

Supplementary Materials: Transformative Si₈R₈ Siliconoids

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1. NMR Spectra

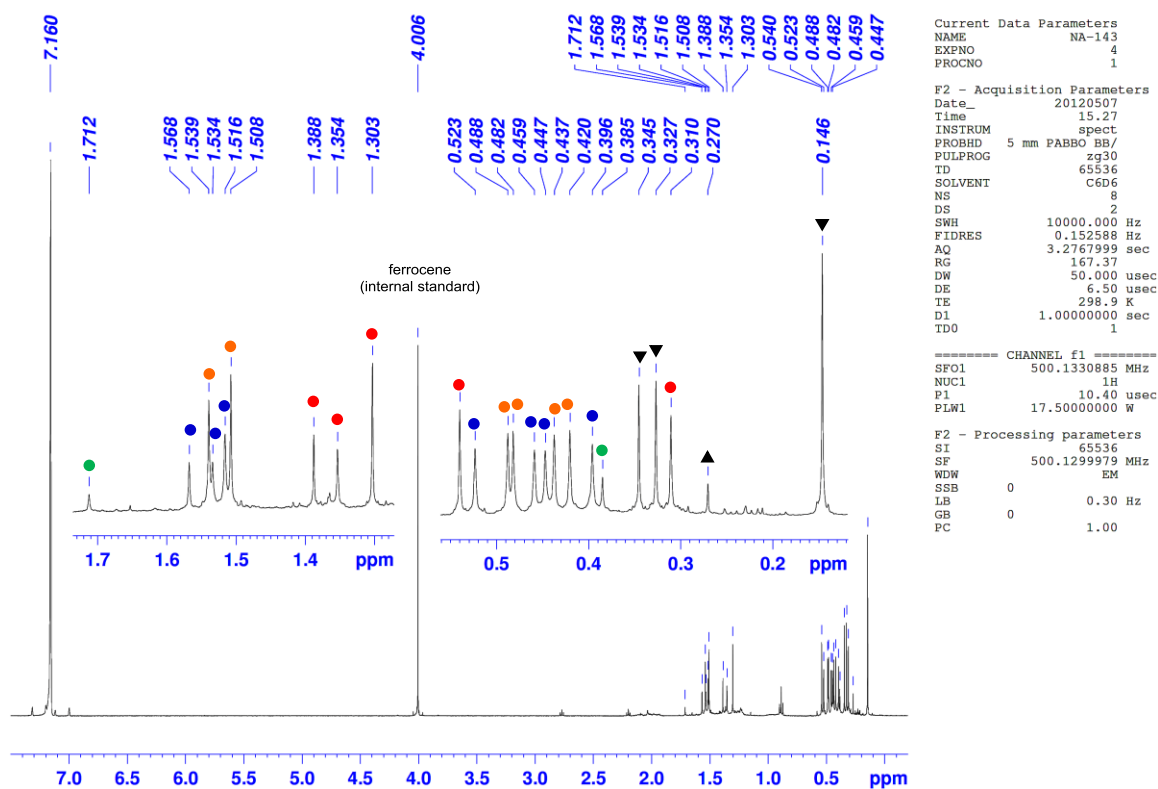
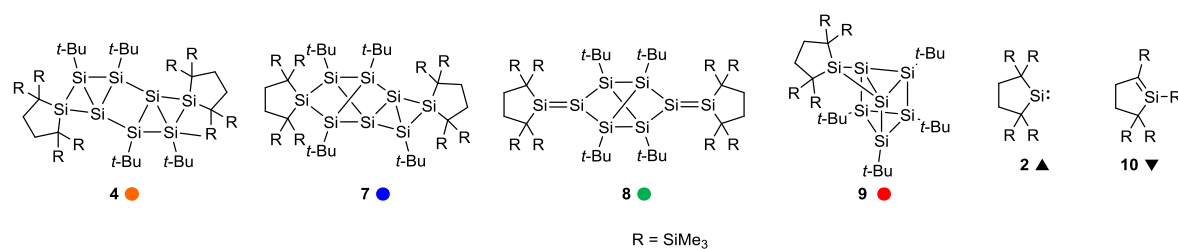


Figure S1. ¹H NMR spectrum of the reaction mixture after heating 4 for 3 h (C₆D₆, rt).

