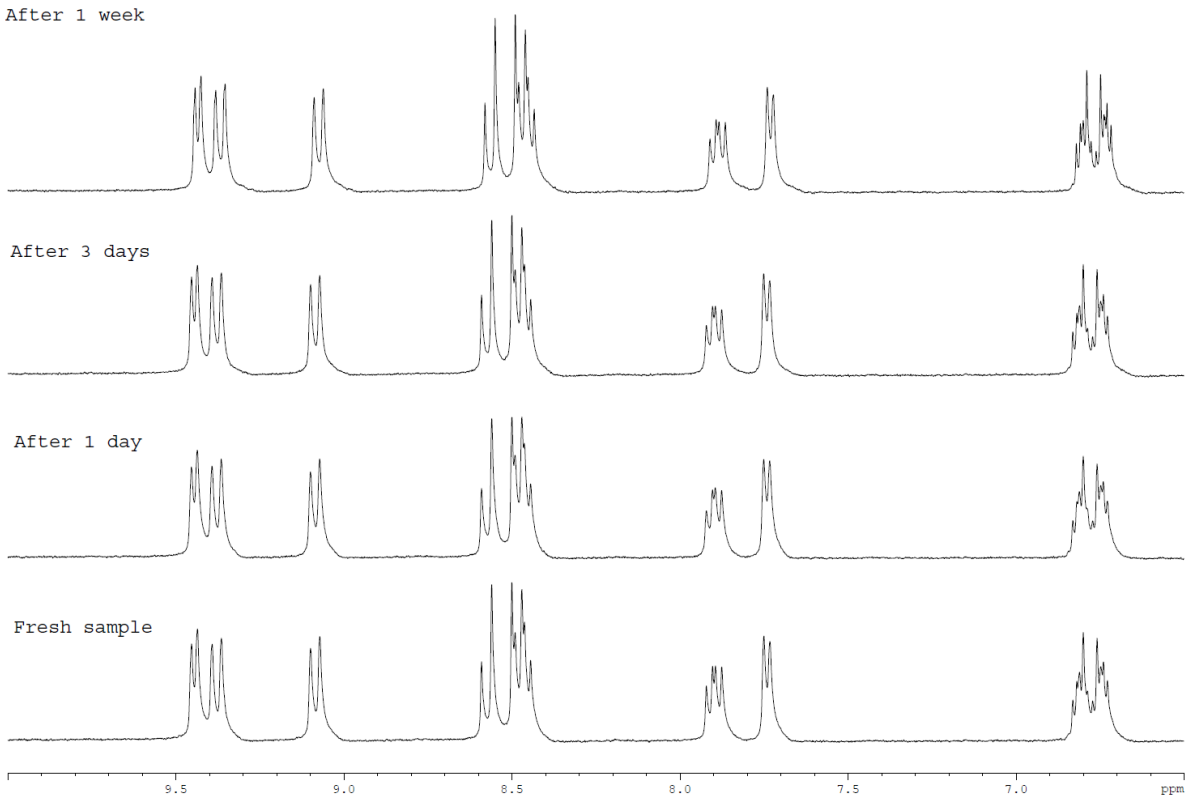


Figure S1. Hydrolytic stability of complex **2** at room temperature in CD_3CN/D_2O 5:1.

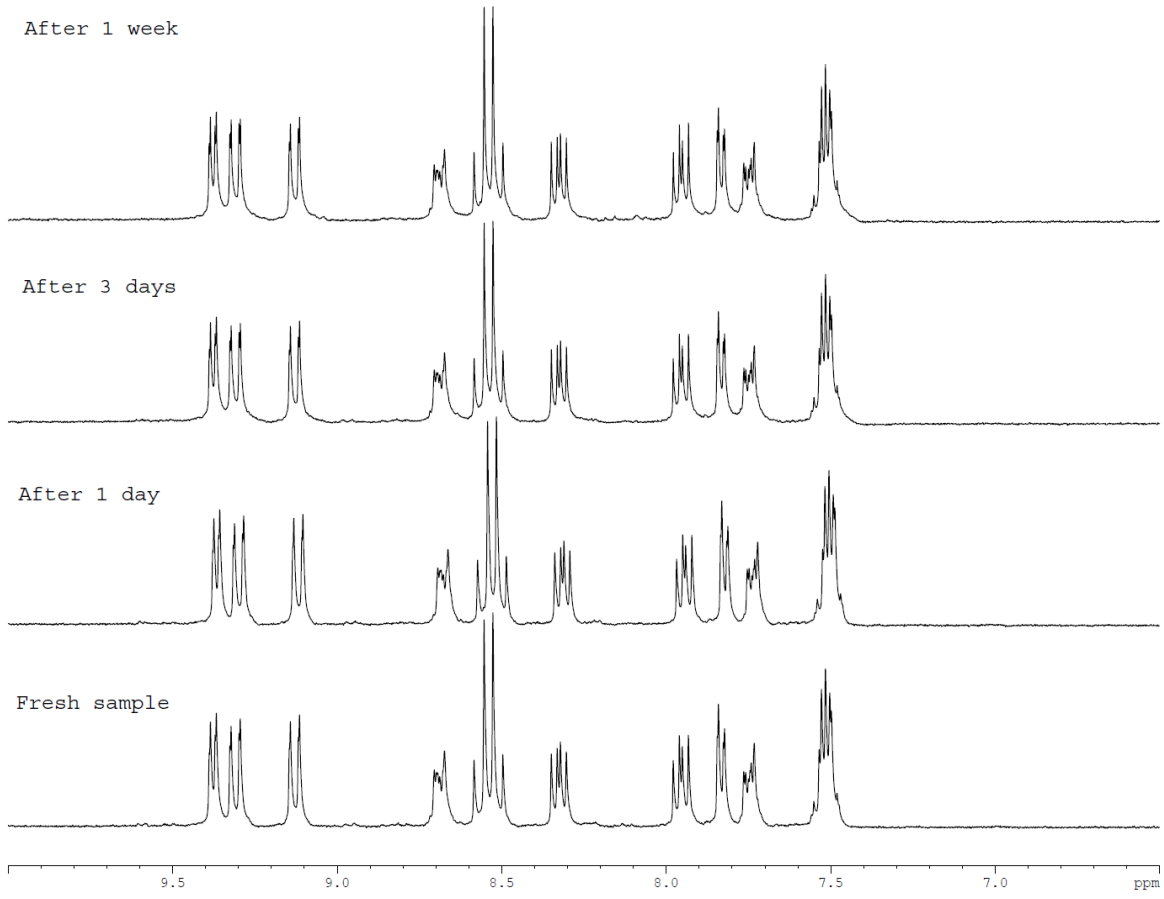


Figure S2. Hydrolytic stability of complex **4** at room temperature in CD_3CN/D_2O 5:1.

III.) UV/Vis and CD Spectroscopy

UV-monitored thermal denaturation. The melting studies were carried out in 1 cm path length quartz cells (total volumn 325 µL; 250 µL sample solutions were covered by mineral oil) on a Beckman 800 UV-Vis spectrophotometer equipped with a thermo-programmer. Melting curves were monitored at 260 nm with a heating rate of 1 °C/min. Melting temperatures were calculated from the first derivatives of the heating curves. Experiments were performed in triplicate and mean values with standard deviations were determined.

UV-monitored titration. The absorption of complex **5** at 355 nm was measured in a quartz cuvette with a path length of 1 cm on a Beckman 800 UV-Vis spectrophotometer. The binding constant of the silicon complex **5** to calf thymus DNA (CT-DNA) was determined by UV-monitored titration at room temperature in 5 mM Tris-HCl buffer (pH 7.5) with 20 mM NaCl. For this, complex **5** (20 or 40 µM) in Tris-HCl buffer (1 mL) was titrated with concentrated calf thymus DNA solutions so that the change in overall volume was negligible. A large hypochromicity and modest bathochromic shift of the pyrene $\pi \rightarrow \pi^*$ absorption band was observed. The binding constant (K) of the complex to CT-DNA was obtained by the McGhee-von Hippel method.[4,5] The determination was performed four times and the mean value was determined ± standard deviation to afford $K = (1.7 \pm 0.6) \times 10^6\ M^{-1}$ (Figure S5).

CD spectroscopy. CD measurements were performed on a JASCO J-810 spectrometer in a 1 mm path length quartz cuvette.

