Electronic Supplementary Information

1,3-Diethynylbicyclo[1.1.0]tetrasilanes:
π-Conjugated species with an unsupported Si–Si π-bond
obtained from direct π-extension

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1. Experimental Details

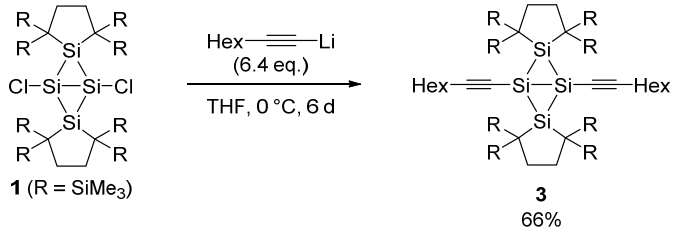
General Procedures

All reactions involving air-sensitive compounds were performed under argon or nitrogen atmosphere using a high-vacuum line and a standard Schlenk techniques, or a glove box, as well as dry and oxygen-free solvents. Reactions at lower temperatures were performed using an EYELA PSL-1400 cryobath. NMR spectra were recorded on a Bruker Avance III 500 FT NMR spectrometer. The ^{1}H and ^{13}C NMR chemical shifts were referenced to residual ^{1}H and ^{13}C shifts of the solvents: C_6D_6 (^{1}H: δ 7.16 and ^{13}C: δ 128.0), toluene-d_8 (^{1}H: δ 2.08).[S1] The ^{29}Si NMR chemical shifts were relative to Me_4Si in ppm (δ 0.00). The 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 spectrometer and JEOL JMS-T100GCV spectrometer. UV-vis spectra were recorded on JASCO V-770 and V-660 spectrometers. X-ray analysis was carried out using a Bruker AXS APEXII CCD diffractometer.

Materials

Dry and degassed hexane, and THF were prepared using a VAC 103991 solvent purifier. Benzene-d_6 was dried by molecular sieves 4Å after degassing through three freeze-pump-thaw cycles. Toluene-d_8 and 3-methylpentane were dried in a tube covered with potassium mirror and then distilled under reduced pressure prior to use. Hexamethyldisiloxane was dried by lithium aluminum hydride after degassing through three freeze-pump-thaw cycles. 1,3-Dichlorobicyclo[1.1.0]tetrasilane **1** was prepared according to the published procedure.[S2] 1-Octynyllithium and lithium phenylacetylide were prepared by the reactions of the corresponding alkyne with butyl lithium in THF. 1-Octyne, phenylacetylene and butyl lithium were commercially available and used without further purification.

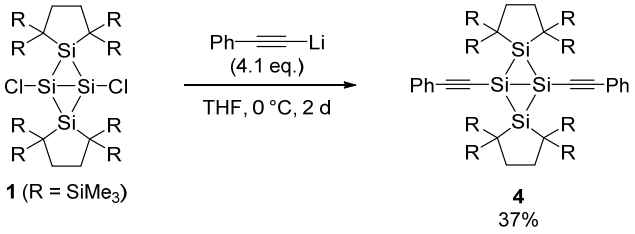
Synthesis of 1,3-Dioctynylbicyclo[1.1.0]tetrasilane 3 [TN864,865]



To a Schlenk tube (30 mL) equipped with a magnetic stir bar, 1,3-dichlorobicyclotetrasilane **1** (30.1 mg, 34.5 μmol) and 1-octynyllithium (25.5 mg, 220 μmol) were charged. To the Schlenk tube, dry and degassed THF (3.0 mL, cooled down to –27 °C) was added and the mixture was stirred at 0 °C for 6 days. The color of the resulting solution turned from orange to dark red. After the volatiles were removed in vacuo at 0 °C, the crude was extracted with hexane and the filtrate was concentrated in vacuo. Recrystallization from hexamethyldisiloxane provided reddish purple crystals of **3** (23.4 mg, 22.9 μmol) in 66% yield.

3: reddish purple crystals; mp 174-176 ˚C (decomp.); ^{1}H NMR (500 MHz, C_6D_6, 296 K) 0.53 (s, 72H, SiC*H*$_3$), 0.91 (t, *J* = 7.0 Hz, 6H, C*H*$_3$ (octynyl)), 1.16-1.24 (m, 4H, C*H*$_2$ (octynyl)), 1.26-1.38 (m, 8H, C*H*$_2$ (octynyl)), 1.50 (tt, *J* = 7.5 Hz, *J* = 7.0 Hz, 4H, C*H*$_2$ (octynyl)), 2.05 (s, 8H, C*H*$_2$ (silacyclopentane ring)), 2.30 (t, *J* = 7.0 Hz, 4H, C*H*$_2$ (octynyl)); ^{13}C NMR (126 MHz, C_6D_6, 297 K) 5.3 (Si*C*H$_3$), 13.8 (*C*), 14.5 (*C*H$_3$ (octynyl)), 21.6 (*C*H$_2$ (octynyl)), 23.2 (*C*H$_2$ (octynyl)), 28.6 (*C*H$_2$ (octynyl)), 29.2 (*C*H$_2$ (octynyl)), 31.9 (*C*H$_2$ (octynyl)), 34.9 (*C*H$_2$ (silacyclopentane ring)), 88.5 (Si*C*≡), 130.3 (Hex*C*≡); ^{29}Si NMR (99 MHz, C_6D_6, 296 K) −8.0 (*Si*), 4.7 (*Si*Me$_3$), 83.3 (*Si*C≡); UV-vis (hexane, 293 K) λ_{max}/nm (ε) 518 (5.6×10^3), 475 (sh, 4.6×10^3), 340 (1.9×10^3), 248 (4.1×10^4), 212 (4.3×10^4); UV-vis (KBr matrix, 293 K) λ_{max}/nm 552, 340, 249; HRMS (FD) Calcd for $C_{48}H_{106}Si_{12}$ [M^+], 1018.55257; Found, 1018.55232; Anal. Calcd for $C_{48}H_{106}Si_{12}$: C, 56.50; H, 10.47%. Found: C, 56.22; H, 10.78%.

Synthesis of 1,3-Diphenylethynylbicyclo[1.1.0]tetrasilane 4 [TN575,577]



To a Schlenk tube (30 mL) equipped with a magnetic stir bar, 1,3-dichlorobicyclotetrasilane **1** (30.0 mg, 34.4 μmol) and lithium phenylacetylide (17.9 mg, 142 μmol) were charged. To the Schlenk tube, dry and degassed THF (5.0 mL, cooled down to –27 °C) was added and the mixture was stirred at 0 °C for 2 days. The color of the resulting suspension turned from orange to purple. After the volatiles were removed in vacuo at 0 °C, the crude was extracted with hexane and the filtrate was concentrated in vacuo. The residue was washed with hexane to provide a blue solid of **4** (12.9 mg, 12.8 μmol) in 37% yield.

4: a blue solid; mp 63-65 ˚C (decomp.); ^{1}H NMR (500 MHz, C_6D_6, 295 K) 0.54 (s, 72H, SiCH_3), 2.05 (s, 8H, CH_2), 6.94-6.99 (m, 2H, aryl), 7.01-7.05 (m, 4H, aryl), 7.64-7.68 (m, 4H, aryl); ^{13}C NMR (126 MHz, C_6D_6, 296 K) 5.2 (Si*C*H$_3$), 14.1 (*C*), 34.9 (*C*H$_2$), 98.6 (Si*C*≡), 123.8 (aryl), 127.2 (Ph*C*≡), 128.9 (aryl), 129.5 (aryl), 131.7 (aryl); ^{29}Si NMR (99 MHz, C_6D_6, 294 K) −6.1 (*Si*), 4.9 (*Si*Me$_3$), 91.5 (*Si*C≡); UV-vis (hexane, 293 K) λ_{max}/nm (ε) 560 (7.8× 10^3), 503 (sh, 4.9 × 10^3), 312 (2.4 × 10^4), 298 (sh, 2.2 × 10^4), 277 (2.2 × 10^4), 247 (3.8 × 10^4); UV-vis (KBr matrix, 293 K) λ_{max}/nm 602, 317, 247, 214; HRMS (APCI_positive) Calcd for $C_{48}H_{90}Si_{12}$ [M$^+$], 1002.42682; Found, 1002.42718; Anal. Calcd for $C_{48}H_{90}Si_{12}$: C, 57.41; H, 9.03%. Found: C, 57.60; H, 9.22%.

2. NMR Spectra

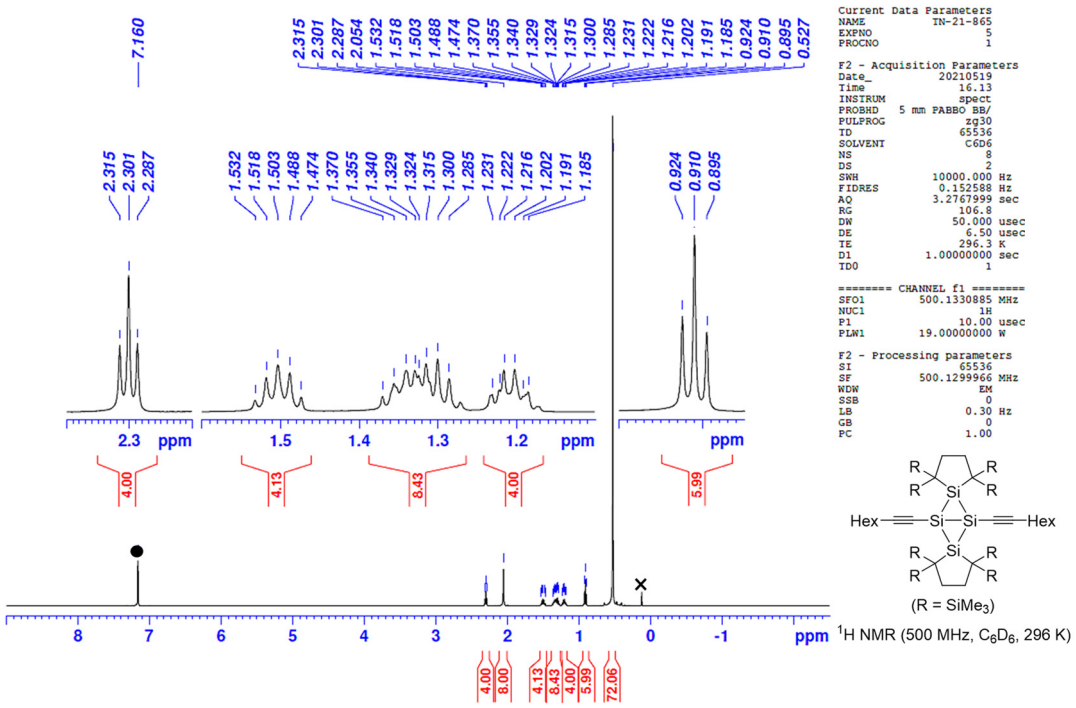


Figure S1. ^{1}H NMR spectrum of **3** in C_6D_6 at 296 K (● = C_6HD_5, × = hexamethyldisiloxane).

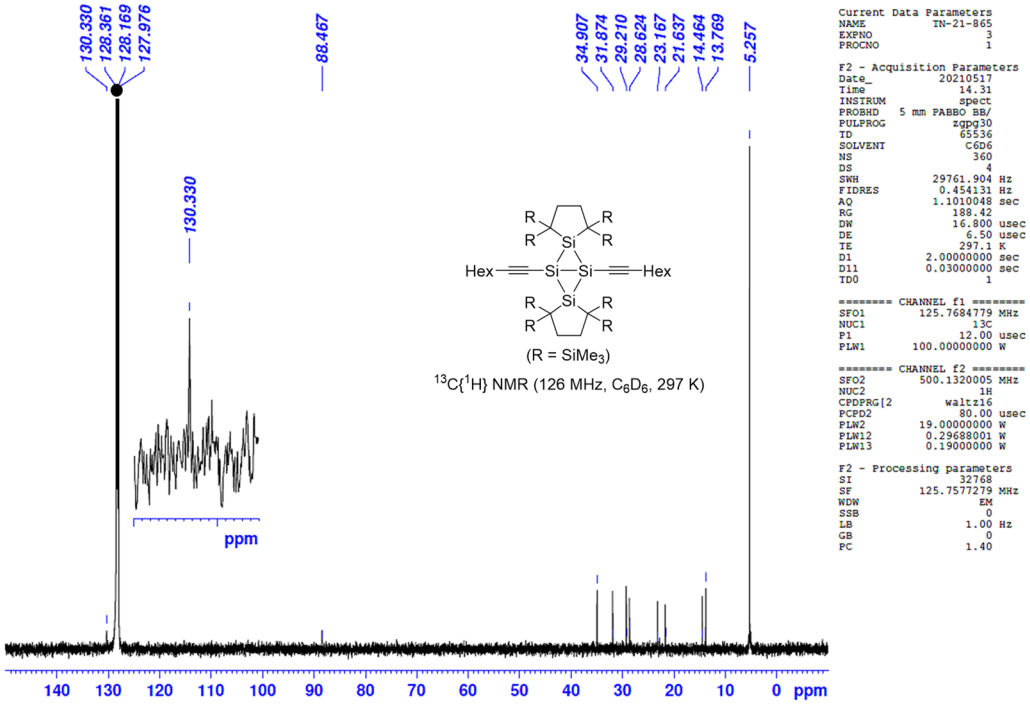


Figure S2. ^{13}C{^{1}H} NMR spectrum of **3** in C_6D_6 in 297 K (● = C_6D_6).

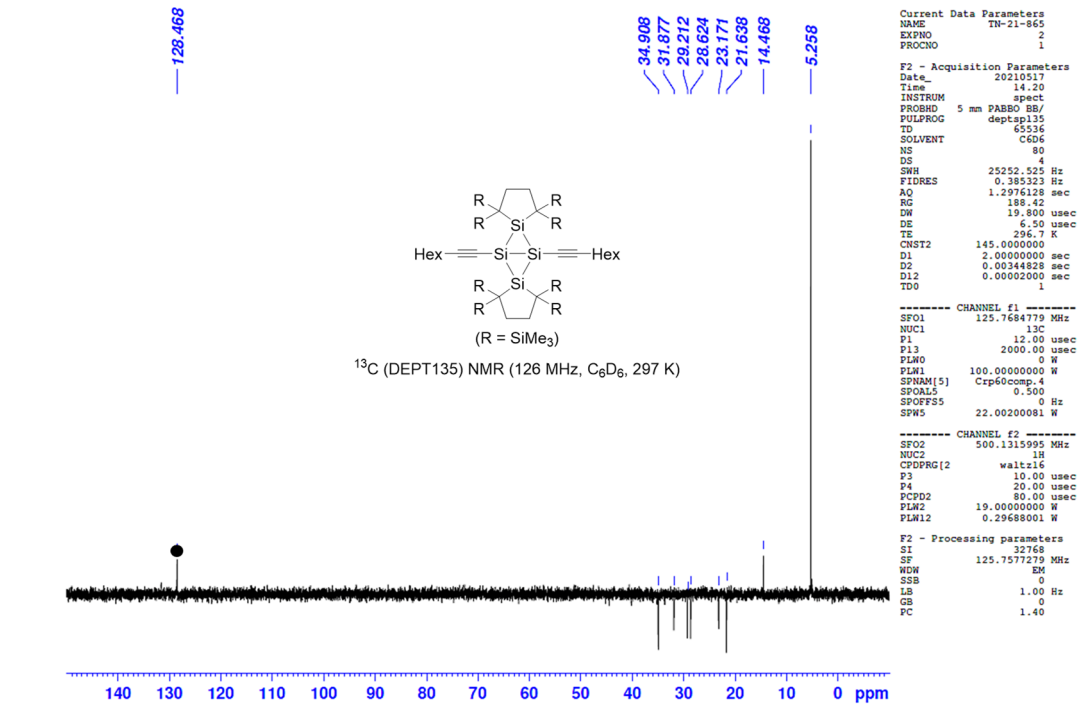


Figure S3. ^{13}C (DEPT135) NMR spectrum of **3** in C_6D_6 at 297 K (● = C_6D_6).

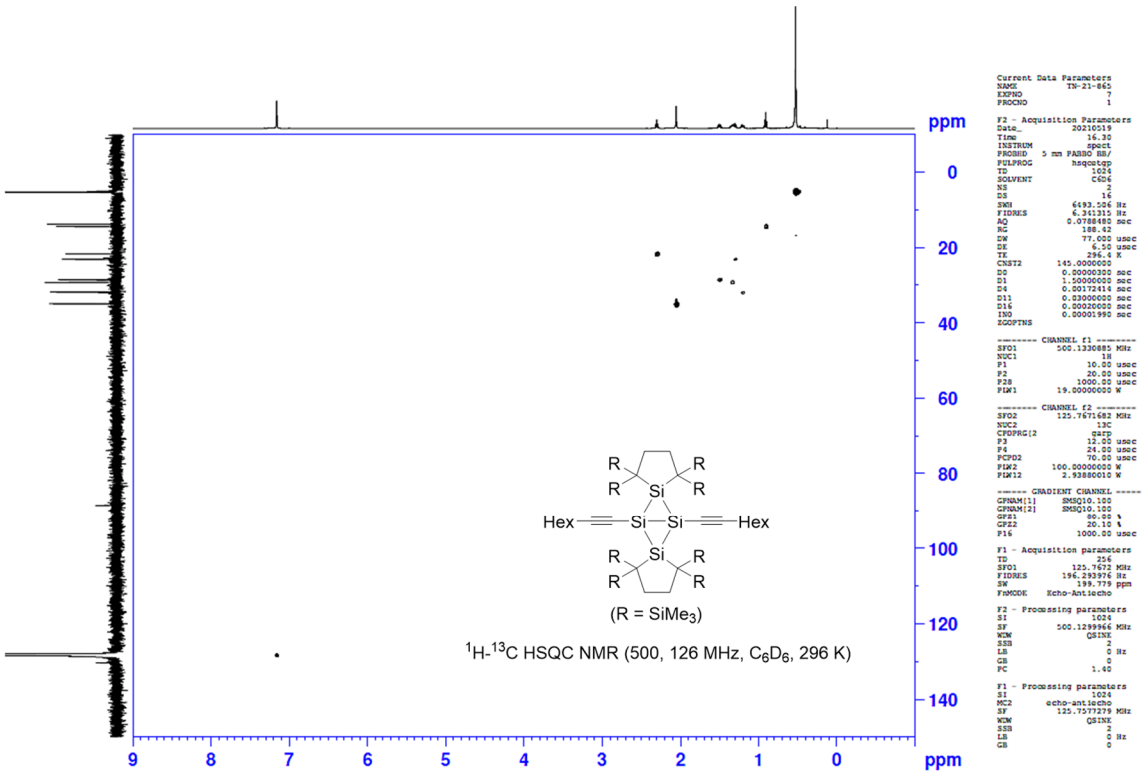


Figure S4. ^{1}H-^{13}C HSQC NMR spectrum of **3** in C_6D_6 at 296 K.

