Electronic Supplementary Information

Naphtho- and anthra-disilacyclobutadienes

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1. Experimental Details

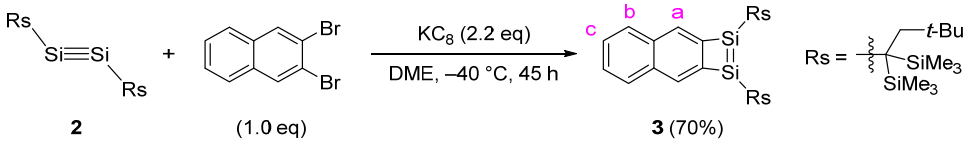
General Procedures

All reactions treating air-sensitive compounds were carried out under an inert atmosphere (N_2 or Ar) using a high-vacuum line and standard Schlenk techniques, or a glove box, as well as dry and oxygen-free solvents. NMR spectra were recorded on a Bruker Avance III 500 FT NMR spectrometer. The ^{1}H NMR chemical shifts were referenced to residual ^{1}H of the solvents; C_6D_6 (^{1}H δ 7.16).[S1] The ^{13}C and ^{29}Si NMR chemical shifts were relative to Me_4Si in ppm (δ 0.00). Sampling of air-sensitive compounds was carried out using a VAC NEXUS 100027 type glove box. Mass spectra were recorded on a Bruker Daltonics SolariX 9.4T. UV-vis spectra were recorded on a JASCO V-660 spectrometer. Measurement of melting point was measured on a SRS OptiMelt MPA100. Elemental analysis was performed with a J-SCIENCE LAB JM-11 at Research and Analytical Center for Giant Molecules, Graduate School of Science, Tohoku University.

Materials

Dimethoxyethane (DME), diethylether, toluene, and hexane were dried and deoxygenated with VAC-103991 type solvent purifiers. Benzene-d_6 (C_6D_6) was dried with molecular sieves 3A. Disilyne **2**[S2] and 2,3-dibromoanthracene [S3] were synthesized according to literature procedures.

Synthesis of Naphtodisilacyclobutadiene 3

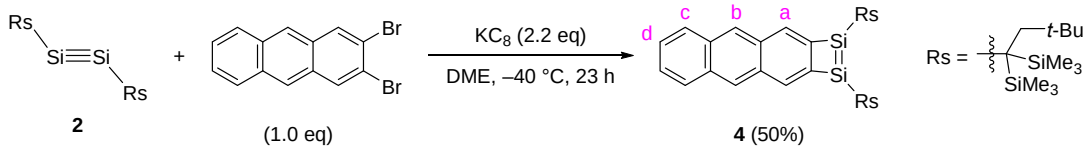


2 (1.0 eq) **3** (70%)

In a Schlenk tube (50 mL) equipped with a magnetic stir bar, disilyne **2** (202 mg, 392 μmol), KC_8 (119 mg, 879 μmol) and 2,3-dibromonaphthalene (113 mg, 394 μmol) were placed. Then, DME (6 mL) was added by vacuum transfer and stirred at −40 ºC for 45 h. The reaction mixture was warmed up to 0 ºC and stirred for 30 minutes. The solvent was changed to hexane (ca. 20 mL) and the insoluble material was filtrated away. Recrystallization of the crude product from Et_2O at −35 ºC gave compound **3** (175 mg, 273 μmol) in 70% as dark-brown powder.

3: dark-brown powder; mp. 65–70 °C (decomp.); ^{1}H NMR (500 MHz, C_6D_6 , 297 K) δ 0.43 (s, 36H, $SiMe_3$), 1.20 (s, 18H, *t*-Bu), 2.22 (s, 4H, CH_2), 6.77 (s, 2H, H^a), 6.97 (dd, J = 5.9, 3.3 Hz, 2H, $H^{b/c}$), 7.15 (dd, J = 5.9, 3.3 Hz, 2H, $H^{c/b}$); ^{13}C{^{1}H} NMR (126 MHz, C_6D_6, 298 K) δ 3.6 ($SiMe_3$), 24.1 ($C(SiMe_3)_2$), 31.4 (*t*-Bu), 34.0 (CMe_3), 45.0 (CH_2), 125.4 (CH), 125.8 (CH), 126.8 (CH), 137.8 (C), 155.4 (C); ^{29}Si{^{1}H} NMR (99 MHz, C_6D_6, 298 K) δ 1.3 ($SiMe_3$), 110.3 (Si=Si); HRMS (APCI) calcd for $[C_{34}H_{65}Si_6]^+$ ([M + H]$^+$), 641.3696; Found, 641.3697; Anal. Calcd for $C_{34}H_{64}Si_6$: C, 63.67; H, 10.06%. Found: C, 63.46; H, 9.95%. UV-vis (hexane, 298 K) λ_{max}/nm (ε) 330 (18000), 446 (5100), 460 (5600), 562 (3300).

Synthesis of Anthradisilacyclobutadiene 4



In a Schlenk tube (50 mL) equipped with a magnetic stir bar, disilyne **2** (197 mg, 382 µmol), KC_8 (115 mg, 852 µmol) and 2,3-dibromoanthracene (131 mg, 391 µmol) were added. Then, DME (10 mL) was added via a vacuum line and stirred at −40 ºC for 23 h. After evaporation of volatiles at room temperature, the residue was filtrated with pentane (ca. 20 mL) by a Schlenk filter. Recrystallization from Et_2O at −35 ºC gave compound **4** (131 mg, 190 µmol) in 50% as dark-purple powder.

4: dark-purple powder; mp. 140–150 °C (decomp.); ^{1}H NMR (500 MHz, C_6D_6 , 297 K) δ 0.44 (s, 36H, $SiMe_3$), 1.23 (s, 18H, *t*-Bu), 2.25 (s, 4H, CH_2), 6.89 (s, 2H, H^a), 7.17 (dd, J = 6.5, 3.2 Hz, 2H, $H^{c/d}$), 7.52 (s, 2H, H^b), 7.60 (dd, J = 6.2, 3.3 Hz, 2H, $H^{d/c}$); ^{13}C{^{1}H} NMR (126 MHz, C_6D_6, 298 K) δ 3.6 ($SiMe_3$), 24.0 ($C(SiMe_3)_2$), 31.5 (*t*-Bu), 34.1 (CMe_3), 45.0 (CH_2), 123.9 (CH), 124.5 (CH), 125.4 (CH), 128.2 (CH), 133.3 (C), 136.0 (C), 155.3 (C); ^{29}Si{^{1}H} NMR (99 MHz, C_6D_6, 298 K) δ 1.5 ($SiMe_3$), 105.0 (Si=Si); HRMS (APCI) calcd for $[C_{38}H_{66}Si_6]^+$ ([M + H]$^+$), 690.37746; Found, 690.37787; Anal. Calcd for $C_{38}H_{66}Si_6$: C, 66.01; H, 9.62%. Found: C, 65.70; H, 9.61%.; UV-vis (hexane, 298 K) λ_{max}/nm (ε) 375 (9400), 508 (3000), 532 (3200).

2. NMR and UV-vis Spectra

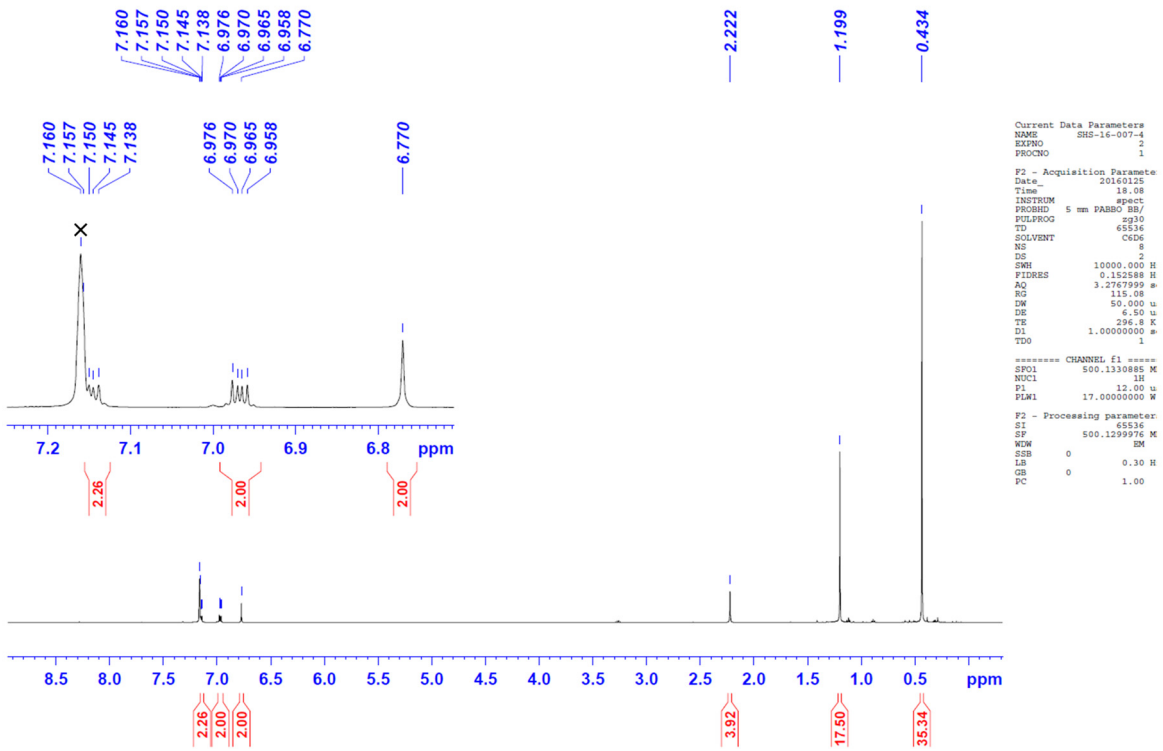


Fig. S1 ^{1}H NMR spectrum of **3** (in C_6D_6, 297 K). (× = C_6D_5H).

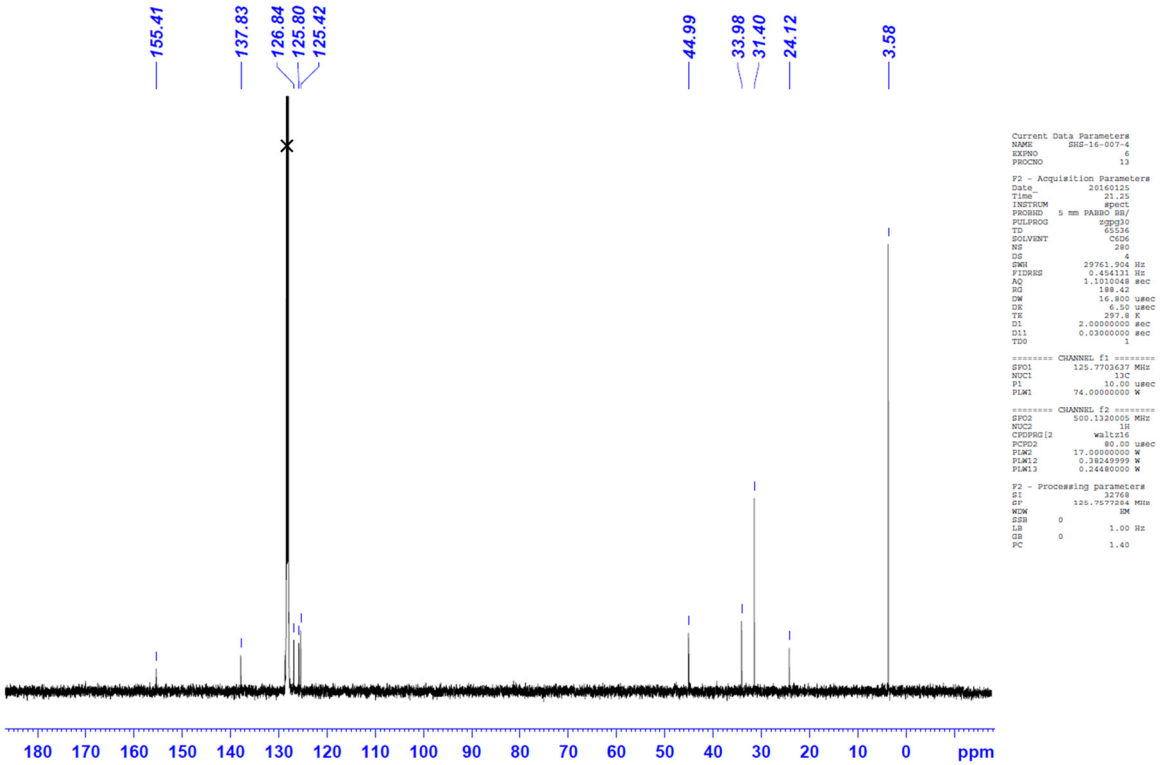


Fig. S2 $^{13}C\{^{1}H\}$ NMR spectrum of **3** (in C_6D_6, 298 K). (× = C_6D_6).

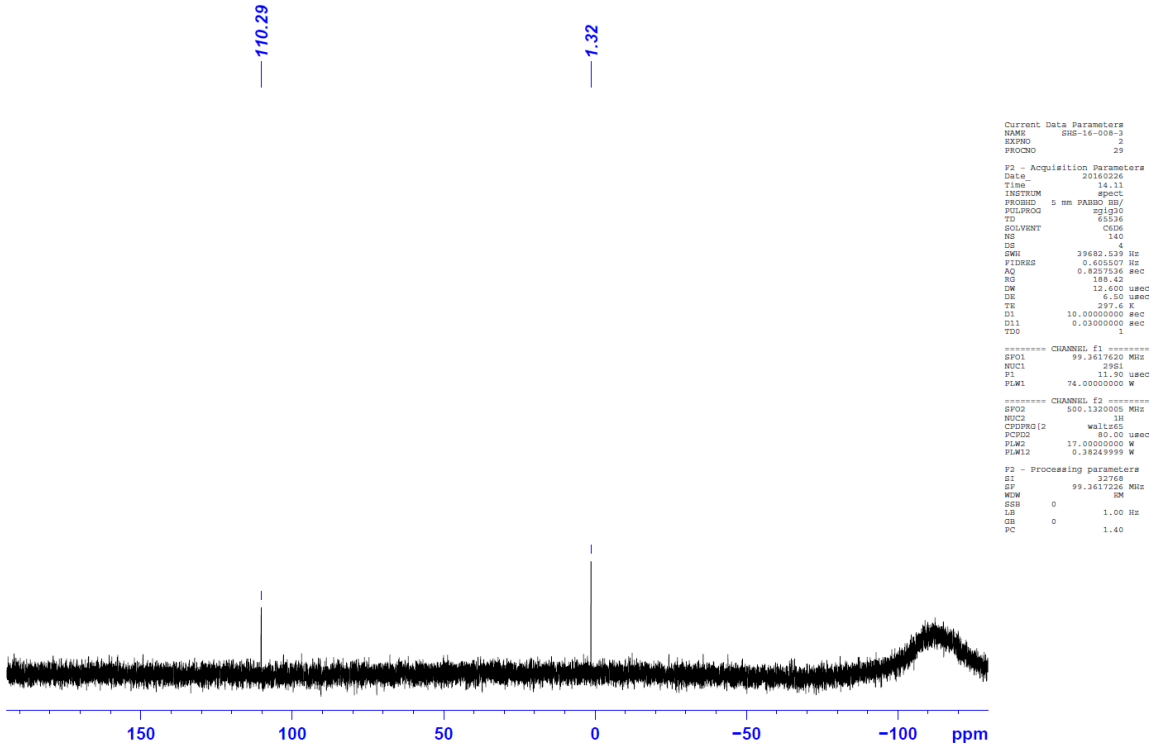


Fig. S3 $^{29}Si\{^{1}H\}$ NMR spectrum of **3** (in C_6D_6, 298 K).

