Making Silole Photovoltaically Active by Attaching Carbazolyl Donor Groups to the Silolyl Acceptor Core

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General Information. All the chemicals and solvents used in this study were purchased from Aldrich in the highest available purities and used as received without further purification. ^{1}H NMR spectra were measured on a Varian Mercury 300 spectrometer with tetramethylsilane (TMS; δ = 0 ppm) as an internal standard. UV–vis absorption spectra were measured on a Milton Roy Spectropic 3000 Array spectrophotometer. FT-IR spectra were taken on a Perkin-Elmer 16PC spectrometer. Mass spectra were recorded on a Finnigan TSQ 7000 triple quadrupole spectrometer operating in a chemical ionization (CI) mode with methane as the carrier gas. PL spectra were recorded on a Perkin Elmer LS

55 spectrometer. Thermal analyses were carried out on a thermal gravimetric analysis (TGA) apparatus of Perkin Elmer TGA 7 and a differential scanning calorimeter (DSC) of Setaram DSC 92 at a heating rate of 10 °C/min under nitrogen.

X-ray diffraction intensity data were collected at 100 K on a Bruker-Nonius Smart Apex CCD diffractometer with graphite-monochromated Mo Kα radiation. Single crystal of CzHPS was grown from a mixture of chloroform and acetone. The intensity data were processed using the SAINT and SADABS routines. The structure solution and refinement were carried out by the SHELXTL suite of X-ray programs (Version 6.10).

LED devices and PV cells were fabricated in the usual manner with sequential vacuum evaporation of various layers on 30 Ω/□ indium-tin oxide (ITO)-coated glass substrates. The ITO glasses were pre-cleaned in ultrasonic assisted detergent followed by rinsing with deionized water before being dried in oven at 100 °C. After 25 min of UV-ozone treatment, the substrates were transferred into a vacuum chamber with a base pressure of 2×10^{-4} pa for device preparation.

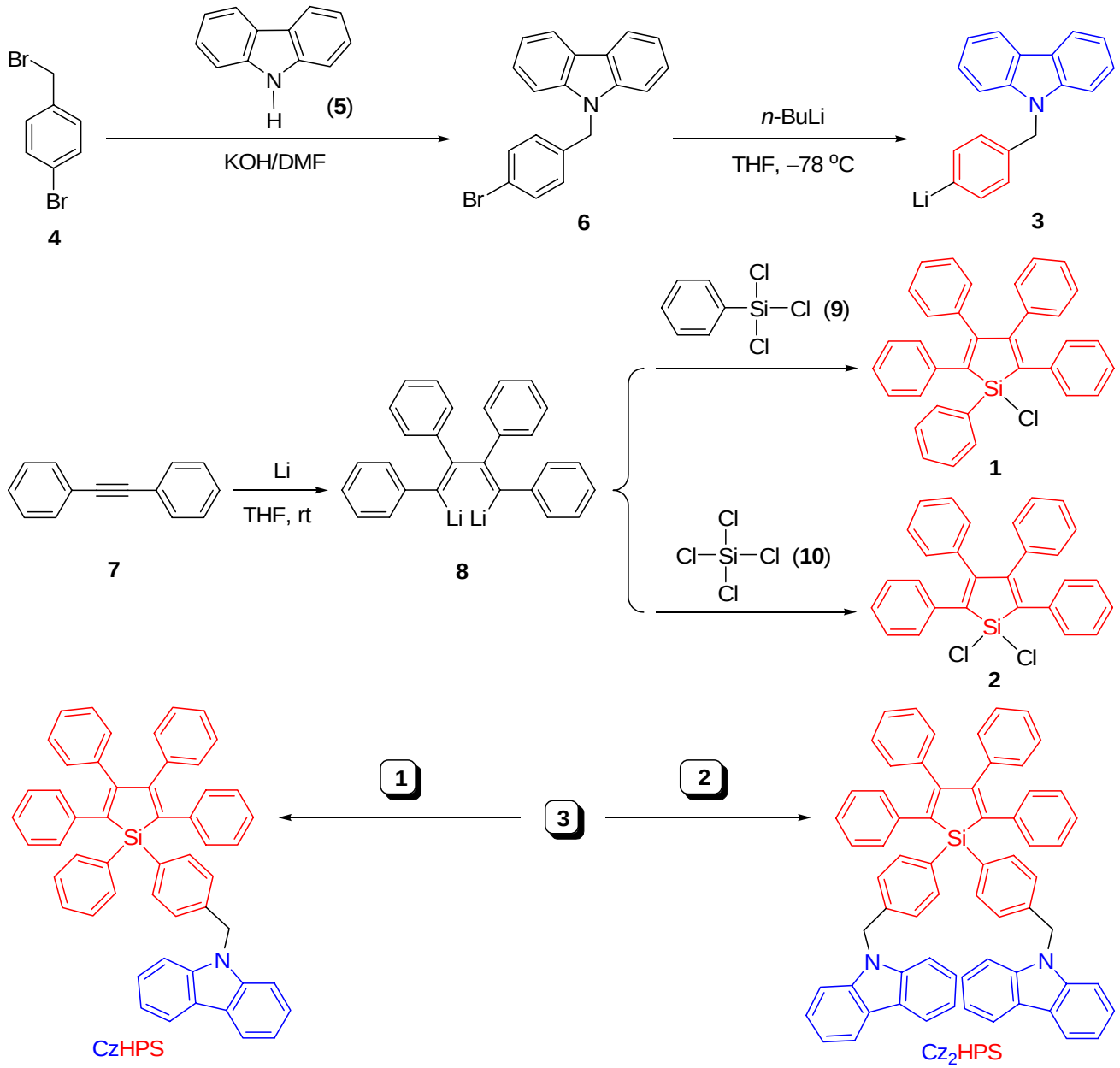
The PV cells were illuminated under a UV light of 365 nm with a power of 15 mW/cm^2 obtained from a lamp of B-100A Blak-Ray. The EL spectra and the current–voltage–luminance characteristics of the LED devices and the current–voltage cures of the PV cells were measured with a Spectrascan PR650 photometer and a computer-controlled HP4145B Semiconductor Parameter Analyzer under ambient conditions.