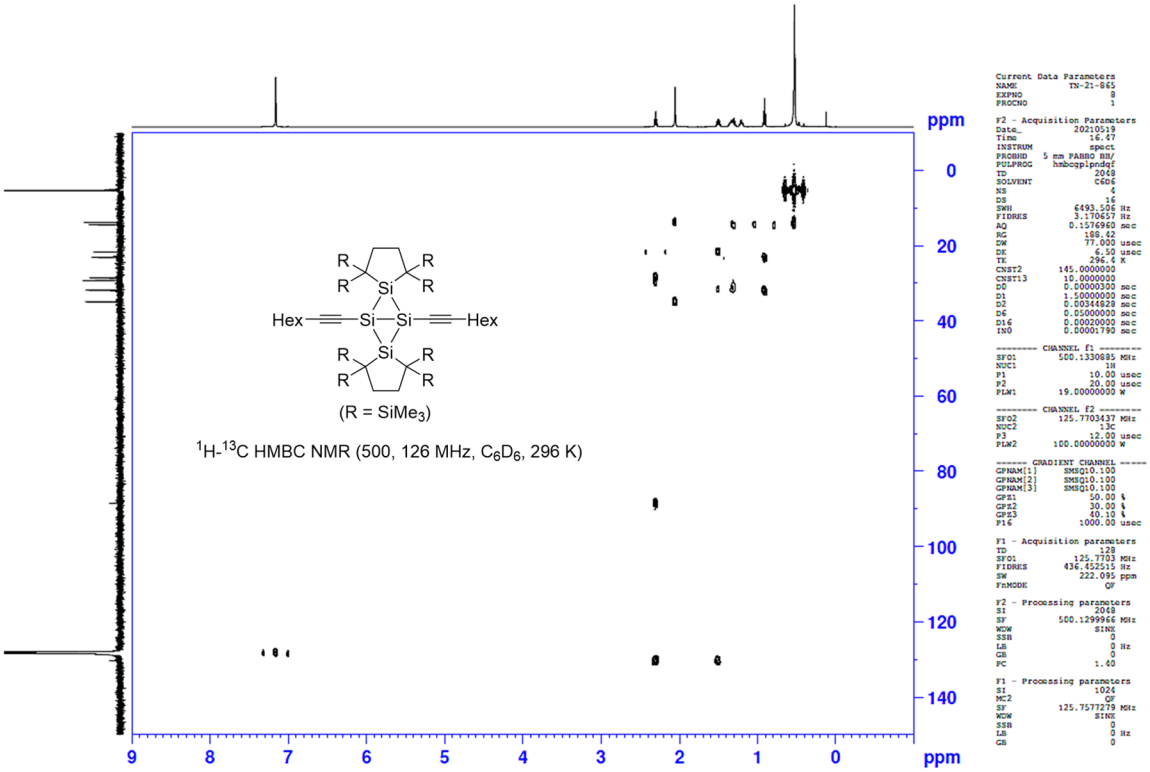


Figure S5. ^{1}H-^{13}C HMBC NMR spectrum of **3** in C_6D_6 at 296 K.

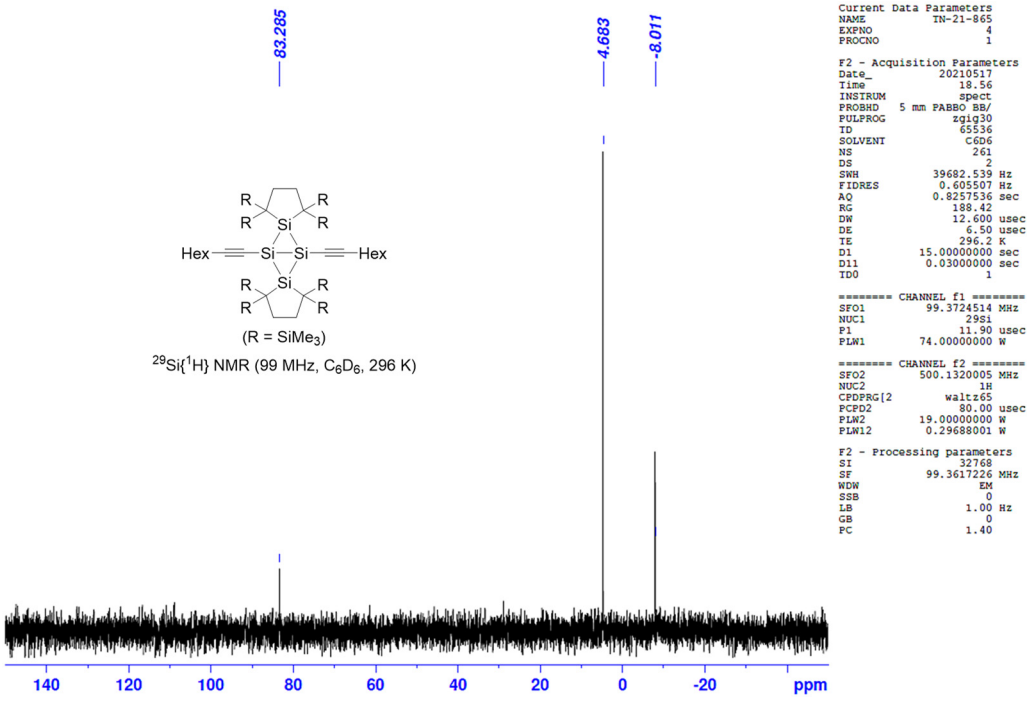


Figure S6. ^{29}Si{^{1}H} NMR spectrum of **3** in C_6D_6 at 296 K.

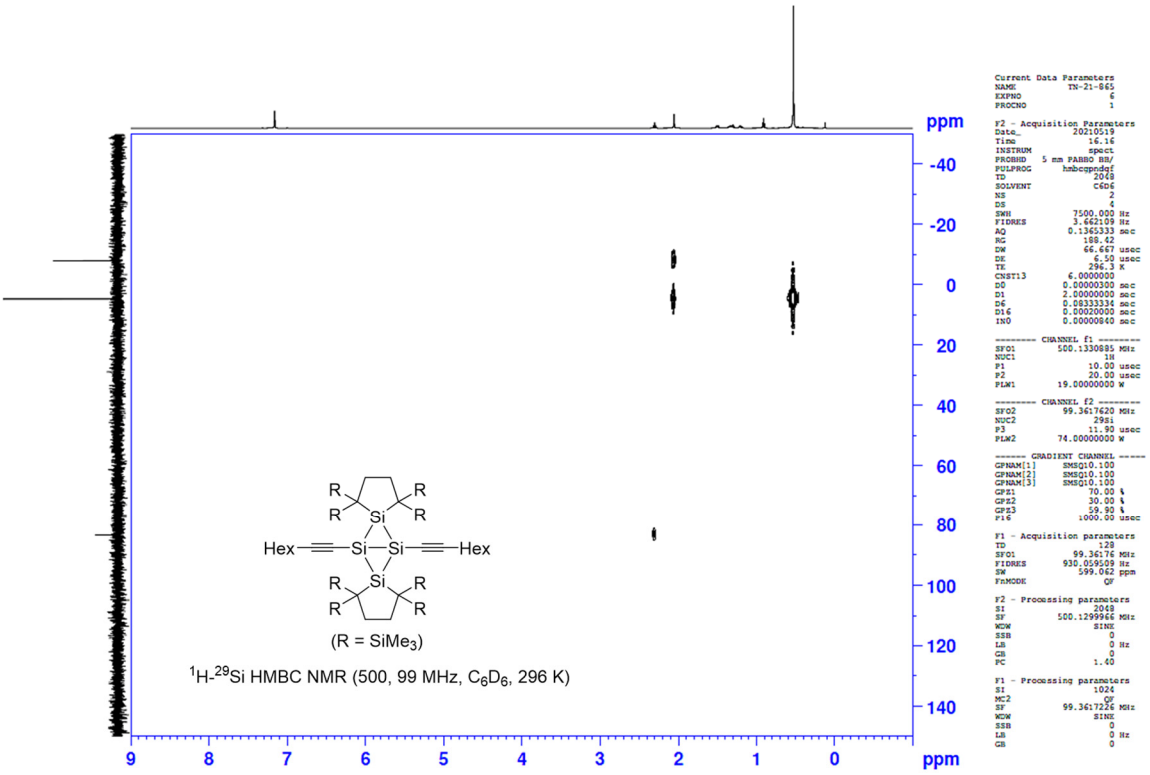


Figure S7. ^{1}H-^{29}Si HMBC NMR spectrum of **3** in C_6D_6 at 296 K.

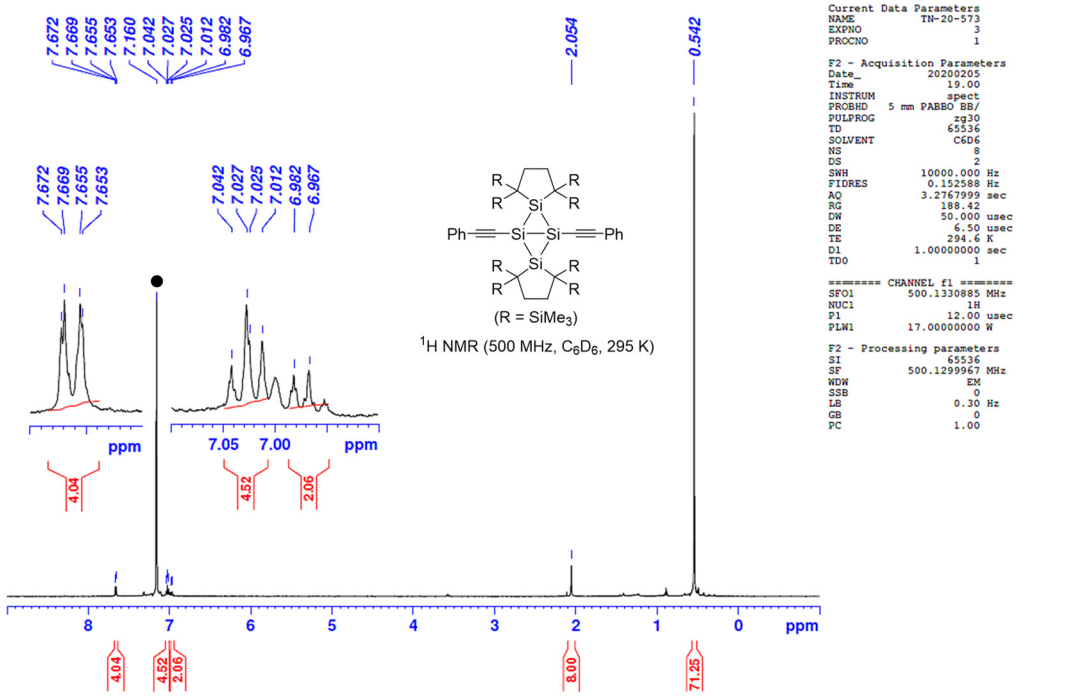


Figure S8. ^{1}H NMR spectrum of **4** in C_6D_6 at 295 K (● = C_6HD_5).

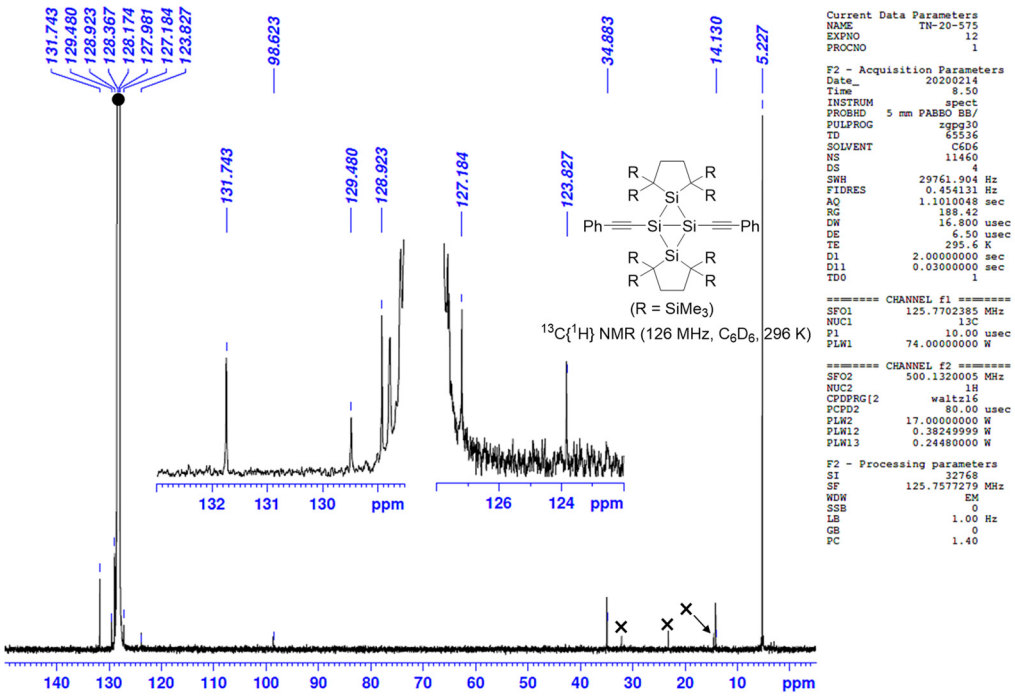


Figure S9. $^{13}C\{^{1}H\}$ NMR spectrum of **4** in C_6D_6 in 296 K (● = C_6D_6, × = hexane).

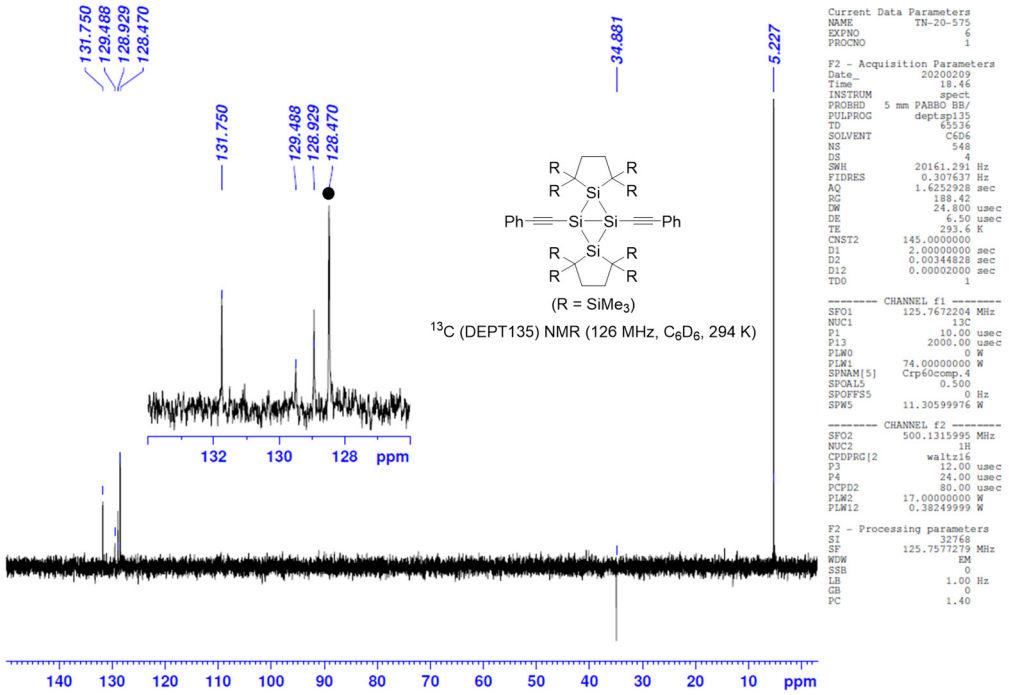


Figure S10. ^{13}C (DEPT135) NMR spectrum of **4** in C_6D_6 at 294 K (● = C_6D_6).

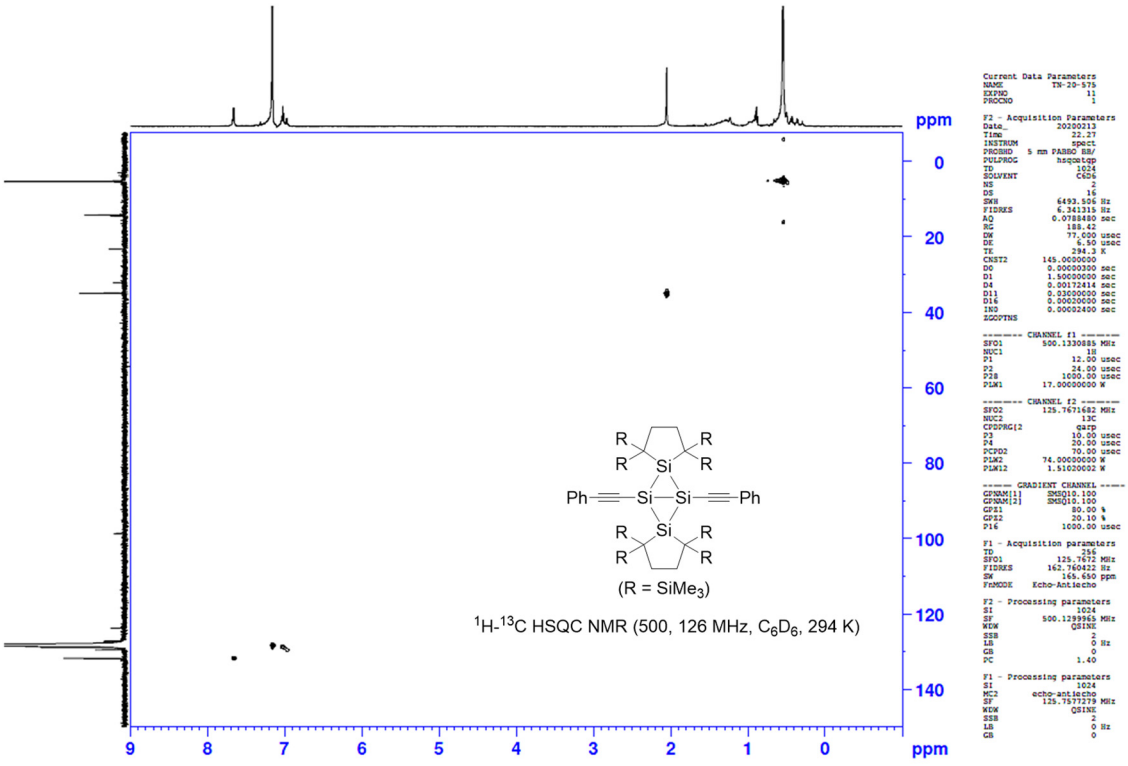


Figure S11. ^{1}H-^{13}C HSQC NMR spectrum of **4** in C_6D_6 at 294 K.

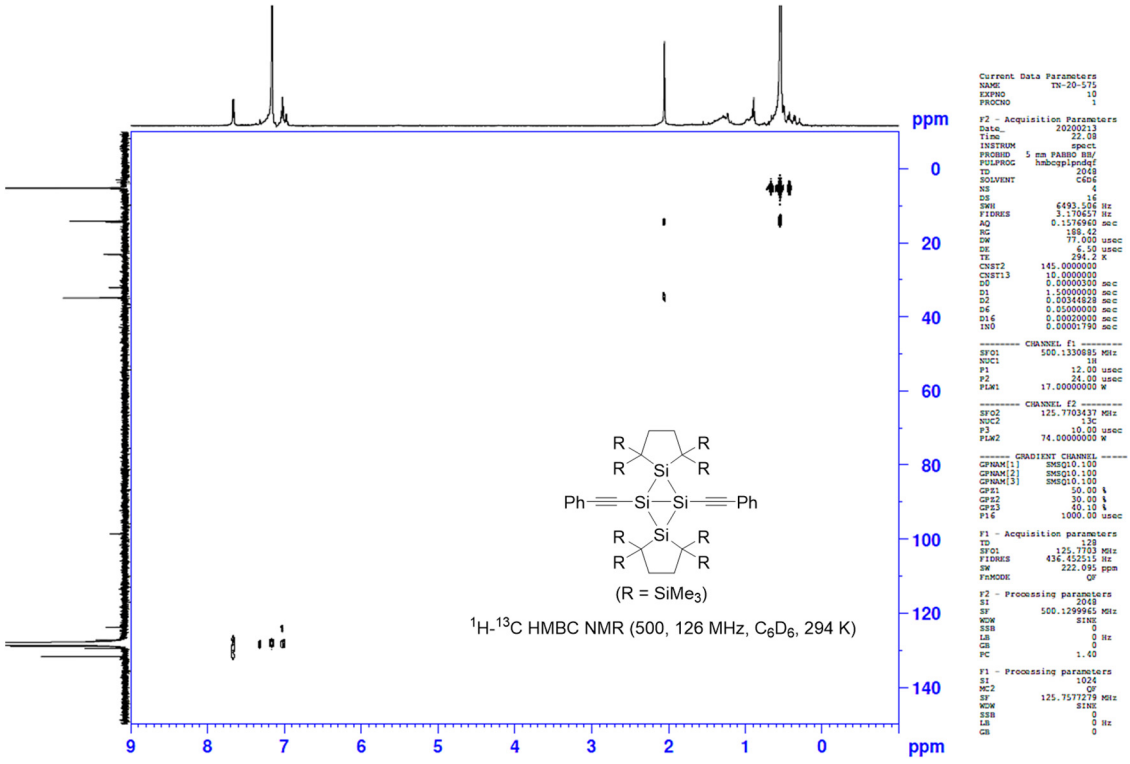


Figure S12. ^{1}H-^{13}C HMBC NMR spectrum of **4** in C_6D_6 at 294 K.

