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Silicon Phthalocyanines as N-Type Semiconductors in Organic Thin Film Transistors

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Supporting Information

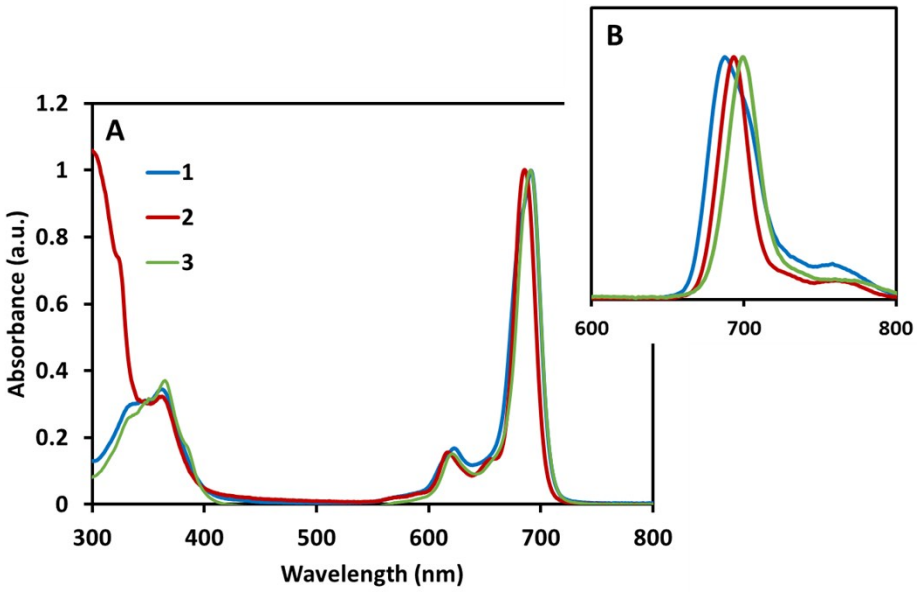

Figure S1: (A) Normalized UV-Vis absorption and (B) normalized fluorescence in toluene solution for **1 (**blue) **2** (red) and **3** (green).

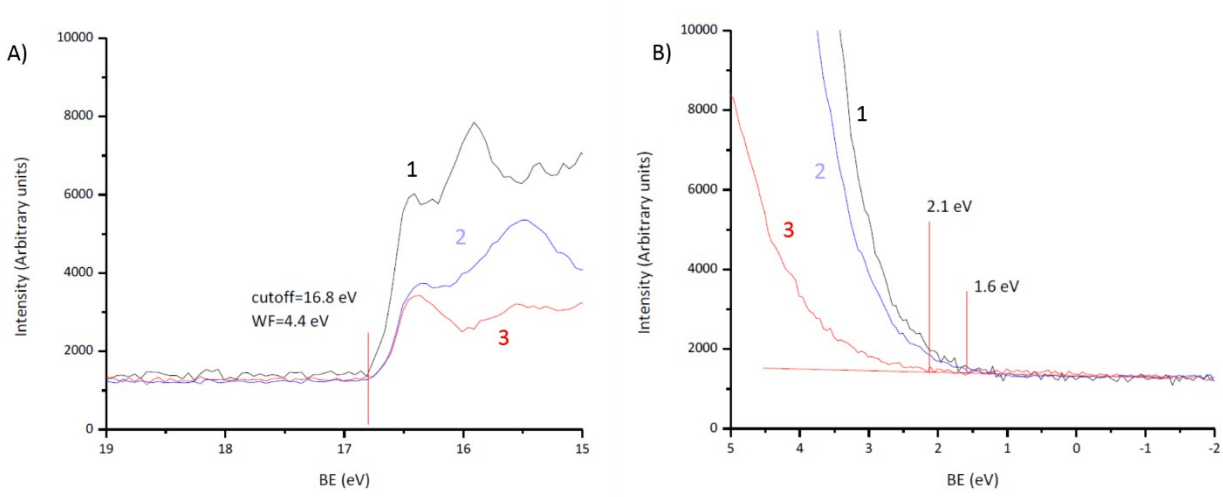

Figure S2: Ultraviolet photoelectron spectroscopy (UPS) for 1 (black), 2 (blue) and 3 (red) where A) is a close of the high binding energy peak used to determine the work function and B) are the low binding energy peaks used to determine the HOMO offset.

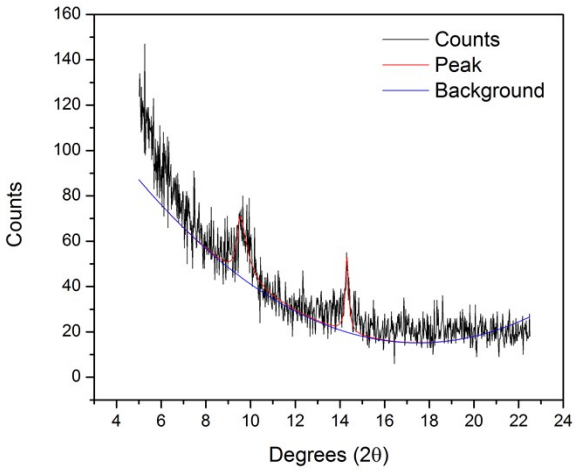

Figure S3: X-ray diffraction pattern for 25 nm thick film of **1** deposited on ODTS treated SiO_2 at 200 °C. Peaks and background were manually assigned to term peak intensity above background.

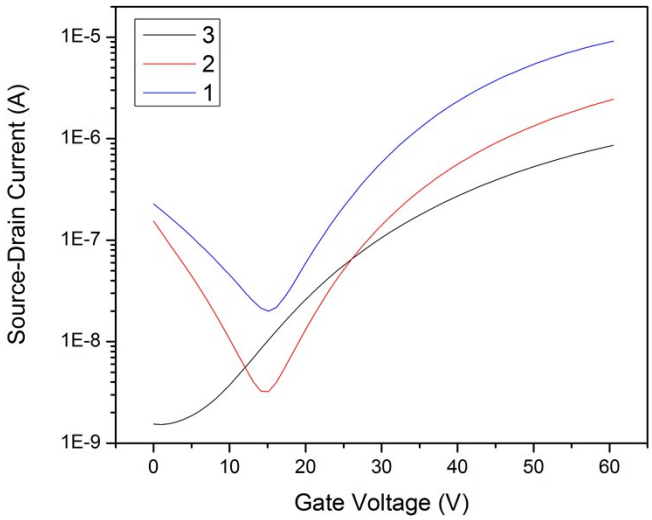

Figure S4: Sample transfer curves for OTFTs using three different active SiPcs with channel length L = 2.5 μm

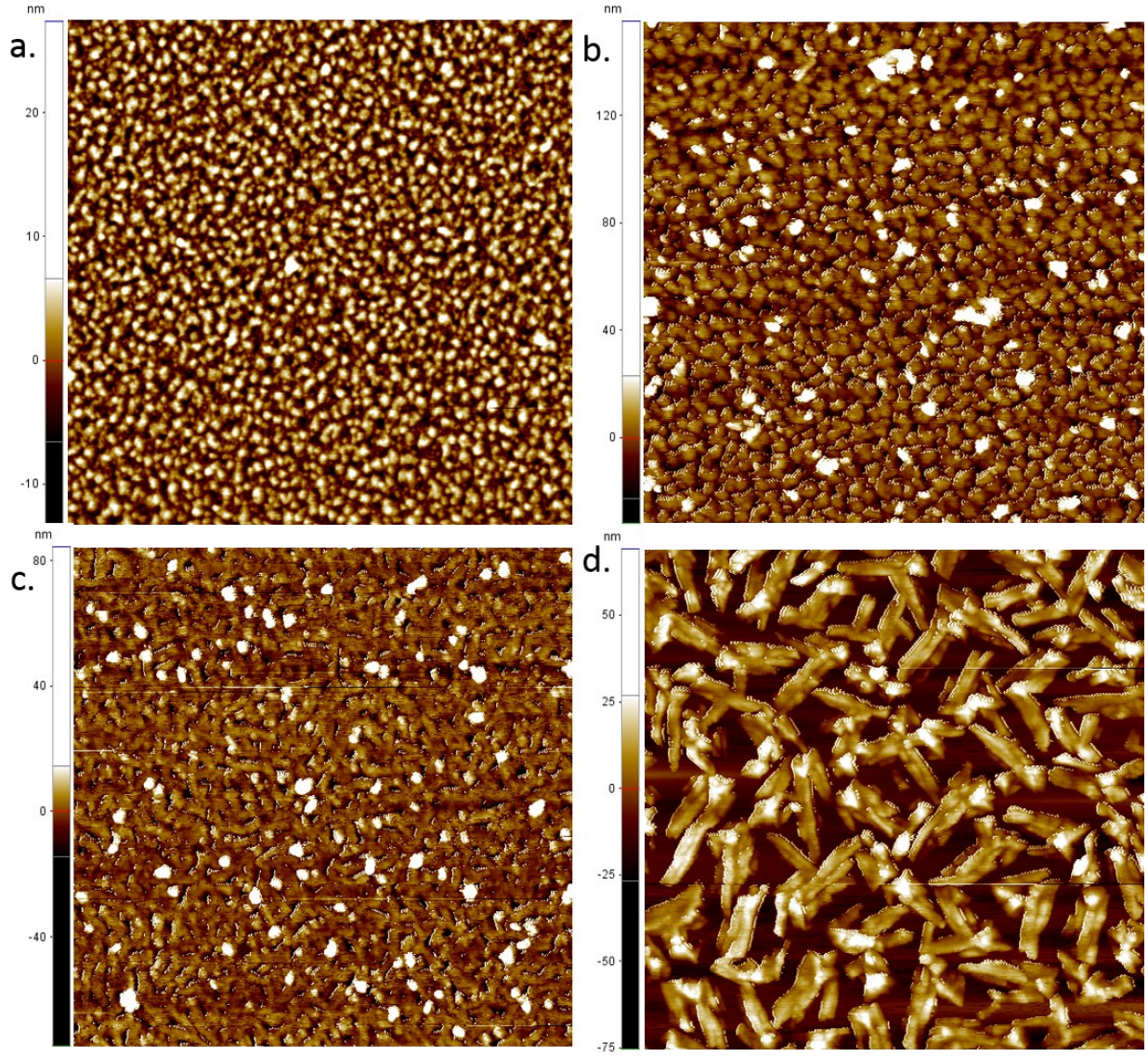

Figure S5: Atomic force microscopy (AFM) images of **1** deposited on different surfaces: a. Plasma treated, room temperature substrate; b. OTS-treated, room temperature substrate; c. OTS-treated, 200 ºC substrate; d. OTS-treated, 250 ºC substrate. All images are 4x4 µm.

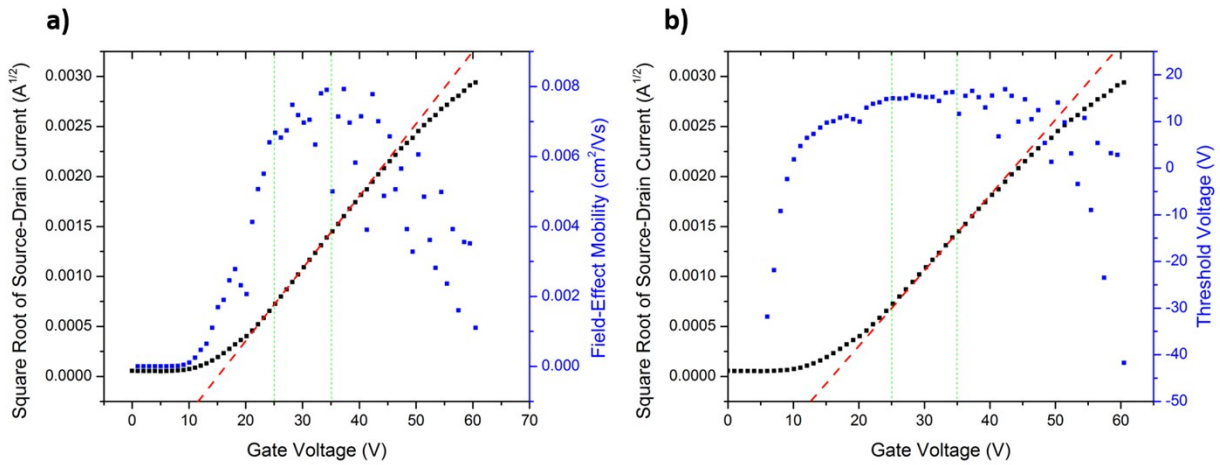

Figure S6: **a)** Saturation region electron field-effect mobility (μ_e) and **b)** threshold voltage (V_T) compared with the square root of source-drain current as a function of gate bias (V_{GS}) for an OTFT using **1** as the active semiconducting layer deposited at 200 ºC on an ODTS surface treated dielectric (L = 20 µm). The green lines represent the bounds used to fit this data linearly to **Equation 1**, resulting in a line of best fit (red, dashes) with slope proportional to the calculated μ_e and x-intercept equal to the reported V_T.

Table S1. Crystal data and structure refinement for Bis(benzoate) SiPc.