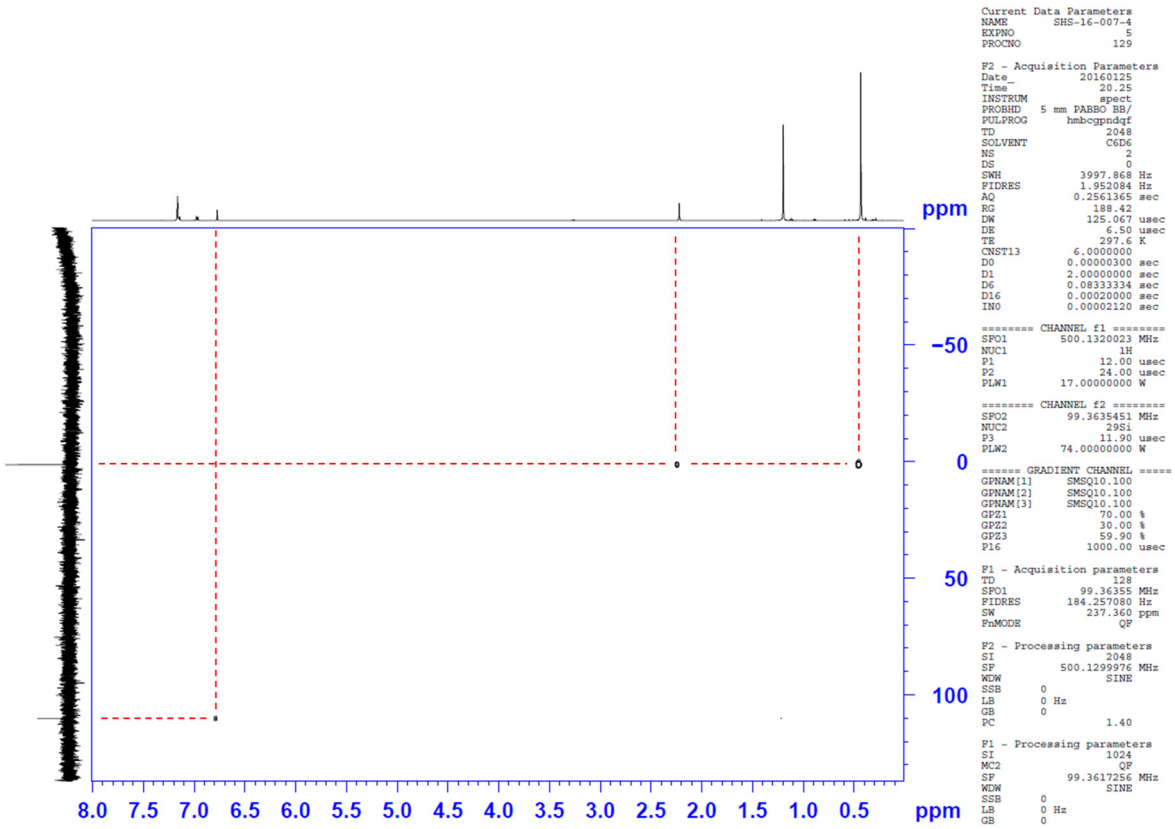


Fig. S4 ^{1}H-^{29}Si HMBC NMR spectrum of **3** (in C_6D_6, 298 K).

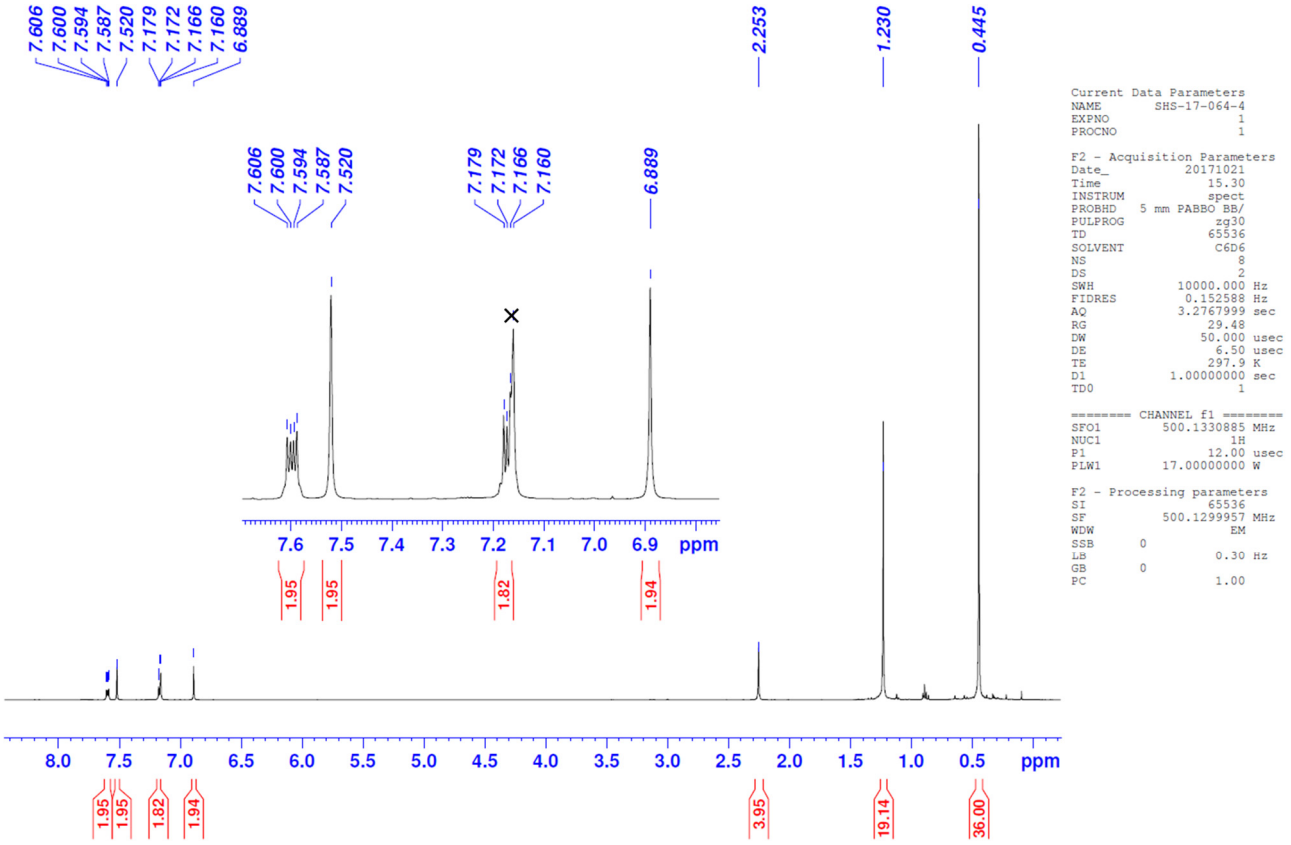


Fig. S5 ^{1}H NMR spectrum of **4** (in C_6D_6, 298 K). (× = C_6D_5H).

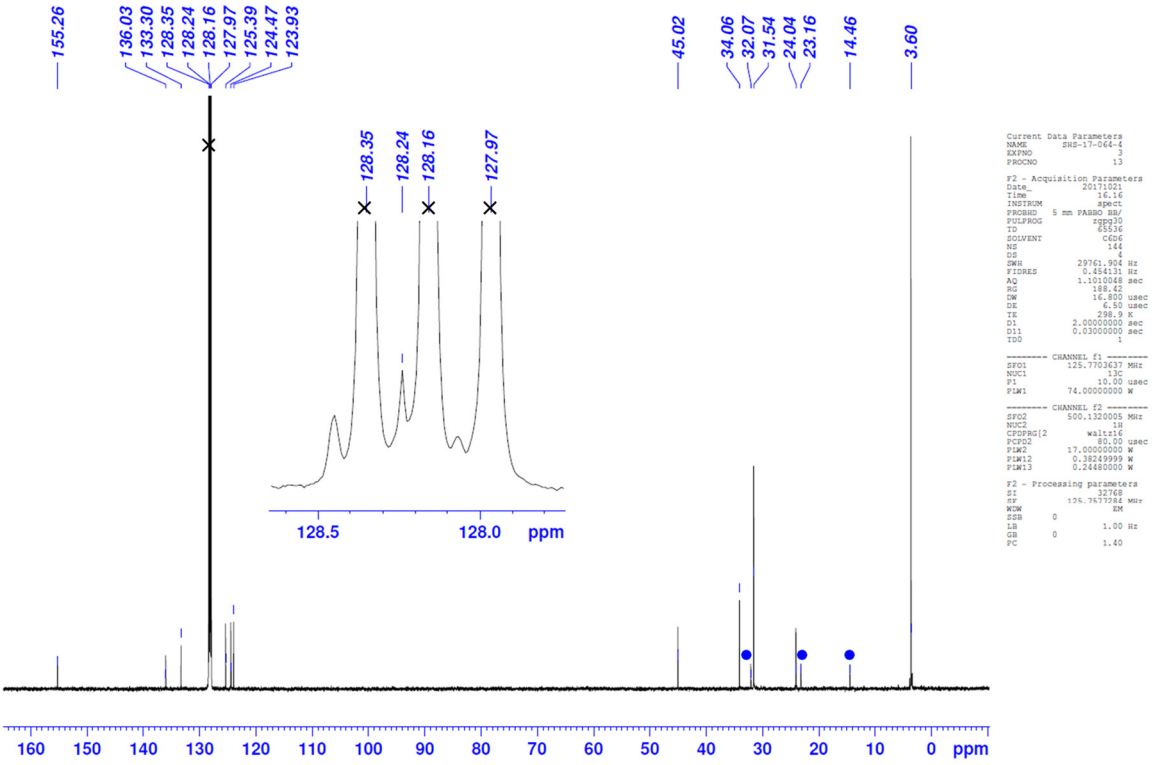


Fig. S6 $^{13}C\{^{1}H\}$ NMR spectrum of **4** (in C_6D_6, 299 K). (× = C_6D_6, • = hexane).

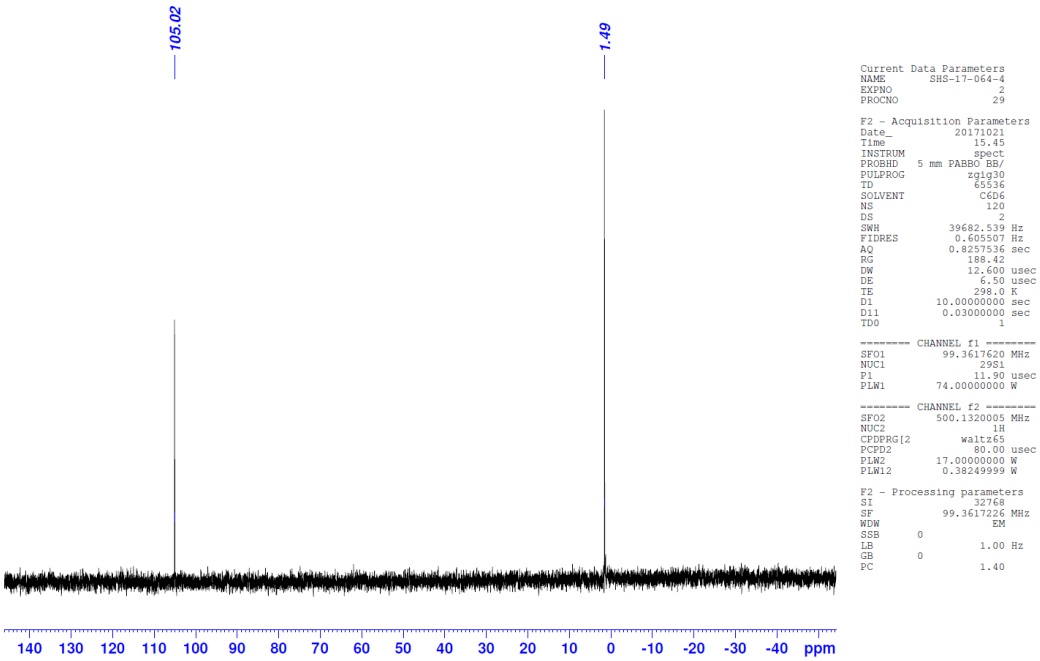


Fig. S7 $^{29}Si\{^{1}H\}$ NMR spectrum of **4** (in C_6D_6, 298 K).

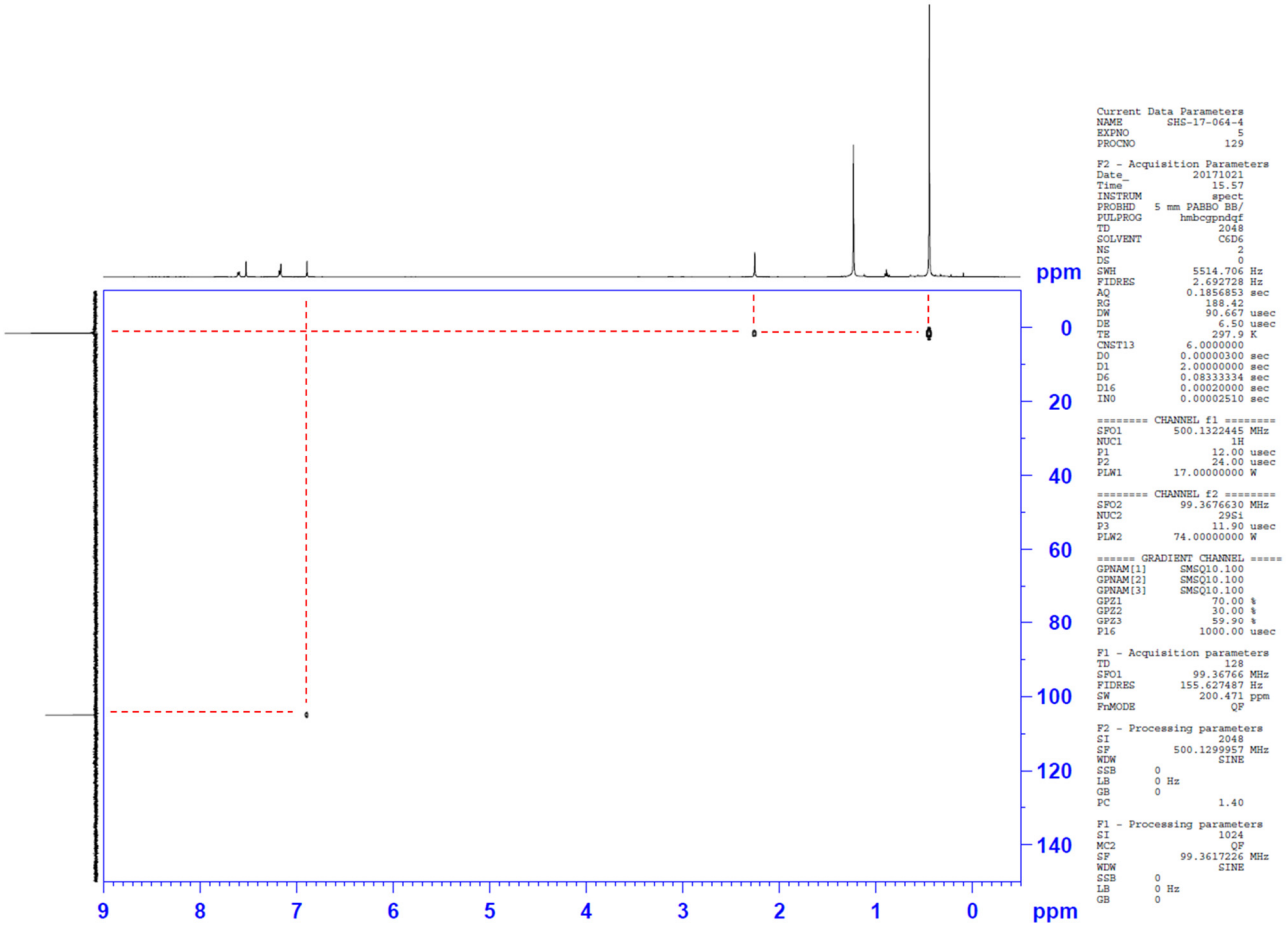


Fig. S8 ^{1}H-^{29}Si HMBC NMR spectrum of **4** (in C_6D_6, 298 K).