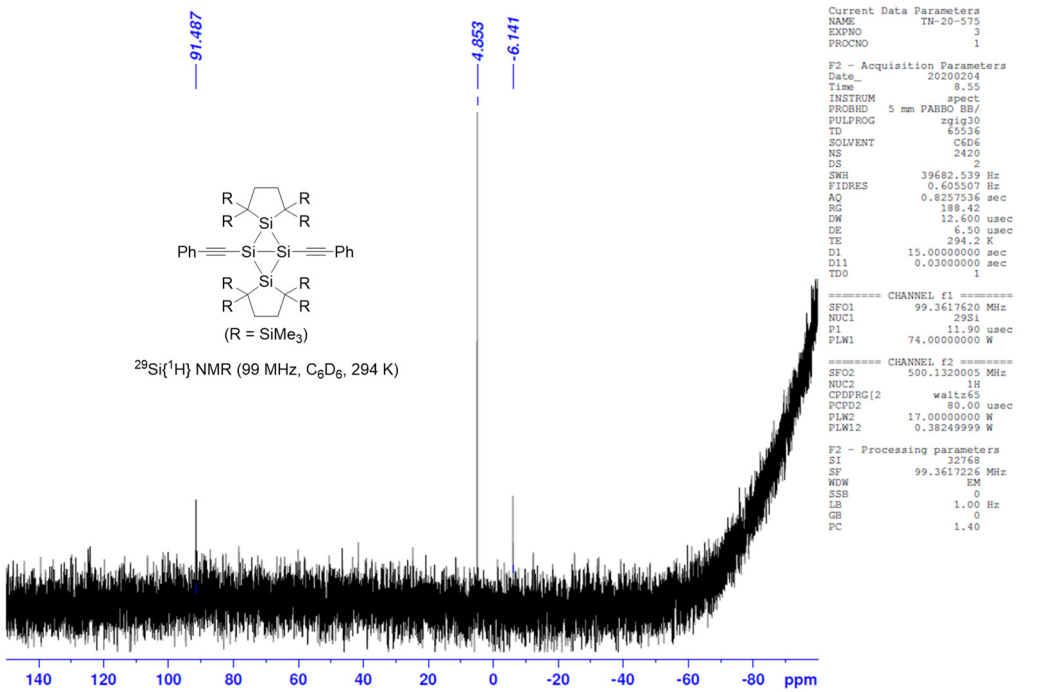


Figure S13. $^{29}Si\{^{1}H\}$ NMR spectrum of **4** in C_6D_6 at 294 K.

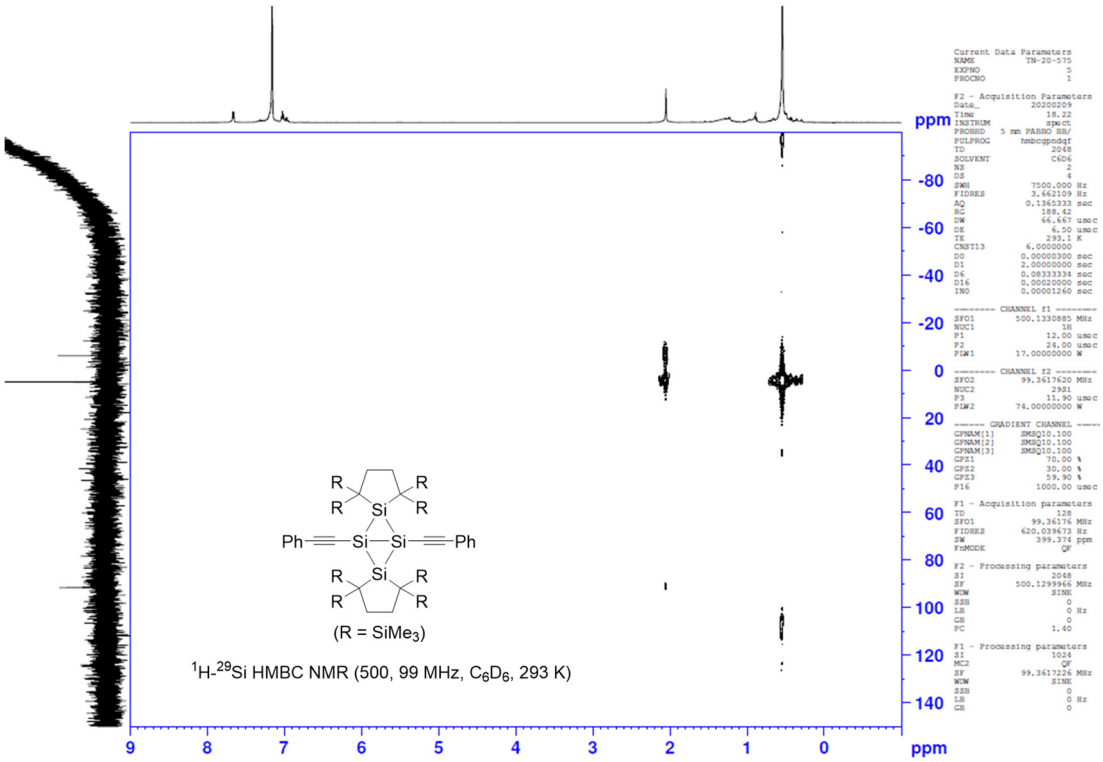


Figure S14. ^{1}H-^{29}Si HMBC NMR spectrum of **4** in C_6D_6 at 293 K.

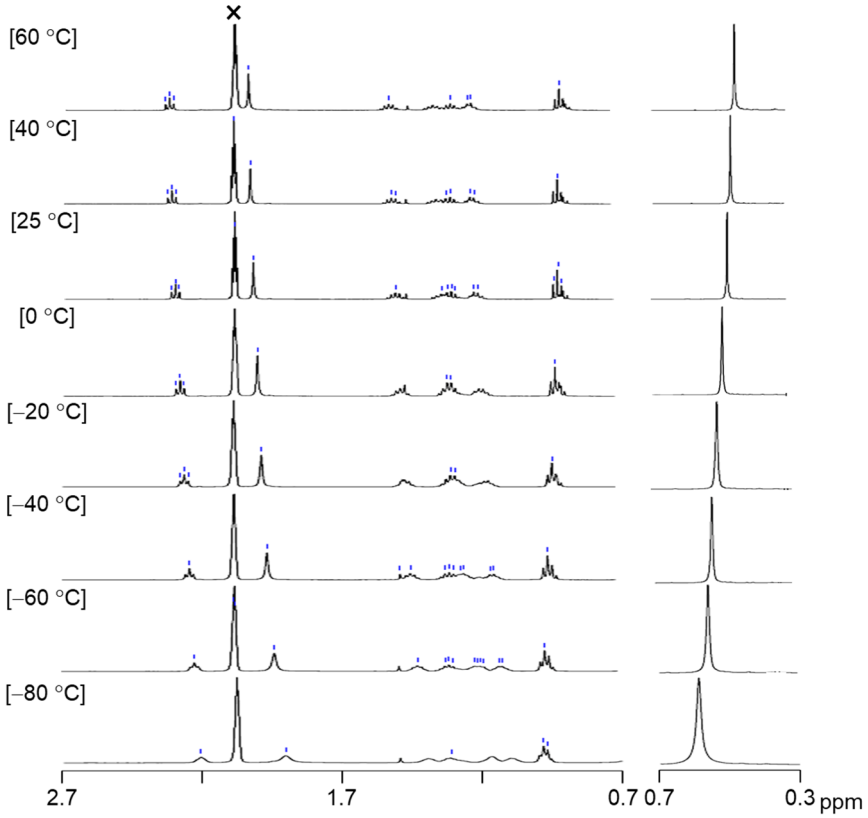


Figure S15. ^{1}H NMR spectra of **3** in toluene-d_8 at variable temperatures (× = C_7D_7H).

Table S1. ^{29}Si Chemical Shifts of **3** at Variable Temperatures.

Temperature/°C	^{29}Si chemical shift/ppm[a,b]			note
	Bridgehead Si	Bridge Si	$SiMe_3$	
60	87.6	–7.3	4.8	TN880_NMR27
50	86.3	–7.5	4.6	TN880_NMR25
40	85.3	–7.7	4.6	TN880_NMR23
30	84.4	–8.0	4.6	TN880_NMR21
25	83.4	–8.1	4.5	TN880_NMR2
0	80.4	–8.6	4.6	TN880_NMR18
–10	78.9	–8.8	4.6	TN880_NMR17
–20	77.1	–9.2	4.6	TN880_NMR9
–30	75.3	–9.4	4.5	TN880_NMR15
–40	73.2	–9.6	4.4	TN880_NMR5

a. These values were obtained by measurement of the ^{1}H-^{29}Si HMBC 2D NMR spectra in toluene-d_8.

b. Spectral resolution is 0.39 ppm.

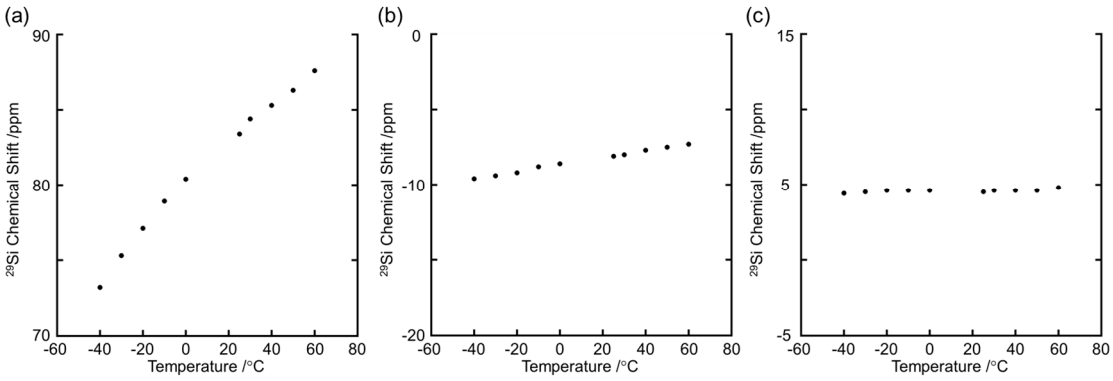


Figure S16. A plot of observed ^{29}Si chemical shift of **3** vs measurement temperature (a: bridgehead Si, b: bridge Si, c: $SiMe_3$).

3. X-ray Diffraction Analysis

Single crystals suitable for X-ray diffraction study were obtained by recrystallization in an inert atmosphere using the following conditions; from hexamethyldisiloxane at room temperature for **3**, from toluene at −27 °C for **4**. For data collection, the single crystals coated by Apiezon grease were mounted on the glass fibre 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 using a graphite monochromated Mo-Kα radiation. An empirical absorption correction based on the multiple measurements of equivalent reflections was applied using the program SADABS[S3] and the structures were solved by direct methods and refined by full-matrix least squares against F^2 using all data (SHELXL-2018/3).[S4] Molecular structure was analysed by Yadokari-XG software.[S5]

Crystal data of **3** [tn87a] (100 K) [CCDC-2095782]: $C_{48}H_{106}Si_{12}$; Fw 1020.40; triclinic; *P*-1, a = 11.9028(5) Å, b = 12.0034(5) Å, c = 12.1944(5) Å, α = 79.1540(10)°, β = 81.4440(10)°, γ = 62.7870(10)°, V = 1517.81(11) Å^3, Z = 1, D_{calc} = 1.116 Mg/m^3, $R1$ = 0.0304 ($I > 2\sigma(I)$), $wR2$ = 0.0786 (all data), GOF = 1.045.

Crystal data of **4** [tn53b] (100 K) [CCDC-2095783]: $C_{48}H_{90}Si_{12}$; Fw 1004.27; monoclinic; $P2_1/c$, a = 10.9137(5) Å, b = 23.4184(12) Å, c = 11.4842(6) Å, β = 90.4870(10)°, V = 2935.0(3) Å^3, Z = 2, D_{calc} = 1.136 Mg/m^3, $R1$ = 0.0400 ($I > 2\sigma(I)$), $wR2$ = 0.1013 (all data), GOF = 1.076.

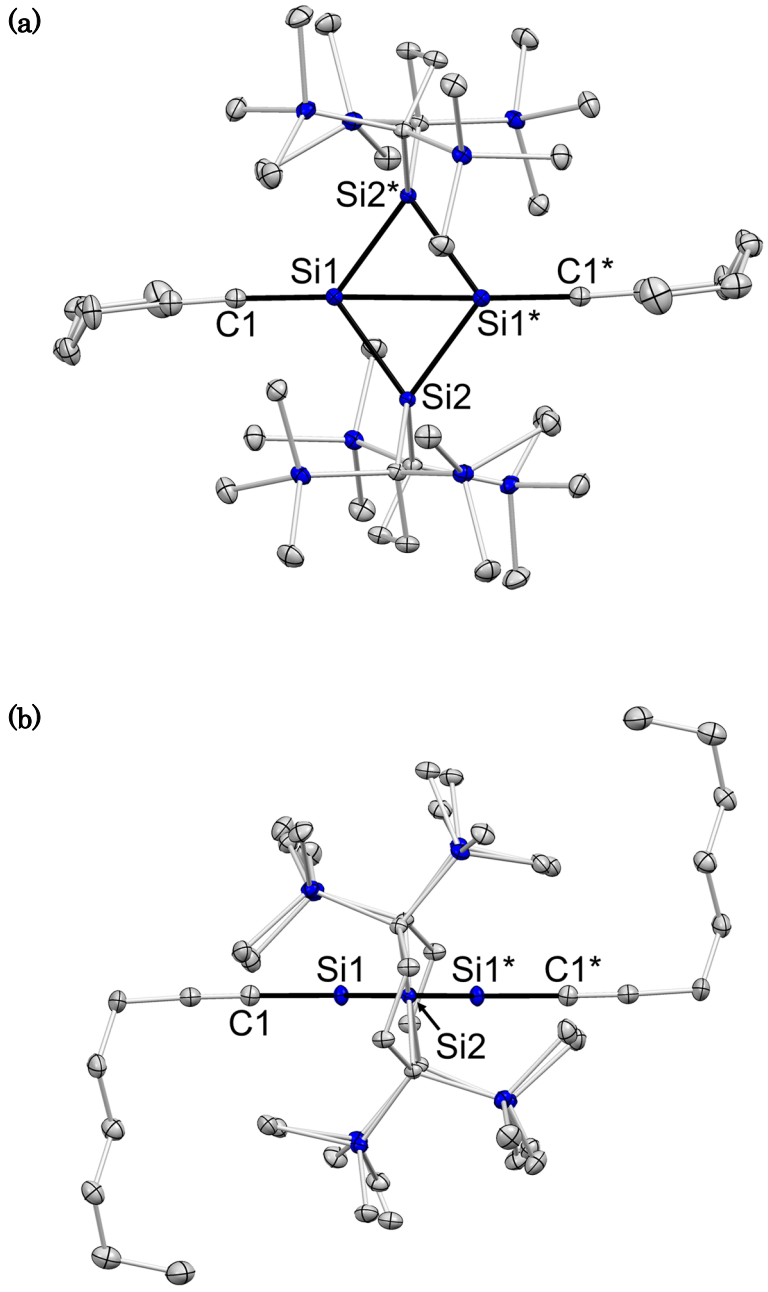


Figure S17. ORTEPs of **3** (a: top view, b: side view). Thermal ellipsoids are shown at the 50% probability level. Hydrogen atoms were omitted for clarity.

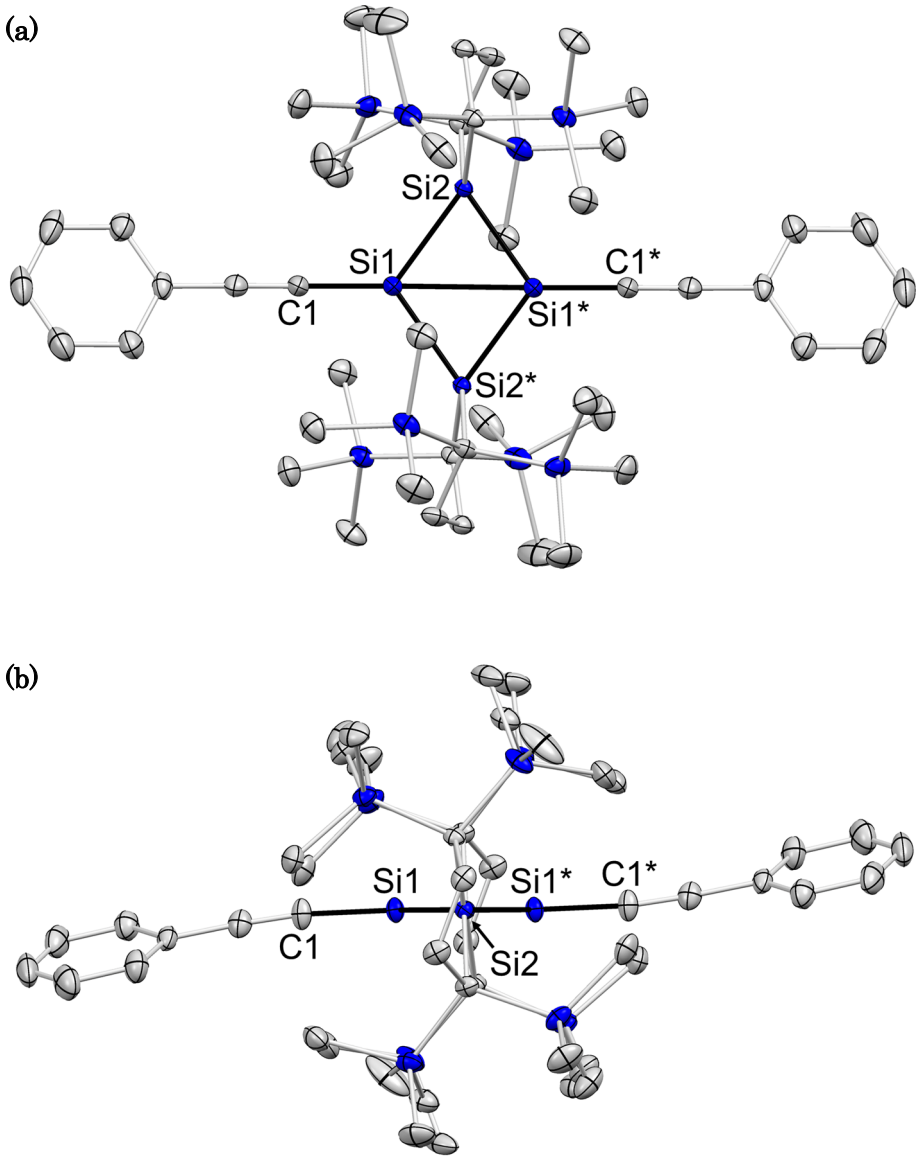


Figure S18. ORTEPs of **4** (a: top view, b: side view). Thermal ellipsoids are shown at the 50% probability level. Hydrogen atoms were omitted for clarity.

