Electronic Supplementary Information

AEE-active Cyclic Tetraphenylsilole Derivatives with ~100% Solid-State Fluorescence Quantum Efficiency

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1. General experimental details

The ¹H and ¹³C NMR spectra were measured on a Bruker Avance III 500 or a Bruker Avance III 400 spectromerer using CDCl₃ as solvent and tetramethylsilane (TMS: δ =0 ppm) as internal standard. The ²⁹Si NMR spectra were recorded on the Bruker Avance III 500 spectromer using CDCl₃ as solvent and TMS as internal standard. Exact mass measurement electrospray ionization-time of flight (EMM-ESI-TOF) mass spectra of compounds **1a** and **2** were recorded on a Waters (Micromass) LCT[®] mass spectrometer using CH₃CN as solvent with 3-10 mM NH₄OAC. The melting points of **1a** and **2** were measured on a Thomas Hoover Capillary Melting Point Apparatus. Elemental analysis (C and H) was determined by CE-440 Elemental Analyzer. FT-IR spectra were recorded on a Bruker Tensor27 spectrophotometer using PIKE ATR (Attenuated Total Reflectance).

Triethylamine, sodium bicarbonate, 1,3-dichloro-1,1,3,3-tetramethyldisiloxane were purchased from Sigma Aldrich and used as received without further purification. Dichloro(methyl)phenyl-silane was purchased from Gelest, Inc and used directly. The compound 1,1-dichloro-2,3,4,5-tetraphenylsilole was synthesized according to a literature procedure and purified by crystallization in Et_2O .^[1] The hydrolysis of 1,1-dichloro-2,3,4,5-tetraphenylsilole gives a yellow powder of 1,1-dihydroxy-2,3,4,5-tetraphenylsilole according to a literature procedure.^[2]

2,2-Phenylmethyl-6,6-phenylmethyl-4,4,8,8-bis(1,4-(1,2,3,4-tetraphenyl-1,3-butadiene)) Cyclotetrasiloxanes (1a and 1b): A solution of dichlorophenylmethylsilane (0.68 mL, 4.20 mmol) was added at -20 °C (ice-NaCl bath) to a 50-mL round-bottom flask containing 1,1-dihydroxy-2,3,4,5-tetraphenylsilole (1.755g, 4.20 mmol), triethylamine (1.17 mL, 8.40 mmol) and THF (25 mL). It then was allowed to warm up to room temperature and stirred for 3 hours. The reaction mixture was filtered and washed with THF (80 mL). After removing the solvent under reduced pressure, Et₂O (30 mL) was added and a yellow precipitate (0.26 g) of a mixture of 1a and 1b was formed. While the compound 1b could not be separated from 1a neither by crystallization nor flash chromatography (only a 5.7:1 mixture with 1b as a major component could be obtained), yellow crystals of the latter (0.09 g, yield: 4%) were isolated after flash column chromatography (eluent: hexane/THF=8:1) and subsequent solvent evaporation. M.p. > 300°C. Elemental analysis (%): calcd for C₇₀H₅₆O₄Si₄: C 78.32, H 5.26; found: C 77.55, H 5.22. UV (1a, THF, 0.86 × 10⁻⁵ mol/L, r.t.), λ_{max} (nm) / ε_{max} (mol⁻¹Lcm⁻¹): 367/1.64 × 10⁴. IR (ν_{max} /cm⁻¹): 3072w (C-H_{4r}), 3055w (C-H_{4r}), 3024w (C-H_{4r}), 2959w (C-H_{4r}), 1593m (C=C_{4r}), 1574w (C=C_{4r}), 1487m, 1441m, 1429m, 1302m, 1263m (Si-C_{Me}), 1115s (Si-C_{Ph}), 1087vs (Si-O-Si), 1072vs (Si-O-Si), 1035s, 1026s, 1006s, 997s, 914m, 786s, 759s, 736s, 713s. NMR of compound 1a: ¹H NMR (500.023 MHz, CDCl₃), δ_H (TMS, ppm): 7.41-7.39 (m, 4H, Ar-H), 7.32-7.29 (m, 2H, Ar-H), 7.18-7.15 (m, 4 H, Ar-H), 7.11-7.08 (m, 4 H, Ar-H), 7.04-6.97 (m, 20 H, Ar-H), 6.92-6.90 (m, 8 H, Ar-H), 6.79-6.77 (m, 8 H, Ar-H), -0.046 (s, 6H, Si-CH₃); ¹³C NMR (125.743 MHz, CDCl₃), *δ*_C (TMS, ppm): 153.82, 138.29, 137.93, 135.78, 133.38, 132.75, 129.80, 129.75, 129.02, 127.98, 127.64, 127.38, 126.44, 125.72, -1.34; ²⁹Si NMR (99.3796 MHz, CDCl₃), δ_{Si} (TMS, ppm): -30.68, -41.87. The aforementioned 1:5.7 mixture of **1a** and **1b** with TMS as an external standard was used to extract spectral data of 1b. NMR of compound 1b: ¹H NMR (500.023 MHz, CDCl₃), δ_H (TMS, ppm): 7.24-7.20 (m, 6H, Ar-H), 7.17-7.14 (m, 6H, Ar-H), 7.05-6.94 (m, 22H, Ar-H), 6.89-6.85 (m, 4H, Ar-H), 6.80-6.77 (m, 4H, Ar- \underline{H}), 6.75-6.73 (m, 8 H, Ar- \underline{H}), 0.12 (s, 6H, Si-C \underline{H}_3); ¹³C NMR (125.743 MHz, CDCl₃), δ_C (TMS, ppm): 153.89, 153.71, 138.59, 138.04, 137.90, 135.51, 133.28, 132.82, 129.66, 129.09, 128.89, 128.07, 127.90, 127.52, 127.35, 126.45, 126.40, 125.82, 125.61, -1.19; ²⁹Si NMR (99.3796 MHz, CDCl₃), δ_{Si} (TMS, ppm): -31.04, -42.25. EMM-ESI-TOF-MS: m/z calcd. for [C₇₀H₅₆O₄Si₄+NH₄]⁺: 1090.3594; found 1090.3601.