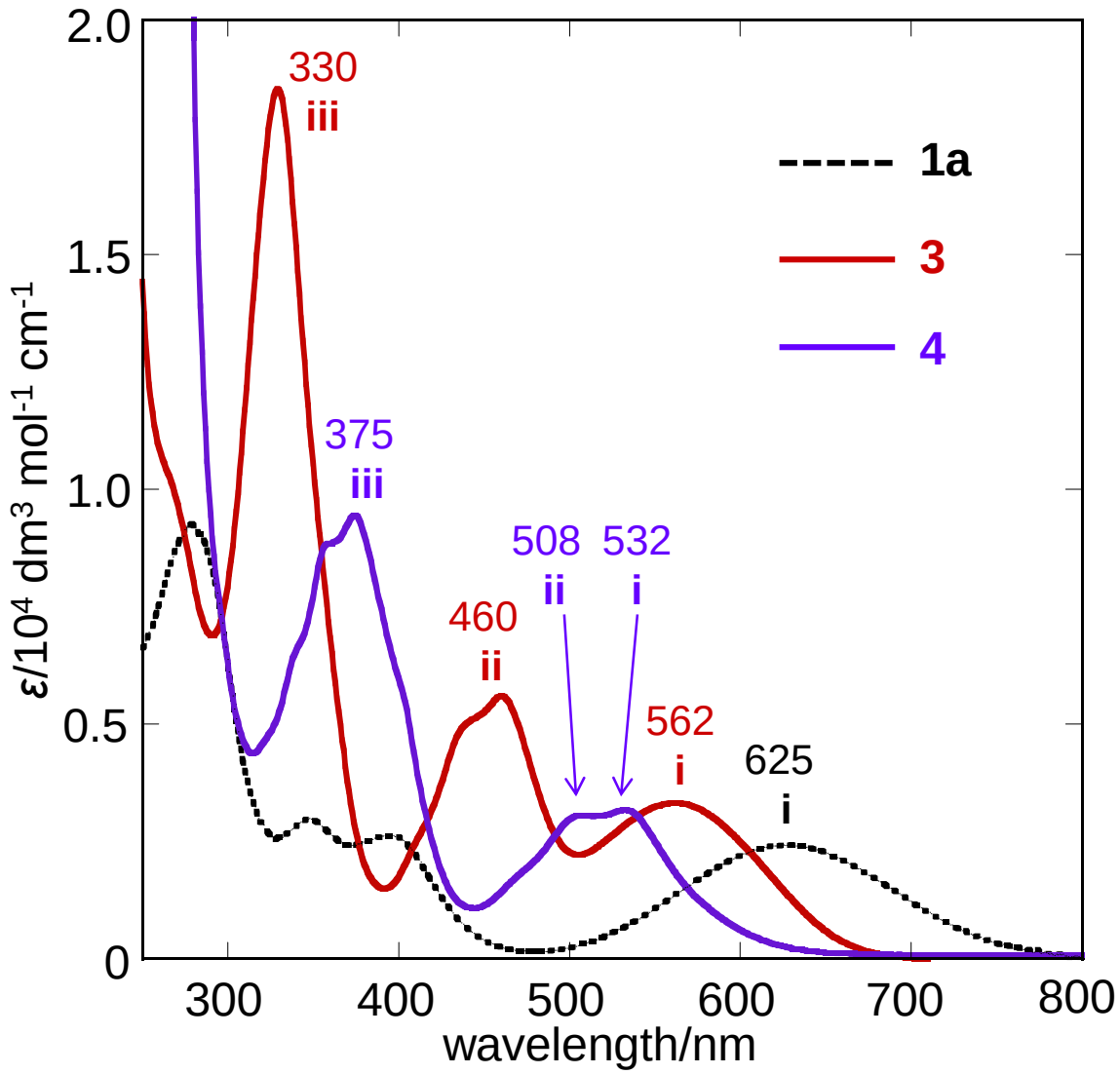


Fig. S9 UV-vis absorption spectra of **1a**[S4], **3**, and **4** in hexane solution at room temperature. The marks **i**, **ii**, and **iii** in the figure indicate band-i, band-ii, and band-iii, respectively.

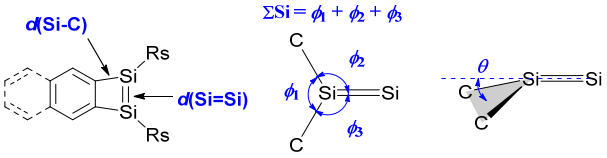
3. Single Crystal X-ray Diffraction Analysis

Single crystals suitable for X-ray diffraction study were obtained by recrystallization from toluene at –35 °C for **3** and **4**. The single crystals for data collection coated by Apiezon® grease was mounted on a glass fiber and then transferred to the cold nitrogen gas stream of the diffractometer. X-ray diffraction data were collected on a Bruker AXS APEX II CCD diffractometer with graphite monochromated Mo-Kα radiation. An empirical absorption correction based on the multiple measurement of equivalent reflections was applied using the program SADABS[S5] and the structures were solved by direct methods and refined by full-matrix least squares against F^2 using all data (SHELEX-2014).[S6] Molecular structures ware analyzed by Yadokari-XG[S7] software.

Crystal data for **3** (CCDC-1958060) (100 K): 0.30 mm × 0.20 mm × 0.02 mm; $C_{34}H_{64}Si_6$; Formula weight 641.39; monoclinic; space group *C*2/*c*; a = 13.861(2) Å, b = 13.3307(19) Å, c = 20.858(3) Å, β = 98.406(3)°, V = 3812.6(10) Å^3, Z = 4, D_{calcd} = 1.117 Mg m^{-3}, 15835 reflections measured, 3547 unique (R_{int} = 0.0461), which were used in all calculations; $R1$ = 0.0370 ($I > 2\sigma(I)$), $wR2$ = 0.1026 (all data), GOF = 1.098, max/min residual electron densities 0.583/–0.258 e/Å^3.

Crystal data for **4** (CCDC-1958061) (100 K): 0.20 mm × 0.10 mm × 0.05 mm; $C_{45}H_{74}Si_6$; Formula weight 783.58; triclinic; space group *P*-1; a = 12.9500(6) Å, b = 13.4087(7) Å, c = 14.2041(7) Å, α = 92.261(1)°, β = 101.164(1)°, γ = 100.116(1)°, V = 2375.2(2) Å^3, Z = 2, D_{calcd} = 1.096 Mg m^{-3}, 35324 reflections measured, 10901 unique (R_{int} = 0.0256), which were used in all calculations; $R1$ = 0.0331 ($I > 2\sigma(I)$), $wR2$ = 0.0891 (all data), GOF = 1.041, max/min residual electron densities 0.467/–0.230 e/Å^3.

Table S1. Structural Parameters around Disilene Moiety in **1a**, **3**, and **4**



Compound	d(Si=Si)[a]/Å	d(Si–C)[b]/Å	ΣSi[c] /°	θ[d]/°
1a[e]	2.2386(8)	1.902(2) 1.915(2)	340.47(7) 335.68(7)	35.3 40.4
3	2.1920(9)	1.8921(16)	349.17(6)	29.3
4	2.1886(5)	1.8758(13) 1.8754(13)	353.37(5) 351.23(5)	19.8 24.0

[a]the lengths of the Si=Si bonds, [b]the lengths of the Si–C bonds connecting the disilene with the benzene rings, [c]angle sums around unsaturated silicon atoms, [d]trans-bent angles of the disilene moieties, [e]ref S4

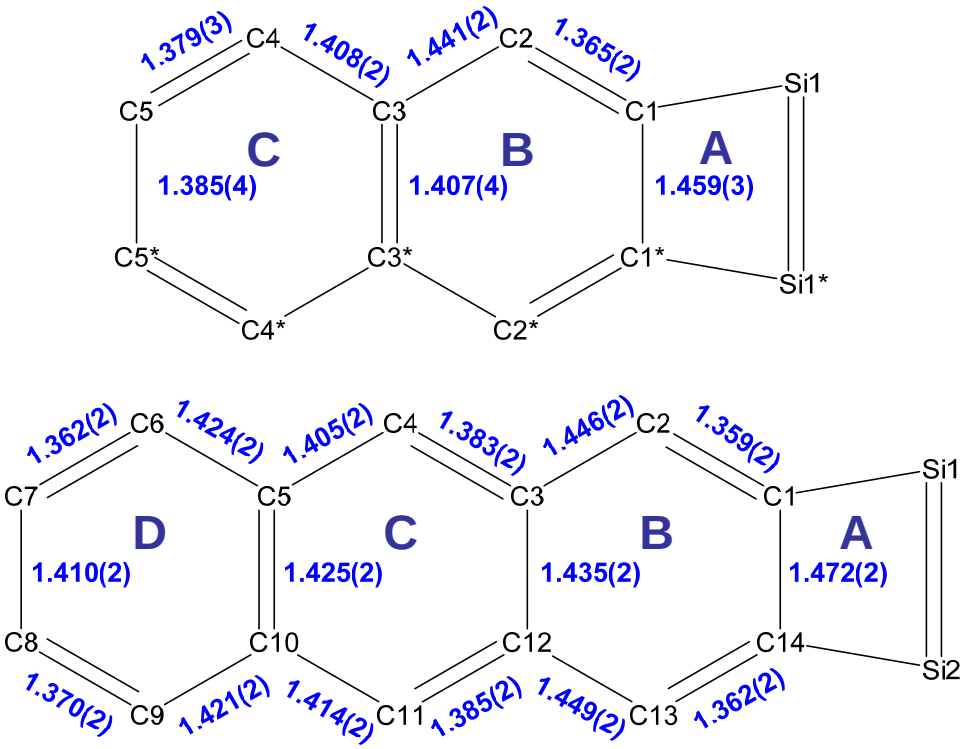


Fig. S10 C(sp^2)–C(sp^2) bond lengths (Å) of **3** and **4**.

4. Theoretical Calculations

All theoretical calculations were performed using Gaussian 09[S8] and GRRM 14[S9] programs. Geometry optimization and frequency analysis were carried out at the B3PW91+D3/6-31G(d) level of theory for all compounds. Atomic coordinates of the optimized structures were listed in Tables S2-S17. No imaginary frequencies were found in the equilibrium structures of all compounds. Forty excited states of $\mathbf{1}_{opt}$ and $\mathbf{3}_{opt}$ and sixty excited states of $\mathbf{4}_{opt}$ calculated at the TD-HCHT407/6-31+G(d,p) level of theory was summarized in Tables S18-S20. NRT analysis of $\mathbf{3}_{m}$ and $\mathbf{4}_{m}$ were carried out at the M06-2X/6-31G(d) level of theory.

Table S2. Atomic Coordinates of $\mathbf{1a}_{opt}$

Atomic Type	Coordinates (Angstroms)		
	X	Y	Z
Si	2.577081628814	2.398203581275	4.517214983814
Si	3.394933912486	0.403222326388	4.148845981485
C	4.089656593706	2.370909409673	5.700637095516
C	4.726557743056	3.215067112977	6.588276703028
H	4.446880503144	4.264430759105	6.665213239046
C	5.751630528491	2.712851757316	7.422239737688
H	6.249105055710	3.379312487591	8.120997353543
C	6.116382040249	1.384906716297	7.353287938545
H	6.907208071765	1.003496913834	7.992782178079
C	5.466808658616	0.511975599155	6.450681765630
H	5.776492911983	-0.530785031266	6.406608896953
C	4.461262379494	0.992991561101	5.635459872647
C	1.998884402578	3.987952406538	3.680591829521
C	2.027336049506	5.160946590546	4.728433865084
H	3.034320334377	5.172880730540	5.165975180290
H	1.945757591842	6.115123503684	4.181792925015
C	1.047260107628	5.273546371125	5.929801701608
C	-0.319954386070	5.823196821567	5.510864457965
H	-0.835021308232	5.174974901037	4.799905291771
H	-0.216495589561	6.812329355216	5.049069611126
H	-0.967422966374	5.928844618629	6.388996886818
C	1.676620300237	6.292205041557	6.894075725643
H	1.001289855100	6.502181066628	7.730742696491
H	1.886836063461	7.239627558264	6.383869409349
H	2.618084265487	5.912573962594	7.307644281061
C	0.870622435674	3.952323798475	6.682331502782
H	1.837898421269	3.541926279687	7.000918796559
H	0.354259880774	3.196480124930	6.080582006980
H	0.271666911334	4.114304937048	7.586532954845
Si	3.377716406698	4.500790223859	2.416088550823
C	4.853548178613	5.219869746851	3.348237656713
H	5.670808960315	5.372794384262	2.633811829456
H	5.216516189143	4.536344450447	4.123982471817
H	4.637002072422	6.186286106367	3.813259152698
C	4.097761142051	3.146283967682	1.318657676205
H	3.357996546364	2.570331321676	0.758946772325
H	4.706983471416	2.447548596358	1.899930839062
H	4.753087707355	3.640472012248	0.589944311317
Si	0.359290254176	3.665769784405	2.751377159903
C	2.716419453847	5.858146975158	1.273721207956
H	3.562909502580	6.306448656750	0.740434153121
H	2.209002854964	6.660441512846	1.818973834172
H	2.022307957564	5.471798670680	0.520612135133
C	-0.893320089411	2.649232625658	3.748261775560
H	-1.646337627390	2.252783130275	3.056194632398
H	-1.422347330475	3.214431301545	4.520098177929
H	-0.414862468949	1.793410988404	4.238522189682
C	0.712570601780	2.608244720092	1.223006659270
H	-0.235816378600	2.241095851743	0.813885930776
H	1.326846679765	1.732931236087	1.463120636022
H	1.220817747948	3.169045662098	0.432001226463
C	-0.459462283318	5.275420190551	2.169975624912
H	-0.323668692491	5.411652448308	1.092574545347
H	-0.057145601301	6.161798906975	2.669027334693
H	-1.536465134112	5.248139811271	2.368897696343
C	2.927082066142	-1.409298350169	3.913468674576
C	4.187328292531	-2.308211077862	4.191519752762
H	4.572158064489	-2.018309108614	5.178155243756
H	3.848052386070	-3.350155573319	4.313785316404
C	5.428712569239	-2.372264630932	3.259312364964

C	5.913880778219	-0.988989123962	2.818380694927
H	6.855825681279	-1.080897526570	2.264613005548
H	6.104979600996	-0.339005307220	3.682503899008
H	5.195615204351	-0.488920709580	2.159476582694
C	6.544341686346	-3.030526294751	4.086936758959
H	7.435475874908	-3.198517505545	3.472173742364
H	6.219452898659	-4.000066733470	4.482565916309
H	6.833171611713	-2.397697221908	4.934066632401
C	5.186954659869	-3.256194215817	2.031867021666
H	4.390773735192	-2.877006037570	1.389098869281
H	4.918647341085	-4.276136525547	2.332006297055
H	6.098470155275	-3.314611472614	1.425821116013
Si	1.728573876297	-1.880570207270	5.364185767518
C	0.346753646407	-0.666393249351	5.782190368576
H	-0.296179110024	-1.156450632243	6.524495299004
H	-0.281954029252	-0.383813300700	4.935605034415
H	0.745000335891	0.248284046328	6.231265056034
C	2.715072280213	-2.082835640684	6.961294633957
H	3.316006141327	-1.194423439510	7.186272097961
H	3.378117572699	-2.953016205905	6.945042029367
H	2.008152808939	-2.221168355016	7.787643207267
C	0.916286729262	-3.549024788530	4.989510657823
H	0.362943833224	-3.875833221759	5.877646114066
H	1.648140185210	-4.328529353728	4.753194774757
H	0.205550781743	-3.494215250795	4.159059945916
Si	2.027410511534	-1.624729273738	2.238955725311
C	0.298431917963	-0.866697620284	2.362530242404
H	0.321280098410	0.145007524178	2.783387442586
H	-0.381178364944	-1.469467129357	2.973608147769
H	-0.133172249852	-0.794144194771	1.357429053607
C	1.830694011730	-3.452083133761	1.764585313072
H	0.787141909054	-3.767717721797	1.862068911722
H	2.437537192605	-4.118846019495	2.384357280996
H	2.129015285999	-3.611451781372	0.722653150303
C	2.851520378799	-0.689180599214	0.809598110143
H	2.125226839811	-0.593650319132	-0.006829867234
H	3.740847199859	-1.177040427713	0.401869224953
H	3.143054793243	0.324083167139	1.109411340042