Chemical Synthesis. The new carbazolylsiloles $Cz_{(2)}$HPS's were prepared according to the synthetic route given in Scheme S1.

*9-(*p-*Bromobenzyl)carbazole (**6**)*: Into a 100 mL round-bottomed flask were added 1.14 g carbazole (**5**; 6.78 mmol), 1.58 g potassium hydroxide (28.25 mmol), and 20 mL DMF. The resultant mixture was stirred for a while, into which 1.44 g 4-bromobenzylbromide (**4**; 5.65 mmol) was added. After stirring at room temperature for 2 h, the reaction mixture was heated to 90 °C for 24 h. The mixture was then cooled to room temperature, into which 3 mL concentrated HCl was added, followed by the addition of 100 mL water. White precipitate formed immediately. The crude product was obtained by filtration

and washing with water until PH equal to 7. After recrystallization from ethanol, **6** was obtained in 56.8% yield (1.08 g). ^{1}H NMR (300 MHz, $CDCl_3$), δ (TMS, ppm): 8.11 (d, 2H), 7.41–7.23 (m, 8H), 6.97 (d, 2H), 5.44 (s, 2H).

Scheme S1



*1-[*p*-(9-Carbazolylmethyl)phenyl]-1,2,3,4,5-pentaphenylsilole (CzHPS)*: Into a solution of 803 mg tolan (**7**; 4.46 mmol) in THF (5 mL) was added under dry nitrogen 22.7 mg lithium shaving (3.30 mmol). The mixture was stirred for 12 h at room temperature and the resultant green-blue colored THF

solution was added dropwise to a solution of phenyltrichlorosilane (**9**; 0.17 mL, 1.49 mmol) in 25 mL THF. The reaction mixture was stirred for 2 h at room temperature and then refluxed for 5 h.