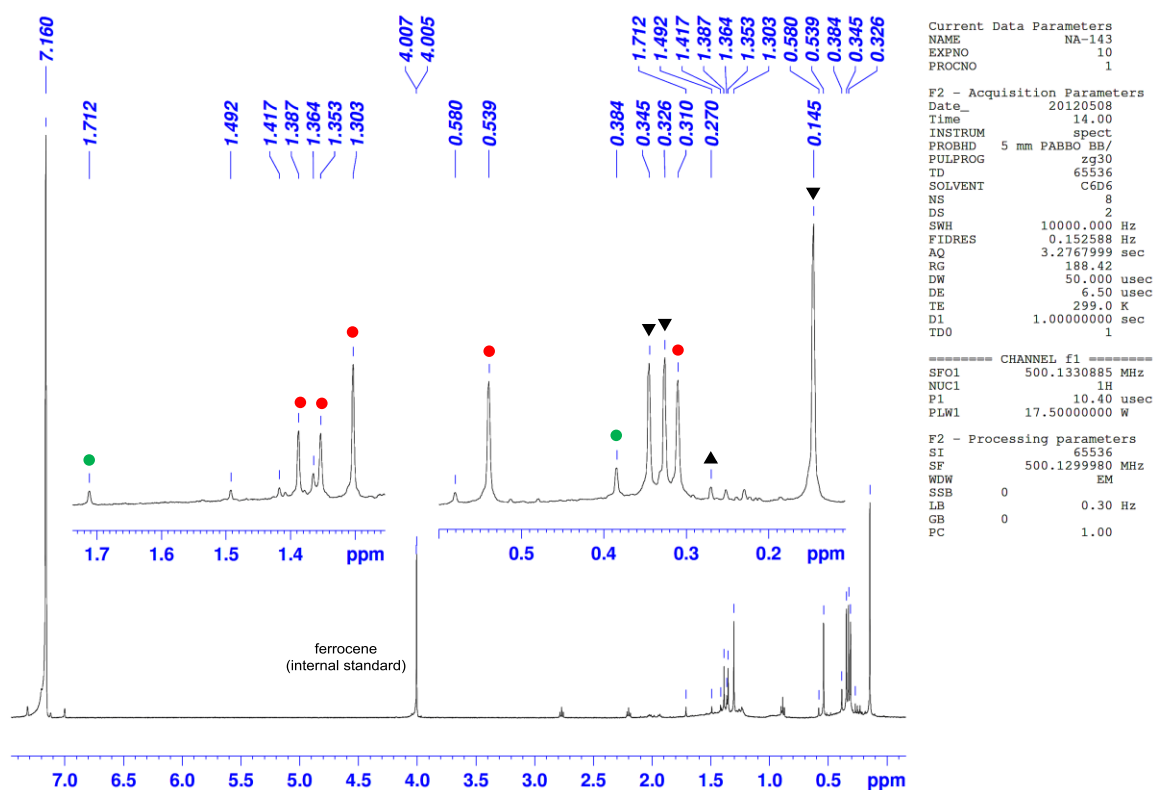
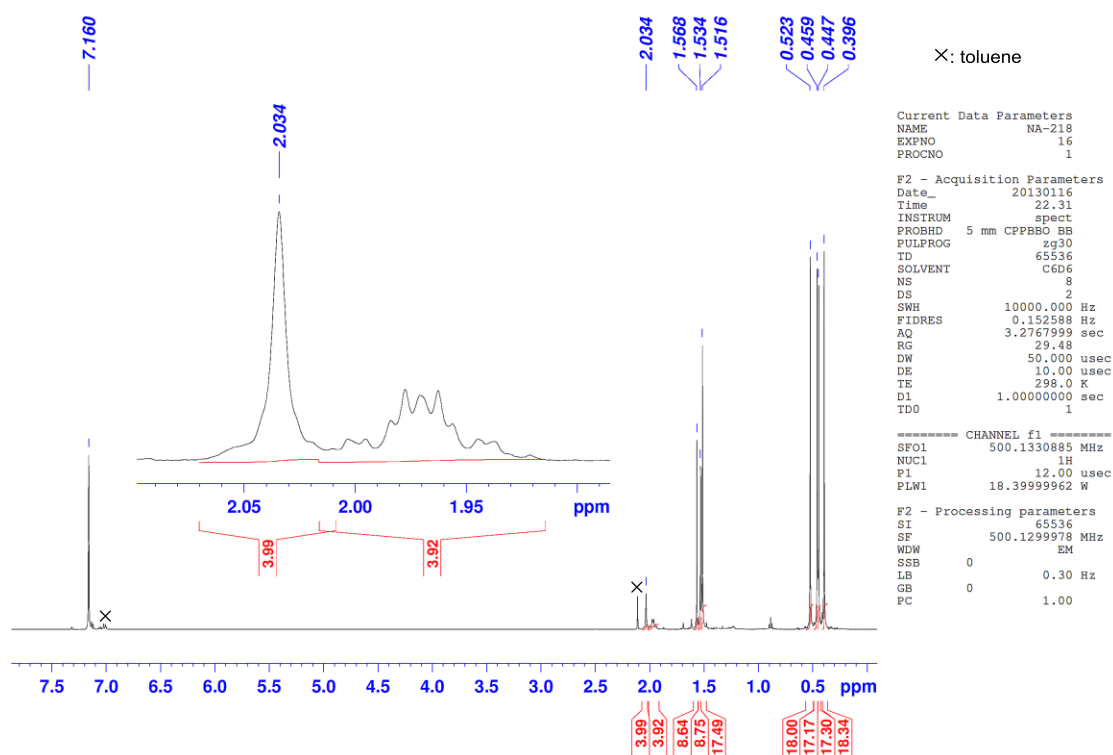