Identification code	Bis(benzoate) SiPc	
Empirical formula	C46 H26 N8 O4 Si	
Formula weight	782.84	
Temperature	147(2) K	
Wavelength	1.54178 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.2516(5) Å	α= 108.442(2)°.
	b = 10.4441(5) Å	β= 112.993(2)°.
	c = 10.6544(5) Å	γ = 97.706(2)°.
Volume	859.00(8) $Å^3$	
Z	1	
Density (calculated)	1.513 Mg/m^3	
Absorption coefficient	1.132 mm^{-1}	
F(000)	404	
Crystal size	0.200 x 0.180 x 0.150 mm^3	
Theta range for data collection	4.671 to 67.825°.	
Index ranges	-11<=h<=10, -12<=k<=12, -12<=l<=12	
Reflections collected	19258	
Independent reflections	3049 [R(int) = 0.0307]	
Completeness to theta = 67.679°	98.3 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7530 and 0.6778	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3049 / 0 / 268	
Goodness-of-fit on F^2	1.059	
Final R indices [I>2sigma(I)]	R1 = 0.0326, wR2 = 0.0815	
R indices (all data)	R1 = 0.0334, wR2 = 0.0821	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.181 and -0.347 $e.Å^{-3}$	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for Bis(benzoate) SiPc. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Si(1)	5000	5000	5000	15(1)
O(1)	5688(1)	3620(1)	5416(1)	18(1)
O(2)	4535(1)	1688(1)	3263(1)	30(1)
N(1)	7227(1)	6161(1)	6222(1)	17(1)
N(2)	7369(1)	7001(1)	8682(1)	19(1)
N(3)	4661(1)	5486(1)	6721(1)	17(1)
N(4)	1780(1)	4181(1)	5621(1)	20(1)
C(1)	7995(2)	6939(1)	7749(2)	18(1)
C(2)	5811(2)	6336(1)	8183(2)	18(1)
C(3)	5056(2)	6432(1)	9157(2)	19(1)
C(4)	5665(2)	7113(2)	10700(2)	23(1)
C(5)	4577(2)	6949(2)	11271(2)	26(1)
C(6)	2916(2)	6165(2)	10342(2)	27(1)
C(7)	2308(2)	5502(2)	8818(2)	23(1)
C(8)	3414(2)	5636(1)	8248(2)	19(1)
C(9)	3200(2)	5044(1)	6747(2)	18(1)
C(10)	1609(2)	3624(1)	4257(2)	18(1)
C(11)	80(2)	2649(1)	3017(2)	19(1)
C(12)	-1410(2)	2080(2)	2954(2)	23(1)
C(13)	-2639(2)	1105(2)	1577(2)	26(1)
C(14)	-2389(2)	712(2)	310(2)	26(1)
C(15)	-911(2)	1297(2)	375(2)	23(1)
C(16)	327(2)	2281(1)	1761(2)	19(1)
C(17)	5558(2)	2336(1)	4556(2)	20(1)
C(18)	6839(2)	1741(2)	5334(2)	20(1)
C(19)	6696(2)	328(2)	4631(2)	29(1)
C(20)	7907(2)	-238(2)	5285(2)	35(1)
C(21)	9258(2)	607(2)	6647(2)	34(1)
C(22)	9408(2)	2012(2)	7348(2)	31(1)
C(23)	8200(2)	2584(2)	6689(2)	23(1)

Table S3. Bond lengths [Å] and angles [°] for Bis(benzoate) SiPc.

Si(1)-O(1)	1.7626(9)
Si(1)-O(1)#1	1.7627(9)
Si(1)-N(3)#1	1.9030(11)
Si(1)-N(3)	1.9030(11)
Si(1)-N(1)	1.9093(11)
Si(1)-N(1)#1	1.9093(11)
O(1)-C(17)	1.3213(17)
O(2)-C(17)	1.2130(17)
N(1)-C(10)#1	1.3808(18)
N(1)-C(1)	1.3852(17)
N(2)-C(2)	1.3201(18)
N(2)-C(1)	1.3211(18)
N(3)-C(9)	1.3823(17)
N(3)-C(2)	1.3870(17)
N(4)-C(10)	1.3178(18)
N(4)-C(9)	1.3206(18)
C(1)-C(16)#1	1.4508(19)
C(2)-C(3)	1.4474(19)
C(3)-C(8)	1.392(2)
C(3)-C(4)	1.398(2)
C(4)-C(5)	1.382(2)
C(4)-H(4A)	0.9500
C(5)-C(6)	1.405(2)
C(5)-H(5A)	0.9500
C(6)-C(7)	1.379(2)
C(6)-H(6A)	0.9500
C(7)-C(8)	1.391(2)
C(7)-H(7A)	0.9500
C(8)-C(9)	1.4401(19)
C(10)-N(1)#1	1.3808(18)
C(10)-C(11)	1.4448(19)
C(11)-C(16)	1.389(2)
C(11)-C(12)	1.393(2)
C(12)-C(13)	1.387(2)

C(12)-H(12A)	0.9500
C(13)-C(14)	1.401(2)
C(13)-H(13A)	0.9500
C(14)-C(15)	1.386(2)
C(14)-H(14A)	0.9500
C(15)-C(16)	1.3967(19)
C(15)-H(15A)	0.9500
C(16)-C(1)#1	1.4509(19)
C(17)-C(18)	1.4947(19)
C(18)-C(23)	1.387(2)
C(18)-C(19)	1.388(2)
C(19)-C(20)	1.384(2)
C(19)-H(19A)	0.9500
C(20)-C(21)	1.387(2)
C(20)-H(20A)	0.9500
C(21)-C(22)	1.378(2)
C(21)-H(21A)	0.9500
C(22)-C(23)	1.389(2)
C(22)-H(22A)	0.9500
C(23)-H(23A)	0.9500

O(1)-Si(1)-O(1)#1	180.0
O(1)-Si(1)-N(3)#1	92.42(4)
O(1)#1-Si(1)-N(3)#1	87.58(4)
O(1)-Si(1)-N(3)	87.58(4)
O(1)#1-Si(1)-N(3)	92.42(4)
N(3)#1-Si(1)-N(3)	180.0
O(1)-Si(1)-N(1)	86.96(4)
O(1)#1-Si(1)-N(1)	93.04(4)
N(3)#1-Si(1)-N(1)	90.60(5)
N(3)-Si(1)-N(1)	89.40(5)
O(1)-Si(1)-N(1)#1	93.04(4)
O(1)#1-Si(1)-N(1)#1	86.96(4)
N(3)#1-Si(1)-N(1)#1	89.40(5)
N(3)-Si(1)-N(1)#1	90.60(5)
N(1)-Si(1)-N(1)#1	180.0

C(17)-O(1)-Si(1)	132.07(9)
C(10)#1-N(1)-C(1)	106.68(11)
C(10)#1-N(1)-Si(1)	126.16(9)
C(1)-N(1)-Si(1)	127.16(9)
C(2)-N(2)-C(1)	120.65(12)
C(9)-N(3)-C(2)	106.58(11)
C(9)-N(3)-Si(1)	126.04(9)
C(2)-N(3)-Si(1)	127.38(9)
C(10)-N(4)-C(9)	121.09(12)
N(2)-C(1)-N(1)	127.69(12)
N(2)-C(1)-C(16)#1	122.46(12)
N(1)-C(1)-C(16)#1	109.85(12)
N(2)-C(2)-N(3)	127.61(12)
N(2)-C(2)-C(3)	122.44(12)
N(3)-C(2)-C(3)	109.94(12)
C(8)-C(3)-C(4)	120.70(13)
C(8)-C(3)-C(2)	106.42(12)
C(4)-C(3)-C(2)	132.87(13)
C(5)-C(4)-C(3)	117.19(14)
C(5)-C(4)-H(4A)	121.4
C(3)-C(4)-H(4A)	121.4
C(4)-C(5)-C(6)	121.70(14)
C(4)-C(5)-H(5A)	119.2
C(6)-C(5)-H(5A)	119.2
C(7)-C(6)-C(5)	121.18(14)
C(7)-C(6)-H(6A)	119.4
C(5)-C(6)-H(6A)	119.4
C(6)-C(7)-C(8)	117.10(14)
C(6)-C(7)-H(7A)	121.4
C(8)-C(7)-H(7A)	121.4
C(7)-C(8)-C(3)	122.09(13)
C(7)-C(8)-C(9)	131.01(13)
C(3)-C(8)-C(9)	106.89(12)
N(4)-C(9)-N(3)	128.14(13)
N(4)-C(9)-C(8)	121.69(12)
N(3)-C(9)-C(8)	110.14(11)

N(4)-C(10)-N(1)#1	127.93(12)
N(4)-C(10)-C(11)	121.98(13)
N(1)#1-C(10)-C(11)	110.08(12)
C(16)-C(11)-C(12)	121.97(13)
C(16)-C(11)-C(10)	106.83(12)
C(12)-C(11)-C(10)	131.17(13)
C(13)-C(12)-C(11)	116.91(14)
C(13)-C(12)-H(12A)	121.5
C(11)-C(12)-H(12A)	121.5
C(12)-C(13)-C(14)	121.40(14)
C(12)-C(13)-H(13A)	119.3
C(14)-C(13)-H(13A)	119.3
C(15)-C(14)-C(13)	121.42(13)
C(15)-C(14)-H(14A)	119.3
C(13)-C(14)-H(14A)	119.3
C(14)-C(15)-C(16)	117.25(14)
C(14)-C(15)-H(15A)	121.4
C(16)-C(15)-H(15A)	121.4
C(11)-C(16)-C(15)	121.03(13)
C(11)-C(16)-C(1)#1	106.49(12)
C(15)-C(16)-C(1)#1	132.45(13)
O(2)-C(17)-O(1)	124.97(13)
O(2)-C(17)-C(18)	122.07(13)
O(1)-C(17)-C(18)	112.96(12)
C(23)-C(18)-C(19)	119.81(13)
C(23)-C(18)-C(17)	121.48(13)
C(19)-C(18)-C(17)	118.60(13)
C(20)-C(19)-C(18)	120.02(15)
C(20)-C(19)-H(19A)	120.0
C(18)-C(19)-H(19A)	120.0
C(19)-C(20)-C(21)	119.93(15)
C(19)-C(20)-H(20A)	120.0
C(21)-C(20)-H(20A)	120.0
C(22)-C(21)-C(20)	120.29(14)
C(22)-C(21)-H(21A)	119.9
C(20)-C(21)-H(21A)	119.9

C(21)-C(22)-C(23)	119.90(15)
C(21)-C(22)-H(22A)	120.0
C(23)-C(22)-H(22A)	120.0
C(18)-C(23)-C(22)	120.03(14)
C(18)-C(23)-H(23A)	120.0
C(22)-C(23)-H(23A)	120.0

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for Bis(benzoate) SiPc. The anisotropic 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}
Si(1)	12(1)	15(1)	16(1)	5(1)	5(1)	4(1)
O(1)	17(1)	18(1)	17(1)	5(1)	6(1)	4(1)
O(2)	31(1)	22(1)	21(1)	4(1)	1(1)	8(1)
N(1)	15(1)	17(1)	18(1)	6(1)	6(1)	5(1)
N(2)	16(1)	19(1)	18(1)	7(1)	6(1)	5(1)
N(3)	15(1)	16(1)	17(1)	6(1)	6(1)	5(1)
N(4)	16(1)	18(1)	21(1)	5(1)	8(1)	4(1)
C(1)	15(1)	17(1)	18(1)	6(1)	5(1)	6(1)
C(2)	17(1)	17(1)	18(1)	7(1)	6(1)	7(1)
C(3)	20(1)	16(1)	20(1)	8(1)	8(1)	7(1)
C(4)	25(1)	21(1)	20(1)	8(1)	8(1)	8(1)
C(5)	35(1)	22(1)	20(1)	7(1)	14(1)	11(1)
C(6)	31(1)	27(1)	30(1)	12(1)	20(1)	12(1)
C(7)	22(1)	22(1)	28(1)	9(1)	13(1)	7(1)
C(8)	20(1)	16(1)	21(1)	7(1)	9(1)	7(1)
C(9)	16(1)	16(1)	21(1)	7(1)	8(1)	6(1)
C(10)	16(1)	15(1)	22(1)	7(1)	8(1)	5(1)
C(11)	16(1)	16(1)	22(1)	6(1)	6(1)	6(1)
C(12)	18(1)	22(1)	27(1)	7(1)	10(1)	5(1)
C(13)	15(1)	24(1)	33(1)	9(1)	8(1)	3(1)
C(14)	16(1)	21(1)	26(1)	4(1)	3(1)	3(1)
C(15)	18(1)	22(1)	21(1)	6(1)	5(1)	6(1)
C(16)	15(1)	18(1)	21(1)	7(1)	6(1)	6(1)
C(17)	20(1)	19(1)	21(1)	7(1)	9(1)	5(1)
C(18)	21(1)	22(1)	21(1)	10(1)	11(1)	7(1)
C(19)	32(1)	22(1)	28(1)	9(1)	11(1)	10(1)
C(20)	42(1)	24(1)	42(1)	14(1)	19(1)	18(1)
C(21)	31(1)	37(1)	43(1)	25(1)	16(1)	20(1)
C(22)	24(1)	34(1)	31(1)	16(1)	7(1)	10(1)
C(23)	24(1)	22(1)	23(1)	10(1)	11(1)	8(1)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for Bis(benzoate) SiPc.

	x	y	z	U(eq)
H(4A)	6781	7666	11330	27
H(5A)	4962	7377	12318	31
H(6A)	2197	6090	10771	32
H(7A)	1184	4977	8185	28
H(12A)	-1577	2348	3814	28
H(13A)	-3672	695	1490	31
H(14A)	-3250	31	-614	31
H(15A)	-746	1039	-487	27
H(19A)	5768	-251	3700	35
H(20A)	7812	-1203	4801	42
H(21A)	10083	216	7099	41
H(22A)	10337	2588	8279	37
H(23A)	8306	3554	7168	27

Table S6. Torsion angles [°] for Bis(benzoate) SiPc.