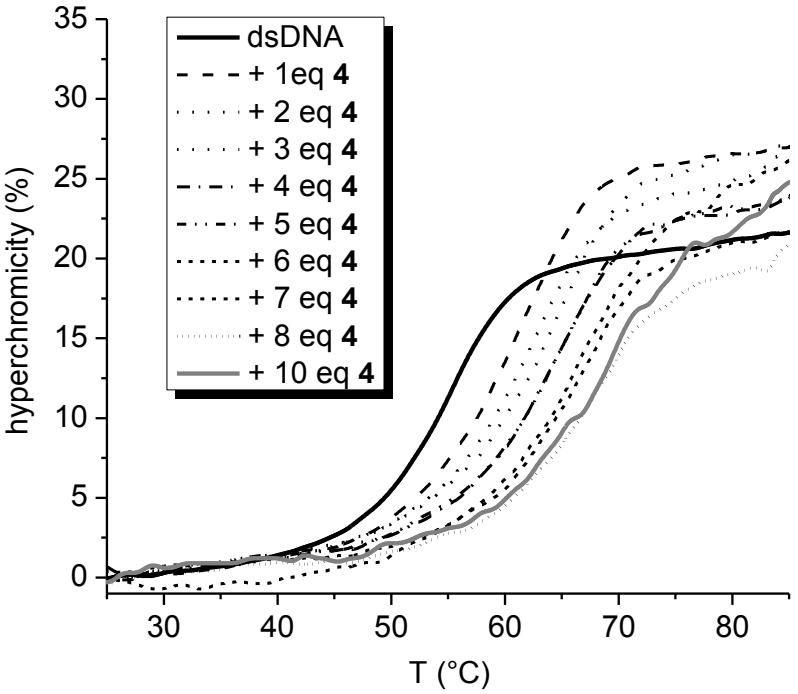


Figure S3. UV-melting curves (λ = 260 nm) of duplex DNA 5'-AGTGCCAAGCTTGCA-3'/3'-TCACGGTTCGAACGT-5' (2 μM) in Tris-HCl buffer (5 mM, pH 7.4) with NaCl (50 mM) and in the presence of the silicon complex **4** at different concentrations (0-20 μM).

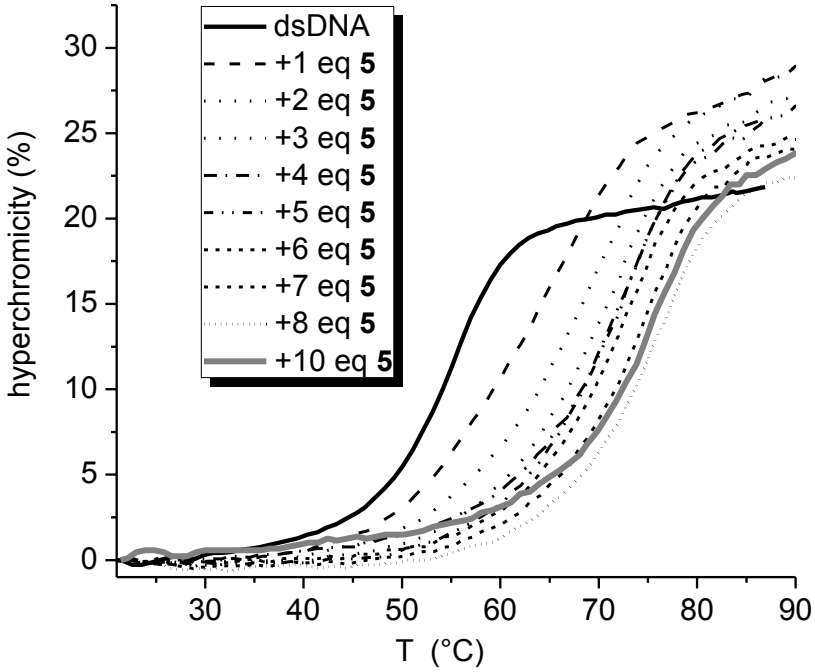


Figure S4. UV-melting curves (λ = 260 nm) of duplex DNA 5'-AGTGCCAAGCTTGCA-3'/3'-TCACGGTTCGAACGT-5' (2 μM) in Tris-HCl buffer (5 mM, pH 7.4) with NaCl (50 mM) and in the presence of the silicon complex **5** at different concentrations (0-20 μM).

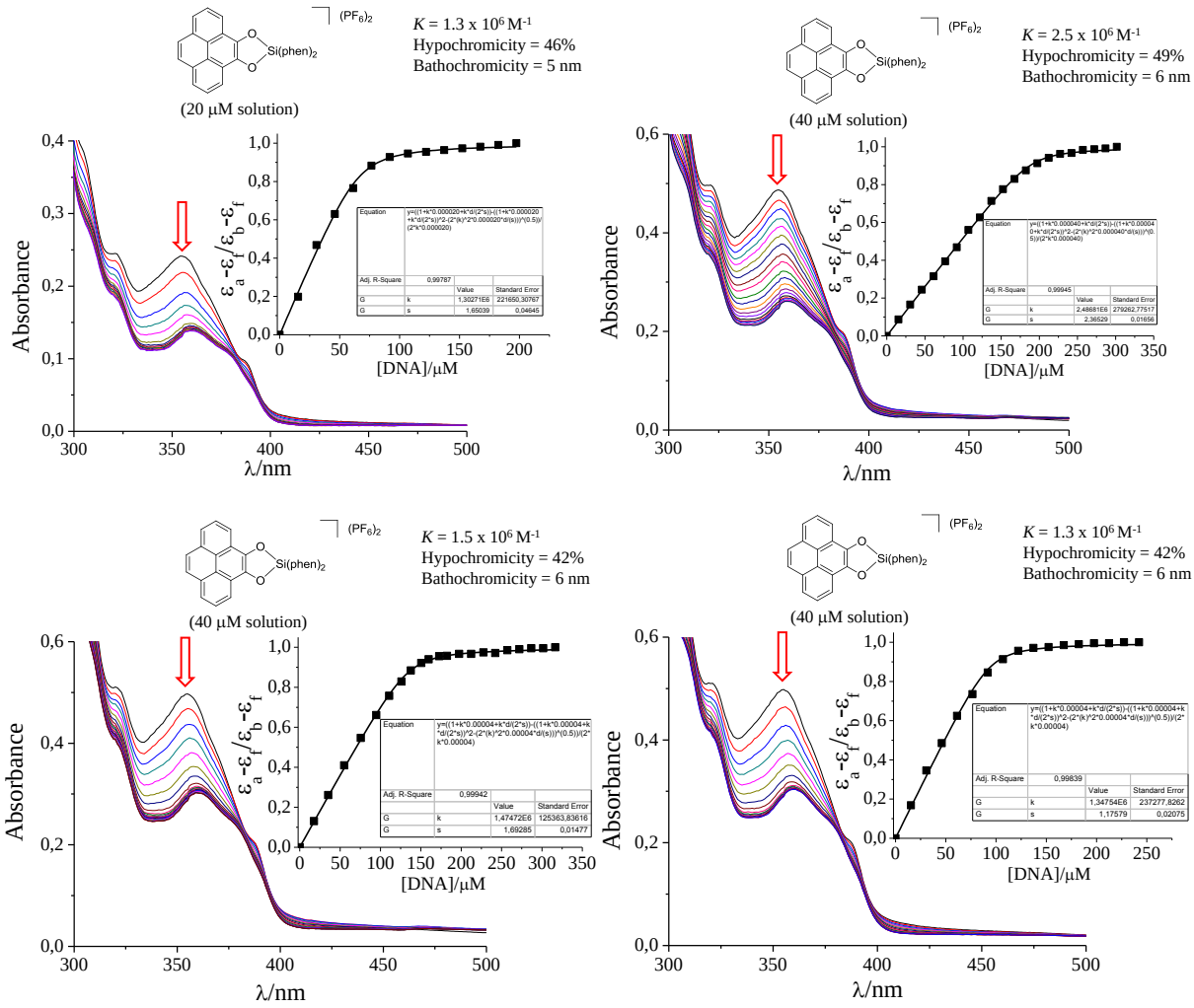


Figure S5. UV-absorption spectra of silicon complex **5** in the absence and presence of increasing concentrations of calf-thymus DNA and determination of binding constants by the McGhee-von Hippel method. The determination was performed four times and the mean value was determined ± standard deviation to afford $K = (1.7 \pm 0.6) \times 10^6$ M^{-1}.

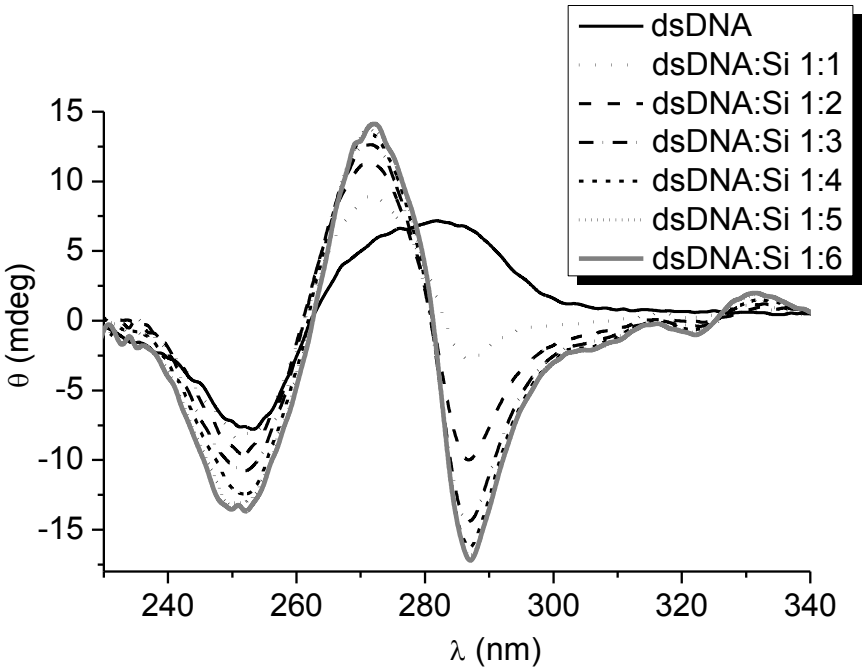


Figure S6. CD spectra of duplex DNA 5'-AGTGCCAAGCTTGCA-3'/3'-TCACGGTTCGAACGT-5' (20 μM) in Tris buffer (5 mM, pH 7.4) with NaCl (50 mM) and different concentrations of 9,10-phenanthrenediolate complex **4** (0-120 μM).