Enthalpie(0K) = -2915.912324877938

Table S3. Atomic Coordinates of $\mathbf{3_{opt}}$

Atomic Type	Coordinates (Angstroms)		
	X	Y	Z
Si	2.642303353902	2.419448460184	4.496808571204
Si	3.374959997404	0.388518975059	4.222375088001
C	4.117988386948	2.393266404352	5.693229789530
C	4.761264508358	3.236507353855	6.546655666076
H	4.517381556423	4.297706507227	6.594428536596
C	5.790718238722	2.746437569352	7.429009797574
C	6.127782439134	1.367670714848	7.401136486242
C	5.429755176987	0.491486136505	6.492937709732
H	5.714379709095	-0.560592964780	6.486825262502
C	4.456157799892	0.974038483627	5.672226111146
C	2.015688394764	3.990610514622	3.670650128878
C	2.037920777788	5.164631862521	4.718429184858
H	3.047944653644	5.189601566070	5.147995469273
H	1.941095920362	6.116392056708	4.170215071397
C	1.065309823843	5.267730473371	5.926828323359
C	-0.309759065770	5.804878382241	5.517258176350
H	-0.825839710522	5.150162950732	4.812934371684
H	-0.218717145593	6.793417077506	5.051496537622
H	-0.950527340281	5.907917526231	6.400556048402
C	1.692572819162	6.292734431155	6.885835232860
H	1.021401315400	6.496900515461	7.727218182728
H	1.890612766178	7.241936161848	6.373989514386
H	2.639975477016	5.920931066502	7.292861028894
C	0.906487523389	3.945929841011	6.682203434778
H	1.878881404374	3.548970757392	7.000289235180
H	0.400396510547	3.181917140604	6.082180094788
H	0.304866139161	4.102676145437	7.585488034638
Si	3.376379414350	4.517637801209	2.390790715590
C	4.851013556712	5.254812685488	3.309413000879
H	5.661339359103	5.416252746521	2.589085090625
H	5.227163954042	4.575732760865	4.082940470535
H	4.627038030906	6.219079921684	3.775384975746
C	4.098015292957	3.156195417304	1.303379309296
H	3.360347874886	2.589478082641	0.731530112113
H	4.690363976530	2.450346901609	1.894145624833
H	4.771447671896	3.641210374598	0.585316230060

Si	0.370709951269	3.645369535974	2.758906407515
C	2.688425347648	5.859813009442	1.247599336901
H	3.522062664500	6.301427751764	0.689237913296
H	2.194500364355	6.668546266887	1.795870646277
H	1.975574298814	5.464796449321	0.517101822805
C	-0.854180459078	2.615133373655	3.775145673538
H	-1.599414117133	2.186907145355	3.093660398369
H	-1.393970180699	3.181955961799	4.538303310167
H	-0.353173686561	1.781091190412	4.280460691133
C	0.719992247117	2.594269175248	1.225562944170
H	-0.229216131088	2.220361931182	0.824432692645
H	1.343948556503	1.723515806621	1.456193081418
H	1.215474467796	3.161976820128	0.431422199639
C	-0.469170390066	5.246963825151	2.186743371930
H	-0.357279710609	5.377749379063	1.105868459669
H	-0.059600217499	6.137561342592	2.672214463380
H	-1.541396617071	5.216553312057	2.409108247852
C	2.916643940107	-1.412903345340	3.930376181571
C	4.177173261749	-2.314618461868	4.201135640876
H	4.556191006304	-2.040007885868	5.194392630815
H	3.836913182494	-3.358075361123	4.305658607586
C	5.423669832536	-2.363521014024	3.274719396649
C	5.908550185442	-0.973786117456	2.854601129808
H	6.850392633970	-1.057787253410	2.299549072132
H	6.097464294552	-0.336314693368	3.727831124453
H	5.189978522446	-0.465011575203	2.202775709168
C	6.535729923103	-3.030196806011	4.100517765556
H	7.430819062891	-3.188041655566	3.488897139634
H	6.210942968968	-4.005572534871	4.481709321057
H	6.818051110150	-2.407159831720	4.957005803667
C	5.190666805947	-3.231810010741	2.034499032909
H	4.401121071655	-2.842776590776	1.389358302315
H	4.918176424632	-4.255107099522	2.319083837230
H	6.107254911168	-3.284032030579	1.435675461625
Si	1.706168277232	-1.909257953277	5.364418680785
C	0.331949776605	-0.688275941655	5.787029200034
H	-0.295927759366	-1.163864483556	6.551154050506
H	-0.314394295663	-0.422031327541	4.948337861507
H	0.738647351979	0.234271786091	6.212740445627
C	2.684069531690	-2.134355491922	6.962974134318
H	3.284677083091	-1.249223941963	7.201644589166
H	3.346495513728	-3.004778882372	6.937988565363
H	1.973949205825	-2.282832861030	7.784709189283
C	0.892329034257	-3.568566417745	4.959555528147
H	0.330056047575	-3.904180033994	5.838762867598
H	1.623955222843	-4.347570650478	4.720889300737
H	0.189407771757	-3.501470542642	4.123609202348
Si	2.029451193620	-1.599599951343	2.245227071778
C	0.296471522828	-0.850871213198	2.367509086613
H	0.308890578520	0.155603534973	2.800715670961
H	-0.384341125804	-1.465460518894	2.965313534785
H	-0.127953923469	-0.768777346938	1.360006573540
C	1.840448874240	-3.419907560084	1.743130778439
H	0.795861370502	-3.737088549063	1.823080707824
H	2.439954408564	-4.094336927324	2.361747453379
H	2.152429830356	-3.565175585208	0.703210452243
C	2.868706151887	-0.637796666817	0.842658678786
H	2.142372871931	-0.494343482091	0.033366327058
H	3.742574625490	-1.136461881651	0.415055563648
H	3.190562040284	0.356203491023	1.174360311026
C	6.471242440693	3.598998155083	8.319118947157
C	7.456290897962	3.112645277636	9.155724051208
H	6.208339049047	4.654164387415	8.335731394853
H	7.973334311692	3.783349783638	9.835260823544
C	7.135948969548	0.894131056396	8.263103274393
C	7.790881857455	1.748558408208	9.127739495017
H	7.390612896523	-0.162911151840	8.238821877274
H	8.563480028543	1.366928951390	9.788237274931

Enthalpie(0K) = -3069.454495122173

Table S4. Atomic Coordinates of $\mathbf{4_{opt}}$

Atomic Type	Coordinates (Angstroms)		
	X	Y	Z
Si	2.674740777974	2.428643411118	4.488507928680
Si	3.368755207821	0.381292135601	4.255150464174
C	4.130892146007	2.400600728226	5.691095082058
C	4.775807532058	3.244531623259	6.534976824362
H	4.542236690611	4.308302731782	6.571665714518
C	5.804367554815	2.757662291243	7.431915274855
C	6.134570069195	1.357069341673	7.416530584340

C	5.422318047536	0.480772906300	6.507364125492
H	5.696452266472	-0.573957566536	6.511333041555
C	4.457786129090	0.965442095285	5.684911610699
C	2.025652914349	3.992622002976	3.671299948052
C	2.045291014226	5.165434862378	4.720843745935
H	3.056354117098	5.195261058734	5.147349824297
H	1.942202501783	6.116922464729	4.173374745094
C	1.075336267784	5.262488518214	5.931845065647
C	-0.302688961078	5.795263656107	5.526417063973
H	-0.818996446771	5.139194103167	4.823530873794
H	-0.216405904934	6.784270483870	5.060720518433
H	-0.941051599528	5.895910953288	6.411697044102
C	1.701069172535	6.288406775162	6.890911762787
H	1.031295878401	6.488173331086	7.734428304343
H	1.893704087016	7.239444631591	6.380395207326
H	2.650945298044	5.919566030517	7.294756959613
C	0.923761541923	3.938962809511	6.685627659708
H	1.897986533592	3.548072410843	7.004748890063
H	0.424178980045	3.172174192117	6.083708495450
H	0.318899917441	4.091002960328	7.587503478967
Si	3.378749049162	4.527559696343	2.385493791654
C	4.851831235494	5.273429262665	3.299020373323
H	5.658737975521	5.440314066024	2.576134433925
H	5.234881287053	4.596031931956	4.070726746493
H	4.623567565073	6.235926059637	3.766540805142
C	4.102876603398	3.163085489849	1.303554332012
H	3.366994627718	2.597446821213	0.728309172406
H	4.690348092305	2.456622287687	1.898805714865
H	4.782116764522	3.644443999649	0.588606073619
Si	0.378589356166	3.639224151842	2.766107694363
C	2.678736377738	5.862571226433	1.242105421745
H	3.505582594655	6.297070100565	0.668344434394
H	2.196086560609	6.676975900722	1.792135055778
H	1.953137241904	5.464976093710	0.525824620423
C	-0.835880450249	2.602737568600	3.788156942223
H	-1.578623626322	2.164728675411	3.110185204441
H	-1.378978341994	3.168920626254	4.549413958429
H	-0.327481793897	1.775434444642	4.297131288946
C	0.727098385822	2.592579952378	1.229813266023
H	-0.222113085351	2.216821762948	0.830406170674
H	1.354226209110	1.723183589277	1.456452306642
H	1.218654829124	3.163575673194	0.435610097721
C	-0.469501826721	5.238486210762	2.200117001393
H	-0.372138650267	5.365780425213	1.117379867837
H	-0.053088899952	6.130454444965	2.677248880019
H	-1.538615713070	5.209146571488	2.436924202983
C	2.916597531943	-1.415080076602	3.938240903233
C	4.177635387517	-2.317733661934	4.204665950812
H	4.555182741363	-2.049799741252	5.200262400961
H	3.837192225292	-3.361811460617	4.301899327901
C	5.425092766787	-2.359819115602	3.279182124748
C	5.908237861512	-0.967213243487	2.866741617630
H	6.848437848452	-1.047418653973	2.308432617038
H	6.098540094405	-0.335246806177	3.743380442706
H	5.187578584883	-0.454676651140	2.220192572381
C	6.537263301289	-3.028877181381	4.102934478374
H	7.433362608345	-3.181790801014	3.491581847879
H	6.213878386406	-4.006880731814	4.478579107092
H	6.817368757086	-2.409643494669	4.962867720260
C	5.194671134551	-3.222451067735	2.034507377537
H	4.406188786148	-2.830939092938	1.389555294183
H	4.922341673300	-4.247263031954	2.313763531403
H	6.112367252071	-3.271328535774	1.437163078122
Si	1.702622715232	-1.921760010213	5.366816435937
C	0.334872795223	-0.695200333088	5.794075471386
H	-0.290178401104	-1.165865646169	6.563483608870
H	-0.315738151820	-0.429320016818	4.958525514337
H	0.747161936875	0.227152597211	6.215307182422
C	2.679054225669	-2.158512266727	6.964159256421
H	3.280708165698	-1.275513161457	7.208221290113
H	3.340303908914	-3.029643666647	6.934252075196
H	1.968518191319	-2.310810811086	7.784801977202
C	0.884835022296	-3.575295202311	4.949469692541
H	0.320569516118	-3.914706340451	5.825938504488
H	1.614625564118	-4.354847098240	4.707079820626
H	0.183204337076	-3.500989575201	4.113156911578
Si	2.032815766992	-1.590294236905	2.249790285313
C	0.299596599642	-0.842639630738	2.372915363963
H	0.310675886841	0.162261893809	2.809596087424
H	-0.382159168245	-1.459606587874	2.967168258062
H	-0.123200334968	-0.757019505261	1.365002691287
C	1.845279426128	-3.407754857109	1.737997238784
H	0.800574593934	-3.725496131533	1.814062124667
H	2.443680970033	-4.085134414091	2.354443961276

H	2.159659918737	-3.547543063085	0.698069594908
C	2.876607571355	-0.620515422289	0.855702558668
H	2.151401999388	-0.466771339259	0.047282365827
H	3.748102356225	-1.120116530805	0.424464074750
H	3.203750040740	0.369098998133	1.195149965031
C	6.474879158290	3.602150108243	8.299174084911
C	7.476340177497	3.129215908358	9.169938600760
H	6.225237303407	4.661734899431	8.310529527765
C	7.118668676663	0.885494771602	8.268597583239
C	7.805445597594	1.739093256630	9.154583134413
H	7.369713900164	-0.173788968394	8.258888906090
C	8.816021130765	1.263929888813	10.037526423439
C	9.465447661911	2.118491423583	10.886681071870
H	9.061632254858	0.204906170785	10.023371162191
H	10.233542134823	1.743195119125	11.555945632716
C	8.171884665564	3.989991662820	10.064797312699
C	9.139409757561	3.500850125513	10.900149740817
H	7.917507524116	5.047003500949	10.070716094867
H	9.663159371972	4.167628952815	11.578359835100

Enthalpie(0K) = -3222.986943921351

Table S5. Atomic Coordinates of benzene

Atomic Type	Coordinates (Angstroms)		
	X	Y	Z
H	-1.029472817182	-1.598678399010	-0.000150657585
C	-1.578860694338	-0.660364138128	0.000061607833
C	-2.988293054105	1.746485332086	0.000603950563
C	-1.593705530174	1.755021069016	0.000418372667
C	-0.888959867035	0.551610978413	0.000147512036
H	-3.537680568606	2.684799813617	0.000816215256
H	-1.055844659182	2.699990804081	0.000485861535
H	0.198333364556	0.558299517431	0.000002992887
C	-3.678196246057	0.534509348795	0.000518060853
H	-4.765488489871	0.527820965108	0.000662621088
C	-2.973450144277	-0.668901463525	0.000247198203
H	-3.511310643732	-1.613870317886	0.000179734665

Sum of electronic and zero-point Energies= -232.058059430870

Table S6. Atomic Coordinates of naphthalene

Atomic Type	Coordinates (Angstroms)		
	X	Y	Z
C	2.426270554377	0.708242231719	-0.000003448626
C	1.242218223902	1.399222501531	0.000002640974
C	0.000009750358	0.711497039336	0.000004887939
C	-0.000009724484	-0.711497761243	0.000003638599
C	1.242235847754	-1.399197671243	0.000001525134
C	2.426171059076	-0.708182516908	-0.000003385671
H	-1.236476979325	2.486309233056	-0.000002057922
H	3.370576801738	1.243874422327	-0.000010467617
H	1.235800988609	2.486287591005	0.000002604157
C	-1.242235618976	1.399197591188	0.000001503378
C	-1.242218592536	-1.399222733849	0.000001602585
H	1.236478726405	-2.486309435186	0.000003215465
H	3.370206667817	-1.244309245342	-0.000009809712
C	-2.426270622763	-0.708241827225	-0.000002506417
C	-2.426170903291	0.708183009033	-0.000003587017
H	-1.235802614184	-2.486287715480	0.000002239856
H	-3.370577124902	-1.243873655598	-0.000008002801
H	-3.370206149642	1.244310444317	-0.000011904477

Sum of electronic and zero-point Energies= -385.569753475335

Table S7. Atomic Coordinates of anthracene

Atomic Type	Coordinates (Angstroms)		
	X	Y	Z
C	3.649011786935	-0.713970902142	-0.000080528230
C	2.473963940641	-1.404757482546	-0.000005581666
C	1.218557583243	-0.718122119409	0.000042878956
C	1.218723753745	0.717891527544	0.000010835157