1-(1.4-(1.2.3.4-Tetramethyl-1.3-butadiene))-3.3.5.5-tetraphenyl Cvclotrisiloxane (2): А solution of dichlorotetramethyldisiloxane (0.524 mL, 2.68 mmol) was added at -20 °C into a 50-mL round-bottom flask containing 1,1dihydroxy-2,3,4,5-tetraphenylsilole (1.12g, 2.68 mmol), triethylamine (0.75 mL, 5.36 mmol) and THF (18 mL). The reaction was started at -20 °C using ice-NaCl bath, then was allowed to warm up to room temperature and stir for 3 hours. The reaction mixture was filtered and washed with THF (60 mL). After removing the solvent under reduced pressure, Et₂O (30 mL) and hexane (10 mL) were added and pale vellow crystals of compound **3** were formed under solvent evaporation. Yield: 0.15 g, 10% (based on 1.1dihydroxyl-2,3,4,5-tetraphenylsilole). M.p. 172.5 °C. Elemental analysis calcd (%) for C₃₂H₃₂O₃Si₃: C 70.03, H 5.88; found: C 69.52, H 5.84. UV (THF, 2.06 × 10⁻⁵ mol/L, r.t.), λ_{max} (nm) / ε_{max} (mol⁻¹Lcm⁻¹): 373/0.73 × 10⁴. IR (v_{max} /cm⁻¹): 3076w (C-H₄r), 3059w (C-H_{Ar}), 3024w (C-H_{Ar}), 2960w (C-H_{Me}), 1595m (C=C_{Ar}), 1573w (C=C_{Ar}), 1493m, 1485m, 1442m, 1303m, 1257m (Si-C_{Me}), 1240s, 1182m, 1155m, 1128m, 1087m (Si-O-Si), 1058m (Si-O-Si), 1020vs (Si-O-Si), 997vs, 933m, 914m, 846m, 806s, 788s, 761s, 748m, 715m. ¹H NMR (500.023 MHz, CDCl₃), δ_H (TMS, ppm): 7.15-7.12 (t, 4H, Ar-<u>H</u>), 7.09-6.99 (m, 12H, Ar-<u>H</u>), 6.82-6.80 (m, 4H, Ar-H), 0.12 (s, 12H, Si-CH₃). ¹³C NMR (125.743 MHz, CDCl₃), δ_C (TMS, ppm): 154.50, 137.90, 137.68, 132.01, 129.59, 128.84, 127.91, 127.53, 126.64, 126.07, 0.76. ²⁹Si NMR (99.3796 MHz, CDCl₃), δ_{Si} (TMS, ppm): -5.37, -29.66. EMM-ESI-TOF-MS: m/z calcd. for [C₃₂H₃₂O₃Si₃+H]⁺: 549.1733; found 549.1736.

2. NMR spectra of Compounds 1a, 1b and 2







---30.68

---41.89

Figure S3. $^{29}Si\{^{1}H\}$ NMR of 1a (99.3796 MHz, CDCl_3/TMS).







Figure S6. ²⁹Si{¹H} NMR 1 (1a:1b = 1:5.7) (99.3796 MHz, CDCl₃/TMS).







3. Infrared Spectra of Compounds 1a and 2



Figure S10. FTIR spectrum of compound 1a.



Figure S11. FTIR spectrum of compound 2.

4. Single Crystal X-ray Crystallography of Compounds 1a, 1b and 2

Suitable single crystals of compounds **1a**, **1b** and **2** were selected under oil under ambient conditions and attached to the tip of a MiTeGenMicroMount[®]. Single crystal X-ray diffraction intensity data were collected in a stream of cold nitrogen at 100K on a Bruker Quazar SMART APEXII diffractometer with Mo K_{α} ($\lambda = 0.71073$ Å) radiation. The intensity data was integrated using SAINT and corrected for absorption using SADABS routines.^[3] The structures were solved using direct methods or charge flipping and refined using SHELXL2013 program.^[4] The details concerning x-ray crystallographic structure solutions and refinement for compounds **1a**, **1b** and **2** are tabulated in Table S1.