IV.) Enantiomers of Silicon Complex 4

The enantiomers of 9,10-phenanthrenediolate complex **4** were resolved with a CHIRALPAK IB HPLC column (250 × 4.6 mm) on an Agilent 1200 Series HPLC System. The flow rate was 1.0 mL/min, the column temperature 40 °C, and UV-absorption was measured at 254 nm. Solvent A = 0.1% TFA, solvent B = MeCN, with a linear gradient of 12% to 24% B in 30 min. Using this method, milligram amounts of the individual enantiomers were obtained. The two enantiomers are configurationally stable at room temperature: Dissolved in MeCN and stored in a glass vial at room temperature on the laboratory bench, no change in the enantiomeric ratio was observed after 3 days. The absolute configurations of the individual enantiomers were assigned based on their CD spectra.[6] See Figures S7-S11.

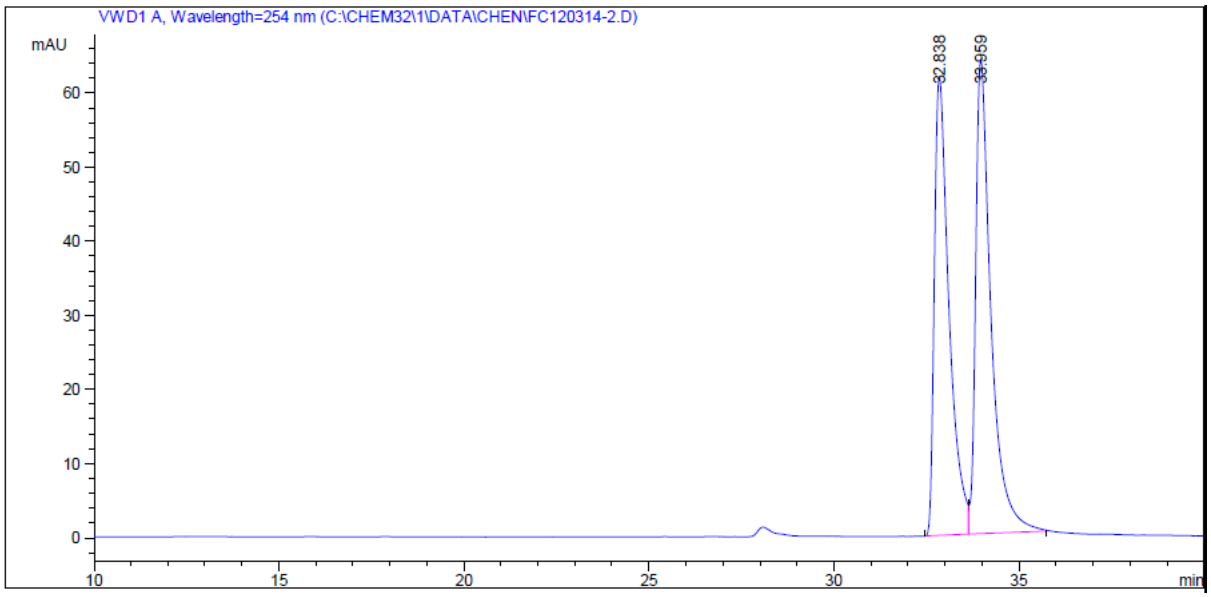


Figure S7. HPLC trace for racemic silicon complex **4**.

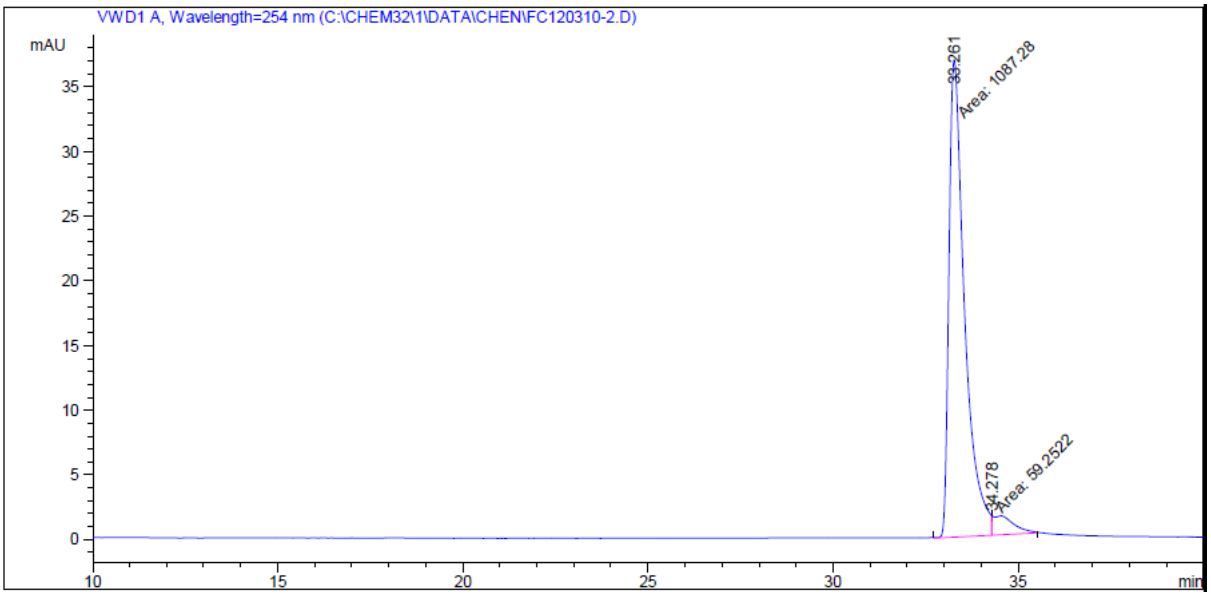


Figure S8. HPLC trace for enantiomer A of complex **4**. Integration of peak areas: 94.8:5.2 e.r.

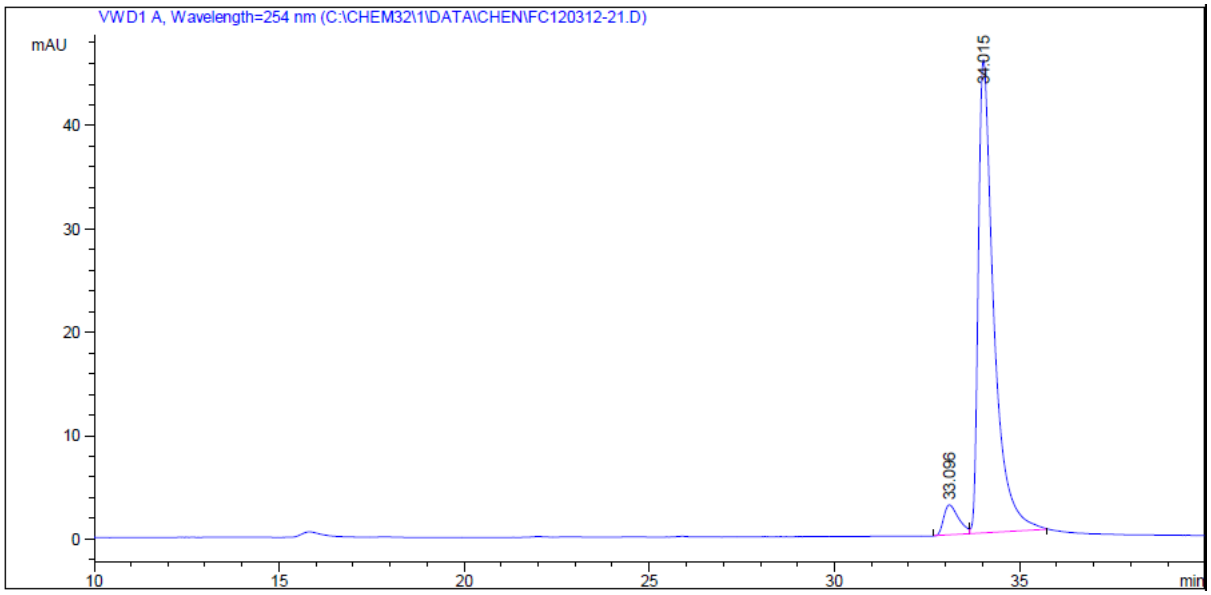


Figure S9. HPLC trace for enantiomer B of complex **4**. Integration of peak areas: 5.8:94.2 e.r.