4. UV-vis Absorption Spectrum [TN575,840,865,867]

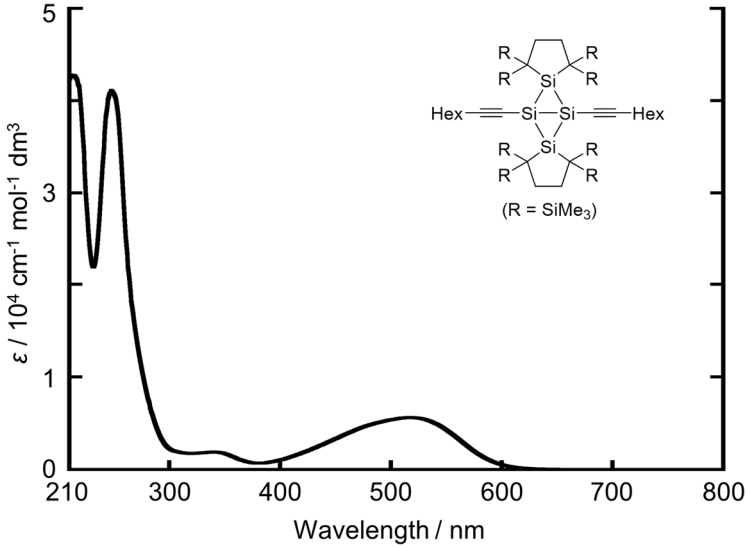


Figure S19. UV-Vis absorption spectrum of **3** in hexane at room temperature. [TN865]

Table S2. UV-vis Absorption Bands of **3** in Hexane at Room Temperature

Absorption maximum / nm	ε / cm^{-1} mol^{-1} dm^3
518	5,600
475 sh [a)]	4,600
340	1,900
248	41,000
212	43,000

a) sh = shoulder

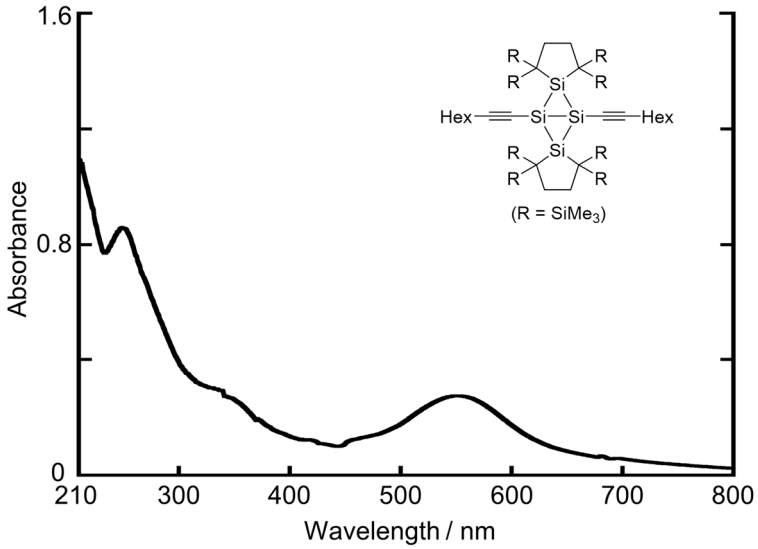


Figure S20. UV-Vis absorption spectrum of **3** in a KBr matrix at room temperature. [TN867]

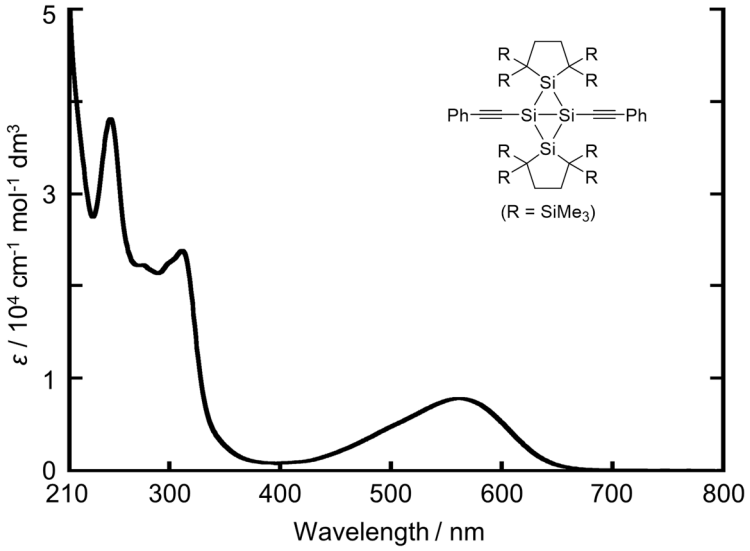


Figure S21. UV-Vis absorption spectrum of **4** in hexane at room temperature. [TN575]

Table S3. UV-vis Absorption Bands of **4** in Hexane at Room Temperature

Absorption maximum / nm	ε / cm^{-1} mol^{-1} dm^3
560	7,800
503 sh [a)]	4,900
312	24,000
298 sh [a)]	22,000
277	22,000
247	38,000

a) sh = shoulder

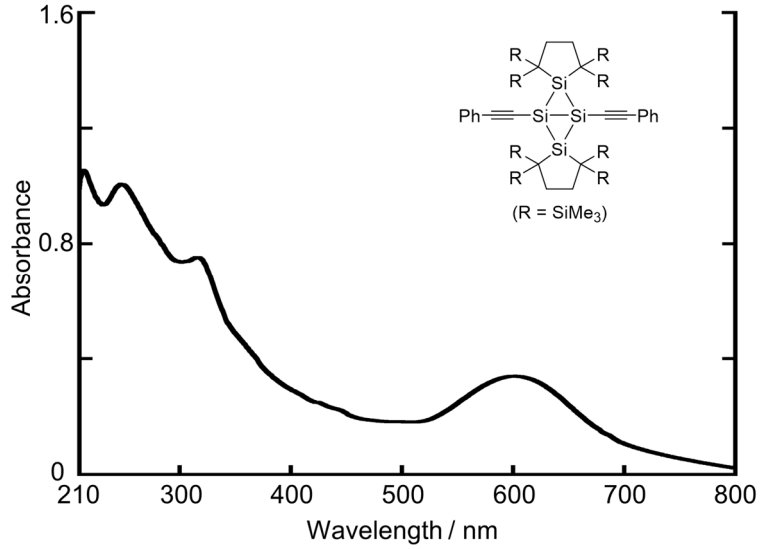


Figure S22. UV-Vis absorption spectrum of **4** in a KBr matrix at room temperature. [TN840]

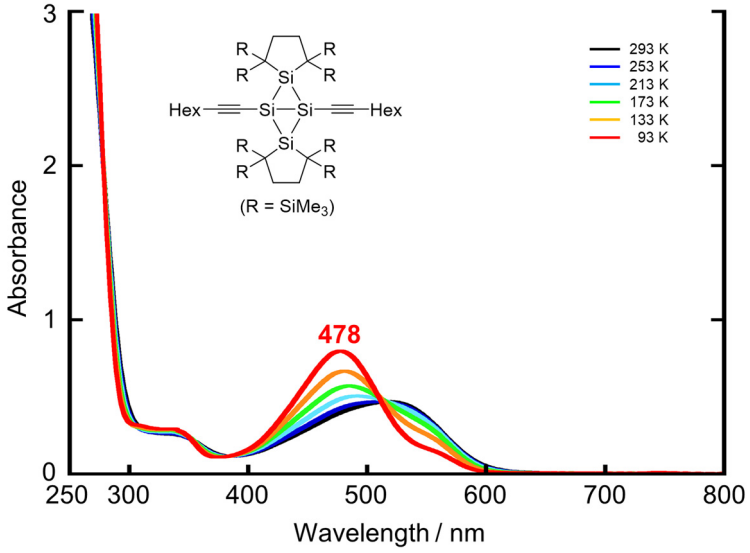


Figure S23. Variable-temperature UV-Vis absorption spectra of **3** in 3-methylpentane at 40 K intervals from 293 K to 93 K. [TN868]

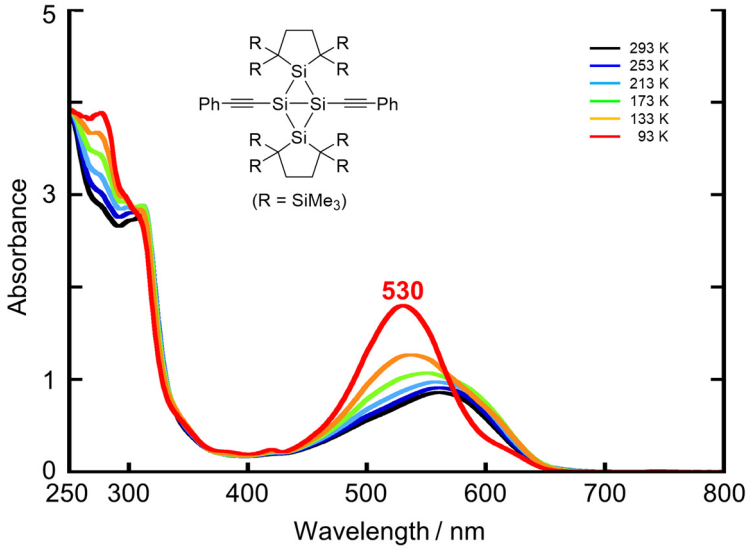


Figure S24. Variable-temperature UV-Vis absorption spectra of **4** in 3-methylpentane at 40 K intervals from 293 K to 93 K. [TN600]

5. Computational Study

All theoretical calculations were performed using a Gaussian 09[S6] program or GRRM14 program.[S7] Geometry optimization was carried out at the ωB97XD/6-311G(d) (**3**$_{opt}$) and ωB97XD/6-311G(d) (SCRF = heptane) (**5**$_p$, **5**$_c$, **5**$_c$**',** and **5**$_c$**''**) level of theory. Frontier Kohn-Sham orbitals and their energy levels of **3**$_{cry}$, **4**$_{cry}$, **5**$_p$, and **5**$_c$ were shown in Figure S26. The atomic coordinates and energies of the optimized structures are summarized in the file named "optimized_structures.xyz". The selected structural parameters of **3**$_{cry}$, **3**$_{opt}$, **5**$_p$, **5**$_c$, **5**$_c$**'**, and **5**$_c$**''** are summarized in Tables S4 and S5. Isotropic chemical shielding tensors were calculated at the GIAO/M06L/6-311+G(2df,p) level of theory (Table S6). Absolute isotropic shielding tensors of ^{29}Si nucleus in tetramethylsilane were calculated to be 361.4 (GIAO/M06L/6-311+G(2df,p)). Natural bond orbital (NBO)[S8] calculations of **3**$_{cry}$ and **4**$_{cry}$ were performed at the ωB97XD/6-311G(d) level of theory. Excitation energies and oscillator strengths of **3**$_{cry}$, **4**$_{cry}$, **5**$_p$, and **5**$_c$ were calculated at the M06-2X/6-311G(d) level of theory (Tables S7-S10).

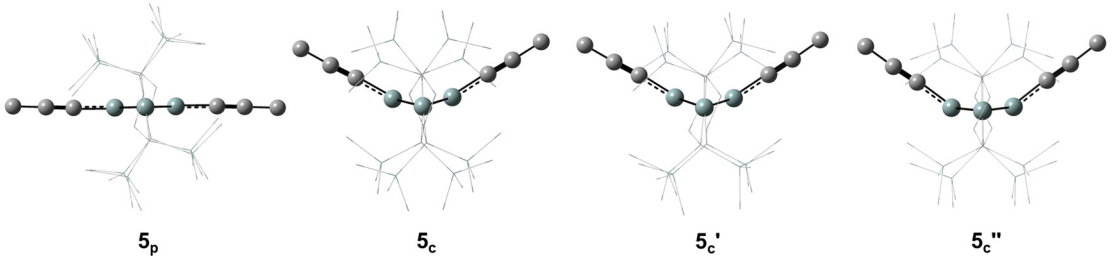
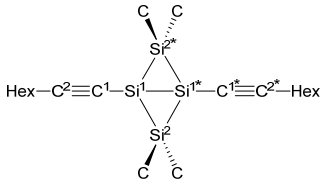


Figure S25. Molecular structures (side view) of **5**$_p$, **5**$_c$, **5**$_c$**',** and **5**$_c$**''** optimized at the ωB97XD/6-311G(d) (SCRF = heptane) level of theory.

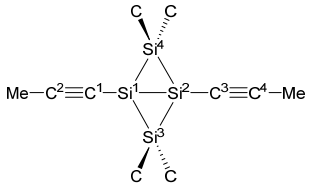
Table S4. Selected Structural Parameters of $\mathbf{3}_{cry}$ and $\mathbf{3}_{opt}$



Cpd	distance/Å					angle/°					note
	Si^1–Si^{1*}	Si^1–Si^2	Si^1–Si^{2*}	Si^1–C^1	C^1–C^2	C^1-Si^1-Si^{1*}	C^2-C^1-Si^1	Si^1-Si^2-Si^{1*}	Si^2-Si^1-Si^{2*}	Si^2-Si^1-Si^{1*}-Si^{2*}	(job name)
XRD											
$\mathbf{3}_{cry}$	2.7112(7)	2.3160(5)	2.3256(5)	1.8207(15)	1.200(2)	178.59(5)	176.51(13)	71.481(18)	108.519(18)	180.00	tn87a
DFT[a]											
$\mathbf{3}_{opt}$	2.67379	2.29718	2.30776	1.81264	1.21154	178.161	174.304	70.990	109.010	180.000	TN120da

a. optimized at the ωB97XD/6-311G(d) level of theory.

Table S5. Selected Structural Parameters of $\mathbf{5}_p$, $\mathbf{5}_c$, $\mathbf{5}_c$' and $\mathbf{5}_c$''



Cpd	distance/Å									angle/°					$E^{b,c}$	$\Delta E^{c,e}$	note
	Si^1–Si^2	Si^1–Si^3	Si^1–Si^4	Si^2–Si^3	Si^2–Si^4	Si^1-C^1	Si^2-C^3	C^1–C^2	C^3–C^4	C^1-Si^1-Si^2	C^3-Si^2-Si^1	C^2-C^1-Si^1	C^4-C^3-Si^2	Si^3-Si^1-Si^2-Si^4	[ΔG][b,d]	[$\Delta\Delta G$][d,e]	(job name)
DFT[a]																	
$\mathbf{5}_p$	2.67959	2.29820	2.30696	2.30696	2.29820	1.81452	1.81452	1.21138	1.21138	178.373	178.373	177.273	177.273	180.000	-4972.787402	0.0	TN116db
															[-4972.896005]	[0.0]	
$\mathbf{5}_c$	2.54519	2.30283	2.31023	2.31023	2.30283	1.81026	1.81026	1.21045	1.21045	148.865	148.865	177.316	177.316	158.584	-4972.790314	-7.6	TN117bb
															[-4972.897349]	[-3.5]	
$\mathbf{5}_c'$	2.52079	2.29977	2.31678	2.31467	2.29824	1.80992	1.80837	1.21003	1.20977	148.704	145.460	175.900	179.070	155.161	-4972.786789	1.6	TN121bb
															[-4972.895845]	[0.4]	
$\mathbf{5}_c''$	2.63320	2.32112	2.32606	2.32606	2.32112	1.81198	1.81198	1.21016	1.21016	142.545	142.545	176.549	176.549	171.213	-4972.783104	11.3	TN124bb
															[-4972.888189]	[20.5]	

a. optimized at the ωB97XD/6-311G(d) (SCRF = heptane) level of theory. b. in hartree. c. Zero-point vibrational energy corrections were included. d. at 298.15 K. e. in kJ mol^{-1}.

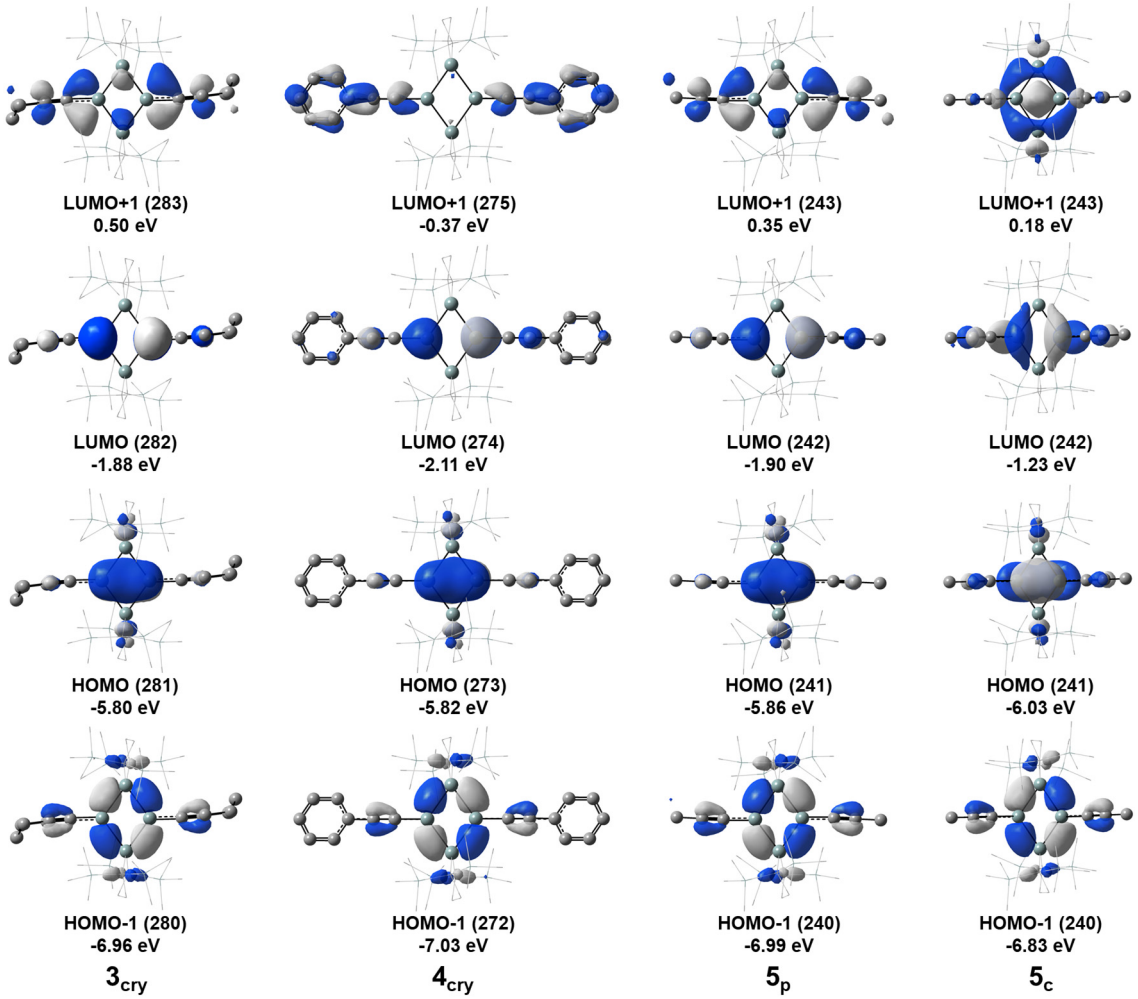


Figure S26. Frontier Kohn-Sham orbitals of $\mathbf{3}_{cry}$, $\mathbf{4}_{cry}$, $\mathbf{5}_{p}$, and $\mathbf{5}_{c}$ at the M06-2X/6-311G(d) level of theory.