N(3)#1-Si(1)-O(1)-C(17)	-34.16(12)
N(3)-Si(1)-O(1)-C(17)	145.84(12)
N(1)-Si(1)-O(1)-C(17)	-124.64(12)
N(1)#1-Si(1)-O(1)-C(17)	55.36(12)
C(2)-N(2)-C(1)-N(1)	-4.2(2)
C(2)-N(2)-C(1)-C(16)#1	176.35(12)
C(10)#1-N(1)-C(1)-N(2)	-176.93(13)
Si(1)-N(1)-C(1)-N(2)	2.6(2)
C(10)#1-N(1)-C(1)-C(16)#1	2.61(14)
Si(1)-N(1)-C(1)-C(16)#1	-177.81(9)
C(1)-N(2)-C(2)-N(3)	2.2(2)
C(1)-N(2)-C(2)-C(3)	-176.90(12)
C(9)-N(3)-C(2)-N(2)	-179.16(13)
Si(1)-N(3)-C(2)-N(2)	1.1(2)
C(9)-N(3)-C(2)-C(3)	0.08(14)
Si(1)-N(3)-C(2)-C(3)	-179.71(8)
N(2)-C(2)-C(3)-C(8)	178.41(12)
N(3)-C(2)-C(3)-C(8)	-0.87(15)
N(2)-C(2)-C(3)-C(4)	-2.4(2)
N(3)-C(2)-C(3)-C(4)	178.30(14)
C(8)-C(3)-C(4)-C(5)	0.5(2)
C(2)-C(3)-C(4)-C(5)	-178.52(14)
C(3)-C(4)-C(5)-C(6)	-1.7(2)
C(4)-C(5)-C(6)-C(7)	1.2(2)
C(5)-C(6)-C(7)-C(8)	0.5(2)
C(6)-C(7)-C(8)-C(3)	-1.7(2)
C(6)-C(7)-C(8)-C(9)	177.31(14)
C(4)-C(3)-C(8)-C(7)	1.2(2)
C(2)-C(3)-C(8)-C(7)	-179.53(12)
C(4)-C(3)-C(8)-C(9)	-178.02(12)
C(2)-C(3)-C(8)-C(9)	1.26(14)
C(10)-N(4)-C(9)-N(3)	-0.5(2)
C(10)-N(4)-C(9)-C(8)	-178.68(12)
C(2)-N(3)-C(9)-N(4)	-177.60(13)

Si(1)-N(3)-C(9)-N(4)	2.2(2)
C(2)-N(3)-C(9)-C(8)	0.73(14)
Si(1)-N(3)-C(9)-C(8)	-179.48(8)
C(7)-C(8)-C(9)-N(4)	-1.9(2)
C(3)-C(8)-C(9)-N(4)	177.17(12)
C(7)-C(8)-C(9)-N(3)	179.61(13)
C(3)-C(8)-C(9)-N(3)	-1.28(15)
C(9)-N(4)-C(10)-N(1)#1	-1.3(2)
C(9)-N(4)-C(10)-C(11)	178.31(12)
N(4)-C(10)-C(11)-C(16)	179.70(12)
N(1)#1-C(10)-C(11)-C(16)	-0.64(15)
N(4)-C(10)-C(11)-C(12)	-2.0(2)
N(1)#1-C(10)-C(11)-C(12)	177.70(13)
C(16)-C(11)-C(12)-C(13)	1.1(2)
C(10)-C(11)-C(12)-C(13)	-177.05(14)
C(11)-C(12)-C(13)-C(14)	0.0(2)
C(12)-C(13)-C(14)-C(15)	-0.9(2)
C(13)-C(14)-C(15)-C(16)	0.8(2)
C(12)-C(11)-C(16)-C(15)	-1.3(2)
C(10)-C(11)-C(16)-C(15)	177.27(12)
C(12)-C(11)-C(16)-C(1)#1	-179.47(12)
C(10)-C(11)-C(16)-C(1)#1	-0.94(14)
C(14)-C(15)-C(16)-C(11)	0.3(2)
C(14)-C(15)-C(16)-C(1)#1	177.97(14)
Si(1)-O(1)-C(17)-O(2)	-21.6(2)
Si(1)-O(1)-C(17)-C(18)	157.56(9)
O(2)-C(17)-C(18)-C(23)	166.10(14)
O(1)-C(17)-C(18)-C(23)	-13.07(19)
O(2)-C(17)-C(18)-C(19)	-10.2(2)
O(1)-C(17)-C(18)-C(19)	170.66(13)
C(23)-C(18)-C(19)-C(20)	0.3(2)
C(17)-C(18)-C(19)-C(20)	176.59(14)
C(18)-C(19)-C(20)-C(21)	0.3(3)
C(19)-C(20)-C(21)-C(22)	-0.5(3)
C(20)-C(21)-C(22)-C(23)	0.2(3)
C(19)-C(18)-C(23)-C(22)	-0.6(2)

C(17)-C(18)-C(23)-C(22)	-176.86(14)
C(21)-C(22)-C(23)-C(18)	0.4(2)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1

Table S7. Crystal data and structure refinement for Bis(1-napthoate) SiPc.

Identification code	Bis(1-napthoate) SiPc	
Empirical formula	C54 H30 N8 O4 Si	
Formula weight	882.95	
Temperature	147(2) K	
Wavelength	1.54178 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.6931(2) Å	α= 104.5910(10)°.
	b = 10.8895(3) Å	β= 109.7420(10)°.
	c = 11.6021(3) Å	γ = 92.1480(10)°.
Volume	991.30(4) $Å^3$	
Z	1	
Density (calculated)	1.479 Mg/m^3	
Absorption coefficient	1.054 mm^{-1}	
F(000)	456	
Crystal size	0.100 x 0.040 x 0.040 mm^3	
Theta range for data collection	4.219 to 67.252°.	
Index ranges	-10<=h<=10, -12<=k<=13, -13<=l<=13	
Reflections collected	35793	
Independent reflections	3512 [R(int) = 0.0507]	
Completeness to theta = 67.252°	98.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7529 and 0.6744	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3512 / 0 / 304	
Goodness-of-fit on F^2	1.074	
Final R indices [I>2sigma(I)]	R1 = 0.0358, wR2 = 0.0881	
R indices (all data)	R1 = 0.0418, wR2 = 0.0916	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.381 and -0.355 $e.Å^{-3}$	

Table S8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for Bis(1-napthoate) SiPc. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Si(1)	5000	5000	5000	17(1)
O(1)	5701(1)	3529(1)	5107(1)	20(1)
O(2)	6543(2)	3551(1)	7160(1)	31(1)
N(1)	3063(2)	4035(1)	3656(1)	18(1)
N(2)	3948(2)	3665(1)	1840(1)	21(1)
N(3)	6052(2)	4961(1)	3800(1)	18(1)
N(4)	8693(2)	6225(1)	5161(1)	21(1)
C(1)	2875(2)	3526(1)	2389(1)	19(1)
C(2)	5400(2)	4362(1)	2505(2)	19(1)
C(3)	6558(2)	4599(2)	1914(2)	21(1)
C(4)	6464(2)	4236(2)	649(2)	24(1)
C(5)	7793(2)	4684(2)	397(2)	30(1)
C(6)	9172(2)	5453(2)	1373(2)	32(1)
C(7)	9281(2)	5802(2)	2633(2)	27(1)
C(8)	7932(2)	5359(2)	2881(2)	21(1)
C(9)	7611(2)	5558(1)	4052(2)	19(1)
C(10)	8362(2)	6414(1)	6215(2)	19(1)
C(11)	9484(2)	7208(1)	7425(2)	21(1)
C(12)	11047(2)	7880(2)	7775(2)	24(1)
C(13)	11783(2)	8593(2)	9034(2)	27(1)
C(14)	11005(2)	8641(2)	9922(2)	28(1)
C(15)	9459(2)	7972(2)	9574(2)	25(1)
C(16)	8712(2)	7254(2)	8304(2)	21(1)
C(17)	6323(2)	3013(2)	6055(2)	20(1)
C(18)	6840(2)	1711(2)	5672(2)	23(1)
C(19)	7859(2)	1333(2)	6684(2)	33(1)
C(20)	8572(3)	198(2)	6511(2)	40(1)
C(21)	8250(3)	-553(2)	5311(2)	40(1)
C(22)	7188(2)	-255(2)	4229(2)	30(1)
C(23)	6842(3)	-1056(2)	2988(2)	40(1)
C(24)	5806(3)	-764(2)	1940(2)	40(1)

C(25)	5060(2)	346(2)	2103(2)	35(1)
C(26)	5357(2)	1154(2)	3295(2)	30(1)
C(27)	6440(2)	910(2)	4403(2)	26(1)

Table S9. Bond lengths [Å] and angles [°] for Bis(1-napthoate) SiPc.

Si(1)-O(1)#1	1.7538(10)
Si(1)-O(1)	1.7538(10)
Si(1)-N(3)#1	1.9004(12)
Si(1)-N(3)	1.9004(12)
Si(1)-N(1)#1	1.9076(13)
Si(1)-N(1)	1.9077(13)
O(1)-C(17)	1.3227(18)
O(2)-C(17)	1.2128(19)
N(1)-C(10)#1	1.382(2)
N(1)-C(1)	1.3845(19)
N(2)-C(1)	1.318(2)
N(2)-C(2)	1.320(2)
N(3)-C(2)	1.381(2)
N(3)-C(9)	1.384(2)
N(4)-C(9)	1.314(2)
N(4)-C(10)	1.318(2)
C(1)-C(16)#1	1.446(2)
C(2)-C(3)	1.444(2)
C(3)-C(8)	1.387(2)
C(3)-C(4)	1.394(2)
C(4)-C(5)	1.384(2)
C(4)-H(4A)	0.9500
C(5)-C(6)	1.397(3)
C(5)-H(5A)	0.9500
C(6)-C(7)	1.384(2)
C(6)-H(6A)	0.9500
C(7)-C(8)	1.394(2)
C(7)-H(7A)	0.9500
C(8)-C(9)	1.444(2)
C(10)-N(1)#1	1.382(2)
C(10)-C(11)	1.439(2)
C(11)-C(16)	1.391(2)
C(11)-C(12)	1.396(2)
C(12)-C(13)	1.380(2)

C(12)-H(12A)	0.9500
C(13)-C(14)	1.403(2)
C(13)-H(13A)	0.9500
C(14)-C(15)	1.383(2)
C(14)-H(14A)	0.9500
C(15)-C(16)	1.392(2)
C(15)-H(15A)	0.9500
C(16)-C(1)#1	1.446(2)
C(17)-C(18)	1.508(2)
C(18)-C(19)	1.379(2)
C(18)-C(27)	1.427(2)
C(19)-C(20)	1.403(3)
C(19)-H(19A)	0.9500
C(20)-C(21)	1.354(3)
C(20)-H(20A)	0.9500
C(21)-C(22)	1.406(3)
C(21)-H(21A)	0.9500
C(22)-C(23)	1.407(3)
C(22)-C(27)	1.447(2)
C(23)-C(24)	1.366(3)
C(23)-H(23A)	0.9500
C(24)-C(25)	1.394(3)
C(24)-H(24A)	0.9500
C(25)-C(26)	1.372(3)
C(25)-H(25A)	0.9500
C(26)-C(27)	1.408(2)
C(26)-H(26A)	0.9500

O(1)#1-Si(1)-O(1)	180.00(7)
O(1)#1-Si(1)-N(3)#1	86.62(5)
O(1)-Si(1)-N(3)#1	93.38(5)
O(1)#1-Si(1)-N(3)	93.38(5)
O(1)-Si(1)-N(3)	86.62(5)
N(3)#1-Si(1)-N(3)	180.00(8)
O(1)#1-Si(1)-N(1)#1	86.86(5)
O(1)-Si(1)-N(1)#1	93.14(5)