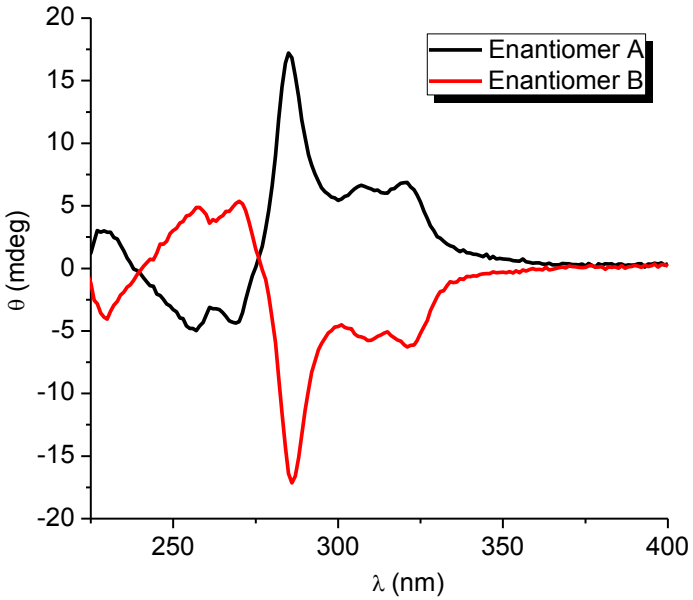


Figure S10. CD spectra of the two enantiomers at 20 μM in Tris-HCl buffer (5 mM, pH 7.4) with NaCl (50 mM). Based on these CD spectra, enantiomer A is assigned the absolute configuration Λ and enantiomer B is assigned as Δ.[6]

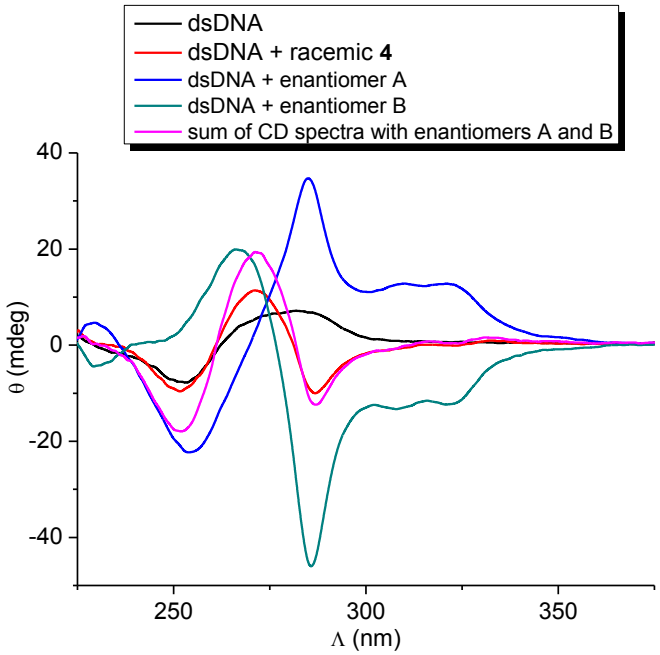


Figure S11. CD spectra of the racemic **4** and the two enantiomers of **4** (each 40 μM) in the presence of DNA (20 μM) in Tris-HCl buffer (5 mM, pH 7.4) with NaCl (50 mM). The CD spectra of the duplex DNA (5'-AGTGCCAAGCTTGCA-3'/3'-TCACGGTTCGAACGT-5') alone and the sum of the CD spectra of the individual enantiomers in the presence of DNA are given for comparison.

V.) Crystal Structure of Silicon Complex 4

The 9,10-phenanthrenediolate complex **4** was crystallized from a MeCN solution layered with Et_2O. Data were collected from a red plate with the dimensions 0.38 x 0.28 x 0.09 mm on a STOE IPDS2 diffractometer using graphite monochromated Mo$K\alpha$ radiation.[7] Crystal data: $C_{38}H_{24}N_4O_2Si$, $2(PF_6)$, 3MeCN, M_r = 1009.80 g mol^{-1}, monoclinic, space group $P2_1/c$, a = 10.9077(5), b = 28.9688(9), c = 14.5670(6) Å, V = 4320.2(3) Å^3, Z = 4, ρ_{calcd} = 1.545 g cm^{-3}, μ = 0.228 mm^{-1}, T = 100(2) K, $2\theta_{max}$ = 50.5°, 24134 total reflections, 7731 independent (R_{int} = 0.033), 4516 observed [$I>2\sigma(I)$]. Data were corrected for absorption effects using indexed faces of the crystal.[7] The structure was solved using direct methods[8] and refined using full matrix least squares on F^2.[9] Final $R1$ [$I>2\sigma$ (I)] = 0.0415, $wR2$ (all data) = 0.0955, largest difference peak (hole) 0.393 (-0.282) e Å^{-3}. CCDC 871583 contains additional supplementary crystallographic data which can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

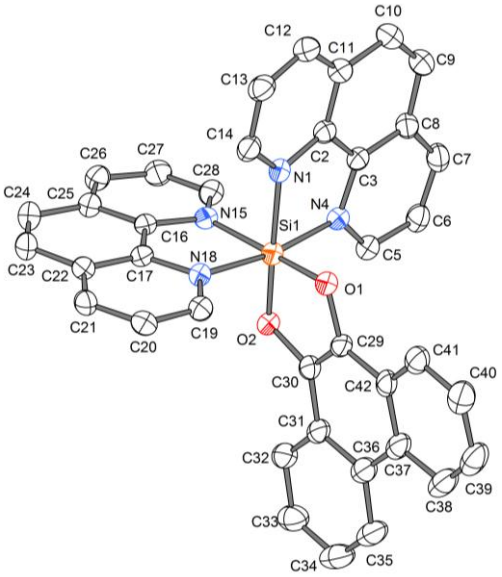


Figure S12. Crystal structure of silicon complex **4**. ORTEP representation with 50% thermal ellipsoids. Two hexafluorophosphate ions and three MeCN molecules are omitted for clarity.

Table S1. Crystal data and structure refinement for silicon complex **4**.

Crystal data:

Identification code	yg546	
Habitus, colour	block, red	
Crystal size	0.38 x 0.20 x 0.09 mm^3	
Crystal system	Monoclinic	
Space group	P $2_1/c$	Z = 4
Unit cell dimensions	a = 10.9077(5) Å	α= 90°.
	b = 28.9688(9) Å	β= 109.451(3)°.
	c = 14.5670(6) Å	γ = 90°.
Volume	4340.2(3) $Å^3$	
Cell determination	16075 peaks with Theta 1.4 to 27.0°.	
Empirical formula	C_{44} H_{33} F_{12} N_7 O_2 P_2 Si	
Formula weight	1009.80	
Density (calculated)	1.545 Mg/m^3	
Absorption coefficient	0.228 mm^{-1}	
F(000)	2056	

Data collection:

Diffractometer type	STOE IPDS 2
Wavelength	0.71073 Å
Temperature	100(2) K
Theta range for data collection	1.41 to 25.25°.
Index ranges	-13<=h<=13, -32<=k<=34, -17<=l<=17
Data collection software	STOE X-AREA
Cell refinement software	STOE X-AREA
Data reduction software	STOE X-RED

Solution and refinement:

Reflections collected	24134
Independent reflections	7731 [R(int) = 0.0326]
Completeness to theta = 25.25°	98.7 %
Observed reflections	4516[I>2sigma(I)]
Reflections used for refinement	7731
Absorption correction	Integration
Max. and min. transmission	0.9831 and 0.9376
Largest diff. peak and hole	0.393 and -0.282 $e.Å^{-3}$
Solution	Direct methods
Refinement	Full-matrix least-squares on F^2
Treatment of hydrogen atoms	Calculated positions, constr. ref.
Programs used	SIR 2011
	SHELXL-97 (Sheldrick, 1997)
	DIAMOND 3.2h
	STOE IPDS2 software
Data / restraints / parameters	7731 / 15 / 616
Goodness-of-fit on F^2	0.823
R index (all data)	wR2 = 0.0955
R index conventional [I>2sigma(I)]	R1 = 0.0415