C	2.474072773283	1.404635871528	0.000003484110
C	3.649043013462	0.713874401784	-0.000053345118
C	-0.000189002726	-1.399667090414	0.000099394594
C	0.000188974271	1.399667418330	0.000024465182
C	-1.218557631269	0.718122319525	0.000060267478
C	-1.218723719691	-0.717891309915	0.000087837841
C	-2.474072541724	-1.404635916854	-0.000017545807
H	-2.468368040179	-2.491618596897	-0.000106976759
C	-3.649042813991	-0.713874731109	-0.000092405409
C	-3.649011792769	0.713970591298	-0.000048965743
C	-2.473964296220	1.404757461084	0.000014427458
H	-0.000645743636	-2.487940238078	0.000076551261
H	4.595508016532	-1.245599996379	-0.000150154135
H	2.467751280605	-2.491681239491	0.000010866932
H	2.468368723079	2.491618509048	0.000055583491
H	4.595293076411	1.245978119266	-0.000086422543
H	0.000645447252	2.487940610924	0.000028425218
H	-4.595292891842	-1.245978509401	-0.000239257480
H	-4.595507995683	1.245599647552	-0.000122276681
H	-2.467752196259	2.491681232606	-0.000004751842

Sum of electronic and zero-point Energies= -539.097967825624

Table S8. Atomic Coordinates of **S1**

Atomic Type	Coordinates (Angstroms)		
	X	Y	Z
C	-1.713027549112	0.707044536937	0.001920992065
C	-0.565845032165	1.442715029638	0.001750350421
C	0.664411620711	0.716107073233	0.001373285907
C	0.664044537615	-0.715902734896	0.001805933917
C	-0.566057599871	-1.442477450308	0.001663674854
C	-1.713065427166	-0.706922835112	0.001391246815
H	1.906111550864	2.482088020382	-0.000360236919
H	-0.546353471326	2.529761863057	0.002148736245
C	1.910885335293	1.394891834565	-0.000498043635
C	1.910528980305	-1.395043847252	0.000860466858
H	-0.546458207643	-2.529552277396	0.000418975020
C	3.097371282944	-0.707231326895	-0.001593686887
C	3.097581906880	0.706921382556	-0.002300490328
H	1.905567260095	-2.482234521362	0.000439287449
H	4.039627518506	-1.246411095076	-0.002951773652
H	4.039966782437	1.245948200837	-0.003594686752
C	-3.229754411684	0.785997603552	-0.001300653389
H	-3.676533800816	1.240209171120	0.887443625864
H	-3.671431058158	1.242000781425	-0.891660936423
C	-3.229732655026	-0.786027446597	-0.003347307070
H	-3.670183123349	-1.239582345407	-0.895603848801
H	-3.677906524487	-1.243082939110	0.883172415841

Sum of electronic and zero-point Energies= -462.885600954160

Table S9. Atomic Coordinates of **S2**

Atomic Type	Coordinates (Angstroms)		
	X	Y	Z
C	-0.263794955743	-0.717925937391	-0.000389272720
C	0.926285345714	-1.407281721438	-0.005838548679
C	2.164231733650	-0.711014363866	-0.003927111020
C	2.166092214445	0.715193235048	0.004912939170
C	0.928452277018	1.413305811317	0.007729218101
C	-0.262887304124	0.725160480387	0.004248492371
H	3.400161135342	-2.485277625826	-0.017172478338
H	0.949391427940	-2.496494160684	-0.011182407815
C	3.407981558805	-1.398199620212	-0.009713857592
C	3.411883528078	1.398834207084	0.009354146838
H	0.952513444594	2.502465541746	0.011879166062
C	4.595012330476	0.707280997406	0.004097482618
C	4.592959153773	-0.710021326377	-0.006103454225
H	3.407452499055	2.485984442750	0.017032276741
H	5.539803663001	1.242240822166	0.007772230768
H	5.536233444037	-1.247526904133	-0.010681312718
Si	-2.108410508718	-1.172677077984	0.004700102549
Si	-2.109963754068	1.173713574478	-0.003088761576
C	-2.660060167041	-2.105508206841	1.550143693991
H	-3.749746540384	-2.206625085345	1.578031578716
H	-2.229180752509	-3.112476057706	1.568594836637

H	-2.342540349378	-1.586548900849	2.459187116398
C	-2.672284118129	-2.114476682207	-1.531521853528
H	-2.240112333987	-3.120789573478	-1.550144534002
H	-3.762143470461	-2.217545165685	-1.546887481404
H	-2.365861536393	-1.599136356704	-2.446415259837
C	-2.668488902784	2.092405425177	-1.555021818098
H	-3.759855215716	2.171613388439	-1.590148295789
H	-2.257395275850	3.107470525811	-1.575367873689
H	-2.335368584805	1.575404033018	-2.459615198511
C	-2.683107764433	2.114378119119	1.530444237436
H	-2.251269746080	3.120588977277	1.554681420596
H	-3.773120139593	2.216537340590	1.539093931768
H	-2.382198720597	1.595975408007	2.445492654656

Sum of electronic and zero-point Energies= -1122.753405271423

Table S10. Atomic Coordinates of **S3**

Atomic Type	Coordinates (Angstroms)		
	X	Y	Z
C	-4.311068865680	-0.713709018702	-0.003321660333
C	-3.135207372997	-1.404246280268	-0.001591137965
C	-1.881237372268	-0.716876036535	0.000752222356
C	-1.881493854415	0.716819952436	0.001747223849
C	-3.135667987469	1.404123911496	0.000277927982
C	-4.311362020701	0.713431145041	-0.002345696799
C	-0.659919222272	-1.395928107094	0.001597553471
C	-0.660430662745	1.396108491157	0.002755646938
C	0.562718816142	0.723761867433	0.002423123672
C	0.562914019776	-0.723327593752	0.002238007323
C	1.806761649532	-1.449296961985	0.002297300959
H	1.786898599030	-2.536213900889	0.002915429779
C	2.943760311085	-0.712764554772	0.001143357020
C	2.943562316748	0.712499216453	-0.000190480009
C	1.806715010834	1.449401307887	0.000847153573
H	-0.662109378516	-2.484294421570	0.001352219632
H	-5.257189845107	-1.246179303714	-0.005555818382
H	-3.129559084370	-2.491315807926	-0.002354505559
H	-3.128932210066	2.491160550134	0.000734705805
H	-5.257633421366	1.245623467440	-0.003983528083
H	-0.661734100362	2.484482005098	0.002879393593
H	1.788416154598	2.536400365138	0.000092501751
C	4.460857021291	0.785856632942	-0.004972138355
H	4.901312435860	1.238838610020	-0.897465059648
H	4.908637283547	1.243961015054	0.881128103842
C	4.460935708534	-0.785860157883	-0.001703288906
H	4.906777399250	-1.239111592704	0.887905313904
H	4.903173758621	-1.243277328693	-0.890927973318

Sum of electronic and zero-point Energies= -616.414584305392

Table S11. Atomic Coordinates of **S4**

Atomic Type	Coordinates (Angstroms)		
	X	Y	Z
C	5.924038784099	0.714307856175	0.000102888127
C	4.749219434519	1.405114451338	-0.005999290790
C	3.493530567691	0.718646641327	-0.004776551037
C	3.493834896628	-0.717752503086	0.002186477432
C	4.749469460447	-1.404559092237	0.008215838200
C	5.924281971022	-0.713901215865	0.007496610866
C	2.274778353307	1.399373119494	-0.009080390142
C	2.275361658581	-1.398437756119	0.003783961376
C	1.054244720114	-0.719085225097	-0.000138726162
C	1.053727458324	0.720122144244	-0.006272386932
C	-0.198137300172	1.416623159587	-0.008010225393
H	-0.172705377750	2.505755620708	-0.011695509330
C	-1.379481263346	0.728563130604	-0.003958457797
C	-1.378425013989	-0.727540864754	-0.000358848794
C	-0.197132809934	-1.415604373410	0.001809094638
H	2.275354912404	2.487770145827	-0.014214740942
H	6.870414887626	1.246310101262	-0.000316749328
H	4.744030119420	2.492092959247	-0.011742532281
H	4.742622678837	-2.491512545441	0.013968520988
H	6.870748518113	-1.245686122817	0.012701557853
H	2.274504782636	-2.486841129205	0.008988814827
H	-0.173121809033	-2.504852657678	0.005097510266

Si	-3.228775241153	1.172623024136	0.004685106650
Si	-3.225545004051	-1.175073351988	-0.003504608564
C	-3.800796749886	2.114956027451	-1.527568250002
H	-4.892694403729	2.190648537079	-1.553499997166
H	-3.393344285275	3.131716617033	-1.532894639888
H	-3.472082624579	1.615408259071	-2.443497532476
C	-3.781987465547	2.093058240180	1.556868274229
H	-3.360885038492	3.104065286938	1.578836744849
H	-4.872593769174	2.183050221020	1.590420252990
H	-3.454951965979	1.572239358658	2.461481661767
C	-3.781728915887	-2.097404038019	-1.553388435739
H	-3.362671489491	-3.109182223519	-1.575374495791
H	-4.872503451323	-2.184910188624	-1.585625146262
H	-3.454506601677	-1.577587576216	-2.458561854155
C	-3.794270074389	-2.111334405014	1.533432698166
H	-4.885581683830	-2.195987432827	1.555202832983
H	-3.378150302275	-3.124474869857	1.548715409800
H	-3.474036841534	-1.601266147545	2.446581297755

Sum of electronic and zero-point Energies= -1276.281766942077

Table S12. Atomic Coordinates of $\mathbf{1a_m}$

Atomic Type	Coordinates (Angstroms)		
	X	Y	Z
C	2.971707154705	0.689777236734	0.051097715747
C	2.971263861553	-0.690622453283	-0.050702558393
C	1.753524448734	-1.402550171747	-0.103120287708
C	0.555691019864	-0.712781685737	-0.049439214387
C	0.556210866765	0.713043261453	0.049329455019
C	1.754330432673	1.402278654968	0.103441851814
H	1.773035179894	-2.486326122698	-0.202405762491
H	1.774253932662	2.485999971783	0.203211945397
C	-2.121948105678	2.682031941987	-0.268704634492
H	-1.765962643872	2.977297332871	-1.261873385159
H	-3.210531367700	2.571123583349	-0.301181603163
H	-1.886178156883	3.489611775233	0.433806966044
C	-2.122593152312	-2.680759439647	0.271707933754
H	-3.210473821680	-2.566099330321	0.314072584356
H	-1.895918946966	-3.488411805408	-0.433673384847
H	-1.758765393823	-2.978058042549	1.261430077610
Si	-1.312291704037	1.064982567730	0.285616421342
Si	-1.312948117427	-1.065294917417	-0.287667868939
H	3.913804340159	1.231312625468	0.096640850786
H	3.913057792185	-1.232748504423	-0.096067469959

Sum of electronic and zero-point Energies= -889.426881106294

Table S13. Atomic Coordinates of $\mathbf{3_m}$

Atomic Type	Coordinates (Angstroms)		
	X	Y	Z
C	1.834151489196	0.708081555538	0.028498827555
C	1.834169493085	-0.711289197987	-0.025861115147
C	0.577803779235	-1.415136611625	-0.055107405108
C	-0.596280008973	-0.730870706448	-0.024385677476
C	-0.595810225293	0.727343605864	0.027189535975
C	0.578054939510	1.411717483702	0.059008684362
H	0.603921218374	-2.501701654082	-0.117285471019
H	0.603711622319	2.498339708781	0.121383409233
C	-3.287096902929	2.683608690310	-0.236304381483
H	-2.934857045463	3.026356585162	-1.212871987486
H	-4.371551970842	2.555294436688	-0.274555372050
H	-3.061598418683	3.456308368395	0.504480141670
C	-3.305480983939	-2.674912455248	0.233083911563
H	-4.379412653813	-2.509654500132	0.349891285963
H	-3.159657071603	-3.428206999632	-0.546350618733
H	-2.902075052022	-3.063388412368	1.171950902649
Si	-2.451995354813	1.063315826410	0.234300209416
Si	-2.453238912510	-1.061936167908	-0.235042564104
C	3.066270306934	1.391286350790	0.055723123821
C	4.260957191590	0.701463799371	0.026492736243
H	3.060305333647	2.477832095741	0.097531043650
H	5.202280237660	1.242094502385	0.045177769338
C	3.066572946939	-1.393769670195	-0.056085657277
C	4.261062770848	-0.703188214641	-0.029601466341
H	3.061473499942	-2.480324620267	-0.098317719514

H	5.202403882734	-1.243791828177	-0.051992228090

Sum of electronic and zero-point Energies= -1042.946336387005

Table S14. Atomic Coordinates of $\mathbf{4_m}$

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	5.525673330900	0.710353304243	-0.023200425630
C	4.344580187409	1.400283652108	-0.049618893363
C	3.097378002492	0.713650970845	-0.026433823740
C	3.097790031624	-0.714381065371	0.024939101055
C	4.345563374459	-1.400350120584	0.051070498352
C	5.526234600016	-0.709646353083	0.028207919366
C	1.865407927817	1.395079920883	-0.050898771971
C	1.866130083507	-1.396201485281	0.047733586457
C	0.657670166708	-0.719893505114	0.021636793113
C	0.657399222307	0.718446498062	-0.025242189139
C	-0.609675477151	1.419757113030	-0.047084994097
H	-0.583541679009	2.506700161173	-0.099460768885
C	-1.777549826596	0.735722805976	-0.019097237750
C	-1.777596113169	-0.737010484190	0.015890663475
C	-0.609500920525	-1.421063407854	0.043845772372
H	1.867046422109	2.482932440111	-0.088825639485
H	6.470279085033	1.245277339778	-0.041267700635
H	4.338774588021	2.486674649939	-0.089284465048
H	4.339103111551	-2.486735804356	0.090356449674
H	6.471284881881	-1.243651563945	0.049268770955
H	1.866873718590	-2.484071577887	0.085655196303
H	-0.584306208535	-2.508001275928	0.098124937304
Si	-3.626506174598	-1.065153555226	0.209287237526
Si	-3.627014959914	1.065900152822	-0.209360198133
C	-4.493096422347	-2.675413586466	-0.233663494771
H	-4.147050640102	-3.040562619828	-1.204204707445
H	-4.286885058359	-3.441308576992	0.519367540220
H	-5.574039463063	-2.522248454582	-0.277595073689
C	-4.486231656502	2.677931557491	0.239923629105
H	-5.570668245262	2.545150513850	0.237204639152
H	-4.172271517347	3.014160417327	1.231642023894
H	-4.235745154115	3.457514497627	-0.485239016221

Sum of electronic and zero-point Energies= -1196.478728303493

Table S15. Atomic Coordinates of **5**

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.511431900441	0.710801010728	-0.000011016021
C	0.634782276522	1.443698729702	-0.000052256044
C	0.634630863226	-1.443737396121	-0.000024325431
C	-0.511571534317	-0.710793815479	-0.000021914449
H	0.656156157720	2.530340233472	0.000009116895
H	0.656069297499	-2.530377705112	-0.000041754975
C	-2.030685239119	-0.675339910257	-0.000024627560
C	-2.030615704473	0.675458619277	0.000061423996
H	-2.809156486979	1.430297696412	0.000203865699
H	-2.809212644121	-1.430189619330	-0.000064463760
C	1.853048830367	-0.688641317980	0.000065416408
C	1.853165240940	0.688562762169	-0.000025998669
H	2.800008003713	-1.222609315741	0.000172301203
H	2.800136084996	1.222435334757	0.000117405765

Sum of electronic and zero-point Energies= -308.132659819679

Table S16. Atomic Coordinates of **6**

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.755091909614	0.724757310253	-0.000388391859
C	-0.629197343214	1.454602660406	0.001348464213
C	0.626599187395	0.712726167696	0.001025151340
C	0.626429638347	-0.712368232135	0.001128341898
C	-0.629269622183	-1.454469259996	0.000517389389