Figure S12. Thermal ellipsoids drawing of compound 1b (all H atoms are omitted)

	1a	1b	2
empirical formula	$C_{70}H_{56}O_4Si_4$	$C_{70}H_{56}Si_4O_4,$ 1.074(C ₄ H ₁₀ O)	$C_{32}H_{32}O_3Si_3$
formula weight	1073.50	1153.10	548.84
crystal dimensions, mm	$0.099 \times 0.093 \times 0.083$	$0.136 \times 0.095 \times 0.074$	$0.199 \times 0.192 \times 0.084$
crystal system	orthorhombic	triclinic	triclinic
space group	$P2_{1}2_{1}2_{1}$	рĪ	<i>p</i> 1
a/Å	13.033(8)	10.476(5)	11.360(4)
b/Å	19.851(11)	12.979(6)	13.726(5)
c/Å	22.521(11)	24.589(11)	19.888(7)
α/°	90	104.557(15)	88.787(14)
β/°	90	92.741(15)	86.10(2)
γ/°	90	100.26(2)	79.312(18)
Volume/Å ³	5827(6)	3169(2)	3040(2)
Z	4	2	4
$\rho_{calc}, mg/mm^3$	1.224	1.208	1.199
F(000)	2256.0	1218.0	1160.0
λ/Å	Μο Κα , 0.71073	Μο Κα , 0.71073	Μο Κα , 0.71073
μ/mm -1	0.152	0.145	0.186
temperature/K	100(1)	100(1)	100(1)
20 range for data collection	2.734 to 51.536°	3.298 to 53.048°	3.02 to 52.814°
reflections collected	58165	44722	52907
independent reflections (R _{int})	11070 (0.1018)	13022 (0.0457)	12420 (0.0450)
data/restraints/parameters	11070/508/846	13022/223/1005	12420/0/693
goodness-of-fit on F2	1.028	1.217	1.046
$R_1, wR_2 [I \ge 2\sigma (I)]$	0.0567, 0.1231	0.0752, 0.1427	0.0399, 0.0979
R_1, wR_2 [all data]	0.0837, 0.1345	0.1033, 0.1509	0.0564, 0.1062
largest diff. peak/hole / e Å-3	0.33/-0.33	0.41/-0.41	0.49/-0.29

Table S1. The crystallographic details of compounds 1a, 1b and 2.

Table S2. Selected bond distances and angles of compounds 1a, 1b and 2.

	1 a	1b	2
d(Si _{Ph-silole} -O) A	1.614(2)	1.6128(15)	1.6298(8)
d(Si _{Ph-silole} -C) Å	1.856(3)	1.860(2)	1.8562(10)
\angle (C-Si _{Ph-silole} -C) °	94.00(10)	93.96(12)	94.34(7)
∠(O-Si _{Ph-silole} -O) °	108.82(13)	108.83(12)	107.37(5)
Planarity (RMSD)	0.107	0.074	0.046, 0.027

Selected bond distances and bond angles are reported in Table S2. In general, the bond distances and bond angles in these compounds are extraordinarily similar to previously reported tetraphenylsilole containing cyclosiloxanes. The bond distances and bond angles reported here are within the typical range of those found in the Cambridge Structural Database (CSD).^[5] The planarity of these compounds was determined by fitting a plane to the Si and O atoms making up the siloxane ring and measuring the root

mean square deviation (RMSD) of those atoms from the plane. These cyclosiloxane rings have comparable planarities to other tetraphenylsilole containing cyclosiloxanes.

5. UV-Vis Absorption and Fluorescence Spectra of Compounds 1a and 2 in THF Solution

UV-Vis absorption spectra were measured on an Agilent 8453 UV-Visible Spectrophotometer under room temperature. Fluorescence spectra were measured on a Horiba Jobin Yvon Fluorolog[®]-3 spectrofluorometer at room temperature. Solutions of \sim 0.01 mg/mL compounds 1a and 2 in HPLC Grade THF were used to test the UV-Vis absorbance and fluorescence spectra at room temperature.



Figure S13. (a) Normalized UV absorption of **2** in THF solution; (b) Normalized fluorescence emission of **2** in THF solution, λ_{ex} = 370 nm; (c) Normalized fluorescence excitation spectrum of **2** in THF solution, $\lambda_{activation}$ =500 nm.

6. Aggregation Enhanced Emission (AEE) of Compounds 1a and 2

Solutions of 10^{-3} mg/mL compounds **1a** and **2** in THF/H₂O mixtures varying with 0-95% water content at room temperature were used to investigate the aggregation enhanced emission properties.



Figure S14. (A) Fluorescence emission spectra of 10^{-3} mg/mL compound **2** in THF/H₂O mixtures with different fractions of H₂O. (B) Plot of I/I₀ at 501 nm versus the water fraction, where I₀ is the fluorescence emission intensity in pure THF solution, λ_{ex} =370 nm. (C) Photograph of **2** in THF/H₂O mixtures containing different volume fractions of water taken under illumination of a UV lamp at 365 nm; from left to right: water fractions 0%-95%.

7. Relative Fluorescence Quantum Yields of Compounds 1a and 2 in THF solution

According to compounds **1a and 2**'s fluorescent emission in a similar region to quinine sulfate, quinine sulfate dihydrate was chosen as a standard reference to measure the fluorescence quantum yield.^[6] To test fluorescence quantum yield, solutions of the standard and test samples with identical absorbance at the same excitation wavelength can be assumed to be absorbing the same number of photons, thus, a simple ratio of the integrated fluorescence intensities of the two solutions (recorded under identical conditions) will yield the ratio of the quantum yield values.^[6]

Compared to a single-point method calculated using the integrated emission intensities from a single sample and standard reference pair at identical UV absorbance, calculating the slope of the linear fitting line generated by plotting the integrated fluorescence intensity against the absorption for multiple concentrations of fluorophores provides much higher accuracy. Hence, we use the following equation to determine the relative fluorescence solution quantum yield.

$$\Phi_{x} = \Phi_{ST} \left(\frac{Grad_{x}}{Grad_{ST}} \right) \left(\frac{\eta_{x}^{2}}{\eta_{ST}^{2}} \right)$$

Where Φ is the fluorescence quantum yield, Grad is the gradient of the linear fitting line from the plot of integrated fluorescence intensity vs absorbance, η is the refractive index of the solvent, the subscripts ST and X denote standard and test sample respectively.