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

	x	y	z	U(eq)	Occupancy
C2	1.0036(3)	0.33904(8)	0.30730(18)	0.0271(6)	1
C3	1.0932(3)	0.31302(8)	0.27659(18)	0.0270(6)	1
C5	1.1689(3)	0.29791(8)	0.14909(19)	0.0295(6)	1
C6	1.2544(3)	0.26502(9)	0.2056(2)	0.0316(7)	1
C7	1.2587(3)	0.25628(9)	0.2995(2)	0.0321(7)	1
C8	1.1764(3)	0.28106(9)	0.33806(19)	0.0299(6)	1
C9	1.1707(3)	0.27652(9)	0.43462(19)	0.0347(7)	1
C10	1.0876(3)	0.30161(9)	0.4646(2)	0.0361(7)	1
C11	0.9979(3)	0.33362(9)	0.40069(19)	0.0313(7)	1
C12	0.9025(3)	0.35943(9)	0.4230(2)	0.0345(7)	1
C13	0.8219(3)	0.38795(9)	0.35388(19)	0.0337(7)	1
C14	0.8354(3)	0.39155(9)	0.26212(19)	0.0308(7)	1
C16	1.0251(3)	0.45850(8)	0.13628(17)	0.0260(6)	1
C17	0.8897(3)	0.45806(8)	0.08401(18)	0.0266(6)	1
C19	0.7121(3)	0.41128(9)	0.01030(19)	0.0301(6)	1
C20	0.6357(3)	0.45017(9)	-0.02498(19)	0.0315(7)	1
C21	0.6883(3)	0.49368(9)	-0.00368(19)	0.0308(6)	1
C22	0.8204(3)	0.49852(8)	0.05199(18)	0.0289(6)	1
C23	0.8901(3)	0.54131(9)	0.0765(2)	0.0344(7)	1
C24	1.0200(3)	0.54197(9)	0.1264(2)	0.0346(7)	1
C25	1.0927(3)	0.50005(9)	0.15690(18)	0.0293(6)	1
C26	1.2278(3)	0.49693(9)	0.20323(19)	0.0321(7)	1
C27	1.2846(3)	0.45443(9)	0.22424(19)	0.0317(7)	1
C28	1.2095(3)	0.41462(9)	0.20259(19)	0.0306(6)	1
C29	0.8397(3)	0.30756(8)	-0.01366(18)	0.0298(7)	1
C30	0.9254(3)	0.32808(8)	-0.04912(18)	0.0293(6)	1
C31	0.9347(3)	0.31598(9)	-0.14177(18)	0.0321(7)	1
C32	1.0200(3)	0.33809(9)	-0.18165(19)	0.0344(7)	1
C33	1.0215(3)	0.32625(10)	-0.2725(2)	0.0407(7)	1
C34	0.9412(3)	0.29125(11)	-0.3242(2)	0.0447(8)	1
C35	0.8607(3)	0.26837(10)	-0.2862(2)	0.0412(8)	1
C36	0.8518(3)	0.28001(9)	-0.19398(19)	0.0344(7)	1
C37	0.7609(3)	0.25761(9)	-0.1552(2)	0.0356(7)	1
C38	0.6757(3)	0.22225(10)	-0.2041(2)	0.0426(8)	1
C39	0.5901(3)	0.20230(10)	-0.1660(2)	0.0470(9)	1
C40	0.5807(3)	0.21722(10)	-0.0770(2)	0.0423(8)	1
C41	0.6608(3)	0.25212(9)	-0.0270(2)	0.0356(7)	1
C42	0.7525(3)	0.27191(8)	-0.06399(19)	0.0314(7)	1
N1	0.9247(2)	0.36771(7)	0.23807(15)	0.0267(5)	1
N4	1.0893(2)	0.32168(7)	0.18372(15)	0.0267(5)	1
N15	1.0812(2)	0.41602(7)	0.15916(15)	0.0266(5)	1
N18	0.8370(2)	0.41500(7)	0.06482(15)	0.0266(5)	1
O1	0.84101(18)	0.32388(6)	0.07616(12)	0.0292(4)	1
O2	1.00012(17)	0.36177(6)	0.01091(12)	0.0286(4)	1
Si1	0.95822(8)	0.36541(2)	0.11435(5)	0.02718(18)	1
C301	0.3747(6)	0.62816(18)	0.2908(5)	0.138(3)	1
C302	0.4825(5)	0.65605(18)	0.2834(5)	0.129(2)	1
N300	0.2897(5)	0.60505(15)	0.3070(5)	0.150(2)	1
F1	0.5934(2)	0.47864(7)	0.19722(14)	0.0695(6)	1
F2	0.66738(19)	0.55055(7)	0.19245(13)	0.0646(6)	1
F3	0.72879(19)	0.55436(7)	0.35559(14)	0.0664(6)	1
F4	0.6531(2)	0.48208(7)	0.36002(14)	0.0716(6)	1
F5	0.79970(17)	0.49573(6)	0.28349(13)	0.0564(5)	1
F6	0.52180(17)	0.53631(6)	0.26880(13)	0.0580(5)	1
P1	0.66116(8)	0.51652(3)	0.27641(6)	0.0416(2)	1

F7	0.42307(16)	0.65054(6)	0.88971(12)	0.0461(4)	1
F8	0.56633(18)	0.70919(5)	0.93344(12)	0.0506(5)	1
F9	0.72291(17)	0.66015(7)	1.01542(13)	0.0611(5)	1
F10	0.58213(19)	0.60084(6)	0.97267(14)	0.0573(5)	1
F11	0.53521(17)	0.66239(6)	1.04855(12)	0.0498(5)	1
F12	0.60991(17)	0.64701(6)	0.85664(12)	0.0471(4)	1
P2	0.57264(8)	0.65468(3)	0.95258(6)	0.03461(19)	1
C101	0.5972(4)	0.59855(15)	0.5503(3)	0.0699(11)	1
C102	0.5527(4)	0.55535(16)	0.5097(3)	0.0834(13)	1
N100	0.6366(4)	0.63305(13)	0.5865(3)	0.0953(13)	1
C201	0.0907(3)	0.48534(14)	0.3972(2)	0.0509(9)	1
C202	0.0804(4)	0.53389(14)	0.4225(3)	0.0844(14)	1
N200	0.0991(3)	0.44849(11)	0.37607(19)	0.0535(7)	1

Table S3. Bond lengths [Å] and angles [°] for complex **4**.

C2-N1	1.367(3)	C31-C36	1.423(4)
C2-C11	1.391(4)	C32-C33	1.372(4)
C2-C3	1.419(4)	C32-H32	0.9500
C3-N4	1.363(3)	C33-C34	1.387(4)
C3-C8	1.393(4)	C33-H33	0.9500
C5-N4	1.332(3)	C34-C35	1.356(4)
C5-C6	1.394(4)	C34-H34	0.9500
C5-H5	0.9500	C35-C36	1.420(4)
C6-C7	1.377(4)	C35-H35	0.9500
C6-H6	0.9500	C36-C37	1.448(4)
C7-C8	1.404(4)	C37-C38	1.407(4)
C7-H7	0.9500	C37-C42	1.423(4)
C8-C9	1.435(4)	C38-C39	1.363(5)
C9-C10	1.343(4)	C38-H38	0.9500
C9-H9	0.9500	C39-C40	1.403(4)
C10-C11	1.441(4)	C39-H39	0.9500
C10-H10	0.9500	C40-C41	1.375(4)
C11-C12	1.405(4)	C40-H40	0.9500
C12-C13	1.371(4)	C41-C42	1.407(4)
C12-H12	0.9500	C41-H41	0.9500
C13-C14	1.397(4)	N1-Si1	1.956(2)
C13-H13	0.9500	N4-Si1	1.926(2)
C14-N1	1.332(3)	N15-Si1	1.947(2)
C14-H14	0.9500	N18-Si1	1.923(2)
C16-N15	1.365(3)	O1-Si1	1.7081(19)
C16-C25	1.391(4)	O2-Si1	1.7172(19)
C16-C17	1.419(4)	C301-N300	1.229(8)
C17-N18	1.363(3)	C301-C302	1.460(8)
C17-C22	1.388(3)	C302-H30A	0.9800
C19-N18	1.333(3)	C302-H30B	0.9800
C19-C20	1.394(4)	C302-H30C	0.9800
C19-H19	0.9500	F1-P1	1.5852(19)
C20-C21	1.377(4)	F2-P1	1.590(2)
C20-H20	0.9500	F3-P1	1.5842(19)
C21-C22	1.405(4)	F4-P1	1.599(2)
C21-H21	0.9500	F5-P1	1.5978(19)
C22-C23	1.436(4)	F6-P1	1.594(2)
C23-C24	1.361(4)	F7-P2	1.5873(18)
C23-H23	0.9500	F8-P2	1.6009(17)
C24-C25	1.437(4)	F9-P2	1.5970(19)
C24-H24	0.9500	F10-P2	1.5840(18)
C25-C26	1.405(4)	F11-P2	1.5972(18)
C26-C27	1.366(4)	F12-P2	1.5956(18)
C26-H26	0.9500	C101-N100	1.145(5)
C27-C28	1.388(4)	C101-C102	1.400(6)
C27-H27	0.9500	C102-H10A	0.9800
C28-N15	1.330(3)	C102-H10B	0.9800
C28-H28	0.9500	C102-H10C	0.9800
C29-C30	1.348(4)	C201-N200	1.123(4)
C29-O1	1.387(3)	C201-C202	1.468(5)
C29-C42	1.430(4)	C202-H20A	0.9800
C30-O2	1.381(3)	C202-H20B	0.9800
C30-C31	1.430(4)	C202-H20C	0.9800
C31-C32	1.405(4)		