C	-1.755155333342	-0.724700168357	-0.001026789650
H	1.852444118499	2.476127793488	-0.000000514003
H	-0.604549208492	2.540702784841	0.003301026458
C	1.855908348642	1.388864640210	-0.000320289340
C	1.855634500264	-1.388912547656	0.000948936103
H	-0.604545371742	-2.540597885312	0.000308532951
C	3.056979091837	-0.699572224703	-0.000618908057
C	3.057156488689	0.699216610899	-0.001553022521
H	1.851620825295	-2.476168112898	0.000576537968
H	3.995641183575	-1.244817324455	-0.000693229338
H	3.995908932857	1.244405923272	-0.001996724057
C	-3.256268174084	-0.675749573937	-0.000861191395
C	-3.256346204123	0.675645826682	-0.000392890391
H	-4.037067110793	1.426331422682	0.000896955950
H	-4.036875888718	-1.426475274432	-0.000092183410

Sum of electronic and zero-point Energies= -461.657092163119

Table S17. Atomic Coordinates of **7**

Atomic Type	Coordinates (Angstroms)		
	X	Y	Z
C	-4.266528622105	-0.709435687389	-0.002229868192
C	-3.083333510865	-1.400385002053	-0.000245277705
C	-1.840215938212	-0.712121934160	0.001281140143
C	-1.840549580704	0.712333408849	0.000925973339
C	-3.084179353030	1.400152963119	-0.000635858125
C	-4.267012321968	0.708681231936	-0.002377260098
C	-0.601863731737	-1.393035314561	0.002102228286
C	-0.602478689751	1.393511006593	0.001640770281
C	0.604112337800	0.724602511647	0.001769482656
C	0.604356315175	-0.723828612273	0.001827910826
C	1.868651426451	-1.462352017080	0.000705019377
H	1.844004334342	-2.548388250195	0.000126928081
C	2.988976159171	-0.730817632262	-0.000368868355
C	2.988766113492	0.730450072758	0.000117223050
C	1.868752858138	1.462597420340	0.001192561729
H	-0.605714363152	-2.481446936808	0.002236935700
H	-5.210651436308	-1.245454159147	-0.003872706259
H	-3.077426342215	-2.487485017416	0.000189619793
H	-3.077511277795	2.487235132779	-0.000745891456
H	-5.211516472168	1.244001135223	-0.003946156361
H	-0.605421383795	2.481939027853	0.001326420787
H	1.845995631995	2.548737345414	0.000703171323
C	4.481362169851	-0.677676591008	-0.002786570693
C	4.481225761210	0.677400064969	-0.001980386825
H	5.263023176506	-1.427529585017	-0.004591154670
H	5.262676669119	1.427487704926	-0.002598388108

Sum of electronic and zero-point Energies= -615.191594110860

Table S18. Transition Energy, Wavelength, and Oscillator Strengths of the Electronic Transition of **1a$_{opt}$**.

```
Excited State   1:       Singlet-A       1.8677 eV
663.82 nm  f=0.0515  <S**2>=0.000
     163 -> 164       0.70136
     163 -> 169      -0.10699

 Excited State   2:       Singlet-A       2.7890 eV
444.54 nm  f=0.0057  <S**2>=0.000
     163 -> 166       0.70359

 Excited State   3:       Singlet-A       2.9522 eV
419.97 nm  f=0.0002  <S**2>=0.000
     163 -> 167       0.70347

 Excited State   4:       Singlet-A       3.0550 eV
405.85 nm  f=0.0723  <S**2>=0.000
     162 -> 164      -0.15962
     163 -> 165       0.65352
     163 -> 170      -0.17882

 Excited State   5:       Singlet-A       3.0923 eV
400.94 nm  f=0.0006  <S**2>=0.000
     163 -> 168       0.70402

 Excited State   6:       Singlet-A       3.2863 eV
377.27 nm  f=0.0112  <S**2>=0.000
     163 -> 165       0.16361
     163 -> 170       0.68143

 Excited State   7:       Singlet-A       3.4112 eV
363.47 nm  f=0.0352  <S**2>=0.000
     163 -> 169       0.55996
     163 -> 172       0.38741

 Excited State   8:       Singlet-A       3.4576 eV
358.59 nm  f=0.0002  <S**2>=0.000
     163 -> 171       0.68393
     163 -> 174       0.16324

 Excited State   9:       Singlet-A       3.4886 eV
355.39 nm  f=0.0221  <S**2>=0.000
     163 -> 169      -0.29900
     163 -> 172       0.54931
     163 -> 173       0.28519

 Excited State  10:       Singlet-A       3.5141 eV
352.81 nm  f=0.0135  <S**2>=0.000
     163 -> 169       0.17352
     163 -> 172      -0.20621
     163 -> 173       0.64325

 Excited State  11:       Singlet-A       3.5678 eV
347.51 nm  f=0.0026  <S**2>=0.000
     162 -> 164       0.13501
     163 -> 171      -0.14643
     163 -> 174       0.67028

 Excited State  12:       Singlet-A       3.6612 eV
338.64 nm  f=0.0052  <S**2>=0.000
     163 -> 175       0.69540

 Excited State  13:       Singlet-A       3.8126 eV
325.20 nm  f=0.0021  <S**2>=0.000
     162 -> 164       0.13489
     163 -> 176       0.69213

 Excited State  14:       Singlet-A       3.8735 eV
320.09 nm  f=0.0052  <S**2>=0.000
     161 -> 164      -0.21695
     163 -> 177       0.64842
     163 -> 179       0.14077

 Excited State  15:       Singlet-A       3.9338 eV
315.18 nm  f=0.0073  <S**2>=0.000
     159 -> 164       0.12997
     161 -> 164       0.58944
     163 -> 177       0.16478
     163 -> 179       0.28311

 Excited State  16:       Singlet-A       3.9512 eV
313.79 nm  f=0.0025  <S**2>=0.000
     162 -> 164      -0.12932
     163 -> 178       0.68830

 Excited State  17:       Singlet-A       3.9692 eV
312.37 nm  f=0.0089  <S**2>=0.000
     161 -> 164      -0.23237
     163 -> 177      -0.21279
     163 -> 179       0.62819

 Excited State  18:       Singlet-A       4.0069 eV
309.42 nm  f=0.0032  <S**2>=0.000
     163 -> 180       0.68123
     163 -> 181      -0.15192

 Excited State  19:       Singlet-A       4.0122 eV
309.02 nm  f=0.0864  <S**2>=0.000
     158 -> 164       0.14396
     162 -> 164       0.55238
     163 -> 165       0.14659
     163 -> 178       0.15455
     163 -> 180      -0.15240
     163 -> 181      -0.25259

 Excited State  20:       Singlet-A       4.0709 eV
304.56 nm  f=0.0016  <S**2>=0.000
     163 -> 181      -0.11056
     163 -> 182       0.67198
     163 -> 183       0.17190

 Excited State  21:       Singlet-A       4.0769 eV
304.12 nm  f=0.0035  <S**2>=0.000
     163 -> 182      -0.18290
     163 -> 183       0.67975

 Excited State  22:       Singlet-A       4.0881 eV
303.28 nm  f=0.0172  <S**2>=0.000
     158 -> 164       0.13705
     162 -> 164       0.20701
     163 -> 181       0.61151
     163 -> 182       0.10860

 Excited State  23:       Singlet-A       4.1723 eV
297.16 nm  f=0.0053  <S**2>=0.000
     158 -> 164       0.24036
     160 -> 164       0.65932

 Excited State  24:       Singlet-A       4.2067 eV
294.73 nm  f=0.0223  <S**2>=0.000
     158 -> 164       0.10240
     163 -> 184       0.68914
```

```
 Excited State  25:       Singlet-A       4.2208 eV
293.74 nm  f=0.0075  <S**2>=0.000
     159 -> 164      -0.27973
     163 -> 185       0.64580

 Excited State  26:       Singlet-A       4.2775 eV
289.85 nm  f=0.0607  <S**2>=0.000
     157 -> 164      -0.20685
     159 -> 164       0.50654
     163 -> 185       0.22884
     163 -> 186      -0.33903
     163 -> 189       0.10278

 Excited State  27:       Singlet-A       4.2899 eV
289.02 nm  f=0.0229  <S**2>=0.000
     158 -> 164       0.61434
     160 -> 164      -0.21918
     162 -> 164      -0.16007
     163 -> 187       0.10575

 Excited State  28:       Singlet-A       4.3048 eV
288.01 nm  f=0.0131  <S**2>=0.000
     157 -> 164      -0.17814
     159 -> 164       0.23949
     163 -> 185       0.13181
     163 -> 186       0.61485

 Excited State  29:       Singlet-A       4.3109 eV
287.61 nm  f=0.0013  <S**2>=0.000
     163 -> 187       0.69604

 Excited State  30:       Singlet-A       4.4012 eV
281.71 nm  f=0.0001  <S**2>=0.000
     163 -> 188       0.70347

 Excited State  31:       Singlet-A       4.4413 eV
279.16 nm  f=0.0170  <S**2>=0.000
     157 -> 164       0.17693
     163 -> 189       0.67945

 Excited State  32:       Singlet-A       4.4662 eV
277.60 nm  f=0.0022  <S**2>=0.000
     156 -> 164       0.68245
     163 -> 190       0.14475

 Excited State  33:       Singlet-A       4.4743 eV
277.10 nm  f=0.0012  <S**2>=0.000
     156 -> 164      -0.14362
     163 -> 190       0.68995

 Excited State  34:       Singlet-A       4.5534 eV
272.29 nm  f=0.0368  <S**2>=0.000
     155 -> 164      -0.11677
     157 -> 164       0.48719
     159 -> 164       0.15316
     163 -> 189      -0.11978
     163 -> 191       0.38314
     163 -> 192      -0.13284

 Excited State  35:       Singlet-A       4.6194 eV
268.40 nm  f=0.0045  <S**2>=0.000
     155 -> 164       0.13132
     157 -> 164      -0.23452
     163 -> 191       0.56080
     163 -> 192       0.28732

 Excited State  36:       Singlet-A       4.6570 eV
266.23 nm  f=0.0174  <S**2>=0.000
     155 -> 164      -0.18567
     157 -> 164       0.14732
     163 -> 191      -0.15810
     163 -> 192       0.61796
     163 -> 194       0.10127

 Excited State  37:       Singlet-A       4.6866 eV
264.55 nm  f=0.0003  <S**2>=0.000
     163 -> 193       0.69776

 Excited State  38:       Singlet-A       4.7313 eV
262.05 nm  f=0.0031  <S**2>=0.000
     155 -> 164       0.49145
     163 -> 194       0.48876

 Excited State  39:       Singlet-A       4.7359 eV
261.79 nm  f=0.0004  <S**2>=0.000
     154 -> 164       0.70370

 Excited State  40:       Singlet-A       4.7432 eV
261.39 nm  f=0.0027  <S**2>=0.000
     155 -> 164       0.20202
     163 -> 194      -0.32357
     163 -> 195       0.57963
```

Table S19. Transition Energy, Wavelength, and Oscillator Strengths of the Electronic Transition of $\mathbf{3_{opt}}$.

```
Excited State   1:       Singlet-A       2.0950 eV
591.82 nm  f=0.0588  <S**2>=0.000
     176 -> 177       0.69559
     176 -> 182      -0.10468

 Excited State   2:       Singlet-A       2.6598 eV
466.13 nm  f=0.1351  <S**2>=0.000
     175 -> 177      -0.28909
     176 -> 178       0.64121

 Excited State   3:       Singlet-A       2.8932 eV
428.53 nm  f=0.0050  <S**2>=0.000
     176 -> 179       0.70292

 Excited State   4:       Singlet-A       3.0425 eV
407.50 nm  f=0.0000  <S**2>=0.000
     176 -> 180       0.70628

 Excited State   5:       Singlet-A       3.2121 eV
385.99 nm  f=0.0003  <S**2>=0.000
     176 -> 181       0.65846
     176 -> 182       0.25368

 Excited State   6:       Singlet-A       3.3271 eV
372.65 nm  f=0.0100  <S**2>=0.000
     175 -> 177       0.10723
     176 -> 183       0.64035
     176 -> 184      -0.26195

 Excited State   7:       Singlet-A       3.3924 eV
365.47 nm  f=0.3227  <S**2>=0.000
     175 -> 177       0.60473
     176 -> 178       0.25383
     176 -> 183      -0.11672
     176 -> 188       0.15466

 Excited State   8:       Singlet-A       3.4341 eV
361.04 nm  f=0.0516  <S**2>=0.000
     174 -> 177       0.17845
     176 -> 181      -0.22654
     176 -> 182       0.61671

 Excited State   9:       Singlet-A       3.4689 eV
357.41 nm  f=0.0007  <S**2>=0.000
     176 -> 183       0.23654
     176 -> 184       0.58888
     176 -> 185       0.29166

 Excited State  10:       Singlet-A       3.5163 eV
352.60 nm  f=0.0000  <S**2>=0.000
     176 -> 183      -0.10938
     176 -> 184      -0.26428
     176 -> 185       0.64304

 Excited State  11:       Singlet-A       3.5699 eV
347.31 nm  f=0.0039  <S**2>=0.000
     176 -> 186       0.70186

 Excited State  12:       Singlet-A       3.6193 eV
342.56 nm  f=0.0027  <S**2>=0.000
     176 -> 187       0.70168

 Excited State  13:       Singlet-A       3.7062 eV
334.53 nm  f=0.0475  <S**2>=0.000
     175 -> 177      -0.12205
     176 -> 188       0.67077

 Excited State  14:       Singlet-A       3.7454 eV
331.03 nm  f=0.0094  <S**2>=0.000
     176 -> 189       0.70454

 Excited State  15:       Singlet-A       3.9608 eV
313.03 nm  f=0.0043  <S**2>=0.000
     176 -> 191       0.69281
     176 -> 193      -0.11368

 Excited State  16:       Singlet-A       3.9885 eV
310.86 nm  f=0.0085  <S**2>=0.000
     176 -> 190       0.67930
     176 -> 192       0.16442

 Excited State  17:       Singlet-A       4.0088 eV
309.28 nm  f=0.0005  <S**2>=0.000
     176 -> 190      -0.16716
     176 -> 192       0.65160
     176 -> 193      -0.21068

 Excited State  18:       Singlet-A       4.0280 eV
307.81 nm  f=0.0131  <S**2>=0.000
     176 -> 191       0.10515
     176 -> 192       0.20549
     176 -> 193       0.64416
     176 -> 194      -0.13587

 Excited State  19:       Singlet-A       4.0498 eV
306.15 nm  f=0.0066  <S**2>=0.000
     174 -> 177       0.52118
     175 -> 178       0.44692

 Excited State  20:       Singlet-A       4.1180 eV
301.08 nm  f=0.0002  <S**2>=0.000
     176 -> 194      -0.33175
     176 -> 195       0.62097

 Excited State  21:       Singlet-A       4.1339 eV
299.92 nm  f=0.0015  <S**2>=0.000
     176 -> 193       0.10948
     176 -> 194       0.57925
     176 -> 195       0.32971
     176 -> 196       0.16675

 Excited State  22:       Singlet-A       4.1504 eV
298.73 nm  f=0.0020  <S**2>=0.000
     176 -> 194      -0.15559
     176 -> 196       0.68248

 Excited State  23:       Singlet-A       4.1739 eV
297.04 nm  f=0.0084  <S**2>=0.000
     173 -> 177       0.10296
     175 -> 178      -0.10979
     176 -> 197       0.68006

 Excited State  24:       Singlet-A       4.1918 eV
295.78 nm  f=0.0389  <S**2>=0.000
     173 -> 177      -0.28297
     174 -> 177      -0.29743
     175 -> 178       0.40134
     176 -> 197       0.19088
     176 -> 198       0.28074
     176 -> 199       0.11737
```

```
 Excited State   25:       Singlet-A       4.2391 eV
292.47 nm  f=0.0058  <S**2>=0.000
     173 -> 177       0.24849
     174 -> 177       0.10308
     175 -> 178      -0.12149
     176 -> 198       0.63197

 Excited State   26:       Singlet-A       4.2873 eV
289.19 nm  f=0.0188  <S**2>=0.000
     174 -> 178       0.10475
     175 -> 179       0.68623

 Excited State   27:       Singlet-A       4.3226 eV
286.83 nm  f=0.0165  <S**2>=0.000
     173 -> 177       0.35870
     176 -> 199       0.59624

 Excited State   28:       Singlet-A       4.3607 eV
284.32 nm  f=0.0128  <S**2>=0.000
     176 -> 200       0.67783
     176 -> 201       0.15557

 Excited State   29:       Singlet-A       4.3869 eV
282.62 nm  f=0.0110  <S**2>=0.000
     171 -> 177       0.23201
     172 -> 177       0.63041
     173 -> 177       0.12759

 Excited State   30:       Singlet-A       4.3982 eV
281.90 nm  f=0.0849  <S**2>=0.000
     170 -> 177      -0.14421
     171 -> 177      -0.20893
     172 -> 177      -0.12352
     173 -> 177       0.38335
     174 -> 177      -0.17824
     175 -> 178       0.17978
     175 -> 180      -0.16885
     176 -> 199      -0.30751
     176 -> 202       0.18590

 Excited State   31:       Singlet-A       4.4002 eV
281.77 nm  f=0.0057  <S**2>=0.000
     171 -> 177       0.62519
     172 -> 177      -0.26707

 Excited State   32:       Singlet-A       4.4145 eV
280.85 nm  f=0.0048  <S**2>=0.000
     176 -> 200      -0.14970
     176 -> 201       0.67649

 Excited State   33:       Singlet-A       4.4241 eV
280.25 nm  f=0.0092  <S**2>=0.000
     175 -> 180       0.68154

 Excited State   34:       Singlet-A       4.4659 eV
277.62 nm  f=0.0300  <S**2>=0.000
     173 -> 177      -0.12489
     176 -> 202       0.66895

 Excited State   35:       Singlet-A       4.5215 eV
274.21 nm  f=0.0002  <S**2>=0.000
     176 -> 203       0.70028

 Excited State   36:       Singlet-A       4.5634 eV
271.69 nm  f=0.0018  <S**2>=0.000
     176 -> 204       0.70475

 Excited State   37:       Singlet-A       4.5812 eV
270.63 nm  f=0.0003  <S**2>=0.000
     174 -> 178      -0.18442
     175 -> 181       0.66098
     175 -> 182       0.14205

 Excited State   38:       Singlet-A       4.6104 eV
268.92 nm  f=0.0071  <S**2>=0.000
     170 -> 177       0.64254
     174 -> 177      -0.10041
     176 -> 205       0.11015
     176 -> 206      -0.16523

 Excited State   39:       Singlet-A       4.6269 eV
267.96 nm  f=0.0140  <S**2>=0.000
     168 -> 177       0.18172
     169 -> 177       0.53679
     174 -> 178      -0.28588
     175 -> 182      -0.28760

 Excited State   40:       Singlet-A       4.6325 eV
267.64 nm  f=0.0014  <S**2>=0.000
     168 -> 177       0.11880
     169 -> 177       0.38548
     174 -> 178       0.38776
     175 -> 182       0.42612
```