Into another flask were added 500 mg of **6** (1.485 mmol) and 15 mL THF. The mixture was cooled to –78 °C, into which 0.6 mL *n*-BuLi (2.5 M in hexane) was added. After stirring for 0.5 h, the mixture was transferred dropwise at –78 °C to the solution of chlorosilole (**1**) prepared above. The reaction mixture was allowed to warm to room temperature and was then stirred overnight at that temperature. The crude product was obtained by extracting the reaction mixture with diethyl ether three times, followed by washing with 1 M HCl three times and with brine one time. The product was isolated by a silica gel column using hexane/chloroform mixture (2:1 by volume) as the eluent. CzHPS was obtained in ~20% yield after purification. Melting point: 245.0 °C. ^{1}H NMR (300 MHz, $CDCl_3$), δ (TMS, ppm): 8.10 (d, 2H), 7.59 (d, 2H), 7.60 (d, 2H), 7.45–7.21 (m, 9H), 7.12 (d, 2H), 6.99–6.93 (m, 12H), 6.83–6.78 (m, 8H), 5.52 (s, 2H). FT-IR (NaCl), ν (cm^{-1}): 3054.8 (w), 2957.0 (s), 1598.3 (m), 1485.1 (s), 1453.4 (s), 1441.3 (s), 1430.8 (s), 1248.1 (s), 1230.8 (s), 1213.6 (s), 1153.9 (s), 1120.4 (m), 861.0 (m), 749.9 (s), 722.5 (m), 697.6 (s). MS (CI) *m*/*e*: calcd for $C_{53}H_{39}NSi$ 717.3, found 717.1 (M^+). UV-vis (THF), λ (nm)/ε (cm^{-1} M^{-1}): 343/9060, 371/4430.

*1,1-Bis[*p-*(9-carbazolylmethyl)phenyl]-2,3,4,5-tetraphenylsilole (*Cz_2*HPS)*: The synthetic procedure is similar to that described for CzHPS, just replacing phenyltrichlorosilane (**9**) by tetrachlorosilane (**10**). Cz_2HPS was obtained in ~18% yield after purification. Melting point: 304.1 °C. ^{1}H NMR (300 MHz, $CDCl_3$), δ (TMS, ppm): 8.10 (d, 4H), 7.47 (d, 4H), 7.40–7.22 (m, 12H), 7.08 (d, 4H), 6.96–6.90 (m, 12H), 6.78–6.74 (m, 8H), 5.49 (s, 4H). FT-IR (NaCl), ν (cm^{-1}): 3054.0 (w), 2956.5 (s), 1597.7 (m), 1484.6 (s), 1458.7 (s), 1431.4 (s), 1230.4 (s), 1212.8 (s), 1153.7 (s), 1120.4 (m), 860.5 (m), 749.7 (s), 722.2 (m), 696.9 (s). MS (CI) *m*/*e*: calcd for $C_{66}H_{48}N_2Si$ 896.4, found 896.6 (M^+). UV-vis (THF), λ (nm)/ε (cm^{-1} M^{-1}): 343/8650, 371/3880.