N(3)#1-Si(1)-N(1)#1	89.80(5)
N(3)-Si(1)-N(1)#1	90.20(5)
O(1)#1-Si(1)-N(1)	93.14(5)
O(1)-Si(1)-N(1)	86.86(5)
N(3)#1-Si(1)-N(1)	90.20(5)
N(3)-Si(1)-N(1)	89.80(5)
N(1)#1-Si(1)-N(1)	180.0
C(17)-O(1)-Si(1)	134.39(10)
C(10)#1-N(1)-C(1)	106.49(13)
C(10)#1-N(1)-Si(1)	126.44(10)
C(1)-N(1)-Si(1)	126.71(10)
C(1)-N(2)-C(2)	120.72(14)
C(2)-N(3)-C(9)	106.64(12)
C(2)-N(3)-Si(1)	126.90(10)
C(9)-N(3)-Si(1)	126.44(10)
C(9)-N(4)-C(10)	121.20(14)
N(2)-C(1)-N(1)	127.71(14)
N(2)-C(1)-C(16)#1	122.18(14)
N(1)-C(1)-C(16)#1	110.09(13)
N(2)-C(2)-N(3)	127.93(14)
N(2)-C(2)-C(3)	121.95(14)
N(3)-C(2)-C(3)	110.12(13)
C(8)-C(3)-C(4)	121.48(15)
C(8)-C(3)-C(2)	106.53(13)
C(4)-C(3)-C(2)	131.97(15)
C(5)-C(4)-C(3)	117.07(16)
C(5)-C(4)-H(4A)	121.5
C(3)-C(4)-H(4A)	121.5
C(4)-C(5)-C(6)	121.22(15)
C(4)-C(5)-H(5A)	119.4
C(6)-C(5)-H(5A)	119.4
C(7)-C(6)-C(5)	121.96(16)
C(7)-C(6)-H(6A)	119.0
C(5)-C(6)-H(6A)	119.0
C(6)-C(7)-C(8)	116.61(16)
C(6)-C(7)-H(7A)	121.7

C(8)-C(7)-H(7A)	121.7
C(3)-C(8)-C(7)	121.66(15)
C(3)-C(8)-C(9)	106.88(13)
C(7)-C(8)-C(9)	131.45(15)
N(4)-C(9)-N(3)	127.95(14)
N(4)-C(9)-C(8)	122.25(14)
N(3)-C(9)-C(8)	109.80(13)
N(4)-C(10)-N(1)#1	127.65(14)
N(4)-C(10)-C(11)	122.14(14)
N(1)#1-C(10)-C(11)	110.15(13)
C(16)-C(11)-C(12)	121.47(15)
C(16)-C(11)-C(10)	106.92(14)
C(12)-C(11)-C(10)	131.60(15)
C(13)-C(12)-C(11)	116.78(15)
C(13)-C(12)-H(12A)	121.6
C(11)-C(12)-H(12A)	121.6
C(12)-C(13)-C(14)	121.82(16)
C(12)-C(13)-H(13A)	119.1
C(14)-C(13)-H(13A)	119.1
C(15)-C(14)-C(13)	121.38(16)
C(15)-C(14)-H(14A)	119.3
C(13)-C(14)-H(14A)	119.3
C(14)-C(15)-C(16)	116.87(15)
C(14)-C(15)-H(15A)	121.6
C(16)-C(15)-H(15A)	121.6
C(11)-C(16)-C(15)	121.68(15)
C(11)-C(16)-C(1)#1	106.35(14)
C(15)-C(16)-C(1)#1	131.96(15)
O(2)-C(17)-O(1)	123.73(14)
O(2)-C(17)-C(18)	121.51(14)
O(1)-C(17)-C(18)	114.67(13)
C(19)-C(18)-C(27)	119.52(15)
C(19)-C(18)-C(17)	113.92(15)
C(27)-C(18)-C(17)	126.49(15)
C(18)-C(19)-C(20)	122.27(18)
C(18)-C(19)-H(19A)	118.9

C(20)-C(19)-H(19A)	118.9
C(21)-C(20)-C(19)	118.98(18)
C(21)-C(20)-H(20A)	120.5
C(19)-C(20)-H(20A)	120.5
C(20)-C(21)-C(22)	122.34(18)
C(20)-C(21)-H(21A)	118.8
C(22)-C(21)-H(21A)	118.8
C(21)-C(22)-C(23)	121.75(17)
C(21)-C(22)-C(27)	118.86(17)
C(23)-C(22)-C(27)	119.39(17)
C(24)-C(23)-C(22)	121.54(17)
C(24)-C(23)-H(23A)	119.2
C(22)-C(23)-H(23A)	119.2
C(23)-C(24)-C(25)	119.36(18)
C(23)-C(24)-H(24A)	120.3
C(25)-C(24)-H(24A)	120.3
C(26)-C(25)-C(24)	121.17(18)
C(26)-C(25)-H(25A)	119.4
C(24)-C(25)-H(25A)	119.4
C(25)-C(26)-C(27)	121.67(16)
C(25)-C(26)-H(26A)	119.2
C(27)-C(26)-H(26A)	119.2
C(26)-C(27)-C(18)	125.18(15)
C(26)-C(27)-C(22)	116.85(16)
C(18)-C(27)-C(22)	117.97(15)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1

Table S10. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for Bis(1-napthoate) SiPc. The anisotropic 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}
Si(1)	18(1)	17(1)	14(1)	4(1)	6(1)	1(1)
O(1)	24(1)	19(1)	17(1)	6(1)	7(1)	2(1)
O(2)	43(1)	28(1)	19(1)	6(1)	8(1)	9(1)
N(1)	20(1)	18(1)	16(1)	4(1)	7(1)	1(1)
N(2)	23(1)	21(1)	18(1)	5(1)	8(1)	2(1)
N(3)	19(1)	19(1)	16(1)	5(1)	7(1)	1(1)
N(4)	20(1)	22(1)	20(1)	6(1)	7(1)	2(1)
C(1)	23(1)	18(1)	17(1)	6(1)	6(1)	2(1)
C(2)	22(1)	19(1)	18(1)	5(1)	8(1)	4(1)
C(3)	23(1)	21(1)	21(1)	7(1)	10(1)	6(1)
C(4)	27(1)	28(1)	19(1)	6(1)	10(1)	7(1)
C(5)	33(1)	41(1)	23(1)	11(1)	17(1)	12(1)
C(6)	28(1)	44(1)	31(1)	14(1)	19(1)	6(1)
C(7)	23(1)	32(1)	27(1)	9(1)	12(1)	2(1)
C(8)	22(1)	22(1)	21(1)	8(1)	10(1)	5(1)
C(9)	20(1)	18(1)	19(1)	6(1)	7(1)	2(1)
C(10)	19(1)	18(1)	19(1)	7(1)	6(1)	2(1)
C(11)	21(1)	20(1)	20(1)	7(1)	6(1)	2(1)
C(12)	22(1)	25(1)	24(1)	8(1)	6(1)	1(1)
C(13)	22(1)	27(1)	28(1)	7(1)	3(1)	-2(1)
C(14)	28(1)	27(1)	20(1)	2(1)	2(1)	-1(1)
C(15)	27(1)	25(1)	20(1)	4(1)	6(1)	1(1)
C(16)	22(1)	19(1)	21(1)	6(1)	6(1)	2(1)
C(17)	19(1)	22(1)	20(1)	7(1)	6(1)	1(1)
C(18)	23(1)	20(1)	29(1)	8(1)	12(1)	1(1)
C(19)	37(1)	30(1)	35(1)	14(1)	13(1)	8(1)
C(20)	49(1)	36(1)	41(1)	20(1)	14(1)	16(1)
C(21)	47(1)	32(1)	48(1)	17(1)	22(1)	14(1)
C(22)	33(1)	23(1)	37(1)	10(1)	16(1)	1(1)
C(23)	49(1)	25(1)	48(1)	5(1)	23(1)	8(1)
C(24)	46(1)	32(1)	34(1)	-1(1)	14(1)	-3(1)

C(25)	36(1)	31(1)	31(1)	1(1)	7(1)	-3(1)
C(26)	29(1)	22(1)	34(1)	5(1)	10(1)	1(1)
C(27)	24(1)	21(1)	32(1)	6(1)	13(1)	-2(1)

Table S11. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{-3}) for Bis(1-napthoate) SiPc.

	x	y	z	U(eq)
H(4A)	5530	3705	-11	29
H(5A)	7767	4464	-456	36
H(6A)	10061	5745	1166	38
H(7A)	10227	6316	3296	32
H(12A)	11578	7849	7176	29
H(13A)	12846	9064	9306	33
H(14A)	11552	9144	10779	33
H(15A)	8930	8001	10174	30
H(19A)	8086	1859	7527	39
H(20A)	9271	-40	7226	48
H(21A)	8760	-1308	5195	48
H(23A)	7339	-1818	2876	48
H(24A)	5596	-1312	1109	48
H(25A)	4333	547	1375	43
H(26A)	4818	1897	3375	36

Table S12. Torsion angles [°] for Bis(1-napthoate) SiPc.

N(3)#1-Si(1)-O(1)-C(17)	-40.31(14)
N(3)-Si(1)-O(1)-C(17)	139.69(14)
N(1)#1-Si(1)-O(1)-C(17)	49.68(14)
N(1)-Si(1)-O(1)-C(17)	-130.33(14)
C(2)-N(2)-C(1)-N(1)	-0.5(2)
C(2)-N(2)-C(1)-C(16)#1	-178.61(14)
C(10)#1-N(1)-C(1)-N(2)	-177.80(15)
Si(1)-N(1)-C(1)-N(2)	-4.4(2)
C(10)#1-N(1)-C(1)-C(16)#1	0.54(16)
Si(1)-N(1)-C(1)-C(16)#1	173.98(10)
C(1)-N(2)-C(2)-N(3)	4.0(2)
C(1)-N(2)-C(2)-C(3)	-175.95(14)
C(9)-N(3)-C(2)-N(2)	179.15(15)
Si(1)-N(3)-C(2)-N(2)	-2.4(2)
C(9)-N(3)-C(2)-C(3)	-0.91(16)
Si(1)-N(3)-C(2)-C(3)	177.54(10)
N(2)-C(2)-C(3)-C(8)	179.85(14)
N(3)-C(2)-C(3)-C(8)	-0.09(17)
N(2)-C(2)-C(3)-C(4)	1.7(3)
N(3)-C(2)-C(3)-C(4)	-178.28(15)
C(8)-C(3)-C(4)-C(5)	-1.0(2)
C(2)-C(3)-C(4)-C(5)	177.00(16)
C(3)-C(4)-C(5)-C(6)	0.7(2)
C(4)-C(5)-C(6)-C(7)	0.2(3)
C(5)-C(6)-C(7)-C(8)	-0.8(3)
C(4)-C(3)-C(8)-C(7)	0.3(2)
C(2)-C(3)-C(8)-C(7)	-178.08(14)
C(4)-C(3)-C(8)-C(9)	179.44(14)
C(2)-C(3)-C(8)-C(9)	1.02(16)
C(6)-C(7)-C(8)-C(3)	0.5(2)
C(6)-C(7)-C(8)-C(9)	-178.31(16)
C(10)-N(4)-C(9)-N(3)	-0.8(2)
C(10)-N(4)-C(9)-C(8)	178.74(14)
C(2)-N(3)-C(9)-N(4)	-178.84(14)

Si(1)-N(3)-C(9)-N(4)	2.7(2)
C(2)-N(3)-C(9)-C(8)	1.56(16)
Si(1)-N(3)-C(9)-C(8)	-176.91(10)
C(3)-C(8)-C(9)-N(4)	178.74(14)
C(7)-C(8)-C(9)-N(4)	-2.3(3)
C(3)-C(8)-C(9)-N(3)	-1.64(17)
C(7)-C(8)-C(9)-N(3)	177.34(16)
C(9)-N(4)-C(10)-N(1)#1	1.0(2)
C(9)-N(4)-C(10)-C(11)	-175.94(14)
N(4)-C(10)-C(11)-C(16)	176.67(14)
N(1)#1-C(10)-C(11)-C(16)	-0.72(17)
N(4)-C(10)-C(11)-C(12)	-1.8(3)
N(1)#1-C(10)-C(11)-C(12)	-179.20(15)
C(16)-C(11)-C(12)-C(13)	-0.1(2)
C(10)-C(11)-C(12)-C(13)	178.15(16)
C(11)-C(12)-C(13)-C(14)	0.1(2)
C(12)-C(13)-C(14)-C(15)	0.1(3)
C(13)-C(14)-C(15)-C(16)	-0.2(2)
C(12)-C(11)-C(16)-C(15)	0.0(2)
C(10)-C(11)-C(16)-C(15)	-178.65(14)
C(12)-C(11)-C(16)-C(1)#1	179.03(14)
C(10)-C(11)-C(16)-C(1)#1	0.36(16)
C(14)-C(15)-C(16)-C(11)	0.2(2)
C(14)-C(15)-C(16)-C(1)#1	-178.57(16)
Si(1)-O(1)-C(17)-O(2)	-0.1(2)
Si(1)-O(1)-C(17)-C(18)	-176.83(10)
O(2)-C(17)-C(18)-C(19)	-12.7(2)
O(1)-C(17)-C(18)-C(19)	164.05(14)
O(2)-C(17)-C(18)-C(27)	170.39(16)
O(1)-C(17)-C(18)-C(27)	-12.8(2)
C(27)-C(18)-C(19)-C(20)	2.2(3)
C(17)-C(18)-C(19)-C(20)	-174.91(16)
C(18)-C(19)-C(20)-C(21)	0.0(3)
C(19)-C(20)-C(21)-C(22)	-1.8(3)
C(20)-C(21)-C(22)-C(23)	-178.86(19)
C(20)-C(21)-C(22)-C(27)	1.3(3)

C(21)-C(22)-C(23)-C(24)	179.83(19)
C(27)-C(22)-C(23)-C(24)	-0.4(3)
C(22)-C(23)-C(24)-C(25)	-0.7(3)
C(23)-C(24)-C(25)-C(26)	0.5(3)
C(24)-C(25)-C(26)-C(27)	0.9(3)
C(25)-C(26)-C(27)-C(18)	178.74(16)
C(25)-C(26)-C(27)-C(22)	-1.9(2)
C(19)-C(18)-C(27)-C(26)	176.83(16)
C(17)-C(18)-C(27)-C(26)	-6.4(3)
C(19)-C(18)-C(27)-C(22)	-2.6(2)
C(17)-C(18)-C(27)-C(22)	174.18(15)
C(21)-C(22)-C(27)-C(26)	-178.58(16)
C(23)-C(22)-C(27)-C(26)	1.6(2)
C(21)-C(22)-C(27)-C(18)	0.8(2)
C(23)-C(22)-C(27)-C(18)	-178.95(16)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1

Table S13. Crystal data and structure refinement for Bis(9-anthronoate) SiPc.