In this study, quantum yields of compounds **1a** and **2** were investigated in HPLC Grade THF using quinine sulfate in $0.1N H_2SO_4$ as a standard. All measurements were carried out at room temperature. The UV-Vis absorbance in the studied range (350-650 nm) was kept below 0.1 using 10 mm path length 23-Q-10 Starna Quartz Cells to avoid re-absorption effects.^[7] The fluorescence intensity was kept below 3×10^6 according to the limitation of the detector and acquisition of better signal to noise ratio. The quantum yield of quinine sulfate in 0.1N H₂SO₄ reported is $0.577^{[8]}$ under excitation wavelength 350 nm. The refractive indexes of THF and 0.1N H₂SO₄ at room temperature are 1.406 and 1.33, respectively. The following parameters were used for the acquisition of fluorescence data.

Fluorescence Emission mode: Activate: 350nm, Slit: 1.2nm Start: 360nm, End: 700nm, Inc: 1, Slit: 1 nm

After subtracting background fluorescence, the integrated fluorescence intensities of all samples were calculated from 370 nm to 650 nm.



Figure S15. (A) UV-Vis Absorbance Cross Point of quinine sulfate and compound 1a at 350 nm. (B) Fluorescence Emission Intensity of quinine sulfate and compound 1a at λ_{ex} = 350 nm. (C) Linear Fit of Integrated Fluorescence Intensity of quinine sulfate and compound 1a.

$$\Phi(1a)_{\text{THF solution}} = 0.577 \left(\frac{1.6893 \times 10^6}{1.3842 \times 10^9}\right) \left(\frac{1.406}{1.33}\right)^2 = 0.0008$$



Figure S16. (A) UV-Vis Absorbance Cross Point of quinine sulfate and compound **2** at 350 nm. (B) Fluorescence Emission Intensity of quinine sulfate and compound **2** at λ_{ex} = 350 nm. (C) Linear Fit of Integrated Fluorescence Intensity of quinine sulfate and compound **2**.

$$\Phi(2)_{\text{THF solution}} = 0.577 \left(\frac{1.7347 \times 10^6}{1.3668 \times 10^9}\right) \left(\frac{1.406}{1.33}\right)^2 = 0.0008$$

8. Absolute Solid State Fluorescence Quantum Yields of Compounds Dichlorotetraphenylsilole, 1a and 2 as Crystals

The absolute solid state fluorescence quantum yields of compounds **dichlorotetraphenylsilole**, **1a** and **2** as **crystals** were determined on a calibrated integrating sphere (Labsphere) according to the method described by de Mello et al.,^[9] using a 325 nm CW light from a He-Cd laser for optical pumping, an Ocean Optics USB2000 miniature fiber optics CCD spectrometer and the same procedure reported elsewhere.^[10] The solid state quantum yield is calculated by the number of photons emitted divided by the number of photons absorbed. The calculation of the number of photons (the integration of the spectral peaks) was carried out using Matlab. The detailed principle and procedure of the measurement are shown below.

The quantum efficiency, η , is defined as (number of photons emitted)/(number of photons absorbed). A standard technique for measuring solid state PL quantum efficiencies with the use of an integrating sphere includes three measurements. For the first measurement (see figure below, experiment (a)), the sphere is empty and laser light (number of photons L_a) alone is detected. For the second measurement (see figure below, experiment (b)), the sample is placed inside the sphere and the laser beam is directed on to the sphere wall. In this experiment, we assume that a fraction μ (determined by the integrating sphere) of the laser light scattered from the sphere wall is absorbed by the sample. Then the detected signal is composed of scattered laser light (number of photons L_b) and light emitted after the absorption of scattered laser light (number of photons P_b).



In the third measurement (see figure above, experiment (c)), the collimated laser beam is directed on to the sample. A fraction, α , of this incident light will be absorbed by the sample. A fraction $(1-\alpha)$ will either be transmitted or reflected and strikes the interior surface of the sphere. A faction, μ (determined by the integrating sphere), of this scattered light is then absorbed by the sample. Hence the detected signal comes from the laser light (number of photons L_c) and emitted PL (number of photons P_c). According to the literature,^[9] the absolute solid state quantum efficiency can be calculated by:

$$\eta = \frac{P_c - P_b(1 - \alpha)}{L_a \alpha} = \frac{P_c \cdot L_b - P_b \cdot L_c}{L_a(L_b - L_c)}$$

The CCD spectrometer is used to capture the detected light intensity. The detected light intensity is then corrected by instrument spectral response function. After this, the corrected light intensity is divided by the corresponding photon energy at specific wavelength to obtain the spectrum with y axis as number of photons. The integral of the selected wavelength region is calculated to obtain the total number of photons (L_a , L_b , L_c , P_b , P_c). The above equation is used to calculate the absolute solid state quantum yield.