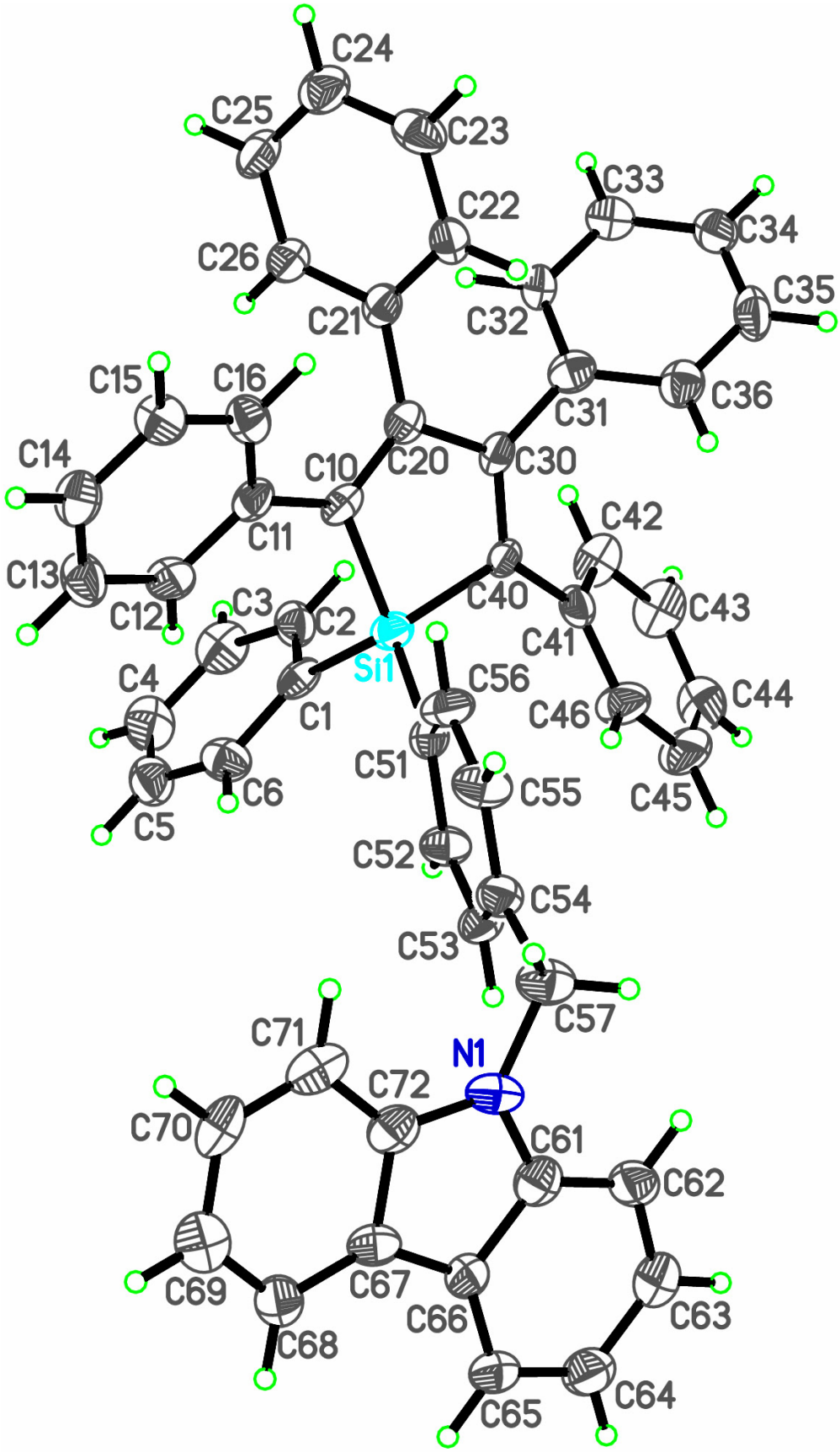


Figure S1. Molecular structure of CzHPS with the atom-labeling schemes for Tables S1–S5.

Table 1. Crystal data and structure refinement for CzHPS.

Empirical formula	C53 H39 N Si	
Formula weight	717.94	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	Cc	
Unit cell dimensions	a = 14.3168(12) Å	α = 90°.
	b = 14.7242(12) Å	β = 102.536(2)°.
	c = 18.7652(15) Å	γ = 90°.
Volume	3861.5(5) $Å^3$	
Z	4	
Density (calculated)	1.235 Mg/m^3	
Absorption coefficient	0.100 mm^{-1}	
F(000)	1512	
Crystal size	0.40 x 0.35 x 0.20 mm^3	
Theta range for data collection	2.01 to 25.00°.	
Index ranges	-16<=h<=16, -17<=k<=17, -22<=l<=13	
Reflections collected	9454	
Independent reflections	5093 [R(int) = 0.0537]	
Completeness to theta = 25.00°	98.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00 and 0.80	
Refinement method	Full-matrix least-squares on F^2	

Data / restraints / parameters	5093 / 2 / 496
Goodness-of-fit on F^2	0.996
Final R indices [I>2sigma(I)]	R1 = 0.0554, wR2 = 0.0928
R indices (all data)	R1 = 0.0776, wR2 = 0.0994
Absolute structure parameter	-0.07(16)
Largest diff. peak and hole	0.296 and -0.245 e.$Å^{-3}$

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

	x	y	z	U(eq)
Si(1)	7271(1)	3446(1)	4479(1)	26(1)
N(1)	7176(2)	7974(2)	3383(2)	36(1)
C(1)	8553(3)	3174(3)	4902(2)	27(1)
C(2)	8860(3)	2270(3)	4943(2)	32(1)
C(3)	9756(3)	2027(3)	5327(3)	41(1)
C(4)	10380(3)	2675(3)	5690(3)	45(1)
C(5)	10093(3)	3577(3)	5644(2)	40(1)
C(6)	9205(3)	3820(3)	5249(2)	35(1)
C(10)	6437(3)	3145(3)	5088(2)	26(1)
C(11)	6320(3)	3677(3)	5731(2)	27(1)
C(12)	7078(3)	4194(3)	6115(2)	32(1)
C(13)	6990(3)	4714(3)	6711(2)	38(1)
C(14)	6132(3)	4738(3)	6934(2)	36(1)
C(15)	5376(3)	4251(3)	6559(2)	36(1)
C(16)	5458(3)	3723(3)	5965(2)	33(1)
C(20)	5946(3)	2400(3)	4799(2)	25(1)
C(21)	5294(3)	1893(2)	5177(2)	27(1)
C(22)	4309(3)	1877(3)	4919(2)	29(1)
C(23)	3738(3)	1442(3)	5326(2)	37(1)
C(24)	4139(3)	1017(3)	5971(2)	40(1)
C(25)	5116(3)	1013(3)	6228(2)	40(1)