Table S6. Theoretical Isotropic ^{29}Si Chemical Shifts of $\mathbf{3}_{cry}$, $\mathbf{4}_{cry}$, $\mathbf{5}_{p}$, $\mathbf{5}_{c}$, $\mathbf{5}_{c}'$, and $\mathbf{5}_{c}''$

Compound	$SiMe_3$	Bridge Si	Bridgehead Si	note
$\mathbf{3}_{cry}$[a,b]	7.5 (353.9)[c]	−17.1 (378.5)	137.2 (224.2)	nmrTN120_tn87a2
$\mathbf{4}_{cry}$[a,b]	8.0 (353.4)[c]	−15.9 (377.3)	129.9 (231.5)	nmr_TN100_tn53b_a
$\mathbf{5}_{p}$[a,b]	3.6 (357.8)[c]	−21.3 (382.7)	133.7 (227.7)	nmrTN116db1
$\mathbf{5}_{c}$[a,b]	2.7 (358.7)[c]	−15.3 (376.7)	−25.7 (387.1)	nmrTN117bb1
$\mathbf{5}_{c}'$[a,b]	3.6 (357.8)[c]	−16.8 (378.2)	−29.4 (390.8)	nmrTN121bb1
		−17.5 (378.9)	−44.9 (406.3)	
$\mathbf{5}_{c}''$[a,b]	3.7 (357.7)[c]	18.2 (343.2)	−27.4 (388.8)	nmrTN124bb1

a. GIAO/M06L/6-311+G(2df,p) level of theory. Absolute chemical shift for tetramethylsilane = 361.4. b. the absolute chemical shift is shown in the parentheses. c. average values.

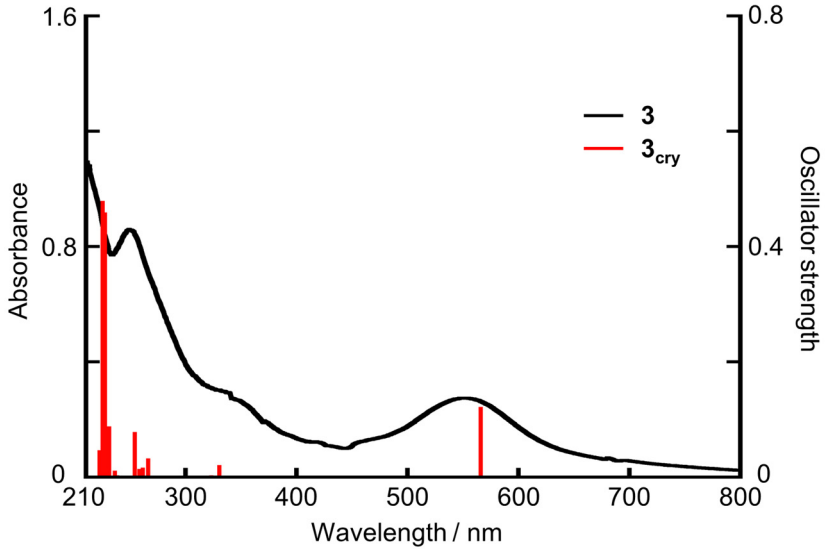


Figure S27. Experimental UV-vis absorption spectrum of **3** in a KBr matrix at room temperature (black) and theoretical band positions of $\mathbf{3}_{cry}$ calculated at the TD-M06-2X/6-311G(d) level of theory (red bar). [tdTN120_tn87a2]

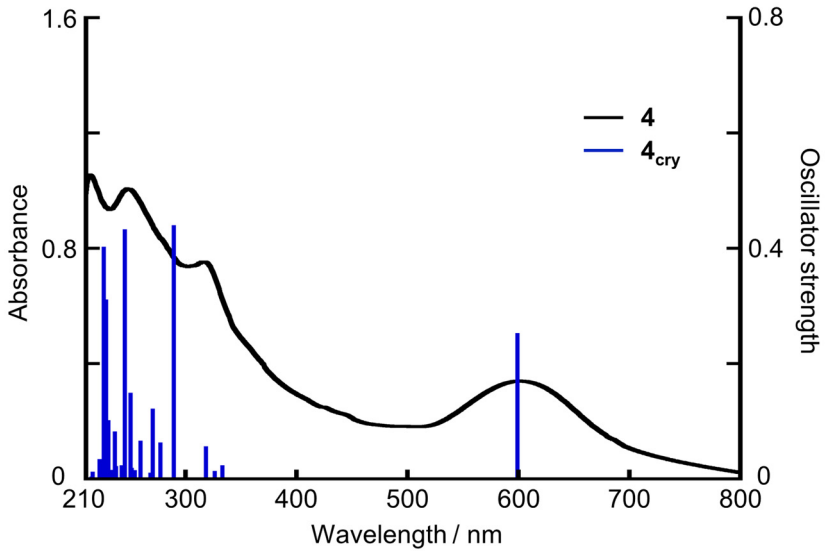


Figure S28. Experimental UV-vis absorption spectrum of **4** in a KBr matrix at room temperature (black) and theoretical band positions of $\mathbf{4}_{cry}$ calculated at the TD-M06-2X/6-311G(d) level of theory (blue bar). [td_TN100_tn53b_d]

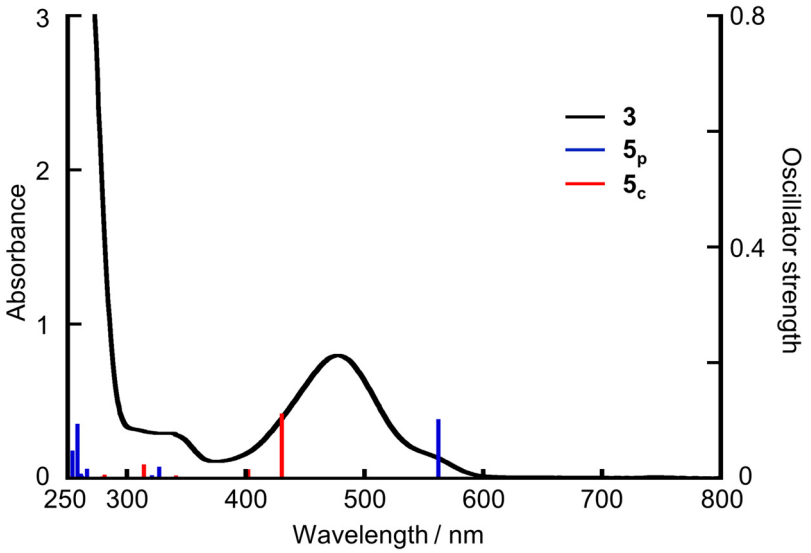


Figure S29. Experimental UV-vis absorption spectrum of **3** in 3-methylpentane at 93 K (black) and theoretical band positions of $\mathbf{5_p}$ (blue bar) and $\mathbf{5_c}$ (red bar) calculated at the TD-M06-2X/6-311G(d) level of theory. [tdTN116db1, tdTN117bb1]

Table S7. Transition Energy, Wavelength, and Oscillator Strengths of the Electronic Transition of $\mathbf{3}_{\mathbf{cry}}$ (The 281th orbital is highest occupied orbital shown in Figure S26) [tdTN120_tn87a2]

Excited State	1:	Singlet-A	2.1894 eV	566.29 nm	f=0.1218
<S**2>=0.000					
281 -> 282	0.70400				
This state for optimization and/or second-order correction.					
Total Energy, E(TD-HF/TD-KS) = -5365.40034799					
Copying the excited state density for this state as the 1-particle RhoCI density.					
Excited State	2:	Singlet-A	2.4748 eV	500.98 nm	f=0.0000
<S**2>=0.000					
280 -> 282	0.69830				
Excited State	3:	Singlet-A	3.7583 eV	329.90 nm	f=0.0211
<S**2>=0.000					
272 -> 282	-0.11190				
276 -> 282	-0.14545				
279 -> 282	0.34366				
281 -> 284	0.56640				
Excited State	4:	Singlet-A	3.8429 eV	322.63 nm	f=0.0034
<S**2>=0.000					
272 -> 282	-0.10406				
279 -> 282	0.51078				
281 -> 284	-0.38319				
281 -> 286	-0.18874				
Excited State	5:	Singlet-A	3.8683 eV	320.51 nm	f=0.0000
<S**2>=0.000					
281 -> 283	0.69629				
Excited State	6:	Singlet-A	3.9886 eV	310.85 nm	f=0.0005
<S**2>=0.000					
269 -> 282	-0.11870				
272 -> 282	0.15346				
274 -> 282	0.16207				
276 -> 282	0.56065				
277 -> 282	0.13700				
279 -> 282	0.19980				
281 -> 286	0.14294				
Excited State	7:	Singlet-A	4.0500 eV	306.13 nm	f=0.0000
<S**2>=0.000					
281 -> 285	0.70060				
Excited State	8:	Singlet-A	4.5832 eV	270.52 nm	f=0.0000
<S**2>=0.000					
278 -> 282	0.69377				
Excited State	9:	Singlet-A	4.6547 eV	266.36 nm	f=0.0325
<S**2>=0.000					
274 -> 282	0.22164				
276 -> 282	-0.21454				
277 -> 282	0.59868				
280 -> 283	-0.12008				
Excited State	10:	Singlet-A	4.7524 eV	260.89 nm	f=0.0164
<S**2>=0.000					
255 -> 282	0.14380				
269 -> 282	0.31318				
270 -> 282	0.14869				
279 -> 282	0.17967				
281 -> 286	0.46183				
281 -> 289	0.15284				
Excited State	11:	Singlet-A	4.7605 eV	260.44 nm	f=0.0000
<S**2>=0.000					
256 -> 282	-0.16463				
257 -> 282	0.34415				
269 -> 288	0.11172				
273 -> 282	0.43028				
275 -> 282	-0.30276				
Excited State	12:	Singlet-A	4.7677 eV	260.05 nm	f=0.0000
<S**2>=0.000					
257 -> 282	0.13972				
273 -> 282	0.23849				
275 -> 282	0.62722				
Excited State	13:	Singlet-A	4.7722 eV	259.80 nm	f=0.0142
<S**2>=0.000					
255 -> 282	-0.12009				
269 -> 282	-0.26273				
270 -> 282	-0.11321				
274 -> 282	0.31873				
276 -> 282	-0.21253				
277 -> 282	-0.28704				
281 -> 286	0.31550				
281 -> 287	0.12555				
Excited State	14:	Singlet-A	4.8005 eV	258.27 nm	f=0.0142
<S**2>=0.000					
255 -> 282	0.11407				
269 -> 282	0.23811				
270 -> 282	0.10089				
274 -> 282	0.52493				
277 -> 282	-0.14357				
281 -> 286	-0.19927				
281 -> 287	-0.13629				
Excited State	15:	Singlet-A	4.8771 eV	254.21 nm	f=0.0782
<S**2>=0.000					
269 -> 282	0.14900				
280 -> 285	0.20220				
281 -> 286	-0.10455				
281 -> 287	0.61429				
Excited State	16:	Singlet-A	5.1165 eV	242.32 nm	f=0.0000
<S**2>=0.000					
280 -> 284	0.66376				
281 -> 288	0.11058				
Excited State	17:	Singlet-A	5.2006 eV	238.41 nm	f=0.0000
<S**2>=0.000					
259 -> 282	-0.22107				
264 -> 282	0.21226				
268 -> 282	-0.29507				
271 -> 282	-0.23482				
273 -> 282	-0.17298				
280 -> 284	-0.11026				
281 -> 288	0.35385				
Excited State	18:	Singlet-A	5.2046 eV	238.22 nm	f=0.0033
<S**2>=0.000					
270 -> 282	0.17445				
272 -> 282	0.58762				
276 -> 282	-0.21049				
279 -> 282	0.11894				
280 -> 283	0.11051				
Excited State	19:	Singlet-A	5.2604 eV	235.69 nm	f=0.0115
<S**2>=0.000					
280 -> 285	-0.23388				
281 -> 289	-0.26698				
281 -> 291	0.55664				
Excited State	20:	Singlet-A	5.2709 eV	235.23 nm	f=0.0000
<S**2>=0.000					
256 -> 282	0.12117				
257 -> 282	-0.14016				
268 -> 282	0.15479				
271 -> 282	0.28056				
273 -> 282	0.27884				
281 -> 288	0.48373				
Excited State	21:	Singlet-A	5.3194 eV	233.08 nm	f=0.0000
<S**2>=0.000					
256 -> 282	0.15550				
257 -> 282	-0.21130				
259 -> 282	-0.16737				
264 -> 282	0.29810				
266 -> 282	0.17928				
268 -> 282	-0.23600				
271 -> 282	0.17912				
273 -> 282	0.28890				
281 -> 288	-0.26773				

Excited State 22: Singlet-A 5.3742 eV 230.70 nm f=0.0880
<S**2>=0.000
258 -> 282 -0.32587
260 -> 282 -0.10605
265 -> 282 -0.17302
267 -> 282 0.20476
270 -> 282 0.10968
272 -> 282 -0.16309
274 -> 282 0.13197
280 -> 283 0.42104

Excited State 23: Singlet-A 5.4201 eV 228.75 nm f=0.0000
<S**2>=0.000
256 -> 282 -0.17279
257 -> 282 0.23432
263 -> 282 0.24785
271 -> 282 0.52129
273 -> 282 -0.21217

Excited State 24: Singlet-A 5.4285 eV 228.39 nm f=0.0781
<S**2>=0.000
260 -> 282 -0.13783
262 -> 282 -0.13464
267 -> 282 -0.20803
269 -> 282 -0.19029
270 -> 282 0.52955
272 -> 282 -0.14596
280 -> 283 -0.12165
280 -> 285 0.17297

Excited State 25: Singlet-A 5.4490 eV 227.53 nm f=0.4592
<S**2>=0.000
265 -> 282 -0.12161
267 -> 282 0.12269
270 -> 282 -0.11577
280 -> 285 0.56332
281 -> 287 -0.17080
281 -> 289 -0.11404
281 -> 291 0.18586

Excited State 26: Singlet-A 5.4997 eV 225.44 nm f=0.0000
<S**2>=0.000
280 -> 286 0.62932
280 -> 289 0.19356

Excited State 27: Singlet-A 5.5168 eV 224.74 nm f=0.4792
<S**2>=0.000
258 -> 282 0.26110
265 -> 282 0.29279
267 -> 282 -0.19871
280 -> 283 0.48146
280 -> 285 0.13678

Excited State 28: Singlet-A 5.5678 eV 222.68 nm f=0.0000
<S**2>=0.000
259 -> 282 -0.19050
261 -> 282 0.18507
263 -> 282 0.14678
264 -> 282 0.37656
266 -> 282 -0.10314
268 -> 282 0.48430

Excited State 29: Singlet-A 5.5727 eV 222.48 nm f=0.0465
<S**2>=0.000
258 -> 282 -0.35256
265 -> 282 0.56120
267 -> 282 0.12014
270 -> 282 -0.14496

Excited State 30: Singlet-A 5.7273 eV 216.48 nm f=0.0000
<S**2>=0.000
261 -> 282 0.11943
263 -> 282 0.47840
264 -> 282 -0.29406
266 -> 282 0.33956
271 -> 282 -0.12746

Excited State 31: Singlet-A 5.7308 eV 216.35 nm f=0.0000
<S**2>=0.000
256 -> 282 0.11080
259 -> 282 0.20557
261 -> 282 0.52110
263 -> 282 0.12175
266 -> 282 -0.26795
268 -> 282 -0.23503

Excited State 32: Singlet-A 5.7361 eV 216.15 nm f=0.0014
<S**2>=0.000
258 -> 282 0.33816
262 -> 282 0.19579
265 -> 282 0.16902
267 -> 282 0.48797
270 -> 282 0.20504

Excited State 33: Singlet-A 5.8225 eV 212.94 nm f=0.0000
<S**2>=0.000
257 -> 282 0.12520
259 -> 282 0.12420
261 -> 282 0.22432
263 -> 282 -0.31923
264 -> 282 0.10886
266 -> 282 0.43929
280 -> 287 -0.25035

Excited State 34: Singlet-A 5.8448 eV 212.13 nm f=0.0027
<S**2>=0.000
254 -> 282 0.10154
260 -> 282 0.20497
262 -> 282 0.60464
267 -> 282 -0.23013
269 -> 282 -0.12183

Excited State 35: Singlet-A 5.8712 eV 211.17 nm f=0.0000
<S**2>=0.000
261 -> 282 0.19107
266 -> 282 0.20316
280 -> 287 0.57925
280 -> 289 0.15781

Excited State 36: Singlet-A 5.8878 eV 210.58 nm f=0.0000
<S**2>=0.000
281 -> 290 0.40951
281 -> 292 -0.35153
281 -> 293 0.13856
281 -> 298 0.19211
281 -> 301 0.23320
281 -> 302 0.17527

Excited State 37: Singlet-A 5.9040 eV 210.00 nm f=0.0269
<S**2>=0.000
260 -> 282 0.20922
269 -> 282 -0.13841
281 -> 289 0.34130
281 -> 291 0.23239
281 -> 294 -0.21222
281 -> 296 -0.28585
281 -> 308 -0.11670
281 -> 312 -0.14696

Excited State 38: Singlet-A 5.9217 eV 209.37 nm f=0.0055
<S**2>=0.000
260 -> 282 0.56885
262 -> 282 -0.17938
267 -> 282 0.16987
270 -> 282 0.11938
281 -> 289 -0.16570

Excited State 39: Singlet-A 5.9401 eV 208.73 nm f=0.0000
<S**2>=0.000
259 -> 282 0.52188
261 -> 282 -0.23785
263 -> 282 0.19947
264 -> 282 0.29277
271 -> 282 -0.14241

Excited State 40: Singlet-A 5.9778 eV 207.41 nm f=0.0148
<S**2>=0.000
281 -> 286 -0.22638
281 -> 289 0.41552
281 -> 291 0.19039
281 -> 294 0.20051
281 -> 296 0.25911
281 -> 297 -0.13955

281 -> 312 0.13744

Excited State 41: Singlet-A 6.0316 eV 205.56 nm f=0.0071
<S**2>=0.000
254 -> 282 0.30898
255 -> 282 -0.29883
269 -> 282 0.31892
280 -> 288 -0.25077
281 -> 294 -0.11275
281 -> 296 -0.12536

Excited State 42: Singlet-A 6.0476 eV 205.01 nm f=0.0000
<S**2>=0.000
281 -> 290 0.49939
281 -> 292 0.30250
281 -> 293 -0.29032
281 -> 301 -0.11985

Excited State 43: Singlet-A 6.1234 eV 202.48 nm f=0.0000
<S**2>=0.000
256 -> 282 0.57212
257 -> 282 0.36532
261 -> 282 -0.11366

Excited State 44: Singlet-A 6.1365 eV 202.04 nm f=0.0134
<S**2>=0.000
254 -> 282 0.54152
255 -> 282 0.24840
260 -> 282 -0.15662
272 -> 282 -0.15633
279 -> 284 -0.10229
280 -> 288 0.19146