N1-C2-C11	124.6(2)	C11-C2-C3	120.5(2)
N1-C2-C3	114.9(2)	N4-C3-C8	124.0(2)

N4-C3-C2	114.7(2)	C25-C26-H26	120.3
C8-C3-C2	121.3(2)	C26-C27-C28	120.6(3)
N4-C5-C6	121.5(2)	C26-C27-H27	119.7
N4-C5-H5	119.2	C28-C27-H27	119.7
C6-C5-H5	119.2	N15-C28-C27	122.0(2)
C7-C6-C5	120.4(3)	N15-C28-H28	119.0
C7-C6-H6	119.8	C27-C28-H28	119.0
C5-C6-H6	119.8	C30-C29-O1	114.9(2)
C6-C7-C8	119.3(2)	C30-C29-C42	123.4(2)
C6-C7-H7	120.4	O1-C29-C42	121.8(3)
C8-C7-H7	120.4	C29-C30-O2	114.0(2)
C3-C8-C7	116.7(2)	C29-C30-C31	122.0(2)
C3-C8-C9	117.4(3)	O2-C30-C31	123.9(3)
C7-C8-C9	126.0(2)	C32-C31-C36	120.3(3)
C10-C9-C8	121.5(3)	C32-C31-C30	122.9(2)
C10-C9-H9	119.2	C36-C31-C30	116.8(3)
C8-C9-H9	119.2	C33-C32-C31	120.5(3)
C9-C10-C11	121.7(3)	C33-C32-H32	119.8
C9-C10-H10	119.2	C31-C32-H32	119.8
C11-C10-H10	119.2	C32-C33-C34	119.9(3)
C2-C11-C12	116.3(2)	C32-C33-H33	120.1
C2-C11-C10	117.5(3)	C34-C33-H33	120.1
C12-C11-C10	126.1(3)	C35-C34-C33	120.9(3)
C13-C12-C11	119.7(3)	C35-C34-H34	119.5
C13-C12-H12	120.2	C33-C34-H34	119.5
C11-C12-H12	120.2	C34-C35-C36	121.8(3)
C12-C13-C14	120.1(3)	C34-C35-H35	119.1
C12-C13-H13	120.0	C36-C35-H35	119.1
C14-C13-H13	120.0	C35-C36-C31	116.6(3)
N1-C14-C13	122.2(3)	C35-C36-C37	122.3(3)
N1-C14-H14	118.9	C31-C36-C37	121.1(3)
C13-C14-H14	118.9	C38-C37-C42	116.6(3)
N15-C16-C25	124.4(2)	C38-C37-C36	123.4(3)
N15-C16-C17	115.1(2)	C42-C37-C36	119.9(2)
C25-C16-C17	120.4(2)	C39-C38-C37	121.9(3)
N18-C17-C22	123.9(2)	C39-C38-H38	119.0
N18-C17-C16	114.3(2)	C37-C38-H38	119.0
C22-C17-C16	121.7(2)	C38-C39-C40	121.1(3)
N18-C19-C20	121.4(2)	C38-C39-H39	119.5
N18-C19-H19	119.3	C40-C39-H39	119.5
C20-C19-H19	119.3	C41-C40-C39	119.1(3)
C21-C20-C19	120.3(3)	C41-C40-H40	120.4
C21-C20-H20	119.9	C39-C40-H40	120.4
C19-C20-H20	119.9	C40-C41-C42	120.3(3)
C20-C21-C22	119.4(2)	C40-C41-H41	119.9
C20-C21-H21	120.3	C42-C41-H41	119.9
C22-C21-H21	120.3	C41-C42-C37	120.9(3)
C17-C22-C21	116.7(2)	C41-C42-C29	122.3(3)
C17-C22-C23	117.5(2)	C37-C42-C29	116.8(3)
C21-C22-C23	125.9(2)	C14-N1-C2	117.2(2)
C24-C23-C22	121.1(3)	C14-N1-Si1	129.59(18)
C24-C23-H23	119.5	C2-N1-Si1	113.19(17)
C22-C23-H23	119.5	C5-N4-C3	118.2(2)
C23-C24-C25	121.5(3)	C5-N4-Si1	127.24(18)
C23-C24-H24	119.3	C3-N4-Si1	114.47(18)
C25-C24-H24	119.3	C28-N15-C16	117.3(2)
C16-C25-C26	116.3(2)	C28-N15-Si1	129.38(18)
C16-C25-C24	117.8(2)	C16-N15-Si1	113.21(18)
C26-C25-C24	125.8(2)	C19-N18-C17	118.3(2)
C27-C26-C25	119.4(2)	C19-N18-Si1	126.99(17)
C27-C26-H26	120.3	C17-N18-Si1	114.60(18)

C29-O1-Si1	108.59(16)	F3-P1-F4	90.43(12)
C30-O2-Si1	109.01(16)	F1-P1-F4	89.54(12)
O1-Si1-O2	93.44(9)	F2-P1-F4	179.26(13)
O1-Si1-N18	93.28(9)	F6-P1-F4	89.08(11)
O2-Si1-N18	93.87(9)	F5-P1-F4	90.39(11)
O1-Si1-N4	92.98(9)	F10-P2-F7	91.35(10)
O2-Si1-N4	92.98(9)	F10-P2-F12	90.27(10)
N18-Si1-N4	170.42(9)	F7-P2-F12	89.82(9)
O1-Si1-N15	175.42(10)	F10-P2-F9	90.01(11)
O2-Si1-N15	89.16(9)	F7-P2-F9	178.64(11)
N18-Si1-N15	82.78(9)	F12-P2-F9	90.21(10)
N4-Si1-N15	90.64(9)	F10-P2-F11	89.77(10)
O1-Si1-N1	88.55(9)	F7-P2-F11	90.13(10)
O2-Si1-N1	175.34(10)	F12-P2-F11	179.94(13)
N18-Si1-N1	90.22(9)	F9-P2-F11	89.83(10)
N4-Si1-N1	82.70(9)	F10-P2-F8	178.77(12)
N15-Si1-N1	89.13(9)	F7-P2-F8	89.87(10)
N300-C301-C302	173.5(8)	F12-P2-F8	89.63(9)
C301-C302-H30A	109.5	F9-P2-F8	88.76(10)
C301-C302-H30B	109.5	F11-P2-F8	90.33(10)
H30A-C302-H30B	109.5	N100-C101-C102	177.4(5)
C301-C302-H30C	109.5	C101-C102-H10A	109.5
H30A-C302-H30C	109.5	C101-C102-H10B	109.5
H30B-C302-H30C	109.5	H10A-C102-H10B	109.5
F3-P1-F1	179.97(16)	C101-C102-H10C	109.5
F3-P1-F2	90.12(12)	H10A-C102-H10C	109.5
F1-P1-F2	89.91(12)	H10B-C102-H10C	109.5
F3-P1-F6	90.22(11)	N200-C201-C202	178.5(4)
F1-P1-F6	89.77(11)	C201-C202-H20A	109.5
F2-P1-F6	90.42(11)	C201-C202-H20B	109.5
F3-P1-F5	90.73(11)	H20A-C202-H20B	109.5
F1-P1-F5	89.29(11)	C201-C202-H20C	109.5
F2-P1-F5	90.10(11)	H20A-C202-H20C	109.5
F6-P1-F5	178.92(12)	H20B-C202-H20C	109.5