Identification code	Bis(9-anthronoate) SiPc	
Empirical formula	C62 H34 N8 O4 Si	
Formula weight	983.06	
Temperature	147(2) K	
Wavelength	1.54178 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 10.9435(2) Å	α= 84.533(1)°.
	b = 11.4401(2) Å	β= 83.930(1)°.
	c = 18.8824(3) Å	γ = 77.144(1)°.
Volume	2285.51(7) $Å^3$	
Z	2	
Density (calculated)	1.428 Mg/m^3	
Absorption coefficient	0.977 mm^{-1}	
F(000)	1016	
Crystal size	0.110 x 0.090 x 0.080 mm^3	
Theta range for data collection	2.359 to 67.893°.	
Index ranges	-12<=h<=13, -13<=k<=13, -22<=l<=22	
Reflections collected	88968	
Independent reflections	8124 [R(int) = 0.0405]	
Completeness to theta = 67.679°	98.3 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7530 and 0.6688	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8124 / 0 / 679	
Goodness-of-fit on F^2	1.036	
Final R indices [I>2sigma(I)]	R1 = 0.0319, wR2 = 0.0808	
R indices (all data)	R1 = 0.0370, wR2 = 0.0842	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.249 and -0.361 $e.Å^{-3}$	

Table S14. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for Bis(9-anthronoate) SiPc. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Si(1A)	0	5000	10000	14(1)
O(1A)	106(1)	3588(1)	9668(1)	18(1)
O(2A)	-1241(1)	3812(1)	8821(1)	29(1)
N(1A)	1625(1)	5014(1)	9539(1)	17(1)
N(2A)	2961(1)	3818(1)	10410(1)	19(1)
N(3A)	743(1)	4095(1)	10807(1)	16(1)
N(4A)	-1104(1)	3879(1)	11592(1)	20(1)
C(1A)	2767(1)	4433(1)	9790(1)	18(1)
C(2A)	2012(1)	3691(1)	10880(1)	17(1)
C(3A)	2201(1)	3039(1)	11569(1)	19(1)
C(4A)	3288(1)	2445(1)	11884(1)	24(1)
C(5A)	3129(1)	1853(1)	12551(1)	28(1)
C(6A)	1929(2)	1859(1)	12896(1)	29(1)
C(7A)	852(1)	2459(1)	12586(1)	25(1)
C(8A)	1013(1)	3050(1)	11912(1)	19(1)
C(9A)	119(1)	3713(1)	11430(1)	18(1)
C(10A)	-1902(1)	4486(1)	11140(1)	19(1)
C(11A)	-3241(1)	4745(1)	11324(1)	21(1)
C(12A)	-3964(1)	4467(1)	11942(1)	25(1)
C(13A)	-5250(1)	4902(1)	11954(1)	28(1)
C(14A)	-5800(1)	5586(1)	11369(1)	28(1)
C(15A)	-5078(1)	5855(1)	10754(1)	24(1)
C(16A)	-3783(1)	5426(1)	10741(1)	20(1)
C(17A)	-442(1)	3192(1)	9176(1)	18(1)
C(18A)	-15(1)	1868(1)	9104(1)	18(1)
C(19A)	1260(1)	1353(1)	8931(1)	21(1)
C(20A)	2220(1)	2038(1)	8819(1)	25(1)
C(21A)	3447(1)	1503(2)	8666(1)	32(1)
C(22A)	3813(2)	246(2)	8599(1)	37(1)
C(23A)	2934(2)	-439(2)	8689(1)	34(1)
C(24A)	1634(1)	82(1)	8861(1)	25(1)

C(25A)	725(2)	-613(1)	8974(1)	28(1)
C(26A)	-535(1)	-114(1)	9154(1)	24(1)
C(27A)	-1456(2)	-833(1)	9297(1)	29(1)
C(28A)	-2684(2)	-342(1)	9466(1)	32(1)
C(29A)	-3079(2)	915(1)	9525(1)	29(1)
C(30A)	-2229(1)	1638(1)	9409(1)	24(1)
C(31A)	-930(1)	1160(1)	9215(1)	20(1)
Si(1B)	5000	5000	5000	15(1)
O(1B)	5116(1)	6381(1)	5292(1)	18(1)
O(2B)	4861(1)	6168(1)	6488(1)	28(1)
N(1B)	6536(1)	5023(1)	4425(1)	17(1)
N(2B)	5768(1)	6327(1)	3404(1)	19(1)
N(3B)	4070(1)	5950(1)	4269(1)	17(1)
N(4B)	1928(1)	6170(1)	4810(1)	23(1)
C(1B)	6665(1)	5658(1)	3769(1)	18(1)
C(2B)	4574(1)	6456(1)	3643(1)	18(1)
C(3B)	3590(1)	7241(1)	3267(1)	20(1)
C(4B)	3633(1)	7988(1)	2641(1)	25(1)
C(5B)	2509(1)	8689(1)	2439(1)	29(1)
C(6B)	1371(1)	8640(1)	2845(1)	31(1)
C(7B)	1325(1)	7901(1)	3466(1)	28(1)
C(8B)	2464(1)	7203(1)	3674(1)	21(1)
C(9B)	2785(1)	6394(1)	4298(1)	20(1)
C(10B)	2262(1)	5489(1)	5392(1)	20(1)
C(11B)	1342(1)	5177(1)	5947(1)	22(1)
C(12B)	34(1)	5438(1)	6004(1)	28(1)
C(13B)	-568(1)	4967(1)	6611(1)	30(1)
C(14B)	111(1)	4255(1)	7143(1)	28(1)
C(15B)	1413(1)	3992(1)	7084(1)	25(1)
C(16B)	2017(1)	4465(1)	6472(1)	20(1)
C(17B)	5026(1)	6774(1)	5937(1)	19(1)
C(18B)	5117(1)	8064(1)	5924(1)	18(1)
C(19B)	6184(1)	8446(1)	5582(1)	20(1)
C(20B)	7230(1)	7654(1)	5240(1)	24(1)
C(21B)	8248(1)	8061(1)	4927(1)	29(1)
C(22B)	8310(1)	9286(1)	4933(1)	31(1)

C(23B)	7344(1)	10070(1)	5256(1)	28(1)
C(24B)	6253(1)	9684(1)	5593(1)	21(1)
C(25B)	5265(1)	10474(1)	5936(1)	23(1)
C(26B)	4213(1)	10101(1)	6281(1)	21(1)
C(27B)	3218(1)	10921(1)	6641(1)	27(1)
C(28B)	2197(1)	10558(1)	6977(1)	31(1)
C(29B)	2096(1)	9344(1)	6967(1)	30(1)
C(30B)	3019(1)	8531(1)	6633(1)	25(1)
C(31B)	4127(1)	8867(1)	6279(1)	19(1)

Table S15. Bond lengths [Å] and angles [°] for Bis(9-anthronoate) SiPc.

Si(1A)-O(1A)#1	1.7641(9)
Si(1A)-O(1A)	1.7641(9)
Si(1A)-N(1A)#1	1.8979(11)
Si(1A)-N(1A)	1.8979(11)
Si(1A)-N(3A)#1	1.9082(10)
Si(1A)-N(3A)	1.9082(10)
O(1A)-C(17A)	1.3215(15)
O(2A)-C(17A)	1.2134(16)
N(1A)-C(10A)#1	1.3843(17)
N(1A)-C(1A)	1.3874(17)
N(2A)-C(2A)	1.3169(17)
N(2A)-C(1A)	1.3197(17)
N(3A)-C(9A)	1.3799(17)
N(3A)-C(2A)	1.3800(17)
N(4A)-C(9A)	1.3171(17)
N(4A)-C(10A)	1.3214(17)
C(1A)-C(16A)#1	1.4424(19)
C(2A)-C(3A)	1.4473(18)
C(3A)-C(8A)	1.3879(19)
C(3A)-C(4A)	1.3934(19)
C(4A)-C(5A)	1.386(2)
C(4A)-H(4AA)	0.9500
C(5A)-C(6A)	1.402(2)
C(5A)-H(5AA)	0.9500
C(6A)-C(7A)	1.383(2)
C(6A)-H(6AA)	0.9500
C(7A)-C(8A)	1.3950(19)
C(7A)-H(7AA)	0.9500
C(8A)-C(9A)	1.4453(18)
C(10A)-N(1A)#1	1.3843(17)
C(10A)-C(11A)	1.4398(19)
C(11A)-C(12A)	1.3920(19)
C(11A)-C(16A)	1.3920(19)
C(12A)-C(13A)	1.382(2)

C(12A)-H(12A)	0.9500
C(13A)-C(14A)	1.400(2)
C(13A)-H(13A)	0.9500
C(14A)-C(15A)	1.383(2)
C(14A)-H(14A)	0.9500
C(15A)-C(16A)	1.3915(19)
C(15A)-H(15A)	0.9500
C(16A)-C(1A)#1	1.4425(19)
C(17A)-C(18A)	1.4964(18)
C(18A)-C(19A)	1.4056(19)
C(18A)-C(31A)	1.4097(19)
C(19A)-C(20A)	1.432(2)
C(19A)-C(24A)	1.4343(19)
C(20A)-C(21A)	1.359(2)
C(20A)-H(20B)	0.9500
C(21A)-C(22A)	1.419(2)
C(21A)-H(21B)	0.9500
C(22A)-C(23A)	1.357(2)
C(22A)-H(22B)	0.9500
C(23A)-C(24A)	1.431(2)
C(23A)-H(23B)	0.9500
C(24A)-C(25A)	1.393(2)
C(25A)-C(26A)	1.390(2)
C(25A)-H(25B)	0.9500
C(26A)-C(27A)	1.426(2)
C(26A)-C(31A)	1.4364(19)
C(27A)-C(28A)	1.353(2)
C(27A)-H(27B)	0.9500
C(28A)-C(29A)	1.419(2)
C(28A)-H(28B)	0.9500
C(29A)-C(30A)	1.364(2)
C(29A)-H(29B)	0.9500
C(30A)-C(31A)	1.428(2)
C(30A)-H(30A)	0.9500
Si(1B)-O(1B)	1.7565(8)
Si(1B)-O(1B)#2	1.7565(8)

Si(1B)-N(1B)	1.9056(11)
Si(1B)-N(1B)#2	1.9056(11)
Si(1B)-N(3B)	1.9078(11)
Si(1B)-N(3B)#2	1.9078(11)
O(1B)-C(17B)	1.3244(15)
O(2B)-C(17B)	1.2145(16)
N(1B)-C(10B)#2	1.3818(17)
N(1B)-C(1B)	1.3851(17)
N(2B)-C(1B)	1.3157(18)
N(2B)-C(2B)	1.3171(17)
N(3B)-C(9B)	1.3814(17)
N(3B)-C(2B)	1.3822(16)
N(4B)-C(9B)	1.3216(18)
N(4B)-C(10B)	1.3219(18)
C(1B)-C(16B)#2	1.4460(18)
C(2B)-C(3B)	1.4437(19)
C(3B)-C(8B)	1.3890(19)
C(3B)-C(4B)	1.3928(19)
C(4B)-C(5B)	1.380(2)
C(4B)-H(4BA)	0.9500
C(5B)-C(6B)	1.401(2)
C(5B)-H(5BA)	0.9500
C(6B)-C(7B)	1.383(2)
C(6B)-H(6BA)	0.9500
C(7B)-C(8B)	1.395(2)
C(7B)-H(7BA)	0.9500
C(8B)-C(9B)	1.4507(18)
C(10B)-N(1B)#2	1.3818(17)
C(10B)-C(11B)	1.4497(18)
C(11B)-C(16B)	1.3886(19)
C(11B)-C(12B)	1.390(2)
C(12B)-C(13B)	1.384(2)
C(12B)-H(12B)	0.9500
C(13B)-C(14B)	1.400(2)
C(13B)-H(13B)	0.9500
C(14B)-C(15B)	1.383(2)

C(14B)-H(14B)	0.9500
C(15B)-C(16B)	1.3944(19)
C(15B)-H(15B)	0.9500
C(16B)-C(1B)#2	1.4460(18)
C(17B)-C(18B)	1.4990(18)
C(18B)-C(19B)	1.4089(19)
C(18B)-C(31B)	1.4100(19)
C(19B)-C(20B)	1.429(2)
C(19B)-C(24B)	1.4376(19)
C(20B)-C(21B)	1.358(2)
C(20B)-H(20A)	0.9500
C(21B)-C(22B)	1.419(2)
C(21B)-H(21A)	0.9500
C(22B)-C(23B)	1.356(2)
C(22B)-H(22A)	0.9500
C(23B)-C(24B)	1.430(2)
C(23B)-H(23A)	0.9500
C(24B)-C(25B)	1.390(2)
C(25B)-C(26B)	1.393(2)
C(25B)-H(25A)	0.9500
C(26B)-C(27B)	1.428(2)
C(26B)-C(31B)	1.4355(19)
C(27B)-C(28B)	1.353(2)
C(27B)-H(27A)	0.9500
C(28B)-C(29B)	1.419(2)
C(28B)-H(28A)	0.9500
C(29B)-C(30B)	1.357(2)
C(29B)-H(29A)	0.9500
C(30B)-C(31B)	1.4320(19)
C(30B)-H(30B)	0.9500