Table S20. Transition Energy, Wavelength, and Oscillator Strengths of the Electronic Transition of $\mathbf{4_{opt}}$.

```
Excited State   1:       Singlet-A       2.2098 eV
561.07 nm  f=0.0654  <S**2>=0.000
     189 -> 190       0.68649
     189 -> 195       0.11389

 Excited State   2:       Singlet-A       2.2308 eV
555.79 nm  f=0.1679  <S**2>=0.000
     188 -> 190       0.29986
     189 -> 191       0.63034

 Excited State   3:       Singlet-A       2.9151 eV
425.31 nm  f=0.4895  <S**2>=0.000
     188 -> 190       0.61237
     189 -> 191      -0.26806
     189 -> 194      -0.12492

 Excited State   4:       Singlet-A       2.9596 eV
418.92 nm  f=0.0047  <S**2>=0.000
     189 -> 192       0.70026

 Excited State   5:       Singlet-A       3.1117 eV
398.45 nm  f=0.0013  <S**2>=0.000
     189 -> 193       0.66235
     189 -> 194       0.24514

 Excited State   6:       Singlet-A       3.1143 eV
398.12 nm  f=0.0118  <S**2>=0.000
     188 -> 191       0.66124
     189 -> 195      -0.20019

 Excited State   7:       Singlet-A       3.2881 eV
377.07 nm  f=0.0040  <S**2>=0.000
     189 -> 195      -0.35772
     189 -> 196       0.59866

 Excited State   8:       Singlet-A       3.3257 eV
372.81 nm  f=0.0793  <S**2>=0.000
     189 -> 193      -0.20722
     189 -> 194       0.59212
     189 -> 197      -0.23152

 Excited State   9:       Singlet-A       3.4168 eV
362.86 nm  f=0.0721  <S**2>=0.000
     187 -> 190      -0.20963
     188 -> 191       0.16453
     189 -> 190      -0.10084
     189 -> 195       0.52465
     189 -> 196       0.35246

 Excited State  10:       Singlet-A       3.4431 eV
360.10 nm  f=0.0182  <S**2>=0.000
     189 -> 194       0.19883
     189 -> 197       0.65832

 Excited State  11:       Singlet-A       3.5560 eV
348.67 nm  f=0.0000  <S**2>=0.000
     189 -> 198       0.63912
     189 -> 199      -0.29656

 Excited State  12:       Singlet-A       3.6493 eV
339.75 nm  f=0.0064  <S**2>=0.000
     189 -> 200       0.69795

 Excited State  13:       Singlet-A       3.6545 eV
339.26 nm  f=0.0352  <S**2>=0.000
     186 -> 190      -0.12793
     189 -> 198       0.28092
     189 -> 199       0.60410
     189 -> 200      -0.10075

 Excited State  14:       Singlet-A       3.6925 eV
335.77 nm  f=0.0012  <S**2>=0.000
     189 -> 201       0.70606

 Excited State  15:       Singlet-A       3.7592 eV
329.82 nm  f=0.0326  <S**2>=0.000
     187 -> 191      -0.11472
     188 -> 192       0.67974
     188 -> 195       0.11657

 Excited State  16:       Singlet-A       3.7768 eV
328.28 nm  f=0.0080  <S**2>=0.000
     189 -> 202       0.69711

 Excited State  17:       Singlet-A       3.8274 eV
323.94 nm  f=0.0051  <S**2>=0.000
     189 -> 203       0.70533

 Excited State  18:       Singlet-A       3.8937 eV
318.42 nm  f=0.0003  <S**2>=0.000
     188 -> 193       0.68761
     188 -> 194       0.15909

 Excited State  19:       Singlet-A       3.9814 eV
311.41 nm  f=0.0022  <S**2>=0.000
     189 -> 204       0.67157
     189 -> 206       0.21182

 Excited State  20:       Singlet-A       4.0006 eV
309.92 nm  f=0.0001  <S**2>=0.000
     186 -> 191       0.32890
     188 -> 193      -0.12085
     188 -> 194       0.60749

 Excited State  21:       Singlet-A       4.0065 eV
309.46 nm  f=0.0003  <S**2>=0.000
     189 -> 205       0.70175

 Excited State  22:       Singlet-A       4.0142 eV
308.87 nm  f=0.0005  <S**2>=0.000
     187 -> 191       0.45952
     188 -> 195       0.53127

 Excited State  23:       Singlet-A       4.0587 eV
305.48 nm  f=0.0581  <S**2>=0.000
     187 -> 190      -0.35536
     189 -> 204      -0.15310
     189 -> 206       0.56804

 Excited State  24:       Singlet-A       4.0741 eV
304.32 nm  f=0.0577  <S**2>=0.000
     187 -> 190       0.52901
     189 -> 195       0.12681
     189 -> 204      -0.14462
     189 -> 206       0.34429
```

```
 Excited State  25:       Singlet-A       4.0775 eV
304.07 nm  f=0.0046  <S**2>=0.000
     186 -> 190      -0.23537
     188 -> 196       0.37597
     189 -> 207       0.52222

 Excited State  26:       Singlet-A       4.0793 eV
303.94 nm  f=0.0003  <S**2>=0.000
     186 -> 190       0.16759
     187 -> 191       0.12837
     188 -> 196       0.56567
     189 -> 207      -0.35044

 Excited State  27:       Singlet-A       4.1478 eV
298.92 nm  f=0.1235  <S**2>=0.000
     186 -> 190       0.50932
     189 -> 207       0.18956
     189 -> 208      -0.39345

 Excited State  28:       Singlet-A       4.1754 eV
296.94 nm  f=0.0176  <S**2>=0.000
     186 -> 190       0.14892
     189 -> 207       0.10376
     189 -> 208       0.26292
     189 -> 209       0.61020
     189 -> 210       0.10574

 Excited State  29:       Singlet-A       4.1829 eV
296.41 nm  f=0.0293  <S**2>=0.000
     186 -> 190       0.18463
     189 -> 207       0.15929
     189 -> 208       0.44567
     189 -> 209      -0.33624
     189 -> 210       0.33231

 Excited State  30:       Singlet-A       4.1988 eV
295.28 nm  f=0.0137  <S**2>=0.000
     186 -> 190      -0.14541
     188 -> 197      -0.39720
     189 -> 207      -0.10213
     189 -> 208      -0.19364
     189 -> 210       0.50807

 Excited State  31:       Singlet-A       4.1996 eV
295.23 nm  f=0.0077  <S**2>=0.000
     186 -> 190      -0.10150
     188 -> 197       0.58269
     189 -> 208      -0.14193
     189 -> 210       0.33687

 Excited State  32:       Singlet-A       4.2438 eV
292.16 nm  f=0.0005  <S**2>=0.000
     189 -> 211       0.70550

 Excited State  33:       Singlet-A       4.2737 eV
290.11 nm  f=0.0042  <S**2>=0.000
     189 -> 212       0.70346

 Excited State  34:       Singlet-A       4.2945 eV
288.70 nm  f=0.0008  <S**2>=0.000
     186 -> 191       0.42197
     188 -> 194      -0.17789
     188 -> 198       0.28407
     188 -> 199       0.43644

 Excited State  35:       Singlet-A       4.3392 eV
285.73 nm  f=0.0001  <S**2>=0.000
     188 -> 198       0.61709
     188 -> 199      -0.34007

 Excited State  36:       Singlet-A       4.3604 eV
284.34 nm  f=0.0003  <S**2>=0.000
     185 -> 190      -0.29698
     189 -> 213       0.63550

 Excited State  37:       Singlet-A       4.3942 eV
282.15 nm  f=0.0200  <S**2>=0.000
     184 -> 191      -0.11963
     185 -> 190       0.60947
     189 -> 213       0.27564

 Excited State  38:       Singlet-A       4.3951 eV
282.10 nm  f=0.0018  <S**2>=0.000
     189 -> 214       0.70255

 Excited State  39:       Singlet-A       4.4298 eV
279.89 nm  f=0.0155  <S**2>=0.000
     185 -> 191       0.12290
     188 -> 200       0.68435

 Excited State  40:       Singlet-A       4.4417 eV
279.14 nm  f=0.0097  <S**2>=0.000
     184 -> 190      -0.23081
     185 -> 191       0.57376
     188 -> 200      -0.15442
     189 -> 215       0.27560

 Excited State  41:       Singlet-A       4.4494 eV
278.65 nm  f=0.0885  <S**2>=0.000
     185 -> 191      -0.24812
     189 -> 215       0.63579

 Excited State  42:       Singlet-A       4.4791 eV
276.81 nm  f=0.0049  <S**2>=0.000
     188 -> 201       0.70048

 Excited State  43:       Singlet-A       4.4850 eV
276.44 nm  f=0.0337  <S**2>=0.000
     183 -> 190      -0.28793
     184 -> 190       0.56866
     185 -> 191       0.22044
     189 -> 216      -0.12294

 Excited State  44:       Singlet-A       4.4881 eV
276.25 nm  f=0.0022  <S**2>=0.000
     189 -> 216       0.68647

 Excited State  45:       Singlet-A       4.4981 eV
275.64 nm  f=0.0131  <S**2>=0.000
     183 -> 190       0.63038
     184 -> 190       0.28346

 Excited State  46:       Singlet-A       4.5336 eV
273.48 nm  f=0.0212  <S**2>=0.000
     183 -> 191       0.10774
     184 -> 191       0.63998
     185 -> 190       0.11471
     186 -> 191       0.10918
     188 -> 199      -0.12792
```

```
 Excited State  47:       Singlet-A       4.5650 eV
271.60 nm  f=0.0013  <S**2>=0.000
     183 -> 191       0.39272
     184 -> 191      -0.20152
     186 -> 191       0.24290
     188 -> 194      -0.14048
     188 -> 199      -0.21325
     188 -> 202       0.38802

 Excited State  48:       Singlet-A       4.5809 eV
270.65 nm  f=0.0007  <S**2>=0.000
     183 -> 191      -0.47253
     188 -> 202       0.50218

 Excited State  49:       Singlet-A       4.5852 eV
270.40 nm  f=0.0179  <S**2>=0.000
     189 -> 217       0.67904
     189 -> 218      -0.16029

 Excited State  50:       Singlet-A       4.6012 eV
269.46 nm  f=0.0192  <S**2>=0.000
     188 -> 203      -0.15192
     189 -> 217       0.13100
     189 -> 218       0.66735

 Excited State  51:       Singlet-A       4.6089 eV
269.01 nm  f=0.0005  <S**2>=0.000
     188 -> 203       0.68400
     189 -> 218       0.13828

 Excited State  52:       Singlet-A       4.6287 eV
267.86 nm  f=0.0028  <S**2>=0.000
     182 -> 190       0.32079
     183 -> 191      -0.15763
     186 -> 191       0.14257
     188 -> 199      -0.12968
     189 -> 219       0.54152

 Excited State  53:       Singlet-A       4.6509 eV
266.58 nm  f=0.0119  <S**2>=0.000
     181 -> 191       0.10438
     182 -> 190       0.60453
     189 -> 219      -0.29178

 Excited State  54:       Singlet-A       4.6643 eV
265.82 nm  f=0.0072  <S**2>=0.000
     180 -> 191      -0.12037
     183 -> 191       0.28180
     184 -> 191       0.10152
     186 -> 191      -0.27934
     188 -> 194       0.15239
     188 -> 198       0.12446
     188 -> 199       0.28878
     188 -> 202       0.20212
     188 -> 205       0.11700
     189 -> 219       0.30531
     189 -> 221       0.12465

 Excited State  55:       Singlet-A       4.6872 eV
264.52 nm  f=0.0931  <S**2>=0.000
     181 -> 190       0.48795
     182 -> 191       0.41482
     187 -> 191       0.11040
     188 -> 195      -0.10368
     189 -> 220       0.19534

 Excited State  56:       Singlet-A       4.6909 eV
264.31 nm  f=0.0011  <S**2>=0.000
     181 -> 190      -0.13017
     182 -> 191      -0.15710
     189 -> 220       0.67398

 Excited State  57:       Singlet-A       4.7274 eV
262.26 nm  f=0.0202  <S**2>=0.000
     181 -> 190      -0.46928
     182 -> 191       0.48712
     188 -> 204       0.11148

 Excited State  58:       Singlet-A       4.7459 eV
261.25 nm  f=0.0054  <S**2>=0.000
     189 -> 221       0.68031

 Excited State  59:       Singlet-A       4.7590 eV
260.53 nm  f=0.0021  <S**2>=0.000
     188 -> 204       0.69097

 Excited State  60:       Singlet-A       4.7933 eV
258.66 nm  f=0.0010  <S**2>=0.000
     181 -> 191      -0.33481
     188 -> 205       0.59213
     189 -> 222      -0.15662
```