Figure S17. Solid state fluorescence of **1a** at $\lambda_{ex} = 325$ nm.



Figure S18. Solid state fluorescence of 2 at $\lambda_{ex} = 325$ nm.



Figure S19. Solid state fluorescence of **dichlorotetraphenylsilole** at $\lambda_{ex} = 325$ nm.

9. Excited state UV-Vis Calculations and Molecular Orbitals of 1a, 1b and 2

All calculations reported herein were performed using Gaussian 09 package^[11] utilizing density functional theory at B3LYP/6-31G (d) with empirical dispersion-force correction ^[12] for MO calculations and geometry optimization. The polarizable continuum model (PCM) ^[13] was employed to account for possible solvent effects in the geometry optimization routine. The nature of stationary points on the PES (potential energy surface) was determined by calculations of full Hessian matrix followed by frequency calculations. All structures reported were found to be true minima on the PSE with no negative frequencies. Excited State UV-Vis calculations were performed using TD-DFT ^[14]/CAM-B3LYP ^[15]/cc-pVTZ. ^[16]

Table S3. Excitation energies (given as wavelengths λ in [nm]) and oscillator strengths (in brackets) are given for the five energetically lowest-lying excited states of **1a**, **1b** and **2** (single molecule) as calculated by TD-DFT/CAM-B3LYP/cc-pVTZ.

	1a			1	b			2	
	transitions	E [a]	λ_{ex} (osc)	transitions	E [a]	λ_{ex} (osc)	transitions	E [a]	$\lambda_{ex}(osc)$
$S_1{}^{[b]}$	HOMO → LUMO, LUMO+1	3.36	369 (0.02)	HOMO→LUMO, LUMO+1	3.36	369 (0.02)	HOMO→LUMO	2.20	563 (0.31)
$S_2{}^{\left[b\right]}$	HOMO→LUMO, LUMO+1	3.40	365 (0.46)	HOMO→LUMO, LUMO+1	3.40	365 (0.46)	HOMO-1, HOMO-2, HOMO-3→LUMO	3.74	331 (0.20)
$S_3^{[b]}$	HOMO-1, HOMO- 2→LUMO; HOMO-1, HOMO- 2→LUMO+1	4.33	286 (0.28)	HOMO-1, HOMO- 2→LUMO; HOMO-1, HOMO- 2→LUMO+1	4.33	286 (0.28)	HOMO-1, HOMO-2, HOMO-3, HOMO- 4→LUMO	3.88	320 (0.06)
S4 ^[b]	HOMO-1, HOMO-2 →LUMO; HOMO-1, HOMO-2→ LUMO+1	4.34	285 (0.00)	HOMO-1, HOMO- 2→LUMO; HOMO-1, HOMO- 2→LUMO+1	4.34	286 (0.00)	HOMO-3, HOMO- 4→LUMO; HOMO-3→LUMO+1; HOMO→LUMO+2	4.34	286 (0.06)
$S_5^{[b]}$	HOMO-1, HOMO- 2→LUMO; HOMO-1, HOMO-2→ LUMO+1	4.52	275 (0.47)	HOMO-1, HOMO- 2→LUMO; HOMO-1, HOMO- 2→LUMO+1	4.52	275 (0.47)	HOMO→LUMO+1	4.38	283 (0.13)

[a] Excitation energy given in eV; [b] excited states.



Figure S20. (a) HOMO-2; (b) HOMO-1; (c) HOMO; (d) LUMO; (e) LUMO+1 in compound 1a.



Figure S21. (a) HOMO-2; (b) HOMO-1; (c) HOMO; (d) LUMO; (e) LUMO+1 in compound 1b.



Figure S22. (a) HOMO-4; (b) HOMO-3; (c) HOMO-2; (d) HOMO-1; (e) HOMO; (f) LUMO; (g) LUMO+1; (h) LUMO+2 in compound **2**.

10. Optimized Geometries of Compounds 1a, 1b and 2.

The nature of stationary points on the PES (potential energy surface) was determined by calculations of full Hessian matrix followed by frequency calculations. All structures reported were found to be true minima on the PSE with no negative frequencies.

Table S4. Optimized geometry of compound 1a (single molecule) at B3LYP/6-31G (d).