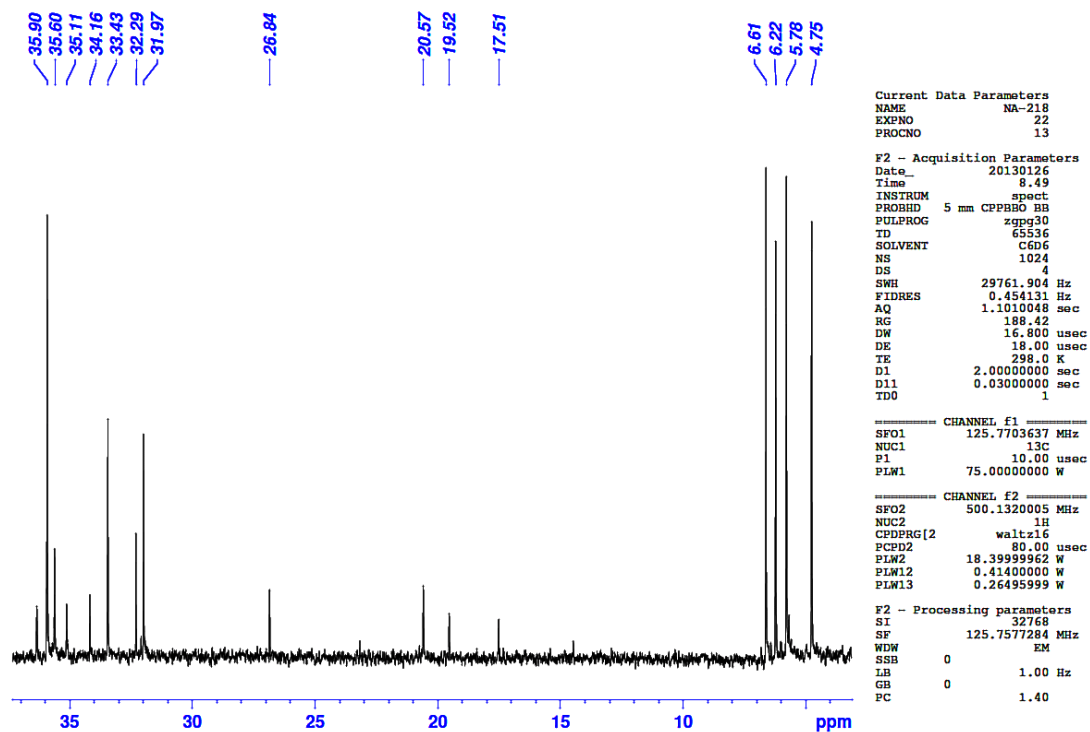