Excited State 45: Singlet-A 6.1659 eV 201.08 nm f=0.0025
<S**2>=0.000
255 -> 282 0.45960
280 -> 288 -0.43761

Excited State 46: Singlet-A 6.1921 eV 200.23 nm f=0.0000
<S**2>=0.000
281 -> 292 0.40174
281 -> 293 0.47295
281 -> 298 0.21848

Excited State 47: Singlet-A 6.2427 eV 198.61 nm f=0.1251
<S**2>=0.000
272 -> 284 -0.11497
274 -> 284 -0.10660
276 -> 284 -0.29830
279 -> 284 0.54962

Excited State 48: Singlet-A 6.2710 eV 197.71 nm f=0.0000
<S**2>=0.000
256 -> 282 -0.10329
257 -> 282 0.18860
258 -> 283 0.31777
259 -> 291 -0.12378
264 -> 291 0.11510
272 -> 283 -0.15035
274 -> 283 0.14571
276 -> 283 -0.14234
277 -> 283 0.15638
279 -> 283 0.10981
281 -> 298 0.10463

Excited State 49: Singlet-A 6.3279 eV 195.93 nm f=0.0000
<S**2>=0.000
253 -> 282 -0.13453
272 -> 283 -0.15667
274 -> 283 -0.15691
276 -> 283 -0.30566
279 -> 283 0.46880
280 -> 286 0.11150
280 -> 291 0.12557

Excited State 50: Singlet-A 6.3397 eV 195.57 nm f=0.0000
<S**2>=0.000
253 -> 282 0.47822
276 -> 285 0.17198
279 -> 285 0.42721
280 -> 291 0.10679

Excited State 51: Singlet-A 6.3483 eV 195.30 nm f=0.0052
<S**2>=0.000
252 -> 282 0.68416

Excited State 52: Singlet-A 6.3488 eV 195.29 nm f=0.0000
<S**2>=0.000
253 -> 282 0.45835
258 -> 283 -0.10717
276 -> 285 -0.17048
279 -> 283 0.12927
279 -> 285 -0.38768
281 -> 292 0.11576

Excited State 53: Singlet-A 6.3696 eV 194.65 nm f=0.0090
<S**2>=0.000
255 -> 282 0.11659
258 -> 291 -0.13504
259 -> 283 0.20693
264 -> 283 -0.19193
268 -> 283 0.16221
278 -> 285 0.13284
280 -> 288 0.31499
281 -> 295 0.14857
281 -> 297 0.10067
281 -> 306 0.18517

Excited State 54: Singlet-A 6.4165 eV 193.23 nm f=0.0000
<S**2>=0.000
278 -> 284 -0.11736
281 -> 290 -0.14307
281 -> 292 0.15494
281 -> 293 -0.35959
281 -> 298 0.45208
281 -> 301 0.14164
281 -> 302 0.14926
281 -> 303 -0.11872

Excited State 55: Singlet-A 6.4448 eV 192.38 nm f=0.6027
<S**2>=0.000
276 -> 284 0.48132
277 -> 284 0.17457
279 -> 284 0.29965
281 -> 294 0.22084

Excited State 56: Singlet-A 6.4861 eV 191.15 nm f=0.1196
<S**2>=0.000
276 -> 284 -0.16703
277 -> 284 -0.10127
279 -> 284 -0.10664
281 -> 294 0.45652
281 -> 295 0.38594
281 -> 297 0.12275
281 -> 312 -0.10000

Excited State 57: Singlet-A 6.5251 eV 190.01 nm f=0.0000
<S**2>=0.000
251 -> 282 -0.18996
276 -> 283 0.20785
276 -> 285 -0.33431
280 -> 289 -0.18940
280 -> 291 0.40090

Excited State 58: Singlet-A 6.5429 eV 189.50 nm f=0.0000
<S**2>=0.000
241 -> 282 -0.12968
249 -> 282 0.11904
251 -> 282 0.62977
280 -> 291 0.10763

Excited State 59: Singlet-A 6.5593 eV 189.02 nm f=0.0012
<S**2>=0.000
278 -> 285 0.11749
281 -> 294 -0.29651
281 -> 295 0.31558
281 -> 296 0.41927
281 -> 305 0.13950

Excited State 60: Singlet-A 6.6176 eV 187.36 nm f=0.0000
<S**2>=0.000
275 -> 284 0.11561
276 -> 283 -0.12246
276 -> 285 -0.14926

278 -> 284 0.56146
281 -> 298 0.18486

Excited State 61: Singlet-A 6.6351 eV 186.86 nm f=0.0162
<S**2>=0.000
274 -> 284 -0.12304
276 -> 284 -0.11128
277 -> 284 0.24624
278 -> 285 0.31532
281 -> 295 -0.28166
281 -> 297 0.31211
281 -> 306 0.12596

Excited State 62: Singlet-A 6.6603 eV 186.15 nm f=0.0001
<S**2>=0.000
275 -> 284 0.14674
276 -> 283 0.15403
276 -> 285 0.28218
278 -> 284 0.17577
279 -> 283 0.15394
281 -> 300 0.28868
281 -> 301 0.20141
281 -> 302 0.20002
281 -> 304 0.16239
281 -> 311 0.10881

Excited State 63: Singlet-A 6.6607 eV 186.14 nm f=0.0311
<S**2>=0.000
274 -> 284 -0.11544
277 -> 284 0.37873
278 -> 285 0.10598
281 -> 295 0.21505
281 -> 296 -0.22102
281 -> 297 -0.37123
281 -> 305 -0.10152
281 -> 308 0.12553

Excited State 64: Singlet-A 6.6885 eV 185.37 nm f=0.0073
<S**2>=0.000
276 -> 284 -0.11548
277 -> 284 0.36359
278 -> 283 0.16130
278 -> 285 -0.34302
281 -> 296 0.12392
281 -> 297 0.23002
281 -> 306 -0.15532

Table S8. Transition Energy, Wavelength, and Oscillator Strengths of the Electronic Transition of $\mathbf{4}_{\mathbf{cry}}$ (The 273th orbital is highest occupied orbital shown in Figure S26) [td_TN100_tn53b_d]

Excited State 1: Singlet-A 2.0683 eV 599.46 nm f=0.2531
<S**2>=0.000
273 -> 274 0.70253
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -5355.85581669
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 2.4338 eV 509.42 nm f=0.0000
<S**2>=0.000
272 -> 274 0.69128

Excited State 3: Singlet-A 3.5927 eV 345.10 nm f=0.0000
<S**2>=0.000
273 -> 275 0.54687
273 -> 277 0.39382
273 -> 280 -0.14822

Excited State 4: Singlet-A 3.7244 eV 332.90 nm f=0.0235
<S**2>=0.000
260 -> 274 0.10504
265 -> 274 -0.11439
269 -> 274 -0.37159
273 -> 276 0.15090
273 -> 278 0.52565

Excited State 5: Singlet-A 3.8058 eV 325.78 nm f=0.0139
<S**2>=0.000
269 -> 274 0.46444
271 -> 274 0.17930
273 -> 278 0.39781
273 -> 282 -0.16517

Excited State 6: Singlet-A 3.8962 eV 318.22 nm f=0.0566
<S**2>=0.000
254 -> 274 -0.11254
260 -> 274 -0.12464
265 -> 274 0.40284
267 -> 274 -0.30580
271 -> 274 -0.34001
272 -> 275 -0.10428
273 -> 278 0.12889
273 -> 282 -0.12747

Excited State 7: Singlet-A 4.0407 eV 306.84 nm f=0.0000
<S**2>=0.000
273 -> 275 -0.16230
273 -> 277 0.29352
273 -> 280 -0.16112
273 -> 281 0.59153

Excited State 8: Singlet-A 4.2487 eV 291.81 nm f=0.0000
<S**2>=0.000
273 -> 275 -0.38431
273 -> 277 0.41740
273 -> 280 -0.12836
273 -> 281 -0.35826

Excited State 9: Singlet-A 4.2873 eV 289.19 nm f=0.4400
<S**2>=0.000
265 -> 274 0.24723
267 -> 274 -0.24980
269 -> 274 -0.20276
271 -> 274 0.53926

Excited State 10: Singlet-A 4.3311 eV 286.26 nm f=0.0000
<S**2>=0.000
240 -> 274 0.10632
270 -> 274 0.64426

Excited State 11: Singlet-A 4.4757 eV 277.02 nm f=0.0634
<S**2>=0.000
244 -> 274 0.10564
264 -> 274 -0.14064
265 -> 274 0.13539
272 -> 275 0.11886
273 -> 276 0.55163
273 -> 278 -0.11255
273 -> 283 0.13621
273 -> 284 -0.14103

Excited State 12: Singlet-A 4.4769 eV 276.94 nm f=0.0000
<S**2>=0.000
268 -> 274 0.68956

Excited State 13: Singlet-A 4.5948 eV 269.83 nm f=0.1220
<S**2>=0.000
244 -> 274 0.14681
253 -> 274 0.15208
254 -> 274 0.12377
264 -> 274 -0.26872
265 -> 274 0.24810
267 -> 274 0.30395
269 -> 274 -0.12778
272 -> 275 0.25537
273 -> 276 -0.23240
273 -> 282 -0.12188

Excited State 14: Singlet-A 4.6313 eV 267.71 nm f=0.0106
<S**2>=0.000
244 -> 274 -0.10742
253 -> 274 -0.11278
254 -> 274 -0.12052

264 -> 274 0.16503
265 -> 274 0.33405
267 -> 274 0.46356
272 -> 275 -0.19983
273 -> 276 0.15259

Excited State 15: Singlet-A 4.6386 eV 267.29 nm f=0.0000
<S**2>=0.000
261 -> 274 0.16217
266 -> 274 0.65404

Excited State 16: Singlet-A 4.7365 eV 261.76 nm f=0.0000
<S**2>=0.000
244 -> 275 -0.10417
246 -> 274 -0.23948
247 -> 274 -0.25549
253 -> 275 -0.12415
261 -> 274 0.39774
266 -> 274 -0.24187
270 -> 274 0.14825
272 -> 276 -0.14520

Excited State 17: Singlet-A 4.7933 eV 258.66 nm f=0.0664
<S**2>=0.000
264 -> 274 -0.22088
265 -> 274 0.10323
269 -> 274 0.18215
273 -> 278 0.11476
273 -> 282 0.56737
273 -> 285 -0.10833

Excited State 18: Singlet-A 4.8816 eV 253.98 nm f=0.0153
<S**2>=0.000
244 -> 274 0.12292
253 -> 274 0.14658
254 -> 274 0.10206
264 -> 274 0.53631
265 -> 274 0.13823
272 -> 275 0.22937
273 -> 282 0.17956

Excited State 19: Singlet-A 4.9323 eV 251.37 nm f=0.0192
<S**2>=0.000
262 -> 274 0.36958
262 -> 276 0.13036
263 -> 275 0.19007
270 -> 280 -0.14392
271 -> 279 -0.13658
273 -> 279 0.40983
273 -> 283 0.23572

Excited State 20: Singlet-A 4.9356 eV 251.20 nm f=0.0000
<S**2>=0.000
262 -> 275 0.21034
263 -> 274 0.40911
263 -> 276 0.14436
270 -> 279 -0.17070
271 -> 280 -0.14071
273 -> 277 0.15536
273 -> 280 0.40836

Excited State 21: Singlet-A 4.9528 eV 250.33 nm f=0.1494
<S**2>=0.000
253 -> 274 -0.10538
262 -> 274 -0.17485
272 -> 275 0.14065
272 -> 281 -0.22063
273 -> 279 -0.15687
273 -> 283 0.51844
273 -> 284 0.11692

Excited State 22: Singlet-A 5.0674 eV 244.67 nm f=0.4331
<S**2>=0.000
244 -> 274 -0.12720
253 -> 274 -0.22746
254 -> 274 -0.14857
260 -> 274 -0.19832
272 -> 275 0.43787
272 -> 277 0.19371
273 -> 276 0.13478
273 -> 283 -0.22155

Excited State 23: Singlet-A 5.0972 eV 243.24 nm f=0.0000
<S**2>=0.000
272 -> 276 0.19025
272 -> 278 0.64463

Excited State 24: Singlet-A 5.1128 eV 242.50 nm f=0.0000
<S**2>=0.000
243 -> 274 -0.11701
246 -> 274 0.21341
247 -> 274 0.10981
257 -> 274 0.13996
259 -> 274 0.23793
261 -> 274 0.51016
272 -> 276 0.18470

Excited State 25: Singlet-A 5.1273 eV 241.81 nm f=0.0237
<S**2>=0.000
245 -> 274 -0.15853
258 -> 274 0.28933
260 -> 274 0.51652
265 -> 274 0.12933
269 -> 274 0.14885
272 -> 275 0.15755
273 -> 282 -0.13633

Excited State 26: Singlet-A 5.2284 eV 237.13 nm f=0.0000
<S**2>=0.000
259 -> 274 -0.13017
262 -> 275 -0.11177
263 -> 274 -0.43140
273 -> 277 0.18603
273 -> 280 0.48043

Excited State 27: Singlet-A 5.2293 eV 237.09 nm f=0.0222
<S**2>=0.000
262 -> 274 -0.43459
263 -> 275 -0.11707
273 -> 279 0.52004

Excited State 28: Singlet-A 5.2635 eV 235.55 nm f=0.0821
<S**2>=0.000
253 -> 274 0.11331
270 -> 277 0.12019
273 -> 276 0.17137
273 -> 283 -0.11467
273 -> 284 0.58527

Excited State 29: Singlet-A 5.2682 eV 235.35 nm f=0.0000
<S**2>=0.000
246 -> 274 -0.12746
249 -> 274 0.12082
250 -> 274 0.12985
259 -> 274 0.58375
261 -> 274 -0.12718
272 -> 276 -0.11797
273 -> 280 0.10418

Excited State 30: Singlet-A 5.3128 eV 233.37 nm f=0.0157
<S**2>=0.000
248 -> 274 0.12693
251 -> 274 0.12770
254 -> 274 0.26577
256 -> 274 0.12034
258 -> 274 0.51968
260 -> 274 -0.29434

Excited State 31: Singlet-A 5.3854 eV 230.22 nm f=0.1019
<S**2>=0.000
251 -> 274 0.17423
253 -> 274 -0.18172
254 -> 274 0.40137
256 -> 274 -0.35521
258 -> 274 -0.12376
272 -> 277 0.25605
272 -> 280 -0.11000
272 -> 281 0.13620

Excited State 32: Singlet-A 5.4184 eV 228.82 nm f=0.0000
<S**2>=0.000
249 -> 274 -0.12238
250 -> 274 0.17424
255 -> 274 -0.37302

257 -> 274 0.52913

Excited State 33: Singlet-A 5.4380 eV 227.99 nm f=0.3114
<S**2>=0.000
253 -> 274 0.24587
256 -> 274 0.32589
272 -> 277 0.41967
272 -> 280 -0.17266
272 -> 281 0.23404
273 -> 283 0.10571

Excited State 34: Singlet-A 5.4938 eV 225.68 nm f=0.0000
<S**2>=0.000
246 -> 274 -0.11081
247 -> 274 -0.11556
250 -> 274 0.13920
271 -> 275 0.11689
272 -> 276 0.29163
272 -> 278 -0.15754
272 -> 282 0.48426
272 -> 285 -0.11498

Excited State 35: Singlet-A 5.4973 eV 225.54 nm f=0.4028
<S**2>=0.000
254 -> 274 -0.12611
256 -> 274 -0.11193
272 -> 277 -0.21578
272 -> 281 0.56595
273 -> 283 0.16371
273 -> 284 0.13853

Excited State 36: Singlet-A 5.5617 eV 222.93 nm f=0.0000
<S**2>=0.000
249 -> 274 -0.27670
250 -> 274 0.49449
252 -> 274 -0.17830
255 -> 274 -0.13013
257 -> 274 -0.29882

Excited State 37: Singlet-A 5.5740 eV 222.43 nm f=0.0000
<S**2>=0.000
250 -> 274 0.34925
252 -> 274 0.38873
255 -> 274 0.40334
257 -> 274 0.14675
259 -> 274 -0.14025

Excited State 38: Singlet-A 5.5806 eV 222.17 nm f=0.0345
<S**2>=0.000
248 -> 274 -0.15605
251 -> 274 0.29035
253 -> 274 -0.15843
254 -> 274 0.21893
256 -> 274 0.44610
258 -> 274 -0.20065
260 -> 274 0.14024
272 -> 277 -0.16720

Excited State 39: Singlet-A 5.6223 eV 220.52 nm f=0.0000
<S**2>=0.000
270 -> 276 -0.17862
270 -> 284 0.12113
271 -> 275 -0.32318
271 -> 277 -0.22009
272 -> 276 -0.23978
272 -> 282 0.33186

Excited State 40: Singlet-A 5.6594 eV 219.08 nm f=0.0000
<S**2>=0.000
249 -> 274 0.18843
252 -> 274 0.47396
255 -> 274 -0.38436
257 -> 274 -0.22993
259 -> 274 0.10188

Excited State 41: Singlet-A 5.6771 eV 218.39 nm f=0.0006
<S**2>=0.000
244 -> 274 -0.10403
248 -> 274 0.10779
251 -> 274 0.54505
253 -> 274 0.31186
254 -> 274 -0.16582
256 -> 274 -0.13613

Excited State 42: Singlet-A 5.7390 eV 216.04 nm f=0.0124
<S**2>=0.000
248 -> 274 -0.12415
251 -> 274 -0.16540
253 -> 274 0.12666
254 -> 274 0.15114
270 -> 275 0.32965
270 -> 277 0.24024
271 -> 276 0.18350
271 -> 284 -0.14148
272 -> 277 -0.16006
273 -> 284 -0.17410

Excited State 43: Singlet-A 5.7409 eV 215.97 nm f=0.0000
<S**2>=0.000
246 -> 274 -0.10380
249 -> 274 0.42952
250 -> 274 0.14144
252 -> 274 -0.25499
271 -> 277 -0.13252
272 -> 276 0.24702
272 -> 282 -0.17311
272 -> 283 0.10966

Excited State 44: Singlet-A 5.7632 eV 215.13 nm f=0.0040
<S**2>=0.000
248 -> 274 0.62640
253 -> 274 -0.16431
258 -> 274 -0.15993

Excited State 45: Singlet-A 5.8018 eV 213.70 nm f=0.0000
<S**2>=0.000
246 -> 274 0.21220
247 -> 274 0.24676
249 -> 274 0.38089
250 -> 274 0.16967
252 -> 274 -0.10737
271 -> 275 0.11154
271 -> 277 0.12008
272 -> 276 -0.24832
272 -> 282 0.12781

Excited State 46: Singlet-A 5.8960 eV 210.29 nm f=0.0059
<S**2>=0.000
262 -> 274 0.29265
262 -> 275 -0.12286
262 -> 276 -0.19634
263 -> 274 0.17447
263 -> 275 -0.21203
263 -> 276 -0.11716
270 -> 279 0.12934
270 -> 280 0.20690
271 -> 279 0.22638
271 -> 280 0.12160
272 -> 279 0.11044
272 -> 280 0.16906
273 -> 279 0.12644

Excited State 47: Singlet-A 5.8961 eV 210.28 nm f=0.0021
<S**2>=0.000
262 -> 274 -0.17421
262 -> 275 -0.21076
262 -> 276 0.11684
263 -> 274 0.29297
263 -> 275 0.12368
263 -> 276 -0.19668
270 -> 279 0.21856
270 -> 280 -0.12237
271 -> 279 -0.13292
271 -> 280 0.20728
272 -> 279 0.18683
272 -> 280 -0.10009
273 -> 280 0.11795