C(26)	5687(3)	1450(3)	5828(2)	32(1)
C(30)	6120(3)	2071(2)	4077(2)	25(1)
C(31)	5566(3)	1296(3)	3697(2)	31(1)
C(32)	5598(3)	437(3)	4006(2)	28(1)
C(33)	5130(3)	-291(3)	3616(2)	31(1)
C(34)	4633(3)	-176(3)	2916(2)	34(1)
C(35)	4574(3)	684(3)	2596(2)	39(1)
C(36)	5038(3)	1410(3)	2980(2)	33(1)
C(40)	6777(3)	2535(2)	3812(2)	24(1)
C(41)	7163(3)	2297(3)	3159(2)	28(1)
C(42)	7377(3)	1413(3)	2995(2)	41(1)
C(43)	7767(3)	1227(3)	2403(3)	44(1)
C(44)	7964(3)	1925(3)	1964(3)	42(1)
C(45)	7742(3)	2796(3)	2111(3)	51(1)
C(46)	7346(3)	2985(3)	2704(2)	43(1)
C(51)	7063(3)	4649(2)	4151(2)	27(1)
C(52)	7697(3)	5128(3)	3829(2)	31(1)
C(53)	7482(3)	5990(3)	3552(2)	31(1)
C(54)	6640(3)	6413(3)	3599(2)	31(1)
C(55)	6005(3)	5947(3)	3929(2)	39(1)
C(56)	6212(3)	5080(3)	4196(2)	35(1)
C(57)	6375(3)	7340(3)	3264(3)	39(1)
C(61)	7746(3)	8156(3)	2901(2)	33(1)
C(62)	7738(3)	7766(3)	2219(2)	37(1)
C(63)	8409(3)	8057(3)	1843(2)	39(1)

C(64)	9086(3)	8705(3)	2129(3)	41(1)
C(65)	9105(3)	9092(3)	2797(2)	37(1)
C(66)	8428(3)	8822(3)	3196(2)	32(1)
C(67)	8231(3)	9075(3)	3899(2)	31(1)
C(68)	8607(3)	9697(3)	4433(2)	36(1)
C(69)	8235(3)	9751(3)	5054(3)	44(1)
C(70)	7508(3)	9185(3)	5152(2)	39(1)
C(71)	7110(3)	8559(3)	4626(3)	42(1)
C(72)	7464(3)	8517(3)	3998(2)	34(1)

Table 3. Bond lengths [Å] and angles [°] for CzHPS.

Si(1)-C(40)	1.866(4)
Si(1)-C(10)	1.876(4)
Si(1)-C(51)	1.878(4)
Si(1)-C(1)	1.878(4)
N(1)-C(61)	1.371(5)
N(1)-C(72)	1.391(5)
N(1)-C(57)	1.457(5)
C(1)-C(6)	1.392(5)
C(1)-C(2)	1.398(5)
C(2)-C(3)	1.375(6)
C(3)-C(4)	1.381(6)
C(4)-C(5)	1.388(6)
C(5)-C(6)	1.372(6)
C(10)-C(20)	1.351(5)
C(10)-C(11)	1.478(5)
C(11)-C(12)	1.391(5)
C(11)-C(16)	1.399(5)
C(12)-C(13)	1.383(5)
C(13)-C(14)	1.382(5)
C(14)-C(15)	1.360(6)
C(15)-C(16)	1.385(5)
C(20)-C(21)	1.490(5)
C(20)-C(30)	1.511(5)