Figure S2. ^1H NMR spectrum of the reaction mixture after heating **4** for 22 h (C_6D_6 , rt).

Figure S3. ^1H NMR spectrum of 7 in C_6D_6 at rt. \times = toluene.Figure S4. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of 7 in C_6D_6 at rt.

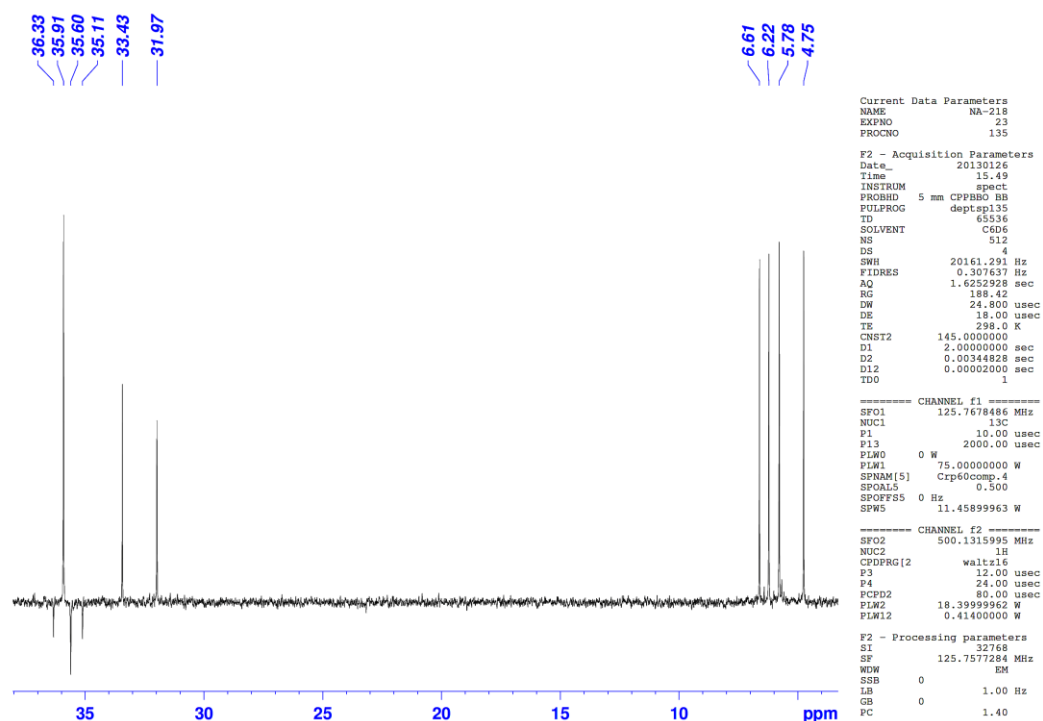


Figure S5. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of 7 using DEPT 135 pulse sequence in C_6D_6 at rt.