Excited State 48: Singlet-A 5.9102 eV 209.78 nm f=0.0000
<S**2>=0.000
269 -> 275 -0.20496
272 -> 276 -0.10083
272 -> 283 0.55473
272 -> 284 0.12467:

Table S9. Transition Energy, Wavelength, and Oscillator Strengths of the Electronic Transition of $\mathbf{5_p}$ (The 241th orbital is highest occupied orbital shown in Figure S26) [tdTN116db1]

Excited State 1: Singlet-AU 2.2067 eV 561.84 nm f=0.1023
<S**2>=0.000
241 -> 242 0.70320
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -4973.38334234
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-AG 2.4947 eV 496.98 nm f=0.0000
<S**2>=0.000
240 -> 242 0.69761

Excited State 3: Singlet-AU 3.7962 eV 326.60 nm f=0.0203
<S**2>=0.000
232 -> 242 -0.11554
239 -> 242 0.40747
241 -> 244 0.53048

Excited State 4: Singlet-AG 3.8037 eV 325.96 nm f=0.0000
<S**2>=0.000
241 -> 243 0.69593

Excited State 5: Singlet-AU 3.8590 eV 321.29 nm f=0.0053
<S**2>=0.000
239 -> 242 0.47933
241 -> 244 -0.44044
241 -> 246 -0.13289
241 -> 250 0.10706

Excited State 6: Singlet-AU 4.0402 eV 306.88 nm f=0.0013
<S**2>=0.000
231 -> 242 0.11222
232 -> 242 -0.16820
234 -> 242 -0.20897
235 -> 242 0.56404
237 -> 242 0.15898
239 -> 242 -0.12028
241 -> 246 -0.10514

Excited State 7: Singlet-AG 4.1716 eV 297.21 nm f=0.0000
<S**2>=0.000
241 -> 245 0.69945

Excited State 8: Singlet-AG 4.5873 eV 270.28 nm f=0.0000
<S**2>=0.000
236 -> 242 0.21117
238 -> 242 0.66342

Excited State 9: Singlet-AU 4.6594 eV 266.09 nm f=0.0164
<S**2>=0.000
234 -> 242 -0.30170
235 -> 242 -0.26762
237 -> 242 0.53884
240 -> 243 -0.12741

Excited State 10: Singlet-AG 4.7251 eV 262.40 nm f=0.0000
<S**2>=0.000
217 -> 242 0.24737
230 -> 242 0.10699
233 -> 242 -0.30194
236 -> 242 0.48650
238 -> 242 -0.18233

Excited State 11: Singlet-AU 4.7350 eV 261.84 nm f=0.0044
<S**2>=0.000
214 -> 242 -0.14281
215 -> 242 0.12641
231 -> 242 0.49660
232 -> 242 -0.10758
237 -> 242 -0.12469
239 -> 242 0.10400
240 -> 248 0.10915
241 -> 247 -0.23882

Excited State 12: Singlet-AG 4.7352 eV 261.83 nm f=0.0000
<S**2>=0.000
217 -> 242 -0.25453
223 -> 242 0.11513
230 -> 242 -0.11841
231 -> 248 0.10068
233 -> 242 0.35785
236 -> 242 0.45293
238 -> 242 -0.12637

Excited State 13: Singlet-AU 4.7500 eV 261.02 nm f=0.0082
<S**2>=0.000
234 -> 242 0.53368
235 -> 242 0.10919
237 -> 242 0.39784
240 -> 243 0.11637

Excited State 14: Singlet-AU 4.8080 eV 257.87 nm f=0.0943
<S**2>=0.000
231 -> 242 0.17320
234 -> 242 -0.11134
240 -> 245 -0.13426
241 -> 246 0.35087
241 -> 247 0.48987
241 -> 250 -0.15387

Excited State 15: Singlet-AU 4.8747 eV 254.34 nm f=0.0481
<S**2>=0.000
231 -> 242 -0.13400
235 -> 242 0.14767
239 -> 242 0.13217
241 -> 246 0.44400
241 -> 247 -0.37809
241 -> 250 -0.19876

Excited State 16: Singlet-AG 5.1141 eV 242.43 nm f=0.0000
<S**2>=0.000
228 -> 242 0.16061
240 -> 244 0.36013
240 -> 247 -0.10339
241 -> 248 0.49761
241 -> 249 -0.12182

Excited State 17: Singlet-AG 5.1658 eV 240.01 nm f=0.0000
<S**2>=0.000
240 -> 244 0.57666
241 -> 248 -0.31451

Excited State 18: Singlet-AU 5.2126 eV 237.85 nm f=0.0122
<S**2>=0.000
231 -> 242 0.11669
240 -> 245 0.15999
241 -> 250 -0.25697
241 -> 251 0.58118

Excited State 19: Singlet-AG 5.2389 eV 236.66 nm f=0.0000
<S**2>=0.000
217 -> 242 -0.12481
218 -> 242 0.15327
223 -> 242 0.12710
227 -> 242 0.18246
228 -> 242 0.37490
230 -> 242 -0.29461
233 -> 242 -0.22153
241 -> 248 -0.28931

Excited State 20: Singlet-AU 5.2443 eV 236.41 nm f=0.0185
<S**2>=0.000
215 -> 242 0.11509
229 -> 242 0.19343
231 -> 242 0.10580
232 -> 242 0.51726
235 -> 242 0.18701
239 -> 242 0.12706
240 -> 243 -0.24190
241 -> 246 -0.10139

Excited State 21: Singlet-AG 5.3108 eV 233.46 nm f=0.0000
<S**2>=0.000
216 -> 242 0.13891
217 -> 242 0.24133

218 -> 242 0.13602
225 -> 242 0.12937
227 -> 242 0.22910
228 -> 242 0.25647
230 -> 242 0.11278
233 -> 242 0.45019

Excited State 22: Singlet-AU 5.3218 eV 232.97 nm f=0.1734
<S**2>=0.000
220 -> 242 0.20634
222 -> 242 -0.10460
224 -> 242 0.19561
232 -> 242 0.29104
234 -> 242 -0.17225
240 -> 243 0.47610

Excited State 23: Singlet-AU 5.4813 eV 226.19 nm f=0.2998
<S**2>=0.000
219 -> 242 -0.11721
220 -> 242 -0.35847
224 -> 242 -0.22192
229 -> 242 0.35863
240 -> 243 0.36568

Excited State 24: Singlet-AU 5.5035 eV 225.28 nm f=0.5221
<S**2>=0.000
240 -> 245 0.64322
241 -> 247 0.15419
241 -> 251 -0.13459

Excited State 25: Singlet-AG 5.5684 eV 222.66 nm f=0.0000
<S**2>=0.000
217 -> 242 -0.12905
223 -> 242 0.28303
228 -> 242 0.20273
230 -> 242 0.52207
240 -> 246 0.20599
240 -> 250 -0.11135

Excited State 26: Singlet-AU 5.5741 eV 222.43 nm f=0.0369
<S**2>=0.000
219 -> 242 0.11661
222 -> 242 -0.20625
224 -> 242 0.30211
226 -> 242 -0.13857
229 -> 242 0.50989
232 -> 242 -0.16862
240 -> 243 -0.11296

Excited State 27: Singlet-AG 5.5827 eV 222.09 nm f=0.0000
<S**2>=0.000
223 -> 242 -0.11117
228 -> 242 -0.11658
230 -> 242 -0.18230
240 -> 246 0.52403
240 -> 250 -0.28277
240 -> 251 -0.13312

Excited State 28: Singlet-AG 5.6516 eV 219.38 nm f=0.0000
<S**2>=0.000
218 -> 242 0.12562
223 -> 242 0.15149
225 -> 242 -0.12386
227 -> 242 0.53547
228 -> 242 -0.34560

Excited State 29: Singlet-AU 5.7248 eV 216.57 nm f=0.0019
<S**2>=0.000
219 -> 242 -0.15276
220 -> 242 -0.21450
222 -> 242 -0.14579
224 -> 242 0.37032
226 -> 242 0.50138

Excited State 30: Singlet-AG 5.7835 eV 214.38 nm f=0.0000
<S**2>=0.000
221 -> 242 0.16732
240 -> 247 0.57145
240 -> 251 -0.15427
241 -> 248 0.12104
241 -> 249 0.23329

Excited State 31: Singlet-AU 5.8061 eV 213.54 nm f=0.0031
<S**2>=0.000
241 -> 246 0.33719
241 -> 250 0.54929
241 -> 251 0.22086

Excited State 32: Singlet-AG 5.8165 eV 213.16 nm f=0.0000
<S**2>=0.000
240 -> 247 -0.25665
241 -> 248 0.12887
241 -> 249 0.58937
241 -> 252 -0.13999

Excited State 33: Singlet-AG 5.8716 eV 211.16 nm f=0.0000
<S**2>=0.000
216 -> 242 -0.14516
218 -> 242 0.17381
221 -> 242 0.50039
225 -> 242 0.33833
228 -> 242 -0.19830
240 -> 247 -0.11927

Excited State 34: Singlet-AG 5.8916 eV 210.44 nm f=0.0000
<S**2>=0.000
216 -> 242 0.11244
217 -> 242 0.13257
218 -> 242 0.12304
221 -> 242 -0.21444
223 -> 242 0.48129
225 -> 242 0.30097
227 -> 242 -0.16932
228 -> 242 -0.14451
230 -> 242 -0.12343

Excited State 35: Singlet-AU 5.9072 eV 209.89 nm f=0.0024
<S**2>=0.000
219 -> 242 0.29298
220 -> 242 0.26152
222 -> 242 0.18141
224 -> 242 -0.16098
226 -> 242 0.40241
229 -> 242 0.17061
240 -> 248 -0.12168

Excited State 36: Singlet-AG 5.9228 eV 209.33 nm f=0.0000
<S**2>=0.000
234 -> 243 -0.10147
241 -> 249 0.17047
241 -> 252 0.48467
241 -> 257 -0.25178
241 -> 259 -0.24412

Excited State 37: Singlet-AU 5.9262 eV 209.21 nm f=0.0112
<S**2>=0.000
220 -> 242 0.14694
224 -> 242 -0.12536
226 -> 242 0.20142
228 -> 243 -0.12080
231 -> 242 -0.17085
240 -> 248 0.24149
241 -> 254 -0.12188
241 -> 255 -0.14943
241 -> 256 -0.23403
241 -> 258 0.20364
241 -> 262 0.17846
241 -> 277 -0.10815

Excited State 38: Singlet-AU 5.9636 eV 207.90 nm f=0.0005
<S**2>=0.000
214 -> 242 0.12231
222 -> 242 0.59701
224 -> 242 0.30521

Excited State 39: Singlet-AG 5.9762 eV 207.46 nm f=0.0000
<S**2>=0.000
217 -> 242 -0.21713
218 -> 242 -0.26691
221 -> 242 -0.20533
223 -> 242 -0.18617
225 -> 242 0.48281
227 -> 242 0.16539

Excited State 40: Singlet-AU 6.0244 eV 205.80 nm f=0.0274
<S**2>=0.000
219 -> 242 -0.10824
231 -> 242 -0.17614
239 -> 244 -0.13921
240 -> 248 0.37634
240 -> 249 -0.10359
241 -> 254 0.17141
241 -> 255 0.14975
241 -> 256 0.23098
241 -> 258 -0.23228
241 -> 277 0.10192

Excited State 41: Singlet-AU 6.0648 eV 204.43 nm f=0.0006
<S**2>=0.000
215 -> 242 -0.14998
219 -> 242 0.52631
220 -> 242 -0.35279
229 -> 242 -0.10678
240 -> 248 0.12588

Excited State 42: Singlet-AG 6.0783 eV 203.98 nm f=0.0000
<S**2>=0.000
217 -> 242 -0.14309
218 -> 242 0.50696
221 -> 242 -0.23340
223 -> 242 -0.22244
227 -> 242 -0.15482
230 -> 242 0.14232
241 -> 252 0.10786

Excited State 43: Singlet-AG 6.1331 eV 202.16 nm f=0.0000
<S**2>=0.000
216 -> 242 0.28144
217 -> 242 0.20227
219 -> 243 0.11198
220 -> 243 0.23351
221 -> 242 0.12697
224 -> 243 0.13786
228 -> 251 -0.12075
229 -> 243 -0.10730
232 -> 243 -0.10785
234 -> 243 0.18758
235 -> 243 0.11900
241 -> 252 0.18733

Excited State 44: Singlet-AG 6.1928 eV 200.21 nm f=0.0000
<S**2>=0.000
216 -> 242 0.56970
217 -> 242 -0.29728
221 -> 242 0.14871

Excited State 45: Singlet-AU 6.1965 eV 200.09 nm f=0.0027
<S**2>=0.000
210 -> 242 -0.12042
214 -> 242 0.36758
215 -> 242 -0.16213
218 -> 243 0.10369
227 -> 243 0.10583
228 -> 243 0.14394
231 -> 242 0.15776
240 -> 248 0.34593

Excited State 46: Singlet-AU 6.2194 eV 199.35 nm f=0.0543
<S**2>=0.000
212 -> 242 -0.10484
214 -> 242 0.22781
215 -> 242 0.42452
219 -> 242 0.14839
232 -> 242 -0.12365
235 -> 244 -0.14506
239 -> 244 -0.36560

Excited State 47: Singlet-AG 6.2270 eV 199.11 nm f=0.0000
<S**2>=0.000
232 -> 243 -0.15815
234 -> 243 -0.12160
235 -> 243 0.21776
239 -> 243 0.53860
240 -> 246 -0.10936
240 -> 250 0.11000
241 -> 253 0.11096

Excited State 48: Singlet-AU 6.2445 eV 198.55 nm f=0.0885
<S**2>=0.000
214 -> 242 0.22044
215 -> 242 0.34210
235 -> 244 0.13265
239 -> 244 0.48205

Excited State 49: Singlet-AG 6.2688 eV 197.78 nm f=0.0000
<S**2>=0.000
235 -> 243 -0.10484
239 -> 243 -0.11219
241 -> 252 0.20319
241 -> 253 0.53499
241 -> 257 0.20818
241 -> 259 0.11316
241 -> 261 -0.22053

Excited State 50: Singlet-AU 6.2842 eV 197.29 nm f=0.0011
<S**2>=0.000
214 -> 242 0.38113
215 -> 242 -0.25749
218 -> 243 -0.14367
227 -> 243 -0.13825
228 -> 243 -0.19207
231 -> 242 0.12092
240 -> 248 -0.15705
241 -> 254 0.15860
241 -> 262 0.12347

Excited State 51: Singlet-AG 6.3593 eV 194.96 nm f=0.0000
<S**2>=0.000
240 -> 251 -0.14062
241 -> 252 0.22696
241 -> 253 -0.37301
241 -> 257 0.38157
241 -> 259 0.17682
241 -> 261 -0.11947
241 -> 263 0.13492

Excited State 52: Singlet-AU 6.4024 eV 193.65 nm f=0.0253
<S**2>=0.000
241 -> 254 0.60067
241 -> 255 -0.16767
241 -> 256 -0.15970

Excited State 53: Singlet-AG 6.4244 eV 192.99 nm f=0.0000
<S**2>=0.000
213 -> 242 0.46720
239 -> 245 0.32069
240 -> 250 0.10689
240 -> 251 -0.19465
241 -> 252 0.11084
241 -> 253 0.10003
241 -> 259 0.10140
241 -> 261 0.15245

Excited State 54: Singlet-AG 6.4252 eV 192.97 nm f=0.0000
<S**2>=0.000
213 -> 242 0.45211
239 -> 245 -0.33911
240 -> 250 -0.12353
240 -> 251 0.25772
241 -> 257 0.11423

Excited State 55: Singlet-AU 6.4294 eV 192.84 nm f=0.0040
<S**2>=0.000
212 -> 242 0.66889
214 -> 242 0.10287

Excited State 56: Singlet-AU 6.4909 eV 191.01 nm f=0.5873
<S**2>=0.000
234 -> 244 -0.18053
235 -> 244 0.51583
237 -> 244 0.27100
239 -> 244 -0.20438

Excited State 57: Singlet-AG 6.4968 eV 190.84 nm f=0.0000
<S**2>=0.000
213 -> 242 -0.19830
235 -> 243 0.12489
235 -> 245 -0.11810

238 -> 244 0.13840
240 -> 251 0.21444
241 -> 252 0.23000
241 -> 259 0.28503
241 -> 261 0.34790
241 -> 266 0.16813

Excited State 58: Singlet-AG 6.5378 eV 189.64 nm f=0.0000
<S**2>=0.000
211 -> 242 0.29070
235 -> 243 0.12264
235 -> 245 -0.28458
237 -> 245 -0.10397
239 -> 245 0.26967
240 -> 247 0.10368
240 -> 250 -0.11180
240 -> 251 0.23526
241 -> 257 0.14140
241 -> 259 -0.14317
241 -> 261 -0.16878

Excited State 59: Singlet-AU 6.5543 eV 189.16 nm f=0.0085
<S**2>=0.000
228 -> 243 0.10336
235 -> 244 -0.11023
236 -> 245 -0.13304
238 -> 245 -0.20551
241 -> 254 -0.10600
241 -> 258 -0.17203
241 -> 262 0.46113
241 -> 269 0.13327

Excited State 60: Singlet-AG 6.5685 eV 188.75 nm f=0.0000
<S**2>=0.000
211 -> 242 0.60663
235 -> 245 0.10552
239 -> 245 -0.13609
241 -> 261 0.15102

Excited State 61: Singlet-AU 6.5799 eV 188.43 nm f=0.0068
<S**2>=0.000
241 -> 255 0.46670
241 -> 256 -0.33198
241 -> 258 -0.12107
241 -> 260 -0.26285
241 -> 265 -0.12997
241 -> 268 -0.12985
241 -> 269 -0.10721

Excited State 62: Singlet-AG 6.6134 eV 187.47 nm f=0.0000
<S**2>=0.000
237 -> 243 -0.12314
238 -> 244 0.57621
241 -> 259 -0.19648
241 -> 264 0.14006

Excited State 63: Singlet-AU 6.6220 eV 187.23 nm f=0.0075
<S**2>=0.000
235 -> 244 0.11683
237 -> 244 -0.32953
238 -> 243 0.11206
241 -> 255 0.17857
241 -> 256 -0.19705
241 -> 260 0.18518
241 -> 268 0.38835

Excited State 64: Singlet-AU 6.6512 eV 186.41 nm f=0.0293
<S**2>=0.000
235 -> 244 -0.22195
237 -> 244 0.43283
238 -> 243 -0.16889
241 -> 255 0.12503
241 -> 258 0.10873
241 -> 260 0.22639
241 -> 268 0.26698

Table S10. Transition Energy, Wavelength, and Oscillator Strengths of the Electronic Transition of **5**$_c$ (The 241th orbital is highest occupied orbital shown in Figure S26) [tdTN117bb1]

Excited State 1: Singlet-B 2.8807 eV 430.39 nm f=0.1121
<S**2>=0.000
240 -> 244 0.11038
241 -> 242 0.68779
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -4973.36122781
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-B 3.0836 eV 402.08 nm f=0.0154
<S**2>=0.000
240 -> 242 0.68349

Excited State 3: Singlet-A 3.6377 eV 340.83 nm f=0.0051
<S**2>=0.000
241 -> 243 0.68177

Excited State 4: Singlet-B 3.9458 eV 314.22 nm f=0.0239
<S**2>=0.000
241 -> 244 0.68675