Table S4. Anisotropic displacement parameters ($Å^2$) for complex **4**.
The anisotropicdisplacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C2	0.0297(16)	0.0230(13)	0.0242(14)	-0.0018(11)	0.0030(13)	-0.0012(12)
C3	0.0313(16)	0.0217(13)	0.0245(14)	-0.0023(11)	0.0046(13)	-0.0020(12)
C5	0.0366(17)	0.0240(14)	0.0278(15)	-0.0022(11)	0.0106(14)	-0.0005(12)
C6	0.0338(17)	0.0242(14)	0.0368(17)	-0.0024(12)	0.0116(14)	0.0034(12)
C7	0.0316(16)	0.0237(14)	0.0362(17)	0.0030(12)	0.0049(14)	0.0013(12)
C8	0.0336(16)	0.0238(13)	0.0287(15)	0.0016(11)	0.0054(14)	-0.0011(12)
C9	0.0403(18)	0.0303(15)	0.0291(16)	0.0041(12)	0.0058(14)	0.0032(13)
C10	0.0443(19)	0.0344(15)	0.0276(15)	0.0049(12)	0.0094(15)	0.0040(14)
C11	0.0383(17)	0.0276(14)	0.0270(15)	-0.0008(11)	0.0095(14)	-0.0024(13)
C12	0.0440(18)	0.0323(15)	0.0285(15)	-0.0033(12)	0.0137(14)	-0.0019(14)
C13	0.0382(18)	0.0320(15)	0.0331(16)	-0.0059(12)	0.0150(15)	0.0011(13)
C14	0.0329(16)	0.0248(14)	0.0317(16)	-0.0044(11)	0.0066(14)	0.0008(12)
C16	0.0348(17)	0.0225(14)	0.0201(13)	-0.0005(10)	0.0082(13)	0.0031(12)
C17	0.0356(17)	0.0233(14)	0.0218(13)	-0.0025(11)	0.0110(13)	-0.0007(12)
C19	0.0332(18)	0.0265(14)	0.0281(15)	-0.0004(11)	0.0069(14)	-0.0021(12)
C20	0.0331(17)	0.0324(15)	0.0263(15)	0.0028(12)	0.0062(13)	0.0021(13)
C21	0.0395(18)	0.0248(14)	0.0290(15)	0.0030(11)	0.0126(14)	0.0065(12)
C22	0.0381(17)	0.0246(14)	0.0242(14)	0.0010(11)	0.0107(13)	0.0026(12)
C23	0.046(2)	0.0222(14)	0.0356(16)	0.0015(12)	0.0149(15)	0.0037(13)
C24	0.0427(19)	0.0230(14)	0.0375(16)	0.0010(12)	0.0126(15)	-0.0016(13)
C25	0.0367(17)	0.0243(14)	0.0271(15)	-0.0007(11)	0.0109(14)	-0.0017(12)
C26	0.0386(18)	0.0276(14)	0.0298(15)	-0.0030(12)	0.0109(14)	-0.0064(13)
C27	0.0301(16)	0.0334(16)	0.0307(15)	-0.0019(12)	0.0090(13)	-0.0010(13)
C28	0.0340(17)	0.0270(14)	0.0303(15)	-0.0021(11)	0.0103(14)	0.0022(12)
C29	0.0380(17)	0.0209(13)	0.0231(15)	-0.0027(11)	0.0006(14)	0.0067(12)
C30	0.0361(17)	0.0214(13)	0.0259(15)	0.0005(11)	0.0044(14)	0.0054(12)
C31	0.0382(17)	0.0238(14)	0.0264(15)	-0.0024(11)	0.0003(14)	0.0123(13)
C32	0.0419(18)	0.0302(15)	0.0292(15)	-0.0009(12)	0.0095(15)	0.0083(13)
C33	0.0450(19)	0.0455(18)	0.0308(17)	-0.0007(13)	0.0113(15)	0.0132(15)
C34	0.046(2)	0.055(2)	0.0290(16)	-0.0092(15)	0.0069(16)	0.0136(17)
C35	0.0416(19)	0.0411(17)	0.0310(17)	-0.0126(14)	-0.0012(15)	0.0121(15)
C36	0.0351(17)	0.0303(15)	0.0298(16)	-0.0034(12)	0.0001(14)	0.0103(13)
C37	0.0374(17)	0.0269(14)	0.0318(16)	-0.0061(12)	-0.0029(14)	0.0117(13)
C38	0.0405(19)	0.0378(17)	0.0399(18)	-0.0150(14)	0.0004(16)	0.0033(15)
C39	0.041(2)	0.0330(16)	0.051(2)	-0.0133(15)	-0.0059(17)	0.0021(15)
C40	0.0326(18)	0.0340(16)	0.050(2)	-0.0017(14)	0.0000(16)	0.0023(14)
C41	0.0356(17)	0.0276(15)	0.0346(16)	-0.0012(12)	-0.0004(14)	0.0062(13)
C42	0.0338(17)	0.0198(13)	0.0320(16)	0.0005(12)	-0.0002(14)	0.0049(12)
N1	0.0320(13)	0.0206(11)	0.0258(12)	-0.0012(9)	0.0074(11)	0.0008(10)
N4	0.0322(13)	0.0222(11)	0.0233(12)	-0.0023(9)	0.0062(11)	-0.0001(10)
N15	0.0319(14)	0.0244(11)	0.0220(11)	-0.0016(9)	0.0071(11)	0.0022(10)
N18	0.0322(14)	0.0215(11)	0.0242(12)	-0.0010(9)	0.0068(11)	-0.0012(10)
O1	0.0379(11)	0.0223(9)	0.0255(10)	-0.0007(7)	0.0079(9)	0.0007(8)
O2	0.0378(11)	0.0219(9)	0.0238(10)	-0.0028(7)	0.0071(9)	-0.0003(8)
Si1	0.0333(4)	0.0212(3)	0.0245(4)	-0.0009(3)	0.0063(3)	0.0021(3)
C301	0.080(4)	0.059(3)	0.217(7)	-0.011(4)	-0.025(4)	0.015(3)
C302	0.102(4)	0.085(4)	0.194(6)	0.065(4)	0.043(4)	0.031(3)
N300	0.078(3)	0.064(3)	0.265(7)	-0.034(3)	0.000(4)	0.008(2)
F1	0.0618(13)	0.0775(14)	0.0688(13)	-0.0344(11)	0.0214(11)	-0.0134(11)
F2	0.0635(13)	0.0708(13)	0.0597(12)	0.0176(10)	0.0208(11)	0.0160(11)
F3	0.0573(13)	0.0653(13)	0.0650(13)	-0.0273(10)	0.0049(11)	0.0037(10)
F4	0.0951(16)	0.0650(13)	0.0657(13)	0.0192(10)	0.0413(13)	0.0286(12)
F5	0.0484(11)	0.0565(11)	0.0609(12)	-0.0022(9)	0.0137(10)	0.0155(9)
F6	0.0421(11)	0.0665(12)	0.0614(12)	-0.0041(10)	0.0118(10)	0.0121(9)
P1	0.0402(5)	0.0433(5)	0.0365(4)	-0.0038(4)	0.0063(4)	0.0077(4)

F7	0.0365(10)	0.0548(11)	0.0427(10)	0.0108(8)	0.0074(9)	-0.0037(8)
F8	0.0636(12)	0.0342(9)	0.0596(11)	0.0016(8)	0.0279(10)	-0.0064(9)
F9	0.0367(11)	0.0909(15)	0.0510(11)	0.0176(10)	0.0084(9)	-0.0042(10)
F10	0.0732(13)	0.0348(9)	0.0729(13)	0.0161(9)	0.0364(11)	0.0131(9)
F11	0.0526(11)	0.0595(11)	0.0406(10)	0.0004(8)	0.0200(9)	-0.0044(9)
F12	0.0547(11)	0.0472(10)	0.0453(10)	0.0001(8)	0.0245(9)	0.0025(9)
P2	0.0339(5)	0.0344(4)	0.0357(4)	0.0063(3)	0.0118(4)	0.0010(3)
C101	0.071(3)	0.058(3)	0.080(3)	0.010(2)	0.024(2)	0.011(2)
C102	0.082(3)	0.099(3)	0.069(3)	-0.008(2)	0.025(3)	-0.004(3)
N100	0.088(3)	0.060(2)	0.117(3)	0.005(2)	0.006(2)	0.002(2)
C201	0.046(2)	0.065(2)	0.0394(19)	-0.0134(17)	0.0109(17)	-0.0048(18)
C202	0.077(3)	0.072(3)	0.096(3)	-0.041(2)	0.018(3)	-0.004(2)
N200	0.0526(19)	0.0625(19)	0.0440(17)	-0.0122(14)	0.0142(15)	-0.0073(15)

Table S5. Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for complex **4**.

	x	y	z	U(eq)	Occupancy
H5	1.1673	0.3035	0.0844	0.035	1
H6	1.3102	0.2485	0.1791	0.038	1
H7	1.3166	0.2337	0.3378	0.038	1
H9	1.2270	0.2553	0.4784	0.042	1
H10	1.0880	0.2982	0.5295	0.043	1
H12	0.8938	0.3571	0.4856	0.041	1
H13	0.7567	0.4053	0.3684	0.040	1
H14	0.7790	0.4116	0.2153	0.037	1
H19	0.6744	0.3815	-0.0048	0.036	1
H20	0.5470	0.4466	-0.0639	0.038	1
H21	0.6357	0.5202	-0.0264	0.037	1
H23	0.8447	0.5696	0.0576	0.041	1
H24	1.0637	0.5708	0.1414	0.042	1
H26	1.2792	0.5241	0.2198	0.039	1
H27	1.3762	0.4521	0.2539	0.038	1
H28	1.2510	0.3855	0.2193	0.037	1
H32	1.0771	0.3614	-0.1455	0.041	1
H33	1.0775	0.3420	-0.2999	0.049	1
H34	0.9426	0.2832	-0.3870	0.054	1
H35	0.8088	0.2439	-0.3224	0.049	1
H38	0.6779	0.2120	-0.2655	0.051	1
H39	0.5359	0.1779	-0.2003	0.056	1
H40	0.5199	0.2034	-0.0515	0.051	1
H41	0.6541	0.2629	0.0327	0.043	1
H30A	0.4504	0.6775	0.2286	0.193	1
H30B	0.5486	0.6358	0.2729	0.193	1
H30C	0.5208	0.6735	0.3438	0.193	1
H10A	0.5295	0.5365	0.5574	0.125	1
H10B	0.6214	0.5399	0.4919	0.125	1
H10C	0.4760	0.5594	0.4515	0.125	1
H20A	0.1098	0.5372	0.4934	0.127	1
H20B	-0.0104	0.5439	0.3950	0.127	1
H20C	0.1347	0.5530	0.3958	0.127	1

Table S6. Torsion angles [°] for complex **4**.