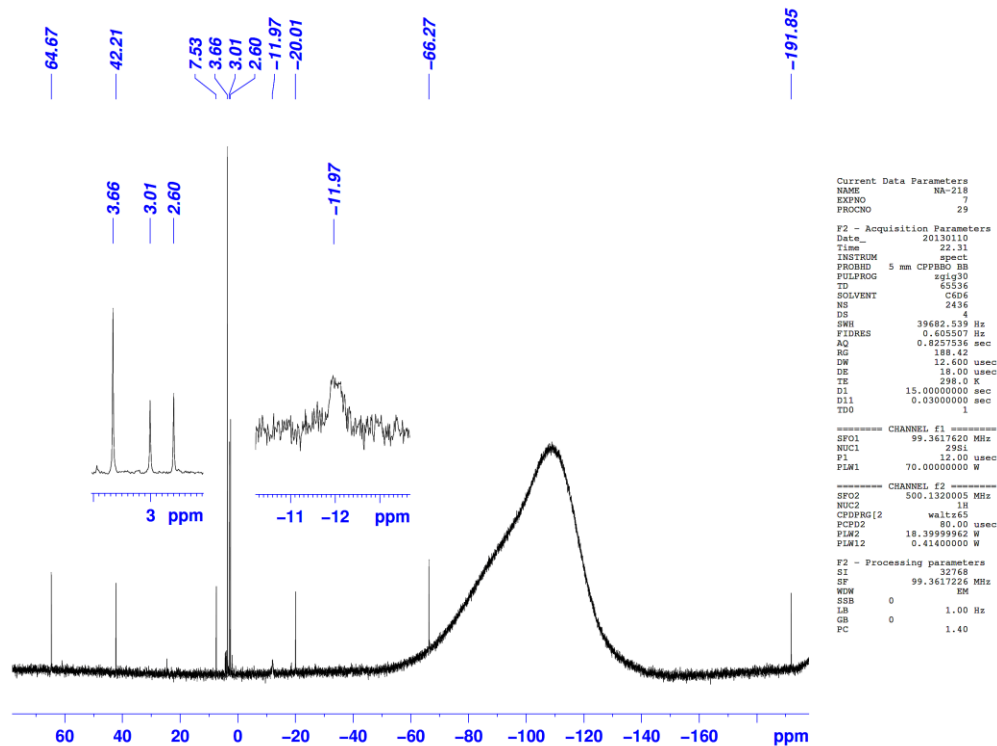
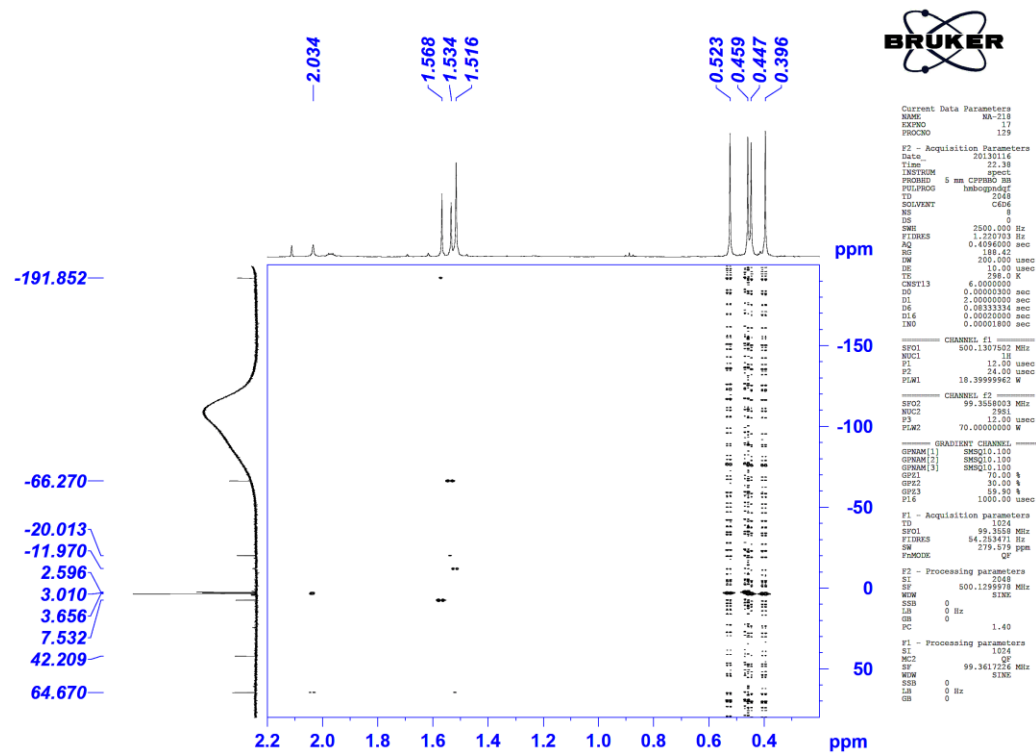


Figure S6. $^{29}\text{Si}\{^1\text{H}\}$ NMR spectrum of 7 using the inverse-gated pulse sequence in C_6D_6 at rt.Figure S7. ^1H - ^{29}Si HMBC 2D NMR spectrum of 7 in C_6D_6 at rt.