Si	-2.322900	-0.017200	-0.019200
0	-1.380200	0.558300	-1.238900
Si	-0.045900	0.581900	-2.220000
0	1.325200	0.264200	-1.347900
Si	2.262500	-0.000600	-0.022000
0	1.308200	-0.267800	1.289700
Si	-0.051700	-0.514300	2.204400
0	-1.368200	-0.587400	1.194100
Č	0 100200	-2 172600	3 060600
Č	-0.231000	-2 321800	4 419700
н	-0.562900	-1 461900	4 996600
C	-0 141300	-3 562800	5.055300
н	-0.402000	-3 653300	6 106700
\hat{C}	0.284700	4 683500	4 340100
с ц	0.264700	-4.083300	4.340100
C	0.330100	-3.049800	2 080800
п	0.022200	-4.337800	2.989800
П	0.962300	-3.425500	2.428000
U U	0.552100	-3.315500	2.360300
Н	0.809200	-3.23/400	1.311900
C	-0.262300	0.903900	3.403600
H	0.603700	1.000500	4.068200
Н	-1.155200	0.771100	4.024600
Н	-0.383900	1.847100	2.859700
С	3.552700	1.340700	0.226200
С	4.769000	0.735000	0.114700
С	4.760600	-0.767700	-0.133300
С	3.538200	-1.355700	-0.264500
С	3.252600	-2.795300	-0.432400
С	2.263900	-3.206400	-1.347400
Η	1.748400	-2.457800	-1.941800
С	1.956800	-4.556500	-1.521100
Н	1.199900	-4.844800	-2.245500
С	2.614600	-5.529800	-0.765400
Н	2.374500	-6.581500	-0.896100
С	3.583000	-5.137400	0.163500
Н	4.094400	-5.884400	0.765100
С	3.899700	-3.789700	0.327200
Н	4.647600	-3.499300	1.057500
С	6.052500	-1.507500	-0.235900
Ċ	6.383600	-2.190600	-1.417200
Ĥ	5 695400	-2 163000	-2 257200
C	7 582400	-2 897100	-1 521800
н	7 823000	-3 414700	-2 446600
C	8 467800	-2 940700	-0 442700
й	9.407000	3 493500	0.522000
\hat{C}	8 148600	2 267000	0.738000
с ц	8.148000	2.207000	1 584500
C	6.055700	-2.290300	0.820000
п	6 710200	-1.550500	1 750800
П	6.719200	-1.023200	1.739800
C	6.070500	1.454800	0.236400
C	6.394100	2.131/00	1.423300
Н	5.692400	2.114500	2.252300
C	7.602200	2.818800	1.54/100
Н	7.836800	3.331800	2.476000
С	8.505100	2.848800	0.482000
Н	9.444800	3.386200	0.576400
С	8.193800	2.180800	-0.704900
Н	8.889700	2.199000	-1.539500
С	6.991100	1.483700	-0.824100
Н	6.761100	0.962100	-1.748700
С	3.282500	2.784900	0.378300
С	2.264700	3.212800	1.251800

Н	1.713400	2.472800	1.823700
С	1.972600	4.567200	1.413600
Н	1.191200	4.867600	2.106400
С	2.675500	5.529200	0.685600
Н	2.445300	6.584500	0.804500
С	3.673200	5.121000	-0.204200
Н	4.219000	5.859700	-0.785700
С	3.975200	3.768700	-0.354900
Н	4.749000	3.466900	-1.053000
С	0.081500	2.310800	-2.926800
С	-1.078100	3.044000	-3.244000
Н	-2.058200	2.621800	-3.034600
С	-0.995800	4.314800	-3.816400
H	-1.904000	4.864800	-4.049500
Ĉ	0 253500	4 879600	-4 084700
Ĥ	0.320000	5 869500	-4 528800
Ĉ	1 416500	4 170300	-3 776500
н	2 390800	4 608500	-3 976700
C	1 328600	2 899600	-3 204000
й	2 243200	2.365700	2 958800
C	0.231800	2.303700	2 534400
U U	-0.231800	-0.730400	-3.334400
п	-0.370900	-1./24300	-3.082300
H	0.653600	-0.779000	-4.1/9000
Н	-1.101100	-0.528600	-4.168/00
C	-3.606100	1.216400	0.567200
С	-4.823900	0.654700	0.322800
С	-4.818900	-0.709900	-0.355500
С	-3.596900	-1.260800	-0.603600
С	-3.301000	-2.517100	-1.321700
С	-3.957000	-2.879400	-2.514900
Н	-4.725000	-2.228100	-2.919100
С	-3.624400	-4.053600	-3.188500
Н	-4.141200	-4.307200	-4.110600
С	-2.632300	-4.900600	-2.686700
Η	-2.378700	-5.818400	-3.210400
С	-1.966100	-4.553100	-1.509200
Н	-1.191000	-5.200400	-1.107900
С	-2.287200	-3.370100	-0.842400
Н	-1.763000	-3.111100	0.073500
С	-6.111500	-1.373000	-0.695000
С	-7.028000	-0.779100	-1.578600
Н	-6.802800	0.190300	-2.013700
С	-8.219700	-1.425100	-1.909100
H	-8.912300	-0.954200	-2.601700
С	-8.524400	-2.668700	-1.350100
H	-9.455800	-3.168100	-1.603000
Ĉ	-7 625800	-3 264400	-0.462300
Ĥ	-7 855300	-4 229800	-0.019000
Ĉ	-6 428200	-2.624100	-0 141700
н	-5 729100	-3 092700	0 545000
C	-6 121700	1 304900	0.667800
č	-6 455400	2 551400	0.114200
н	-5 765500	3.026700	-0 577100
C	7 658200	3 179100	0.440500
с u	7.000000	4 141100	0.440300
n C	-7.900900	2 575000	1 224400
U U	-8.545100	2.373000	1.534400
П	-9.480500	3.064400	1.391800
C III	-8.225500	1.335900	1.893800
Н	-8.906600	0.858500	2.591200
C	-7.026400	0.702500	1.557600
Н	-6.787700	-0.263400	1.993300
С	-3.318400	2.476100	1.282800
C	-2.308900	3.333400	0.802000
Н	-1.781600	3.075100	-0.112200
С	-1.994700	4.519900	1.466000
Н	-1.222600	5.169800	1.063000
С	-2.663800	4.866800	2.641900
Η	-2.415600	5.787300	3.163500
С	-3.651800	4.015700	3.145200
Н	-4.170700	4.268900	4.066200

- $\begin{array}{cccc} C & -3.977400 & 2.837900 & 2.474500 \\ H & -4.741900 & 2.183300 & 2.880100 \end{array}$

Table S5. Optimized geometry of compound 1b (single molecule) at B3LYP/6-31G (d).