C(21)-C(22)	1.389(5)
C(21)-C(26)	1.391(5)
C(22)-C(23)	1.391(5)
C(23)-C(24)	1.371(6)
C(24)-C(25)	1.377(6)
C(25)-C(26)	1.383(5)
C(30)-C(40)	1.342(5)
C(30)-C(31)	1.482(5)
C(31)-C(32)	1.388(5)
C(31)-C(36)	1.404(5)
C(32)-C(33)	1.385(5)
C(33)-C(34)	1.363(6)
C(34)-C(35)	1.396(6)
C(35)-C(36)	1.376(6)
C(40)-C(41)	1.491(5)
C(41)-C(46)	1.386(5)
C(41)-C(42)	1.386(5)
C(42)-C(43)	1.376(5)
C(43)-C(44)	1.383(6)
C(44)-C(45)	1.364(6)
C(45)-C(46)	1.382(5)
C(51)-C(52)	1.386(5)
C(51)-C(56)	1.392(5)
C(52)-C(53)	1.382(5)
C(53)-C(54)	1.376(5)

C(54)-C(55)	1.388(5)
C(54)-C(57)	1.516(5)
C(55)-C(56)	1.379(5)
C(61)-C(62)	1.401(6)
C(61)-C(66)	1.409(6)
C(62)-C(63)	1.378(5)
C(63)-C(64)	1.383(6)
C(64)-C(65)	1.371(6)
C(65)-C(66)	1.405(5)
C(66)-C(67)	1.456(5)
C(67)-C(68)	1.378(5)
C(67)-C(72)	1.415(5)
C(68)-C(69)	1.385(5)
C(69)-C(70)	1.377(6)
C(70)-C(71)	1.379(6)
C(71)-C(72)	1.382(6)

C(40)-Si(1)-C(10)	92.29(18)
C(40)-Si(1)-C(51)	116.62(17)
C(10)-Si(1)-C(51)	110.24(17)
C(40)-Si(1)-C(1)	108.87(17)
C(10)-Si(1)-C(1)	112.60(17)
C(51)-Si(1)-C(1)	114.30(18)
C(61)-N(1)-C(72)	108.8(3)
C(61)-N(1)-C(57)	125.9(4)

C(72)-N(1)-C(57)	125.3(3)
C(6)-C(1)-C(2)	117.0(4)
C(6)-C(1)-Si(1)	123.1(3)
C(2)-C(1)-Si(1)	119.5(3)
C(3)-C(2)-C(1)	121.5(4)
C(2)-C(3)-C(4)	120.6(4)
C(3)-C(4)-C(5)	118.6(4)
C(6)-C(5)-C(4)	120.7(4)
C(5)-C(6)-C(1)	121.6(4)
C(20)-C(10)-C(11)	128.0(3)
C(20)-C(10)-Si(1)	107.0(3)
C(11)-C(10)-Si(1)	124.9(3)
C(12)-C(11)-C(16)	117.0(3)
C(12)-C(11)-C(10)	119.9(3)
C(16)-C(11)-C(10)	123.1(4)
C(13)-C(12)-C(11)	121.6(4)
C(14)-C(13)-C(12)	120.2(4)
C(15)-C(14)-C(13)	119.3(4)
C(14)-C(15)-C(16)	121.0(4)
C(15)-C(16)-C(11)	120.9(4)
C(10)-C(20)-C(21)	122.8(3)
C(10)-C(20)-C(30)	116.5(3)
C(21)-C(20)-C(30)	120.6(3)
C(22)-C(21)-C(26)	119.1(4)
C(22)-C(21)-C(20)	122.4(4)

C(26)-C(21)-C(20)	118.5(4)
C(21)-C(22)-C(23)	119.3(4)
C(24)-C(23)-C(22)	120.8(4)
C(23)-C(24)-C(25)	120.6(4)
C(24)-C(25)-C(26)	118.9(4)
C(25)-C(26)-C(21)	121.3(4)
C(40)-C(30)-C(31)	124.0(3)
C(40)-C(30)-C(20)	115.7(3)
C(31)-C(30)-C(20)	120.2(3)
C(32)-C(31)-C(36)	118.2(4)
C(32)-C(31)-C(30)	122.4(4)
C(36)-C(31)-C(30)	119.3(4)
C(33)-C(32)-C(31)	121.0(4)
C(34)-C(33)-C(32)	120.3(4)
C(33)-C(34)-C(35)	119.8(4)
C(36)-C(35)-C(34)	120.2(4)
C(35)-C(36)-C(31)	120.4(4)
C(30)-C(40)-C(41)	126.7(3)
C(30)-C(40)-Si(1)	108.2(3)
C(41)-C(40)-Si(1)	124.5(3)
C(46)-C(41)-C(42)	118.0(4)
C(46)-C(41)-C(40)	119.1(4)
C(42)-C(41)-C(40)	122.8(4)
C(43)-C(42)-C(41)	120.9(4)
C(42)-C(43)-C(44)	120.3(4)