O(1A)#1-Si(1A)-O(1A)	180.0
O(1A)#1-Si(1A)-N(1A)#1	88.43(4)
O(1A)-Si(1A)-N(1A)#1	91.57(4)
O(1A)#1-Si(1A)-N(1A)	91.57(4)
O(1A)-Si(1A)-N(1A)	88.43(4)

N(1A)#1-Si(1A)-N(1A)	180.0
O(1A)#1-Si(1A)-N(3A)#1	85.16(4)
O(1A)-Si(1A)-N(3A)#1	94.84(4)
N(1A)#1-Si(1A)-N(3A)#1	90.08(4)
N(1A)-Si(1A)-N(3A)#1	89.93(4)
O(1A)#1-Si(1A)-N(3A)	94.84(4)
O(1A)-Si(1A)-N(3A)	85.16(4)
N(1A)#1-Si(1A)-N(3A)	89.92(4)
N(1A)-Si(1A)-N(3A)	90.07(4)
N(3A)#1-Si(1A)-N(3A)	180.0
C(17A)-O(1A)-Si(1A)	134.96(8)
C(10A)#1-N(1A)-C(1A)	106.35(11)
C(10A)#1-N(1A)-Si(1A)	126.81(9)
C(1A)-N(1A)-Si(1A)	126.62(9)
C(2A)-N(2A)-C(1A)	120.93(11)
C(9A)-N(3A)-C(2A)	106.57(10)
C(9A)-N(3A)-Si(1A)	126.82(9)
C(2A)-N(3A)-Si(1A)	126.61(9)
C(9A)-N(4A)-C(10A)	120.89(11)
N(2A)-C(1A)-N(1A)	127.73(12)
N(2A)-C(1A)-C(16A)#1	122.34(12)
N(1A)-C(1A)-C(16A)#1	109.92(11)
N(2A)-C(2A)-N(3A)	127.87(12)
N(2A)-C(2A)-C(3A)	122.01(12)
N(3A)-C(2A)-C(3A)	110.10(11)
C(8A)-C(3A)-C(4A)	121.54(12)
C(8A)-C(3A)-C(2A)	106.56(11)
C(4A)-C(3A)-C(2A)	131.87(13)
C(5A)-C(4A)-C(3A)	117.00(13)
C(5A)-C(4A)-H(4AA)	121.5
C(3A)-C(4A)-H(4AA)	121.5
C(4A)-C(5A)-C(6A)	121.46(13)
C(4A)-C(5A)-H(5AA)	119.3
C(6A)-C(5A)-H(5AA)	119.3
C(7A)-C(6A)-C(5A)	121.41(13)
C(7A)-C(6A)-H(6AA)	119.3

C(5A)-C(6A)-H(6AA)	119.3
C(6A)-C(7A)-C(8A)	117.09(14)
C(6A)-C(7A)-H(7AA)	121.5
C(8A)-C(7A)-H(7AA)	121.5
C(3A)-C(8A)-C(7A)	121.50(13)
C(3A)-C(8A)-C(9A)	106.56(11)
C(7A)-C(8A)-C(9A)	131.91(13)
N(4A)-C(9A)-N(3A)	127.73(12)
N(4A)-C(9A)-C(8A)	122.05(12)
N(3A)-C(9A)-C(8A)	110.21(11)
N(4A)-C(10A)-N(1A)#1	127.76(12)
N(4A)-C(10A)-C(11A)	121.82(12)
N(1A)#1-C(10A)-C(11A)	110.39(11)
C(12A)-C(11A)-C(16A)	121.71(13)
C(12A)-C(11A)-C(10A)	131.78(13)
C(16A)-C(11A)-C(10A)	106.48(12)
C(13A)-C(12A)-C(11A)	116.95(13)
C(13A)-C(12A)-H(12A)	121.5
C(11A)-C(12A)-H(12A)	121.5
C(12A)-C(13A)-C(14A)	121.57(13)
C(12A)-C(13A)-H(13A)	119.2
C(14A)-C(13A)-H(13A)	119.2
C(15A)-C(14A)-C(13A)	121.31(13)
C(15A)-C(14A)-H(14A)	119.3
C(13A)-C(14A)-H(14A)	119.3
C(14A)-C(15A)-C(16A)	117.35(13)
C(14A)-C(15A)-H(15A)	121.3
C(16A)-C(15A)-H(15A)	121.3
C(15A)-C(16A)-C(11A)	121.11(13)
C(15A)-C(16A)-C(1A)#1	132.01(13)
C(11A)-C(16A)-C(1A)#1	106.86(12)
O(2A)-C(17A)-O(1A)	124.69(12)
O(2A)-C(17A)-C(18A)	121.77(12)
O(1A)-C(17A)-C(18A)	113.52(11)
C(19A)-C(18A)-C(31A)	121.24(12)
C(19A)-C(18A)-C(17A)	120.83(12)

C(31A)-C(18A)-C(17A)	117.93(12)
C(18A)-C(19A)-C(20A)	123.04(12)
C(18A)-C(19A)-C(24A)	119.27(12)
C(20A)-C(19A)-C(24A)	117.69(13)
C(21A)-C(20A)-C(19A)	121.34(14)
C(21A)-C(20A)-H(20B)	119.3
C(19A)-C(20A)-H(20B)	119.3
C(20A)-C(21A)-C(22A)	120.79(15)
C(20A)-C(21A)-H(21B)	119.6
C(22A)-C(21A)-H(21B)	119.6
C(23A)-C(22A)-C(21A)	120.01(15)
C(23A)-C(22A)-H(22B)	120.0
C(21A)-C(22A)-H(22B)	120.0
C(22A)-C(23A)-C(24A)	121.15(15)
C(22A)-C(23A)-H(23B)	119.4
C(24A)-C(23A)-H(23B)	119.4
C(25A)-C(24A)-C(23A)	121.84(14)
C(25A)-C(24A)-C(19A)	119.15(13)
C(23A)-C(24A)-C(19A)	119.01(14)
C(26A)-C(25A)-C(24A)	122.01(13)
C(26A)-C(25A)-H(25B)	119.0
C(24A)-C(25A)-H(25B)	119.0
C(25A)-C(26A)-C(27A)	121.93(13)
C(25A)-C(26A)-C(31A)	119.60(13)
C(27A)-C(26A)-C(31A)	118.46(13)
C(28A)-C(27A)-C(26A)	121.78(14)
C(28A)-C(27A)-H(27B)	119.1
C(26A)-C(27A)-H(27B)	119.1
C(27A)-C(28A)-C(29A)	119.95(14)
C(27A)-C(28A)-H(28B)	120.0
C(29A)-C(28A)-H(28B)	120.0
C(30A)-C(29A)-C(28A)	120.47(15)
C(30A)-C(29A)-H(29B)	119.8
C(28A)-C(29A)-H(29B)	119.8
C(29A)-C(30A)-C(31A)	121.33(13)
C(29A)-C(30A)-H(30A)	119.3

C(31A)-C(30A)-H(30A)	119.3
C(18A)-C(31A)-C(30A)	123.26(12)
C(18A)-C(31A)-C(26A)	118.72(13)
C(30A)-C(31A)-C(26A)	117.98(12)
O(1B)-Si(1B)-O(1B)#2	180.0
O(1B)-Si(1B)-N(1B)	87.08(4)
O(1B)#2-Si(1B)-N(1B)	92.92(4)
O(1B)-Si(1B)-N(1B)#2	92.92(4)
O(1B)#2-Si(1B)-N(1B)#2	87.08(4)
N(1B)-Si(1B)-N(1B)#2	180.0
O(1B)-Si(1B)-N(3B)	85.33(4)
O(1B)#2-Si(1B)-N(3B)	94.67(4)
N(1B)-Si(1B)-N(3B)	90.44(5)
N(1B)#2-Si(1B)-N(3B)	89.56(5)
O(1B)-Si(1B)-N(3B)#2	94.67(4)
O(1B)#2-Si(1B)-N(3B)#2	85.33(4)
N(1B)-Si(1B)-N(3B)#2	89.56(5)
N(1B)#2-Si(1B)-N(3B)#2	90.43(5)
N(3B)-Si(1B)-N(3B)#2	180.0
C(17B)-O(1B)-Si(1B)	132.23(8)
C(10B)#2-N(1B)-C(1B)	106.58(11)
C(10B)#2-N(1B)-Si(1B)	126.95(9)
C(1B)-N(1B)-Si(1B)	126.21(9)
C(1B)-N(2B)-C(2B)	121.30(11)
C(9B)-N(3B)-C(2B)	106.43(11)
C(9B)-N(3B)-Si(1B)	127.14(9)
C(2B)-N(3B)-Si(1B)	125.96(9)
C(9B)-N(4B)-C(10B)	120.68(12)
N(2B)-C(1B)-N(1B)	127.77(12)
N(2B)-C(1B)-C(16B)#2	122.22(12)
N(1B)-C(1B)-C(16B)#2	109.97(11)
N(2B)-C(2B)-N(3B)	128.04(12)
N(2B)-C(2B)-C(3B)	121.66(12)
N(3B)-C(2B)-C(3B)	110.24(11)
C(8B)-C(3B)-C(4B)	121.57(13)
C(8B)-C(3B)-C(2B)	106.79(11)

C(4B)-C(3B)-C(2B)	131.55(13)
C(5B)-C(4B)-C(3B)	117.38(13)
C(5B)-C(4B)-H(4BA)	121.3
C(3B)-C(4B)-H(4BA)	121.3
C(4B)-C(5B)-C(6B)	121.07(13)
C(4B)-C(5B)-H(5BA)	119.5
C(6B)-C(5B)-H(5BA)	119.5
C(7B)-C(6B)-C(5B)	121.71(14)
C(7B)-C(6B)-H(6BA)	119.1
C(5B)-C(6B)-H(6BA)	119.1
C(6B)-C(7B)-C(8B)	117.10(13)
C(6B)-C(7B)-H(7BA)	121.4
C(8B)-C(7B)-H(7BA)	121.4
C(3B)-C(8B)-C(7B)	121.16(13)
C(3B)-C(8B)-C(9B)	106.30(12)
C(7B)-C(8B)-C(9B)	132.48(13)
N(4B)-C(9B)-N(3B)	127.52(12)
N(4B)-C(9B)-C(8B)	122.24(12)
N(3B)-C(9B)-C(8B)	110.23(11)
N(4B)-C(10B)-N(1B)#2	127.82(12)
N(4B)-C(10B)-C(11B)	122.02(12)
N(1B)#2-C(10B)-C(11B)	110.16(11)
C(16B)-C(11B)-C(12B)	121.45(13)
C(16B)-C(11B)-C(10B)	106.43(12)
C(12B)-C(11B)-C(10B)	132.09(13)
C(13B)-C(12B)-C(11B)	117.23(14)
C(13B)-C(12B)-H(12B)	121.4
C(11B)-C(12B)-H(12B)	121.4
C(12B)-C(13B)-C(14B)	121.44(14)
C(12B)-C(13B)-H(13B)	119.3
C(14B)-C(13B)-H(13B)	119.3
C(15B)-C(14B)-C(13B)	121.27(13)
C(15B)-C(14B)-H(14B)	119.4
C(13B)-C(14B)-H(14B)	119.4
C(14B)-C(15B)-C(16B)	117.19(13)
C(14B)-C(15B)-H(15B)	121.4

C(16B)-C(15B)-H(15B)	121.4
C(11B)-C(16B)-C(15B)	121.41(13)
C(11B)-C(16B)-C(1B)#2	106.86(11)
C(15B)-C(16B)-C(1B)#2	131.72(13)
O(2B)-C(17B)-O(1B)	124.10(12)
O(2B)-C(17B)-C(18B)	122.59(12)
O(1B)-C(17B)-C(18B)	113.30(11)
C(19B)-C(18B)-C(31B)	121.41(12)
C(19B)-C(18B)-C(17B)	120.36(12)
C(31B)-C(18B)-C(17B)	118.20(11)
C(18B)-C(19B)-C(20B)	123.32(12)
C(18B)-C(19B)-C(24B)	118.95(12)
C(20B)-C(19B)-C(24B)	117.71(12)
C(21B)-C(20B)-C(19B)	121.17(13)
C(21B)-C(20B)-H(20A)	119.4
C(19B)-C(20B)-H(20A)	119.4
C(20B)-C(21B)-C(22B)	121.01(14)
C(20B)-C(21B)-H(21A)	119.5
C(22B)-C(21B)-H(21A)	119.5
C(23B)-C(22B)-C(21B)	120.01(14)
C(23B)-C(22B)-H(22A)	120.0
C(21B)-C(22B)-H(22A)	120.0
C(22B)-C(23B)-C(24B)	121.03(14)
C(22B)-C(23B)-H(23A)	119.5
C(24B)-C(23B)-H(23A)	119.5
C(25B)-C(24B)-C(23B)	121.66(13)
C(25B)-C(24B)-C(19B)	119.27(12)
C(23B)-C(24B)-C(19B)	119.06(13)
C(24B)-C(25B)-C(26B)	122.11(12)
C(24B)-C(25B)-H(25A)	118.9
C(26B)-C(25B)-H(25A)	118.9
C(25B)-C(26B)-C(27B)	121.25(13)
C(25B)-C(26B)-C(31B)	119.53(13)
C(27B)-C(26B)-C(31B)	119.22(13)
C(28B)-C(27B)-C(26B)	121.17(13)
C(28B)-C(27B)-H(27A)	119.4