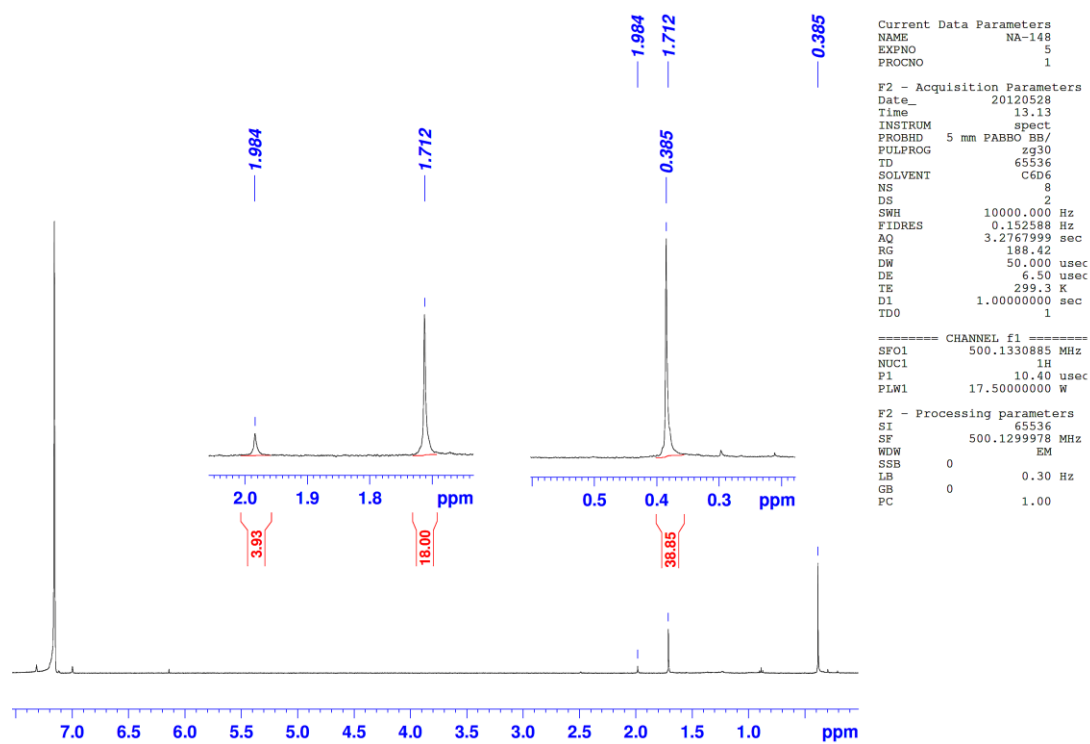
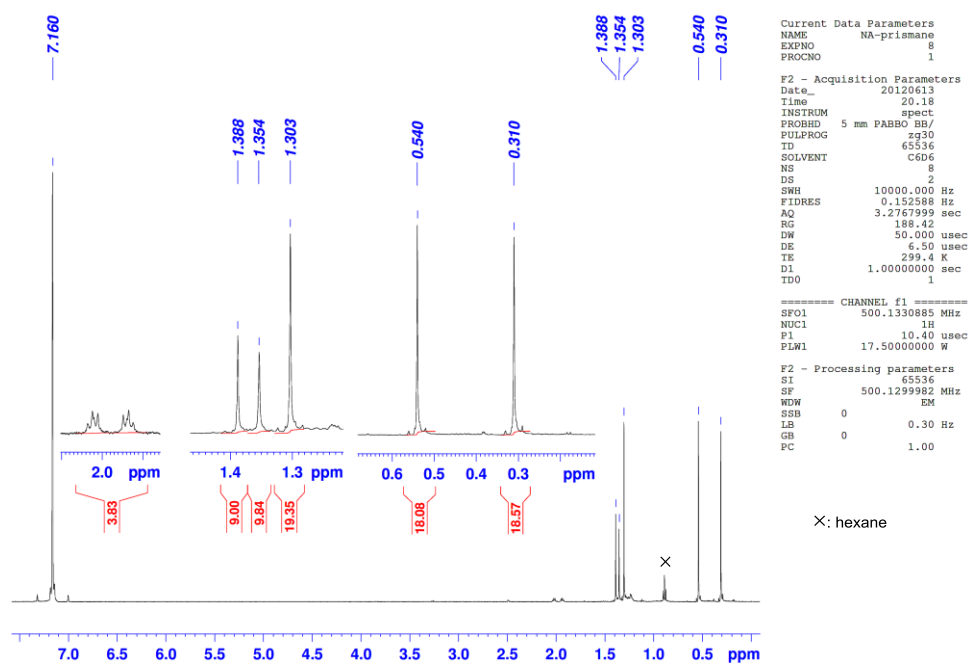
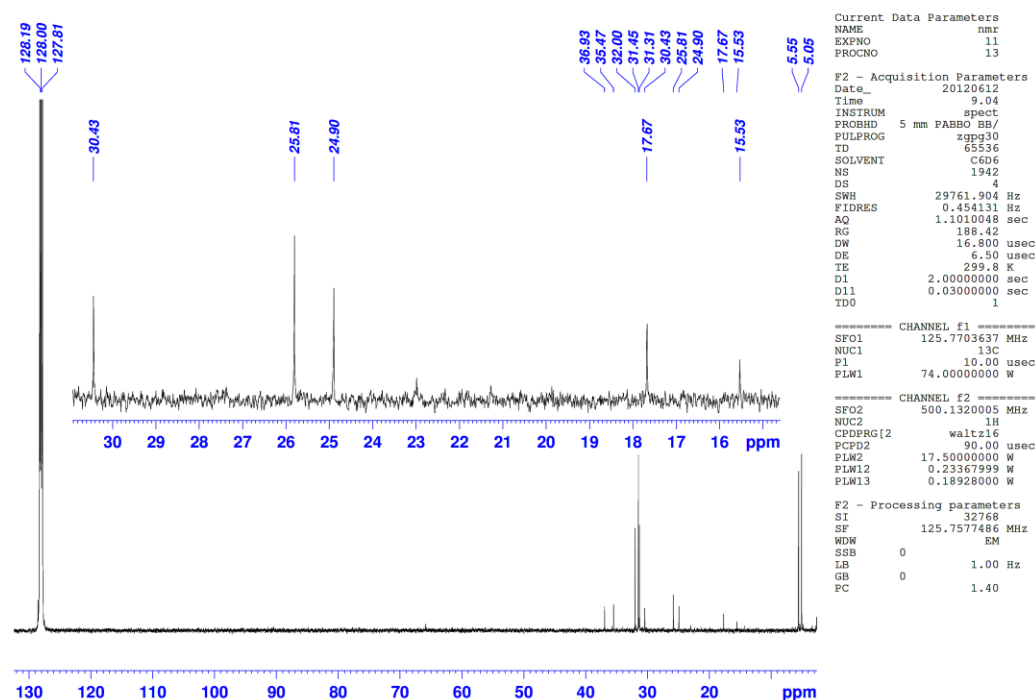