N1-C2-C3-N4	1.9(3)	C36-C31-C32-C33	2.0(4)
C11-C2-C3-N4	-179.7(2)	C30-C31-C32-C33	-177.6(2)
N1-C2-C3-C8	-177.5(2)	C31-C32-C33-C34	-2.0(4)
C11-C2-C3-C8	0.8(4)	C32-C33-C34-C35	0.0(4)
N4-C5-C6-C7	0.0(4)	C33-C34-C35-C36	2.0(4)
C5-C6-C7-C8	-0.4(4)	C34-C35-C36-C31	-1.9(4)
N4-C3-C8-C7	-1.0(4)	C34-C35-C36-C37	176.4(3)
C2-C3-C8-C7	178.3(2)	C32-C31-C36-C35	-0.1(4)
N4-C3-C8-C9	178.8(2)	C30-C31-C36-C35	179.5(2)
C2-C3-C8-C9	-1.8(4)	C32-C31-C36-C37	-178.4(2)
C6-C7-C8-C3	0.9(4)	C30-C31-C36-C37	1.2(4)
C6-C7-C8-C9	-179.0(3)	C35-C36-C37-C38	1.0(4)
C3-C8-C9-C10	0.7(4)	C31-C36-C37-C38	179.3(3)
C7-C8-C9-C10	-179.5(3)	C35-C36-C37-C42	-177.5(2)
C8-C9-C10-C11	1.4(4)	C31-C36-C37-C42	0.7(4)
N1-C2-C11-C12	0.8(4)	C42-C37-C38-C39	-0.5(4)
C3-C2-C11-C12	-177.4(2)	C36-C37-C38-C39	-179.1(3)
N1-C2-C11-C10	179.5(2)	C37-C38-C39-C40	1.8(4)
C3-C2-C11-C10	1.3(4)	C38-C39-C40-C41	-0.9(4)
C9-C10-C11-C2	-2.4(4)	C39-C40-C41-C42	-1.3(4)
C9-C10-C11-C12	176.1(3)	C40-C41-C42-C37	2.5(4)
C2-C11-C12-C13	-0.1(4)	C40-C41-C42-C29	-178.6(2)
C10-C11-C12-C13	-178.6(3)	C38-C37-C42-C41	-1.6(4)
C11-C12-C13-C14	-0.5(4)	C36-C37-C42-C41	177.0(2)
C12-C13-C14-N1	0.4(4)	C38-C37-C42-C29	179.5(2)
N15-C16-C17-N18	0.0(3)	C36-C37-C42-C29	-1.9(4)
C25-C16-C17-N18	177.0(2)	C30-C29-C42-C41	-177.7(2)
N15-C16-C17-C22	-177.1(2)	O1-C29-C42-C41	1.7(4)
C25-C16-C17-C22	-0.1(4)	C30-C29-C42-C37	1.1(4)
N18-C19-C20-C21	-0.2(4)	O1-C29-C42-C37	-179.4(2)
C19-C20-C21-C22	1.5(4)	C13-C14-N1-C2	0.2(4)
N18-C17-C22-C21	-0.2(4)	C13-C14-N1-Si1	177.76(19)
C16-C17-C22-C21	176.6(2)	C11-C2-N1-C14	-0.9(4)
N18-C17-C22-C23	-178.8(2)	C3-C2-N1-C14	177.4(2)
C16-C17-C22-C23	-2.0(4)	C11-C2-N1-Si1	-178.8(2)
C20-C21-C22-C17	-1.2(4)	C3-C2-N1-Si1	-0.5(3)
C20-C21-C22-C23	177.2(3)	C6-C5-N4-C3	-0.1(4)
C17-C22-C23-C24	2.2(4)	C6-C5-N4-Si1	-175.93(19)
C21-C22-C23-C24	-176.3(3)	C8-C3-N4-C5	0.7(4)
C22-C23-C24-C25	-0.3(4)	C2-C3-N4-C5	-178.7(2)
N15-C16-C25-C26	0.9(4)	C8-C3-N4-Si1	177.0(2)
C17-C16-C25-C26	-175.9(2)	C2-C3-N4-Si1	-2.4(3)
N15-C16-C25-C24	178.8(2)	C27-C28-N15-C16	0.0(4)
C17-C16-C25-C24	2.0(4)	C27-C28-N15-Si1	175.61(19)
C23-C24-C25-C16	-1.8(4)	C25-C16-N15-C28	-1.2(4)
C23-C24-C25-C26	175.9(3)	C17-C16-N15-C28	175.7(2)
C16-C25-C26-C27	0.6(4)	C25-C16-N15-Si1	-177.5(2)
C24-C25-C26-C27	-177.1(3)	C17-C16-N15-Si1	-0.6(3)
C25-C26-C27-C28	-1.8(4)	C20-C19-N18-C17	-1.3(4)
C26-C27-C28-N15	1.5(4)	C20-C19-N18-Si1	-176.9(2)
O1-C29-C30-O2	0.3(3)	C22-C17-N18-C19	1.5(4)
C42-C29-C30-O2	179.8(2)	C16-C17-N18-C19	-175.5(2)
O1-C29-C30-C31	-178.7(2)	C22-C17-N18-Si1	177.7(2)
C42-C29-C30-C31	0.8(4)	C16-C17-N18-Si1	0.6(3)
C29-C30-C31-C32	177.6(3)	C30-C29-O1-Si1	-1.3(3)
O2-C30-C31-C32	-1.2(4)	C42-C29-O1-Si1	179.16(19)
C29-C30-C31-C36	-2.0(4)	C29-C30-O2-Si1	0.9(3)
O2-C30-C31-C36	179.2(2)	C31-C30-O2-Si1	179.8(2)

C29-O1-Si1-O2	1.54(16)
C29-O1-Si1-N18	95.63(16)
C29-O1-Si1-N4	-91.62(16)
C29-O1-Si1-N15	126.2(11)
C29-O1-Si1-N1	-174.24(16)
C30-O2-Si1-O1	-1.41(16)
C30-O2-Si1-N18	-94.94(16)
C30-O2-Si1-N4	91.76(16)
C30-O2-Si1-N15	-177.65(16)
C30-O2-Si1-N1	113.7(11)
C19-N18-Si1-O1	-7.3(2)
C17-N18-Si1-O1	176.91(18)
C19-N18-Si1-O2	86.3(2)
C17-N18-Si1-O2	-89.41(18)
C19-N18-Si1-N4	-138.1(6)
C17-N18-Si1-N4	46.1(7)
C19-N18-Si1-N15	175.0(2)
C17-N18-Si1-N15	-0.74(18)
C19-N18-Si1-N1	-95.9(2)
C17-N18-Si1-N1	88.35(18)
C5-N4-Si1-O1	89.5(2)
C3-N4-Si1-O1	-86.49(18)
C5-N4-Si1-O2	-4.1(2)
C3-N4-Si1-O2	179.91(18)
C5-N4-Si1-N18	-139.7(6)
C3-N4-Si1-N18	44.3(7)
C5-N4-Si1-N15	-93.3(2)
C3-N4-Si1-N15	90.71(18)
C5-N4-Si1-N1	177.6(2)
C3-N4-Si1-N1	1.66(18)
C28-N15-Si1-O1	154.2(11)
C16-N15-Si1-O1	-30.0(12)
C28-N15-Si1-O2	-81.0(2)
C16-N15-Si1-O2	94.72(18)
C28-N15-Si1-N18	-175.0(2)
C16-N15-Si1-N18	0.71(18)
C28-N15-Si1-N4	11.9(2)
C16-N15-Si1-N4	-172.31(18)
C28-N15-Si1-N1	94.6(2)
C16-N15-Si1-N1	-89.62(18)
C14-N1-Si1-O1	-85.0(2)
C2-N1-Si1-O1	92.59(18)
C14-N1-Si1-O2	159.6(11)
C2-N1-Si1-O2	-22.7(12)
C14-N1-Si1-N18	8.2(2)
C2-N1-Si1-N18	-174.13(17)
C14-N1-Si1-N4	-178.2(2)
C2-N1-Si1-N4	-0.61(17)
C14-N1-Si1-N15	91.0(2)
C2-N1-Si1-N15	-91.36(18)

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