C(26B)-C(27B)-H(27A)	119.4
C(27B)-C(28B)-C(29B)	119.91(14)
C(27B)-C(28B)-H(28A)	120.0
C(29B)-C(28B)-H(28A)	120.0
C(30B)-C(29B)-C(28B)	120.98(14)
C(30B)-C(29B)-H(29A)	119.5
C(28B)-C(29B)-H(29A)	119.5
C(29B)-C(30B)-C(31B)	121.27(13)
C(29B)-C(30B)-H(30B)	119.4
C(31B)-C(30B)-H(30B)	119.4
C(18B)-C(31B)-C(30B)	123.84(12)
C(18B)-C(31B)-C(26B)	118.72(12)
C(30B)-C(31B)-C(26B)	117.43(12)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+1,-z+2 #2 -x+1,-y+1,-z+1

Table S16. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for Bis(9-anthronoate) SiPc. The anisotropic 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}
Si(1A)	16(1)	13(1)	15(1)	0(1)	-4(1)	-1(1)
O(1A)	21(1)	16(1)	18(1)	-2(1)	-6(1)	-2(1)
O(2A)	31(1)	19(1)	40(1)	0(1)	-19(1)	-4(1)
N(1A)	18(1)	16(1)	17(1)	1(1)	-4(1)	-2(1)
N(2A)	18(1)	19(1)	20(1)	1(1)	-5(1)	-2(1)
N(3A)	18(1)	13(1)	17(1)	-1(1)	-4(1)	-3(1)
N(4A)	20(1)	21(1)	19(1)	2(1)	-4(1)	-2(1)
C(1A)	18(1)	16(1)	20(1)	-2(1)	-4(1)	-2(1)
C(2A)	18(1)	14(1)	20(1)	-1(1)	-6(1)	-2(1)
C(3A)	23(1)	15(1)	19(1)	-1(1)	-6(1)	-3(1)
C(4A)	23(1)	24(1)	25(1)	1(1)	-8(1)	-2(1)
C(5A)	31(1)	27(1)	26(1)	4(1)	-13(1)	-2(1)
C(6A)	36(1)	29(1)	20(1)	6(1)	-9(1)	-6(1)
C(7A)	28(1)	26(1)	20(1)	3(1)	-5(1)	-6(1)
C(8A)	23(1)	16(1)	19(1)	-1(1)	-6(1)	-2(1)
C(9A)	22(1)	15(1)	17(1)	0(1)	-4(1)	-4(1)
C(10A)	21(1)	17(1)	18(1)	0(1)	-2(1)	-3(1)
C(11A)	21(1)	20(1)	22(1)	-1(1)	-2(1)	-4(1)
C(12A)	24(1)	29(1)	21(1)	2(1)	-2(1)	-5(1)
C(13A)	24(1)	35(1)	23(1)	-1(1)	3(1)	-9(1)
C(14A)	19(1)	34(1)	31(1)	-2(1)	-2(1)	-5(1)
C(15A)	20(1)	28(1)	24(1)	1(1)	-4(1)	-3(1)
C(16A)	20(1)	19(1)	21(1)	-2(1)	-3(1)	-4(1)
C(17A)	16(1)	19(1)	19(1)	-1(1)	-2(1)	-5(1)
C(18A)	23(1)	16(1)	15(1)	-2(1)	-5(1)	-2(1)
C(19A)	25(1)	21(1)	15(1)	-2(1)	-4(1)	-2(1)
C(20A)	26(1)	26(1)	22(1)	-3(1)	1(1)	-4(1)
C(21A)	25(1)	39(1)	30(1)	-5(1)	3(1)	-4(1)
C(22A)	27(1)	42(1)	34(1)	-6(1)	4(1)	6(1)
C(23A)	36(1)	28(1)	31(1)	-6(1)	-2(1)	7(1)
C(24A)	30(1)	22(1)	21(1)	-4(1)	-5(1)	2(1)

C(25A)	41(1)	16(1)	25(1)	-4(1)	-8(1)	0(1)
C(26A)	35(1)	18(1)	19(1)	-1(1)	-9(1)	-5(1)
C(27A)	46(1)	18(1)	28(1)	1(1)	-12(1)	-11(1)
C(28A)	41(1)	30(1)	30(1)	5(1)	-10(1)	-20(1)
C(29A)	28(1)	31(1)	29(1)	3(1)	-6(1)	-10(1)
C(30A)	27(1)	21(1)	25(1)	1(1)	-6(1)	-6(1)
C(31A)	26(1)	18(1)	17(1)	0(1)	-7(1)	-5(1)
Si(1B)	18(1)	13(1)	14(1)	0(1)	-1(1)	-3(1)
O(1B)	23(1)	16(1)	16(1)	-2(1)	-1(1)	-5(1)
O(2B)	46(1)	18(1)	19(1)	1(1)	1(1)	-7(1)
N(1B)	21(1)	15(1)	16(1)	0(1)	-1(1)	-4(1)
N(2B)	21(1)	17(1)	19(1)	1(1)	-1(1)	-4(1)
N(3B)	20(1)	15(1)	17(1)	-1(1)	-1(1)	-4(1)
N(4B)	20(1)	25(1)	21(1)	3(1)	-1(1)	-4(1)
C(1B)	22(1)	15(1)	18(1)	-1(1)	1(1)	-5(1)
C(2B)	24(1)	15(1)	16(1)	-1(1)	-1(1)	-5(1)
C(3B)	23(1)	17(1)	19(1)	-1(1)	-3(1)	-5(1)
C(4B)	27(1)	25(1)	21(1)	3(1)	-1(1)	-5(1)
C(5B)	32(1)	28(1)	24(1)	7(1)	-6(1)	-5(1)
C(6B)	26(1)	33(1)	31(1)	7(1)	-7(1)	0(1)
C(7B)	22(1)	32(1)	27(1)	5(1)	-2(1)	-4(1)
C(8B)	23(1)	20(1)	20(1)	0(1)	-3(1)	-5(1)
C(9B)	21(1)	18(1)	20(1)	-1(1)	-2(1)	-4(1)
C(10B)	20(1)	19(1)	20(1)	-1(1)	0(1)	-3(1)
C(11B)	22(1)	21(1)	21(1)	-1(1)	1(1)	-4(1)
C(12B)	23(1)	31(1)	28(1)	2(1)	0(1)	-3(1)
C(13B)	22(1)	35(1)	33(1)	-3(1)	4(1)	-7(1)
C(14B)	29(1)	29(1)	25(1)	-2(1)	7(1)	-10(1)
C(15B)	28(1)	23(1)	22(1)	1(1)	2(1)	-6(1)
C(16B)	23(1)	16(1)	21(1)	-2(1)	1(1)	-4(1)
C(17B)	20(1)	18(1)	18(1)	-2(1)	-1(1)	-3(1)
C(18B)	24(1)	17(1)	15(1)	-1(1)	-6(1)	-4(1)
C(19B)	23(1)	21(1)	15(1)	1(1)	-6(1)	-4(1)
C(20B)	25(1)	23(1)	24(1)	0(1)	-3(1)	-4(1)
C(21B)	24(1)	33(1)	28(1)	1(1)	1(1)	-4(1)
C(22B)	26(1)	37(1)	31(1)	3(1)	-1(1)	-14(1)

C(23B)	31(1)	28(1)	28(1)	2(1)	-6(1)	-13(1)
C(24B)	25(1)	22(1)	19(1)	1(1)	-7(1)	-8(1)
C(25B)	31(1)	17(1)	23(1)	-1(1)	-7(1)	-8(1)
C(26B)	25(1)	19(1)	20(1)	-2(1)	-7(1)	-2(1)
C(27B)	32(1)	19(1)	28(1)	-5(1)	-4(1)	-2(1)
C(28B)	30(1)	27(1)	32(1)	-8(1)	1(1)	1(1)
C(29B)	26(1)	30(1)	32(1)	-4(1)	4(1)	-7(1)
C(30B)	28(1)	22(1)	26(1)	-1(1)	-2(1)	-7(1)
C(31B)	23(1)	19(1)	17(1)	0(1)	-6(1)	-4(1)

Table S17. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{-3}) for Bis(9-anthronoate) SiPc.

	x	y	z	U(eq)
H(4AA)	4101	2446	11651	29
H(5AA)	3849	1434	12780	34
H(6AA)	1854	1442	13353	34
H(7AA)	39	2468	12820	30
H(12A)	-3592	4000	12338	30
H(13A)	-5772	4734	12368	33
H(14A)	-6687	5870	11395	34
H(15A)	-5452	6314	10356	29
H(20B)	1994	2883	8852	30
H(21B)	4067	1977	8604	39
H(22B)	4674	-117	8491	44
H(23B)	3187	-1278	8636	41
H(25B)	975	-1454	8927	33
H(27B)	-1200	-1679	9273	35
H(28B)	-3281	-840	9546	38
H(29B)	-3941	1257	9646	35
H(30A)	-2508	2476	9459	29
H(4BA)	4405	8014	2365	30
H(5BA)	2506	9212	2017	34
H(6BA)	611	9128	2689	37
H(7BA)	551	7871	3740	34
H(12B)	-427	5919	5642	34
H(13B)	-1461	5132	6667	36
H(14B)	-331	3945	7553	34
H(15B)	1875	3511	7446	30
H(20A)	7214	6829	5231	29
H(21A)	8929	7517	4701	35
H(22A)	9027	9557	4711	37
H(23A)	7393	10888	5257	33
H(25A)	5308	11294	5934	28

H(27A)	3275	11737	6646	32
H(28A)	1549	11114	7219	37
H(29A)	1371	9097	7198	36
H(30B)	2929	7724	6634	30

Table S18. Torsion angles [°] for Bis(9-anthronoate) SiPc.

N(1A)#1-Si(1A)-O(1A)-C(17A)	71.00(12)
N(1A)-Si(1A)-O(1A)-C(17A)	-109.00(12)
N(3A)#1-Si(1A)-O(1A)-C(17A)	-19.21(12)
N(3A)-Si(1A)-O(1A)-C(17A)	160.79(12)
O(1A)#1-Si(1A)-N(1A)-C(10A)#1	-87.27(11)
O(1A)-Si(1A)-N(1A)-C(10A)#1	92.73(11)
N(3A)#1-Si(1A)-N(1A)-C(10A)#1	-2.12(11)
N(3A)-Si(1A)-N(1A)-C(10A)#1	177.88(11)
O(1A)#1-Si(1A)-N(1A)-C(1A)	98.93(10)
O(1A)-Si(1A)-N(1A)-C(1A)	-81.07(10)
N(3A)#1-Si(1A)-N(1A)-C(1A)	-175.92(11)
N(3A)-Si(1A)-N(1A)-C(1A)	4.08(11)
C(2A)-N(2A)-C(1A)-N(1A)	0.1(2)
C(2A)-N(2A)-C(1A)-C(16A)#1	-179.07(12)
C(10A)#1-N(1A)-C(1A)-N(2A)	-179.12(13)
Si(1A)-N(1A)-C(1A)-N(2A)	-4.29(19)
C(10A)#1-N(1A)-C(1A)-C(16A)#1	0.17(14)
Si(1A)-N(1A)-C(1A)-C(16A)#1	175.00(8)
C(1A)-N(2A)-C(2A)-N(3A)	3.0(2)
C(1A)-N(2A)-C(2A)-C(3A)	-178.92(12)
C(9A)-N(3A)-C(2A)-N(2A)	178.02(12)
Si(1A)-N(3A)-C(2A)-N(2A)	-1.80(19)
C(9A)-N(3A)-C(2A)-C(3A)	-0.22(14)
Si(1A)-N(3A)-C(2A)-C(3A)	179.96(8)
N(2A)-C(2A)-C(3A)-C(8A)	-178.01(12)
N(3A)-C(2A)-C(3A)-C(8A)	0.35(14)
N(2A)-C(2A)-C(3A)-C(4A)	0.0(2)
N(3A)-C(2A)-C(3A)-C(4A)	178.37(13)
C(8A)-C(3A)-C(4A)-C(5A)	0.7(2)
C(2A)-C(3A)-C(4A)-C(5A)	-177.02(14)
C(3A)-C(4A)-C(5A)-C(6A)	-0.4(2)
C(4A)-C(5A)-C(6A)-C(7A)	-0.2(2)
C(5A)-C(6A)-C(7A)-C(8A)	0.5(2)
C(4A)-C(3A)-C(8A)-C(7A)	-0.5(2)