Si	2.293600	0.291700	0.043600
0	1.327000	0.101200	-1.273000
Si	0.038800	0.414100	-2.265700
0	-1.365300	0.490900	-1.388100
Si	-2.293400	0.291800	-0.043100
0	-1.327200	0.101300	1.273800
Si	-0.038600	0.413500	2.266200
0	1.365300	0.490100	1.388600
Ċ	0.081800	-1 011900	3 473500
Č	-1.080100	-1.636800	3.965400
Ĥ	-2.056600	-1 321700	3 604800
Ĉ	-1 004700	-2.666000	4 905800
н	-1 914500	-3 136900	5 269300
C	0 240300	-3 092700	5 374500
н	0.301700	-3 895100	6 105200
C	1 405700	2 488300	4 808100
й	2 376000	2 821000	5 254200
C	1 324700	1 458800	3 958100
с u	2 241600	1.005000	2 500000
C	0.200100	-1.005900	2 106700
U U	-0.290100	2.000100	3.100/00
п	-0.413200	2.808500	2.370000
п	0.504400	2.314600	3.740000
П	-1.188100	2.048800	5./54/00
C	-3.569300	-1.068500	-0.230300
C	-4./90800	-0.4/0100	-0.134800
C	-4./94400	1.031400	0.126300
C	-3.5/6500	1.640/00	0.185/00
C	-3.289000	3.051500	0.514900
C	-3.938900	3.735400	1.561600
Н	-4.696000	3.221300	2.144500
С	-3.613700	5.056100	1.866700
Н	-4.126000	5.558600	2.683200
С	-2.635300	5.732600	1.132800
Н	-2.388000	6.764000	1.368900
С	-1.974500	5.067600	0.097500
Н	-1.210200	5.578900	-0.481600
С	-2.288500	3.740600	-0.198000
Н	-1.768900	3.232800	-1.005700
С	-6.091300	1.749900	0.293700
С	-6.982600	1.414500	1.326500
Н	-6.733800	0.607300	2.009300
С	-8.180000	2.111800	1.488900
Н	-8.852700	1.843500	2.299200
С	-8.515700	3.146900	0.612700
Н	-9.451500	3.685400	0.735800
С	-7.642100	3.483300	-0.423800
Н	-7.895700	4.284600	-1.112900
С	-6.438900	2.793900	-0.578700
Н	-5.759700	3.061600	-1.383000
С	-6.086600	-1.200400	-0.254000
Ċ	-6.398100	-2.239400	0.637700
H	-5.689900	-2,497500	1,419800
C	-7.601800	-2.936700	0.529300
Ĥ	-7.826900	-3.734200	1.232400
Ċ	-8 512400	-2.612900	-0 479100
й	-9 448700	-3 157500	-0 566000
Ċ	-8 213000	-1 582700	-1 374000
й	_8 91/1800	-1 32/100	-2 162/00
C	-7 01/700	-0.877700	_1 258000
н	-6 702700	_0.073000	-1.95/300
C	-3 281300	-2 483000	-0 543300
4.7	· · · · · · · · · · · · · · · · · · ·	2. TO NAM	

С	-2.256300	-3.153000	0.152800
Н	-1.705300	-2.626800	0.927400
С	-1.955500	-4.487900	-0.119000
Н	-1.173100	-4.984900	0.448000
С	-2.650000	-5.178100	-1.114500
Н	-2.410900	-6.215600	-1.332200
С	-3.650300	-4.519100	-1.834700
Н	-4.188800	-5.041300	-2.621500
С	-3.965200	-3.191400	-1.551000
Н	-4.742500	-2.691400	-2.119600
С	-0.082000	-1.011100	-3.473200
С	1.079700	-1.637200	-3.964300
Ĥ	2.056200	-1.323100	-3.602900
C	1 003900	-2.666300	-4 904800
н	1 913500	-3 138100	-5 267600
C	-0.241200	-3 091600	-5 374500
н	-0.302900	-3 893900	-6 105200
C	1 406300	2 486000	4 808000
н	2 377600	2 818600	-4.898900
C	-2.377000	-2.818000	2 059900
	-1.324900	-1.430700	-3.938800
П	-2.241600	-1.002800	-3.391300
U U	0.290500	2.066/00	-3.105900
H	0.415800	2.868600	-2.369200
H	-0.564800	2.316200	-3./44200
Н	1.18/400	2.048700	-3.735600
С	3.576400	1.640800	-0.185100
С	4.794400	1.031600	-0.126300
С	4.791100	-0.469900	0.134500
С	3.569700	-1.068500	0.230200
С	3.281900	-2.483100	0.543100
С	2.256800	-3.153100	-0.152800
Н	1.705500	-2.626900	-0.927100
С	1.956200	-4.488100	0.119000
Η	1.173800	-4.985100	-0.447800
С	2.651100	-5.178300	1.114200
Η	2.412200	-6.215800	1.331900
С	3.651500	-4.519300	1.834200
Н	4.190300	-5.041500	2.620800
С	3.966200	-3.191500	1.550600
Н	4.743600	-2.691500	2.119000
С	6.087000	-1.200000	0.253400
С	6.398500	-2.238900	-0.638400
H	5.690100	-2.497100	-1.420500
С	7.602200	-2.936100	-0.530400
Ĥ	7.827400	-3.733500	-1.233600
C	8 513000	-2.612200	0 477800
Ĥ	9 449400	-3 156700	0 564500
C	8 213700	-1 582200	1 372900
н	8 91 5700	-1 323500	2 161200
C	7.015300	-0.877200	1 257200
н	6 794300	-0.073600	1.953600
C	6 091100	1 750400	-0.29/100
č	6 / 3 8 9 0 0	2 794300	0.578300
н	5 750000	2.794300	1 382800
n C	7 6 4 1 0 0 0	2 484000	0.422000
U U	7.041900	3.484000	0.423000
П	7.895600	4.285300	1.112000
C	8.515200	3.14/800	-0.613900
Н	9.450800	3.686400	-0./3/300
C	8.179300	2.112700	-1.490000
Н	8.851800	1.844400	-2.300600
С	6.982200	1.415100	-1.327200
Н	6.733200	0.608000	-2.009900
С	3.288600	3.051600	-0.514200
С	2.288200	3.740500	0.199200
Н	1.769100	3.232600	1.007100
С	1.973900	5.067500	-0.096100
Н	1.209800	5.578600	0.483400
С	2.634200	5.732600	-1.131600
Н	2.386700	6.764000	-1.367500
C	3 612500	5.056300	-1 866000