C(45)-C(44)-C(43)	119.4(4)
C(44)-C(45)-C(46)	120.5(4)
C(45)-C(46)-C(41)	120.9(4)
C(52)-C(51)-C(56)	117.3(4)
C(52)-C(51)-Si(1)	123.4(3)
C(56)-C(51)-Si(1)	119.3(3)
C(53)-C(52)-C(51)	121.2(4)
C(54)-C(53)-C(52)	121.2(4)
C(53)-C(54)-C(55)	118.2(4)
C(53)-C(54)-C(57)	121.6(4)
C(55)-C(54)-C(57)	120.1(4)
C(56)-C(55)-C(54)	120.6(4)
C(55)-C(56)-C(51)	121.5(4)
N(1)-C(57)-C(54)	113.3(4)
N(1)-C(61)-C(62)	129.4(4)
N(1)-C(61)-C(66)	109.8(4)
C(62)-C(61)-C(66)	120.8(4)
C(63)-C(62)-C(61)	118.1(4)
C(62)-C(63)-C(64)	121.6(4)
C(65)-C(64)-C(63)	121.0(4)
C(64)-C(65)-C(66)	119.4(4)
C(65)-C(66)-C(61)	119.1(4)
C(65)-C(66)-C(67)	134.6(4)
C(61)-C(66)-C(67)	106.3(4)
C(68)-C(67)-C(72)	118.8(4)

C(68)-C(67)-C(66)	135.0(4)
C(72)-C(67)-C(66)	106.2(4)
C(67)-C(68)-C(69)	119.3(4)
C(70)-C(69)-C(68)	121.2(4)
C(69)-C(70)-C(71)	121.0(4)
C(70)-C(71)-C(72)	118.0(4)
C(71)-C(72)-N(1)	129.5(4)
C(71)-C(72)-C(67)	121.6(4)
N(1)-C(72)-C(67)	108.9(4)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x 10^3$) for CzHPS. 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)	30(1)	26(1)	25(1)	0(1)	11(1)	-3(1)
N(1)	35(2)	27(2)	47(3)	4(2)	12(2)	-6(2)
C(1)	31(3)	32(2)	23(2)	3(2)	16(2)	4(2)
C(2)	29(3)	40(3)	28(3)	-6(2)	7(2)	-2(2)
C(3)	40(3)	45(3)	43(3)	-1(2)	18(3)	10(2)
C(4)	25(3)	67(4)	44(3)	0(3)	8(2)	5(3)
C(5)	32(3)	54(3)	33(3)	-5(2)	7(2)	-6(2)
C(6)	32(3)	35(3)	41(3)	-6(2)	15(2)	-4(2)
C(10)	27(2)	31(2)	22(2)	9(2)	10(2)	6(2)
C(11)	39(3)	25(2)	21(2)	-1(2)	12(2)	1(2)
C(12)	27(2)	42(3)	33(3)	-3(2)	17(2)	-3(2)
C(13)	34(3)	48(3)	33(3)	-13(2)	9(2)	-4(2)
C(14)	42(3)	39(3)	29(3)	-8(2)	12(2)	5(2)
C(15)	35(3)	40(3)	37(3)	-12(2)	19(2)	-1(2)
C(16)	28(2)	35(2)	32(3)	-1(2)	1(2)	0(2)
C(20)	26(2)	23(2)	25(2)	4(2)	5(2)	6(2)
C(21)	40(3)	20(2)	22(2)	-3(2)	7(2)	-2(2)
C(22)	30(3)	28(2)	26(2)	-2(2)	1(2)	0(2)
C(23)	28(2)	41(3)	46(3)	-11(2)	15(2)	-7(2)
C(24)	52(3)	41(3)	33(3)	-3(2)	20(3)	-5(2)
C(25)	54(3)	41(3)	24(2)	7(2)	9(2)	-5(2)