Figure S8. ^1H NMR spectrum of **8** in C_6D_6 at rt.

Figure S9. ^1H NMR spectrum of **9** in C_6D_6 at rt.Figure S10. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **9** in C_6D_6 at rt.

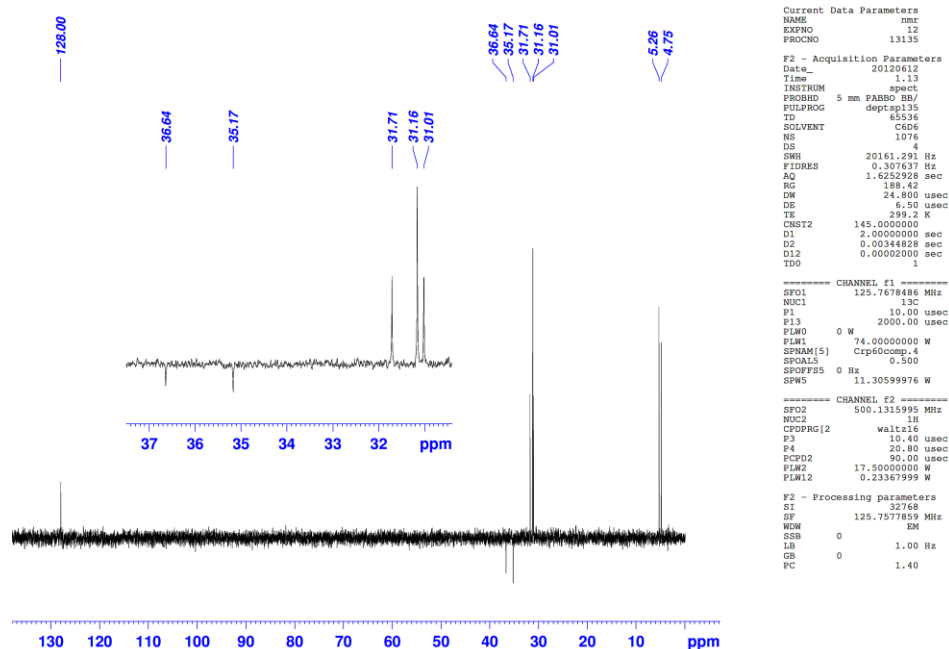


Figure S11. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **9** using DEPT 135 pulse sequence in C_6D_6 at rt.