C(2A)-C(3A)-C(8A)-C(7A)	177.80(12)
C(4A)-C(3A)-C(8A)-C(9A)	-178.60(12)
C(2A)-C(3A)-C(8A)-C(9A)	-0.33(14)
C(6A)-C(7A)-C(8A)-C(3A)	-0.1(2)
C(6A)-C(7A)-C(8A)-C(9A)	177.44(14)
C(10A)-N(4A)-C(9A)-N(3A)	-0.9(2)
C(10A)-N(4A)-C(9A)-C(8A)	-179.75(12)
C(2A)-N(3A)-C(9A)-N(4A)	-178.94(12)
Si(1A)-N(3A)-C(9A)-N(4A)	0.88(19)
C(2A)-N(3A)-C(9A)-C(8A)	0.00(14)
Si(1A)-N(3A)-C(9A)-C(8A)	179.83(8)
C(3A)-C(8A)-C(9A)-N(4A)	179.23(12)
C(7A)-C(8A)-C(9A)-N(4A)	1.4(2)
C(3A)-C(8A)-C(9A)-N(3A)	0.21(14)
C(7A)-C(8A)-C(9A)-N(3A)	-177.64(14)
C(9A)-N(4A)-C(10A)-N(1A)#1	2.0(2)
C(9A)-N(4A)-C(10A)-C(11A)	-175.94(12)
N(4A)-C(10A)-C(11A)-C(12A)	0.1(2)
N(1A)#1-C(10A)-C(11A)-C(12A)	-178.17(14)
N(4A)-C(10A)-C(11A)-C(16A)	177.85(12)
N(1A)#1-C(10A)-C(11A)-C(16A)	-0.42(15)
C(16A)-C(11A)-C(12A)-C(13A)	-0.2(2)
C(10A)-C(11A)-C(12A)-C(13A)	177.32(14)
C(11A)-C(12A)-C(13A)-C(14A)	0.3(2)
C(12A)-C(13A)-C(14A)-C(15A)	0.0(2)
C(13A)-C(14A)-C(15A)-C(16A)	-0.4(2)
C(14A)-C(15A)-C(16A)-C(11A)	0.6(2)
C(14A)-C(15A)-C(16A)-C(1A)#1	-177.65(14)
C(12A)-C(11A)-C(16A)-C(15A)	-0.3(2)
C(10A)-C(11A)-C(16A)-C(15A)	-178.35(12)
C(12A)-C(11A)-C(16A)-C(1A)#1	178.32(12)
C(10A)-C(11A)-C(16A)-C(1A)#1	0.29(14)
Si(1A)-O(1A)-C(17A)-O(2A)	-1.2(2)
Si(1A)-O(1A)-C(17A)-C(18A)	-179.44(9)
O(2A)-C(17A)-C(18A)-C(19A)	122.93(14)
O(1A)-C(17A)-C(18A)-C(19A)	-58.79(16)

O(2A)-C(17A)-C(18A)-C(31A)	-57.09(18)
O(1A)-C(17A)-C(18A)-C(31A)	121.19(12)
C(31A)-C(18A)-C(19A)-C(20A)	-179.52(12)
C(17A)-C(18A)-C(19A)-C(20A)	0.46(19)
C(31A)-C(18A)-C(19A)-C(24A)	0.42(19)
C(17A)-C(18A)-C(19A)-C(24A)	-179.59(12)
C(18A)-C(19A)-C(20A)-C(21A)	178.67(13)
C(24A)-C(19A)-C(20A)-C(21A)	-1.3(2)
C(19A)-C(20A)-C(21A)-C(22A)	1.3(2)
C(20A)-C(21A)-C(22A)-C(23A)	-0.2(2)
C(21A)-C(22A)-C(23A)-C(24A)	-0.8(2)
C(22A)-C(23A)-C(24A)-C(25A)	-178.23(15)
C(22A)-C(23A)-C(24A)-C(19A)	0.8(2)
C(18A)-C(19A)-C(24A)-C(25A)	-0.66(19)
C(20A)-C(19A)-C(24A)-C(25A)	179.29(13)
C(18A)-C(19A)-C(24A)-C(23A)	-179.68(13)
C(20A)-C(19A)-C(24A)-C(23A)	0.27(19)
C(23A)-C(24A)-C(25A)-C(26A)	178.90(14)
C(19A)-C(24A)-C(25A)-C(26A)	-0.1(2)
C(24A)-C(25A)-C(26A)-C(27A)	-177.45(13)
C(24A)-C(25A)-C(26A)-C(31A)	1.1(2)
C(25A)-C(26A)-C(27A)-C(28A)	-179.51(14)
C(31A)-C(26A)-C(27A)-C(28A)	2.0(2)
C(26A)-C(27A)-C(28A)-C(29A)	-1.8(2)
C(27A)-C(28A)-C(29A)-C(30A)	0.2(2)
C(28A)-C(29A)-C(30A)-C(31A)	1.1(2)
C(19A)-C(18A)-C(31A)-C(30A)	178.34(12)
C(17A)-C(18A)-C(31A)-C(30A)	-1.65(19)
C(19A)-C(18A)-C(31A)-C(26A)	0.52(19)
C(17A)-C(18A)-C(31A)-C(26A)	-179.46(11)
C(29A)-C(30A)-C(31A)-C(18A)	-178.69(13)
C(29A)-C(30A)-C(31A)-C(26A)	-0.9(2)
C(25A)-C(26A)-C(31A)-C(18A)	-1.26(19)
C(27A)-C(26A)-C(31A)-C(18A)	177.30(12)
C(25A)-C(26A)-C(31A)-C(30A)	-179.18(12)
C(27A)-C(26A)-C(31A)-C(30A)	-0.63(19)

N(1B)-Si(1B)-O(1B)-C(17B)	-130.40(12)
N(1B)#2-Si(1B)-O(1B)-C(17B)	49.60(12)
N(3B)-Si(1B)-O(1B)-C(17B)	138.92(12)
N(3B)#2-Si(1B)-O(1B)-C(17B)	-41.08(12)
C(2B)-N(2B)-C(1B)-N(1B)	-0.6(2)
C(2B)-N(2B)-C(1B)-C(16B)#2	-178.00(12)
C(10B)#2-N(1B)-C(1B)-N(2B)	-177.05(12)
Si(1B)-N(1B)-C(1B)-N(2B)	-2.65(19)
C(10B)#2-N(1B)-C(1B)-C(16B)#2	0.57(14)
Si(1B)-N(1B)-C(1B)-C(16B)#2	174.98(8)
C(1B)-N(2B)-C(2B)-N(3B)	-0.5(2)
C(1B)-N(2B)-C(2B)-C(3B)	176.42(12)
C(9B)-N(3B)-C(2B)-N(2B)	177.37(12)
Si(1B)-N(3B)-C(2B)-N(2B)	4.82(19)
C(9B)-N(3B)-C(2B)-C(3B)	0.15(14)
Si(1B)-N(3B)-C(2B)-C(3B)	-172.40(8)
N(2B)-C(2B)-C(3B)-C(8B)	-177.73(12)
N(3B)-C(2B)-C(3B)-C(8B)	-0.30(14)
N(2B)-C(2B)-C(3B)-C(4B)	-1.2(2)
N(3B)-C(2B)-C(3B)-C(4B)	176.25(14)
C(8B)-C(3B)-C(4B)-C(5B)	-0.2(2)
C(2B)-C(3B)-C(4B)-C(5B)	-176.37(14)
C(3B)-C(4B)-C(5B)-C(6B)	-0.5(2)
C(4B)-C(5B)-C(6B)-C(7B)	0.6(2)
C(5B)-C(6B)-C(7B)-C(8B)	0.0(2)
C(4B)-C(3B)-C(8B)-C(7B)	0.9(2)
C(2B)-C(3B)-C(8B)-C(7B)	177.85(13)
C(4B)-C(3B)-C(8B)-C(9B)	-176.65(12)
C(2B)-C(3B)-C(8B)-C(9B)	0.32(14)
C(6B)-C(7B)-C(8B)-C(3B)	-0.7(2)
C(6B)-C(7B)-C(8B)-C(9B)	176.03(15)
C(10B)-N(4B)-C(9B)-N(3B)	2.9(2)
C(10B)-N(4B)-C(9B)-C(8B)	-175.69(12)
C(2B)-N(3B)-C(9B)-N(4B)	-178.67(13)
Si(1B)-N(3B)-C(9B)-N(4B)	-6.2(2)
C(2B)-N(3B)-C(9B)-C(8B)	0.06(14)

Si(1B)-N(3B)-C(9B)-C(8B)	172.49(8)
C(3B)-C(8B)-C(9B)-N(4B)	178.56(12)
C(7B)-C(8B)-C(9B)-N(4B)	1.4(2)
C(3B)-C(8B)-C(9B)-N(3B)	-0.24(15)
C(7B)-C(8B)-C(9B)-N(3B)	-177.38(14)
C(9B)-N(4B)-C(10B)-N(1B)#2	3.1(2)
C(9B)-N(4B)-C(10B)-C(11B)	-176.86(12)
N(4B)-C(10B)-C(11B)-C(16B)	-179.81(12)
N(1B)#2-C(10B)-C(11B)-C(16B)	0.20(15)
N(4B)-C(10B)-C(11B)-C(12B)	2.0(2)
N(1B)#2-C(10B)-C(11B)-C(12B)	-177.95(14)
C(16B)-C(11B)-C(12B)-C(13B)	0.6(2)
C(10B)-C(11B)-C(12B)-C(13B)	178.48(14)
C(11B)-C(12B)-C(13B)-C(14B)	-0.2(2)
C(12B)-C(13B)-C(14B)-C(15B)	0.0(2)
C(13B)-C(14B)-C(15B)-C(16B)	-0.1(2)
C(12B)-C(11B)-C(16B)-C(15B)	-0.7(2)
C(10B)-C(11B)-C(16B)-C(15B)	-179.12(12)
C(12B)-C(11B)-C(16B)-C(1B)#2	177.86(13)
C(10B)-C(11B)-C(16B)-C(1B)#2	-0.53(14)
C(14B)-C(15B)-C(16B)-C(11B)	0.5(2)
C(14B)-C(15B)-C(16B)-C(1B)#2	-177.69(14)
Si(1B)-O(1B)-C(17B)-O(2B)	2.0(2)
Si(1B)-O(1B)-C(17B)-C(18B)	-176.58(8)
O(2B)-C(17B)-C(18B)-C(19B)	123.66(15)
O(1B)-C(17B)-C(18B)-C(19B)	-57.73(16)
O(2B)-C(17B)-C(18B)-C(31B)	-54.49(18)
O(1B)-C(17B)-C(18B)-C(31B)	124.13(13)
C(31B)-C(18B)-C(19B)-C(20B)	177.49(12)
C(17B)-C(18B)-C(19B)-C(20B)	-0.60(19)
C(31B)-C(18B)-C(19B)-C(24B)	-0.60(18)
C(17B)-C(18B)-C(19B)-C(24B)	-178.69(11)
C(18B)-C(19B)-C(20B)-C(21B)	-178.97(13)
C(24B)-C(19B)-C(20B)-C(21B)	-0.9(2)
C(19B)-C(20B)-C(21B)-C(22B)	0.3(2)
C(20B)-C(21B)-C(22B)-C(23B)	0.1(2)

C(21B)-C(22B)-C(23B)-C(24B)	0.0(2)
C(22B)-C(23B)-C(24B)-C(25B)	179.01(14)
C(22B)-C(23B)-C(24B)-C(19B)	-0.5(2)
C(18B)-C(19B)-C(24B)-C(25B)	-0.40(18)
C(20B)-C(19B)-C(24B)-C(25B)	-178.59(12)
C(18B)-C(19B)-C(24B)-C(23B)	179.13(12)
C(20B)-C(19B)-C(24B)-C(23B)	0.94(18)
C(23B)-C(24B)-C(25B)-C(26B)	-178.39(13)
C(19B)-C(24B)-C(25B)-C(26B)	1.1(2)
C(24B)-C(25B)-C(26B)-C(27B)	178.75(13)
C(24B)-C(25B)-C(26B)-C(31B)	-0.8(2)
C(25B)-C(26B)-C(27B)-C(28B)	-179.98(14)
C(31B)-C(26B)-C(27B)-C(28B)	-0.4(2)
C(26B)-C(27B)-C(28B)-C(29B)	-0.7(2)
C(27B)-C(28B)-C(29B)-C(30B)	0.9(2)
C(28B)-C(29B)-C(30B)-C(31B)	0.0(2)
C(19B)-C(18B)-C(31B)-C(30B)	179.79(12)
C(17B)-C(18B)-C(31B)-C(30B)	-2.09(19)
C(19B)-C(18B)-C(31B)-C(26B)	0.89(19)
C(17B)-C(18B)-C(31B)-C(26B)	179.02(11)
C(29B)-C(30B)-C(31B)-C(18B)	-179.98(13)
C(29B)-C(30B)-C(31B)-C(26B)	-1.1(2)
C(25B)-C(26B)-C(31B)-C(18B)	-0.18(19)
C(27B)-C(26B)-C(31B)-C(18B)	-179.77(12)
C(25B)-C(26B)-C(31B)-C(30B)	-179.15(12)
C(27B)-C(26B)-C(31B)-C(30B)	1.26(19)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+1,-z+2 #2 -x+1,-y+1,-z+1