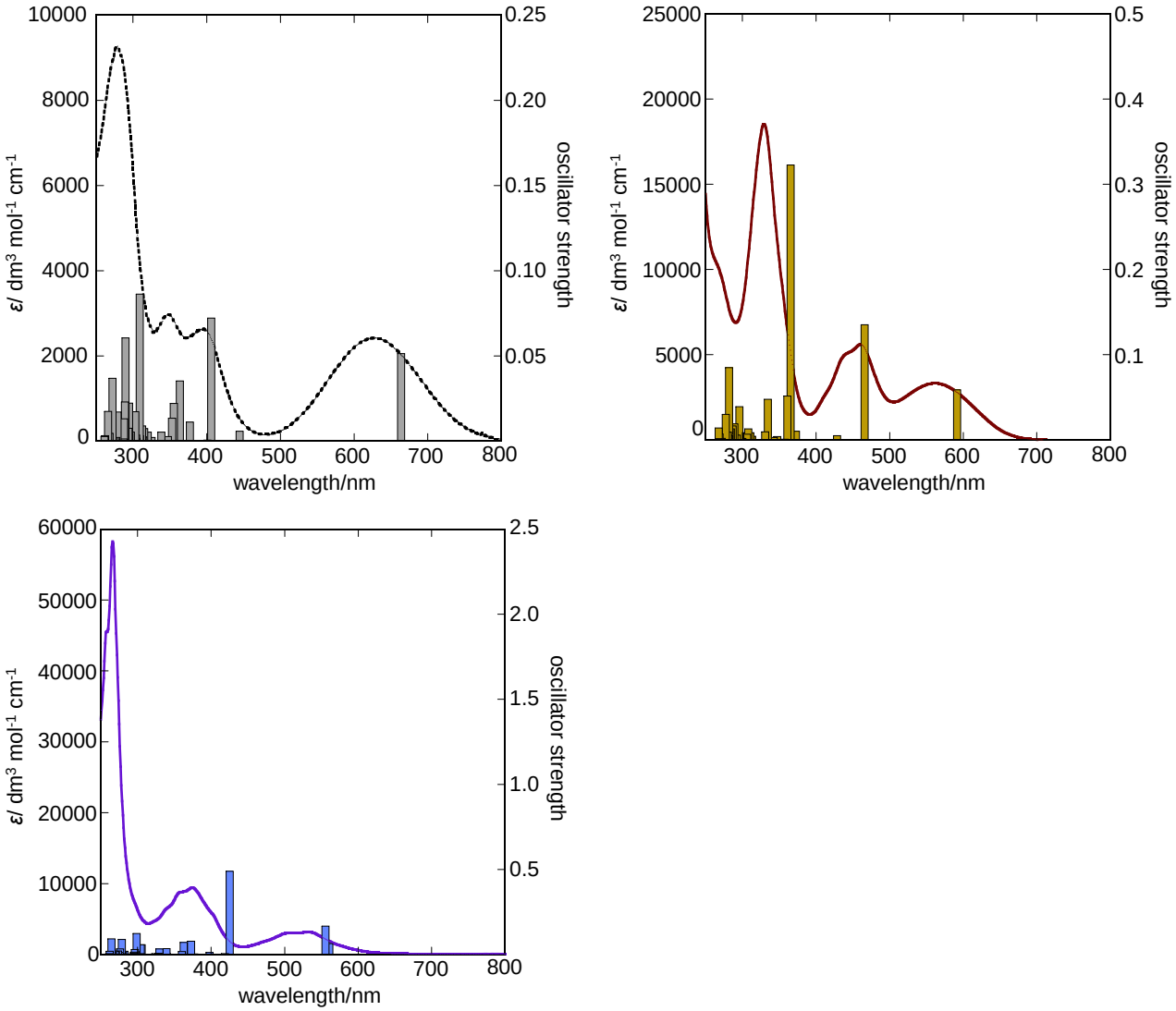


Fig. S11 UV-vis spectra of **1a**[S7], **3**, and **4** in hexane at room temperature. Superimposed vertical bars indicate band positions and oscillator strengths of each compounds calculated at the TD-HCTH407/6-31+G(d,p)//B3PW91+D3/6-31G(d) level of theory.

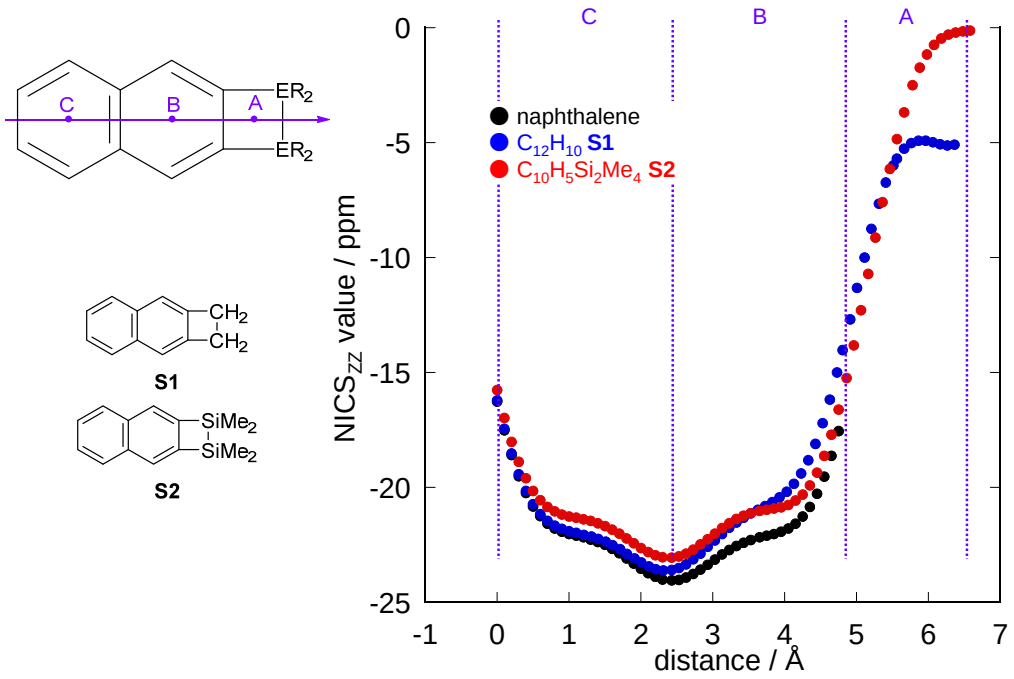


Fig. S12 $NICS_{zz}$-X scans for naphthalene, **S1**, and **S2**; trajectory for the $NICS_{zz}$ plots: trajectories are located 1.7 Å above the least square planes.

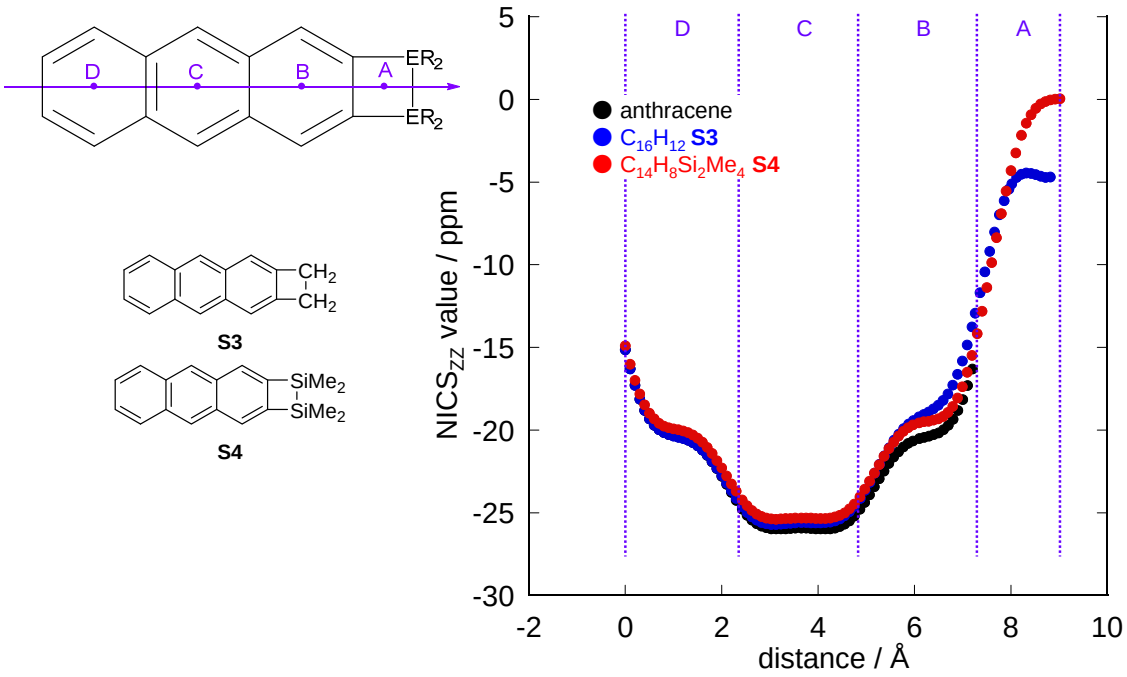


Fig. S13 $NICS_{zz}$-X scans for anthracene, **S3**, and **S4**; trajectory for the $NICS_{zz}$ plots: trajectories are located 1.7 Å above the least square planes.

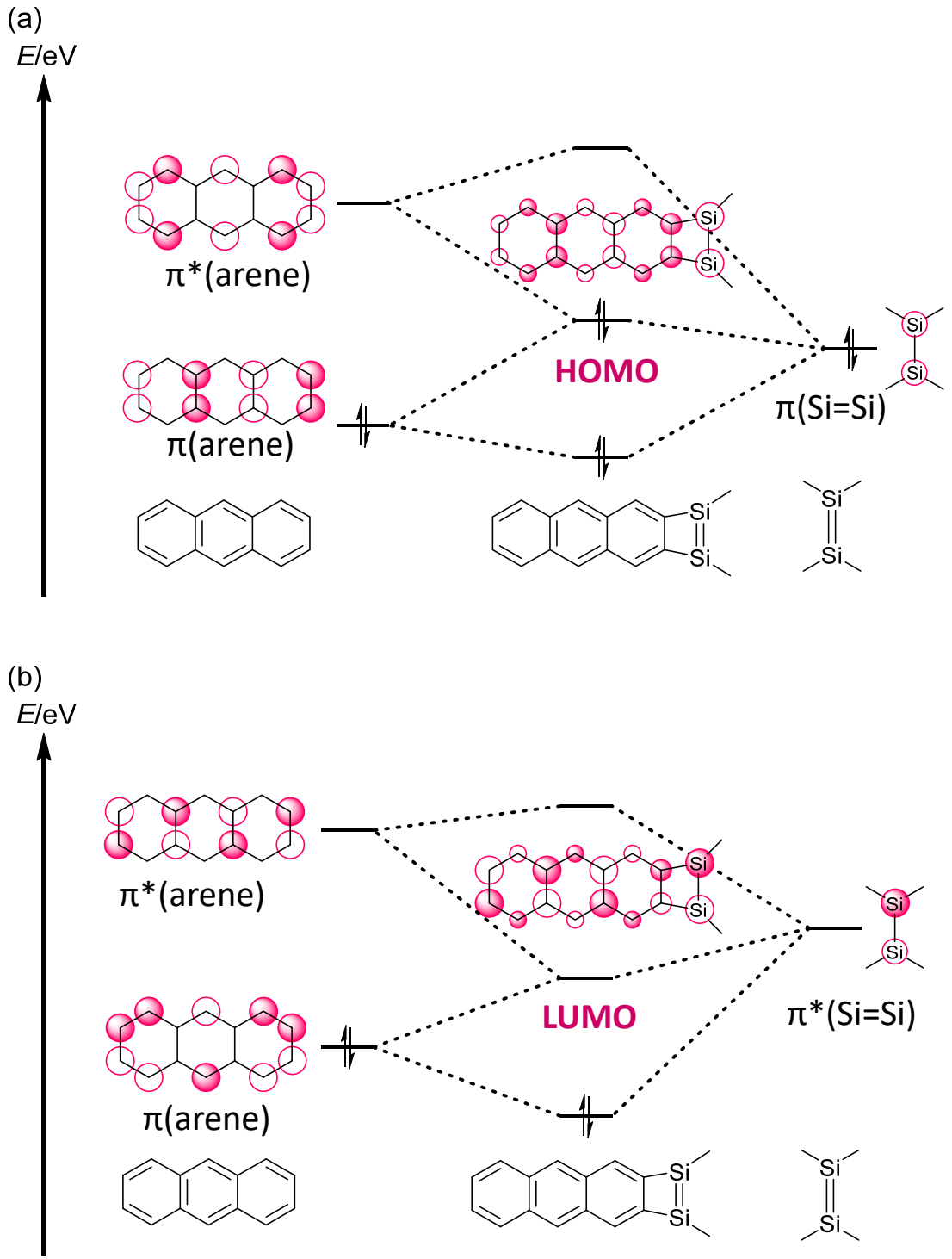


Fig. S14 Diagrams for the orbital interactions to form the HOMO and LUMO of $\mathbf{4}_{\mathbf{opt}}$.

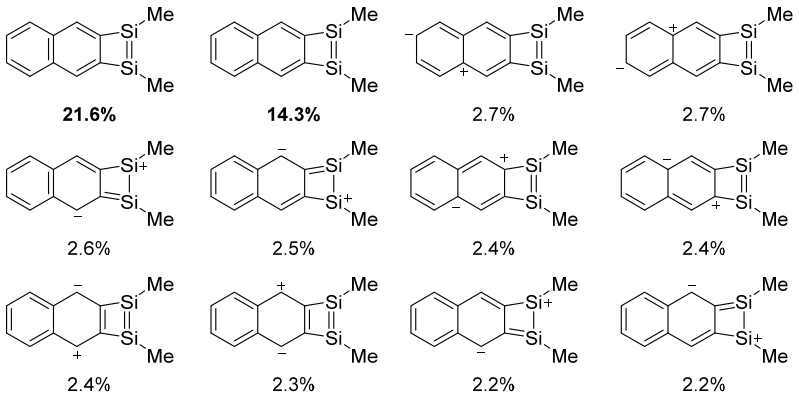


Fig. S15 Major resonance structures of $\mathbf{3_m}$ obtained by natural resonance theory analysis.

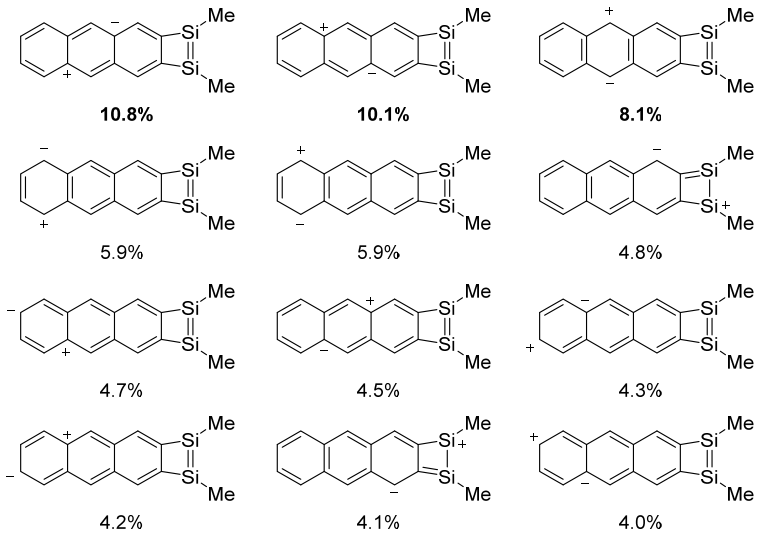


Fig. S16 Major resonance structures of $\mathbf{4_m}$ obtained by natural resonance theory analysis.

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