Excited State 5: Singlet-A 4.4118 eV 281.03 nm f=0.0064
<S**2>=0.000
232 -> 242 0.10939
235 -> 242 -0.10778
236 -> 242 0.14713
239 -> 242 0.37873
240 -> 243 -0.12879
241 -> 245 0.50112

Excited State 6: Singlet-B 4.4502 eV 278.61 nm f=0.0031
<S**2>=0.000
240 -> 244 -0.11076
241 -> 246 0.68716

Excited State 7: Singlet-A 4.4545 eV 278.33 nm f=0.0005
<S**2>=0.000
230 -> 242 -0.15400
235 -> 242 0.24366
236 -> 242 0.19983
238 -> 242 0.26328
239 -> 242 -0.11046
240 -> 243 0.40438
240 -> 245 -0.18803
241 -> 245 0.20342

Excited State 8: Singlet-A 4.6600 eV 266.06 nm f=0.0022
<S**2>=0.000
232 -> 242 0.12124
236 -> 242 0.22133
238 -> 242 0.11880
239 -> 242 0.41889
240 -> 243 0.14957
241 -> 245 -0.39424
241 -> 247 0.16781

Excited State 9: Singlet-A 4.7530 eV 260.85 nm f=0.0003
<S**2>=0.000
230 -> 242 0.12674
235 -> 242 -0.14607
236 -> 242 -0.20533
238 -> 242 -0.20735
240 -> 243 0.50789
241 -> 247 -0.10472
241 -> 248 0.18969

Excited State 10: Singlet-A 4.9405 eV 250.95 nm f=0.0033
<S**2>=0.000
236 -> 242 0.16771
238 -> 242 0.12912
240 -> 243 -0.11207
240 -> 245 -0.22795
241 -> 247 -0.20701
241 -> 248 0.51714

Excited State 11: Singlet-B 5.0316 eV 246.41 nm f=0.0800
<S**2>=0.000

220 -> 242 -0.15552
233 -> 242 -0.13708
234 -> 242 -0.17730
240 -> 244 0.50759
240 -> 246 -0.16854
241 -> 249 -0.23084

Excited State 12: Singlet-A 5.0345 eV 246.27 nm f=0.0000
<S**2>=0.000
235 -> 242 0.10882
236 -> 242 0.13622
238 -> 242 0.17092
239 -> 242 -0.15252
240 -> 245 0.59365
241 -> 248 0.15557

Excited State 13: Singlet-B 5.1029 eV 242.97 nm f=0.0830
<S**2>=0.000
220 -> 242 0.20965
228 -> 242 0.13064
233 -> 242 0.16677
240 -> 244 0.36343
240 -> 246 0.21087
241 -> 249 0.28153
241 -> 252 0.13035

Excited State 14: Singlet-A 5.1506 eV 240.72 nm f=0.0340
<S**2>=0.000
230 -> 242 0.23169
235 -> 242 -0.17731
236 -> 242 0.19175
239 -> 242 -0.26696
241 -> 247 0.40820
241 -> 251 0.16325

Excited State 15: Singlet-A 5.2160 eV 237.70 nm f=0.0286
<S**2>=0.000
230 -> 242 -0.20667
235 -> 242 0.17139
236 -> 242 -0.29717
241 -> 245 0.10026
241 -> 247 0.35842
241 -> 248 0.24745
241 -> 251 0.23554

Excited State 16: Singlet-B 5.2824 eV 234.71 nm f=0.0596
<S**2>=0.000
220 -> 242 -0.24135
223 -> 242 -0.11962
228 -> 242 -0.10305
233 -> 242 -0.23519
237 -> 242 0.14784
240 -> 246 0.13548
241 -> 249 0.44825
241 -> 252 0.15671

Excited State 17: Singlet-A 5.4026 eV 229.49 nm f=0.0031
<S**2>=0.000
230 -> 242 0.12587
235 -> 242 -0.15429
236 -> 242 -0.36545
238 -> 242 0.54506

Excited State 18: Singlet-B 5.4068 eV 229.31 nm f=0.0167
<S**2>=0.000
234 -> 242 0.13139
237 -> 242 0.66565

Excited State 19: Singlet-B 5.4541 eV 227.32 nm f=0.4391
<S**2>=0.000
234 -> 242 -0.18123
240 -> 246 0.57976
241 -> 249 -0.25283

Excited State 20: Singlet-B 5.5190 eV 224.65 nm f=0.1602
<S**2>=0.000
234 -> 242 0.58873
237 -> 242 -0.11400
240 -> 244 0.18455
240 -> 246 0.19538

Excited State 21: Singlet-A 5.5699 eV 222.60 nm f=0.0003
<S**2>=0.000
214 -> 242 -0.10602
230 -> 242 0.31700
235 -> 242 0.52325
239 -> 242 0.12570
240 -> 247 -0.14223

Excited State 22: Singlet-A 5.6766 eV 218.41 nm f=0.0010
<S**2>=0.000
222 -> 242 -0.24592
227 -> 242 0.30682
229 -> 242 0.15718
230 -> 244 -0.13721
231 -> 242 -0.24365
232 -> 242 0.19878
235 -> 244 0.11550
240 -> 248 -0.24179
241 -> 247 -0.10671

Excited State 23: Singlet-B 5.7749 eV 214.70 nm f=0.0022
<S**2>=0.000
218 -> 242 0.14634
225 -> 242 -0.13744
236 -> 243 -0.16220
239 -> 243 -0.28114
240 -> 249 0.44743
240 -> 252 0.21729

Excited State 24: Singlet-A 5.7930 eV 214.03 nm f=0.0050
<S**2>=0.000
230 -> 242 0.21025
240 -> 247 0.58135
240 -> 251 0.24741

Excited State 25: Singlet-B 5.9399 eV 208.73 nm f=0.0215
<S**2>=0.000
218 -> 242 0.10455
225 -> 242 -0.13500
228 -> 242 -0.21012
233 -> 242 0.43844
234 -> 242 -0.11304
239 -> 243 0.25358
241 -> 250 0.14646
241 -> 252 -0.12144
241 -> 258 0.11466

Excited State 26: Singlet-B 5.9629 eV 207.93 nm f=0.0551
<S**2>=0.000
218 -> 242 -0.21465
219 -> 242 -0.10846
223 -> 242 -0.10302
225 -> 242 0.23621
226 -> 242 0.10844
228 -> 242 0.22567
240 -> 244 -0.10055
240 -> 249 0.30333
241 -> 250 0.16256
241 -> 252 -0.18518
241 -> 258 0.15249

Excited State 27: Singlet-A 5.9746 eV 207.52 nm f=0.0022
<S**2>=0.000
222 -> 242 0.10547
227 -> 242 -0.13856
232 -> 242 0.53176
236 -> 242 -0.11242
238 -> 242 -0.10446
239 -> 242 -0.11306
241 -> 247 -0.13316
241 -> 251 0.26522

Excited State 28: Singlet-A 5.9857 eV 207.13 nm f=0.0019
<S**2>=0.000
232 -> 242 -0.28106
241 -> 247 -0.23187
241 -> 248 -0.20597
241 -> 251 0.48972
241 -> 259 0.11130

Excited State 29: Singlet-B 5.9979 eV 206.71 nm f=0.0290
<S**2>=0.000
218 -> 242 -0.12107

220 -> 242 -0.18204
223 -> 242 -0.11341
225 -> 242 0.12373
226 -> 242 0.10030
233 -> 242 0.40144
236 -> 243 -0.13141
239 -> 243 -0.30270
240 -> 249 -0.13356
241 -> 250 -0.18662

Excited State 30: Singlet-B 6.0244 eV 205.80 nm f=0.0705
<S**2>=0.000
220 -> 242 -0.13070
235 -> 243 -0.12127
239 -> 243 0.30861
240 -> 249 0.24686
241 -> 249 -0.16546
241 -> 250 -0.17730
241 -> 252 0.27879
241 -> 258 -0.19756

Excited State 31: Singlet-B 6.0802 eV 203.91 nm f=0.0064
<S**2>=0.000
241 -> 250 0.57953
241 -> 252 0.29203

Excited State 32: Singlet-A 6.1250 eV 202.42 nm f=0.0718
<S**2>=0.000
227 -> 242 0.15211
229 -> 242 0.14016
231 -> 242 -0.24188
239 -> 244 0.15439
240 -> 248 0.45150
240 -> 251 0.11586
241 -> 257 -0.11601
241 -> 259 0.14530

Excited State 33: Singlet-A 6.1557 eV 201.41 nm f=0.0084
<S**2>=0.000
227 -> 244 0.10791
230 -> 242 0.19191
231 -> 244 -0.12642
232 -> 244 0.16159
236 -> 244 0.20397
238 -> 244 0.10803
239 -> 244 0.32308
240 -> 248 -0.20623
241 -> 251 0.16082
241 -> 259 -0.12785

Excited State 34: Singlet-A 6.1894 eV 200.32 nm f=0.0057
<S**2>=0.000
222 -> 242 -0.25156
227 -> 242 0.25477
229 -> 242 -0.20912
231 -> 242 0.50354
232 -> 242 0.11570

Excited State 35: Singlet-B 6.2363 eV 198.81 nm f=0.4857
<S**2>=0.000
235 -> 243 0.19539
236 -> 243 0.36067
238 -> 243 0.43114
239 -> 243 -0.20915
241 -> 252 0.10600

Excited State 36: Singlet-B 6.2608 eV 198.03 nm f=0.0041
<S**2>=0.000
218 -> 244 -0.20244
220 -> 242 0.15796
222 -> 248 0.12876
225 -> 244 0.19314
227 -> 248 -0.14076
228 -> 242 0.26209
228 -> 244 0.13556
231 -> 248 0.10146
234 -> 244 -0.20909
241 -> 252 0.23452

Excited State 37: Singlet-A 6.2669 eV 197.84 nm f=0.0198
<S**2>=0.000
222 -> 244 0.15115
227 -> 244 -0.15810
230 -> 242 -0.12657
236 -> 244 0.12234
239 -> 244 0.31272
239 -> 246 -0.11686
240 -> 248 -0.17429
241 -> 253 0.18241
241 -> 254 0.15612
241 -> 257 -0.14961
241 -> 259 0.26609

Excited State 38: Singlet-A 6.2963 eV 196.91 nm f=0.0001
<S**2>=0.000
222 -> 244 -0.11743
227 -> 244 0.12281
236 -> 244 -0.17527
238 -> 244 -0.11199
239 -> 244 -0.23323
241 -> 253 0.48383
241 -> 254 0.10776
241 -> 259 0.13889
241 -> 260 -0.10550

Excited State 39: Singlet-B 6.3533 eV 195.15 nm f=0.0106
<S**2>=0.000
218 -> 242 0.14107
219 -> 242 0.22938
220 -> 242 -0.11711
223 -> 242 -0.17694
225 -> 242 -0.22705
226 -> 242 0.11683
228 -> 242 0.46878
241 -> 252 -0.10010

Excited State 40: Singlet-A 6.3574 eV 195.02 nm f=0.0282
<S**2>=0.000
222 -> 244 0.11124
227 -> 244 -0.12293
238 -> 244 0.10598
240 -> 248 0.19594
241 -> 253 0.38363
241 -> 254 -0.20592
241 -> 257 0.20031
241 -> 259 -0.22364
241 -> 260 -0.10166

Excited State 41: Singlet-A 6.3930 eV 193.94 nm f=0.0028
<S**2>=0.000
217 -> 242 0.13096
224 -> 242 0.26177
227 -> 242 -0.11173
229 -> 242 0.54406
231 -> 242 0.25428

Excited State 42: Singlet-B 6.4063 eV 193.54 nm f=0.0127
<S**2>=0.000
236 -> 243 -0.23238
238 -> 243 0.21292
241 -> 249 -0.11983
241 -> 250 -0.10328
241 -> 252 0.25476
241 -> 255 0.23456
241 -> 256 -0.22711
241 -> 258 0.25523
241 -> 262 0.18188
241 -> 265 0.12425

Excited State 43: Singlet-B 6.4148 eV 193.28 nm f=0.0051
<S**2>=0.000
219 -> 242 -0.22667
223 -> 242 0.13274
225 -> 242 -0.32942
226 -> 242 0.53334

Excited State 44: Singlet-A 6.4503 eV 192.22 nm f=0.0012
<S**2>=0.000
237 -> 243 0.62383
237 -> 245 0.12165
238 -> 244 -0.13661

Excited State 45: Singlet-B 6.4607 eV 191.91 nm f=0.0227
<S**2>=0.000

235 -> 243 -0.11891
236 -> 243 -0.35402
237 -> 244 -0.13827
238 -> 243 0.38769
239 -> 243 0.10901
241 -> 252 -0.10980
241 -> 255 -0.17753
241 -> 256 0.17873
241 -> 258 -0.14410
241 -> 262 -0.13429

Excited State 46: Singlet-B 6.5334 eV 189.77 nm f=0.1185
<S**2>=0.000
219 -> 242 -0.23106
221 -> 242 -0.12569
223 -> 242 -0.12038
235 -> 243 0.27400
236 -> 243 -0.13518
236 -> 245 0.10536
239 -> 245 0.38377
240 -> 249 -0.12897
241 -> 262 -0.12000

Excited State 47: Singlet-A 6.5393 eV 189.60 nm f=0.0000
<S**2>=0.000
217 -> 242 -0.16295
224 -> 242 0.55972
227 -> 242 -0.23868
229 -> 242 -0.19214
230 -> 242 0.10426
231 -> 242 -0.11693

Excited State 48: Singlet-B 6.5823 eV 188.36 nm f=0.0023
<S**2>=0.000
219 -> 242 0.25194
220 -> 242 -0.10257
221 -> 242 0.27649
223 -> 242 0.31988
225 -> 242 0.17627
226 -> 242 0.17458
235 -> 243 0.33012
238 -> 245 -0.10267

Excited State 49: Singlet-B 6.5909 eV 188.12 nm f=0.0212
<S**2>=0.000
218 -> 242 -0.15622
221 -> 242 -0.15798
223 -> 242 -0.13603
225 -> 242 -0.25148
226 -> 242 -0.17396
235 -> 243 0.35801
236 -> 245 -0.15278
238 -> 245 -0.15509
239 -> 243 0.10976
239 -> 245 -0.14523
241 -> 255 -0.14774

Excited State 50: Singlet-A 6.5910 eV 188.11 nm f=0.0014
<S**2>=0.000
222 -> 242 0.43342
224 -> 242 0.19480
227 -> 242 0.35232
234 -> 243 0.18685
239 -> 246 -0.17672

Excited State 51: Singlet-A 6.6125 eV 187.50 nm f=0.0105
<S**2>=0.000
222 -> 242 -0.31750
227 -> 242 -0.16636
234 -> 243 0.41592
235 -> 244 -0.15740
238 -> 246 0.10956
239 -> 246 -0.24134
241 -> 254 -0.10410

Excited State 52: Singlet-B 6.6320 eV 186.95 nm f=0.0047
<S**2>=0.000
218 -> 242 -0.13852
219 -> 242 0.36839
220 -> 242 0.32346
223 -> 242 -0.35970
226 -> 242 0.19562
228 -> 242 -0.18024

Excited State 53: Singlet-A 6.6437 eV 186.62 nm f=0.0538
<S**2>=0.000
234 -> 243 0.36164
235 -> 246 -0.11344
236 -> 244 0.22899
236 -> 246 -0.18629
238 -> 244 0.11296
238 -> 246 -0.18544
239 -> 244 -0.17592
239 -> 246 0.26838
240 -> 248 -0.10182

Excited State 54: Singlet-B 6.6667 eV 185.98 nm f=0.0171
<S**2>=0.000
218 -> 242 0.27524
220 -> 242 0.13271
223 -> 242 -0.11196
225 -> 242 0.10982
226 -> 242 0.11050
241 -> 256 -0.12100
241 -> 258 -0.27015
241 -> 261 -0.19104
241 -> 262 0.29479
241 -> 265 0.18712

Excited State 55: Singlet-B 6.7094 eV 184.79 nm f=0.0452
<S**2>=0.000
215 -> 242 0.10157
218 -> 242 0.32516
219 -> 242 -0.23725
223 -> 242 -0.20508
225 -> 242 0.12400
239 -> 245 -0.26847
241 -> 258 0.21257
241 -> 262 -0.14316

Excited State 56: Singlet-A 6.7118 eV 184.73 nm f=0.0410
<S**2>=0.000
235 -> 244 -0.12118
236 -> 244 -0.11381
238 -> 244 -0.23402
239 -> 244 0.15138
239 -> 246 0.15544
241 -> 253 0.11695
241 -> 254 -0.26048
241 -> 257 -0.25178
241 -> 259 -0.12517
241 -> 260 0.28491
241 -> 268 0.11867
241 -> 270 0.10813

Excited State 57: Singlet-A 6.7222 eV 184.44 nm f=0.0068
<S**2>=0.000
235 -> 246 0.10348
236 -> 244 0.10142
239 -> 246 -0.16442
240 -> 251 -0.12836
241 -> 254 0.36545
241 -> 259 -0.20559
241 -> 260 0.38057

Excited State 58: Singlet-A 6.7284 eV 184.27 nm f=0.0332
<S**2>=0.000
236 -> 244 -0.10515
240 -> 247 -0.23321
240 -> 248 -0.11977
240 -> 251 0.50425
240 -> 259 0.10685
241 -> 254 0.21083
241 -> 257 0.10302
241 -> 259 -0.13986

Excited State 59: Singlet-B 6.7481 eV 183.73 nm f=0.0068
<S**2>=0.000
218 -> 242 -0.10338
219 -> 242 -0.13533
221 -> 242 0.49172
223 -> 242 -0.14141
225 -> 242 -0.18242
226 -> 242 -0.12894

238 -> 245 -0.12120
241 -> 255 0.19509
241 -> 258 -0.13185
241 -> 261 0.15142

Excited State 60: Singlet-A 6.7517 eV 183.64 nm f=0.0135
<S**2>=0.000
235 -> 244 -0.10334
236 -> 244 -0.14352
238 -> 244 -0.28992
239 -> 244 0.16524
239 -> 246 0.23284
240 -> 251 -0.18653
241 -> 254 0.29593
241 -> 257 0.16300
241 -> 259 -0.13087
241 -> 260 -0.19878
241 -> 268 -0.10479

Excited State 61: Singlet-B 6.7584 eV 183.45 nm f=0.0065
<S**2>=0.000
221 -> 242 -0.23518
225 -> 242 0.11679
239 -> 245 -0.17798
241 -> 255 0.35334
241 -> 258 -0.32191
241 -> 261 0.22636
241 -> 265 -0.13869

Excited State 62: Singlet-A 6.7755 eV 182.99 nm f=0.0088
<S**2>=0.000
216 -> 242 0.19051
217 -> 242 -0.20198
229 -> 242 0.11597
236 -> 246 0.14409
241 -> 257 0.32138
241 -> 259 0.21263
241 -> 260 0.27533
241 -> 263 0.19231
241 -> 264 -0.12039

Excited State 63: Singlet-B 6.7827 eV 182.79 nm f=0.0861
<S**2>=0.000
240 -> 250 0.49767
240 -> 252 -0.21626
240 -> 255 0.10366
240 -> 258 0.22370
241 -> 256 0.10299

Excited State 64: Singlet-A 6.7945 eV 182.48 nm f=0.0191
<S**2>=0.000
216 -> 242 -0.29769
217 -> 242 0.42491
224 -> 242 0.13779
227 -> 242 0.10817
229 -> 242 -0.15546
238 -> 246 -0.11579
241 -> 257 0.18478
241 -> 260 0.16822

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