C(26)	37(3)	33(2)	26(2)	1(2)	9(2)	-3(2)
C(30)	33(2)	23(2)	17(2)	2(2)	3(2)	4(2)
C(31)	31(3)	33(2)	32(3)	0(2)	15(2)	2(2)
C(32)	31(2)	31(2)	20(2)	-2(2)	3(2)	1(2)
C(33)	30(3)	26(2)	39(3)	0(2)	10(2)	4(2)
C(34)	35(3)	39(3)	31(3)	-10(2)	12(2)	-7(2)
C(35)	35(3)	56(3)	23(2)	-9(2)	2(2)	-2(2)
C(36)	33(3)	39(3)	30(3)	-1(2)	10(2)	2(2)
C(40)	33(2)	22(2)	16(2)	2(2)	4(2)	-2(2)
C(41)	28(2)	33(2)	21(2)	-8(2)	5(2)	-6(2)
C(42)	46(3)	43(3)	34(3)	4(2)	11(2)	9(2)
C(43)	48(3)	42(3)	44(3)	-1(2)	15(3)	18(2)
C(44)	41(3)	55(3)	35(3)	-15(2)	19(2)	0(2)
C(45)	73(4)	58(3)	31(3)	-5(2)	29(3)	-18(3)
C(46)	62(3)	37(3)	37(3)	-5(2)	27(3)	-12(2)
C(51)	37(3)	27(2)	19(2)	-7(2)	11(2)	-5(2)
C(52)	24(2)	32(2)	40(3)	2(2)	13(2)	-2(2)
C(53)	36(3)	34(3)	26(2)	0(2)	13(2)	-6(2)
C(54)	35(3)	27(2)	31(2)	-2(2)	9(2)	-5(2)
C(55)	34(3)	31(2)	53(3)	1(2)	13(2)	0(2)
C(56)	40(3)	31(3)	38(3)	4(2)	18(2)	-7(2)
C(57)	37(3)	30(2)	52(3)	5(2)	11(2)	-1(2)
C(61)	36(3)	29(2)	34(3)	5(2)	6(2)	6(2)
C(62)	40(3)	25(2)	42(3)	5(2)	2(2)	-2(2)
C(63)	45(3)	42(3)	31(3)	2(2)	8(2)	5(2)

C(64)	46(3)	40(3)	38(3)	4(2)	14(3)	-4(2)
C(65)	46(3)	28(2)	37(3)	5(2)	9(2)	-6(2)
C(66)	37(3)	28(2)	28(3)	4(2)	3(2)	-2(2)
C(67)	33(3)	23(2)	39(3)	4(2)	12(2)	1(2)
C(68)	35(3)	40(3)	33(3)	-1(2)	6(2)	-2(2)
C(69)	43(3)	44(3)	45(3)	-3(2)	7(3)	5(2)
C(70)	50(3)	45(3)	26(3)	7(2)	13(2)	15(2)
C(71)	42(3)	42(3)	46(3)	15(2)	19(2)	8(2)
C(72)	40(3)	25(2)	37(3)	7(2)	8(2)	7(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for CzHPS.

	x	y	z	U(eq)
H(2A)	8439	1813	4701	39
H(3A)	9947	1408	5342	49
H(4A)	10993	2506	5966	54
H(5A)	10515	4031	5888	48
H(6A)	9032	4444	5212	42
H(12A)	7670	4190	5964	39
H(13A)	7521	5054	6967	46
H(14A)	6071	5091	7345	43
H(15A)	4783	4273	6707	43
H(16A)	4920	3387	5712	39
H(22A)	4028	2160	4468	35
H(23A)	3063	1439	5156	45
H(24A)	3738	723	6243	48
H(25A)	5393	715	6672	48
H(26A)	6362	1448	6002	38
H(32A)	5946	347	4493	33
H(33A)	5156	-873	3838	38
H(34A)	4327	-680	2646	41
H(35A)	4212	769	2113	46
H(36A)	5000	1992	2757	40

H(42A)	7253	929	3297	49
H(43A)	7902	617	2294	52
H(44A)	8252	1799	1564	51
H(45A)	7860	3276	1804	62
H(46A)	7198	3595	2802	51
H(52A)	8289	4858	3799	37
H(53A)	7923	6298	3325	37
H(55A)	5422	6227	3972	46
H(56A)	5765	4771	4416	42
H(57A)	6125	7267	2733	47
H(57B)	5857	7600	3475	47
H(62A)	7283	7312	2021	44
H(63A)	8406	7807	1376	47
H(64A)	9545	8885	1860	49
H(65A)	9571	9539	2987	45
H(68A)	9117	10084	4376	44
H(69A)	8485	10188	5419	53
H(70A)	7277	9225	5589	47
H(71A)	6608	8169	4694	50