Н	4.124400	5.559000	-2.682600
С	3.938000	3.735600	-1.561000
н	4 604000	3 221700	2 144200

Н 4.694900 3.221700 -2.144200

Table S6. Optimized geometry of compound 2 (single molecule) at B3LYP/6-31G (d).

Si	0.959900	0.000300	0.000200
0	1.941700	-0.122500	-1.332600
Si	3.602900	-0.300900	-1.501500
0	4.269400	-0.000200	-0.000400
Si	3.603500	0.301500	1.500800
0	1.942100	0.123400	1.332500
Č	4 226100	-0.966200	2,726300
Ĥ	3 754400	-0.830600	3 706500
н	5 310600	-0.876500	2 860500
н	4 012900	-1 985400	2 384700
C	3 988300	2 056300	2.004700
н	3 563300	2.030300	1 315500
п п	5.071000	2.778800	2.068800
н	3.572000	2.222300	2.008800
C	3.372000	2.270300	2.022400
с ц	3.987000	-2.033300	-2.023400
11	5.060600	-2.778200	-1.31/300
п	3.009000	-2.222000	-2.0/1900
П	3.309000	-2.209000	-3.014300
C	4.225500	0.96/300	-2.726500
н	3./53100	0.832900	-3.706500
H	5.309800	0.8/6800	-2.861500
Н	4.013400	1.986300	-2.383900
C	-0.319300	1.366200	-0.089700
C	-1.539/00	0.761800	-0.033400
С	-1.539500	-0.762100	0.033600
С	-0.318900	-1.366100	0.090200
С	-0.014200	-2.810500	0.058900
С	-0.670900	-3.709100	-0.804800
Н	-1.453400	-3.341700	-1.460600
С	-0.317500	-5.057100	-0.840000
Н	-0.834900	-5.728600	-1.520500
С	0.697500	-5.545600	-0.012500
Н	0.969200	-6.597300	-0.040900
С	1.363700	-4.668400	0.846000
Н	2.155300	-5.034700	1.494500
С	1.018200	-3.316900	0.873600
Н	1.538200	-2.641800	1.547800
С	-2.833000	-1.504100	0.046100
С	-3.749500	-1.394900	-1.013000
Η	-3.524000	-0.744300	-1.853000
С	-4.941400	-2.119900	-1.000700
Н	-5.633800	-2.029800	-1.833500
С	-5.246400	-2.954400	0.077400
Н	-6.178100	-3.513600	0.089000
С	-4.347800	-3.063300	1.141100
Н	-4.577600	-3.706800	1.986200
С	-3.150000	-2.348200	1.122800
Н	-2.451100	-2.438800	1.949300
С	-2.833500	1.503300	-0.046100
С	-3.150600	2.347400	-1.122800
Н	-2.451500	2.438200	-1.949200
С	-4.348600	3.062000	-1.141400
Н	-4.578500	3.705400	-1.986600
C	-5.247500	2.952800	-0.078000
Н	-6.179400	3.511500	-0.089800
C	-4.942400	2.118400	1.000200
H	-5.635000	2.028000	1.832800
C	-3.750200	1.393800	1.012800
Ĥ	-3.524700	0.743300	1.852900
C	-0.015200	2.810800	-0.058200
Č	1.017200	3.317600	-0.872600
Ĥ	1.537700	2.642800	-1.546700

С	1.362200	4.669200	-0.844800
Н	2.153900	5.035900	-1.493000
С	0.695400	5.546100	0.013600
Н	0.966800	6.597900	0.042200
С	-0.319700	5.057100	0.840800
Η	-0.837400	5.728400	1.521100
С	-0.672500	3.709000	0.805400
Η	-1.455000	3.341300	1.460900

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