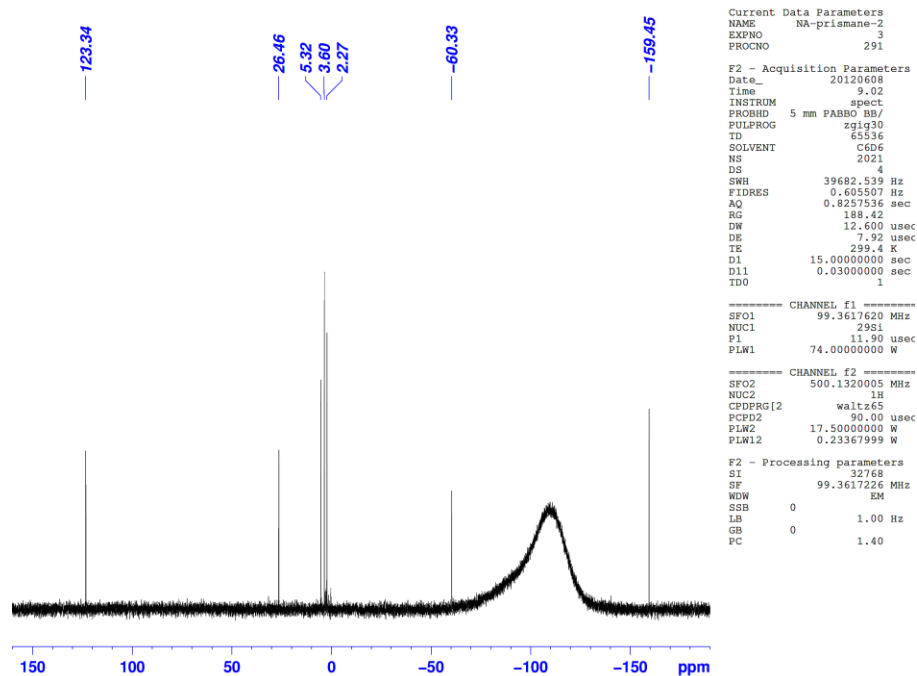
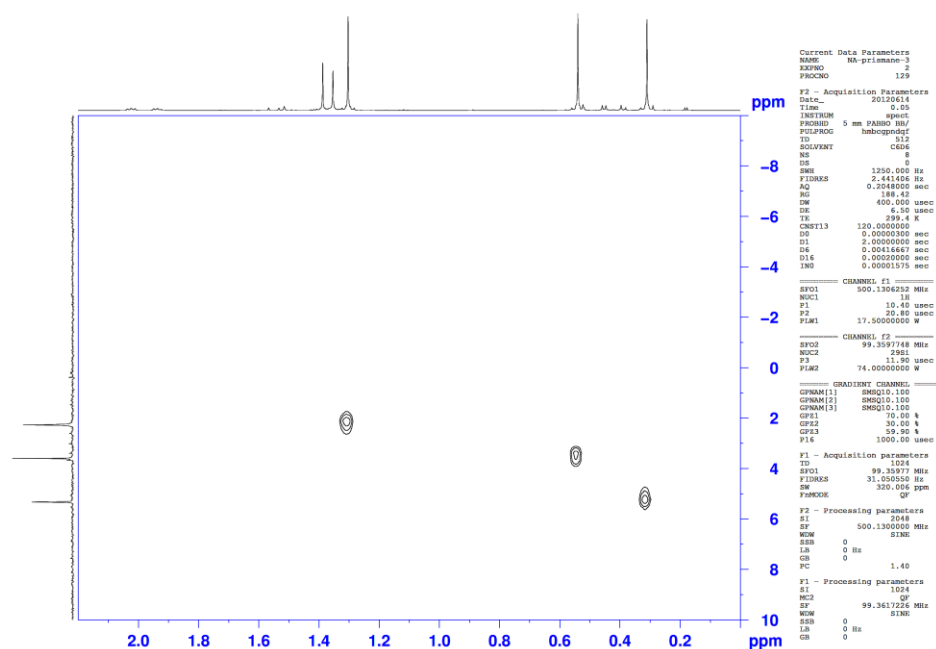
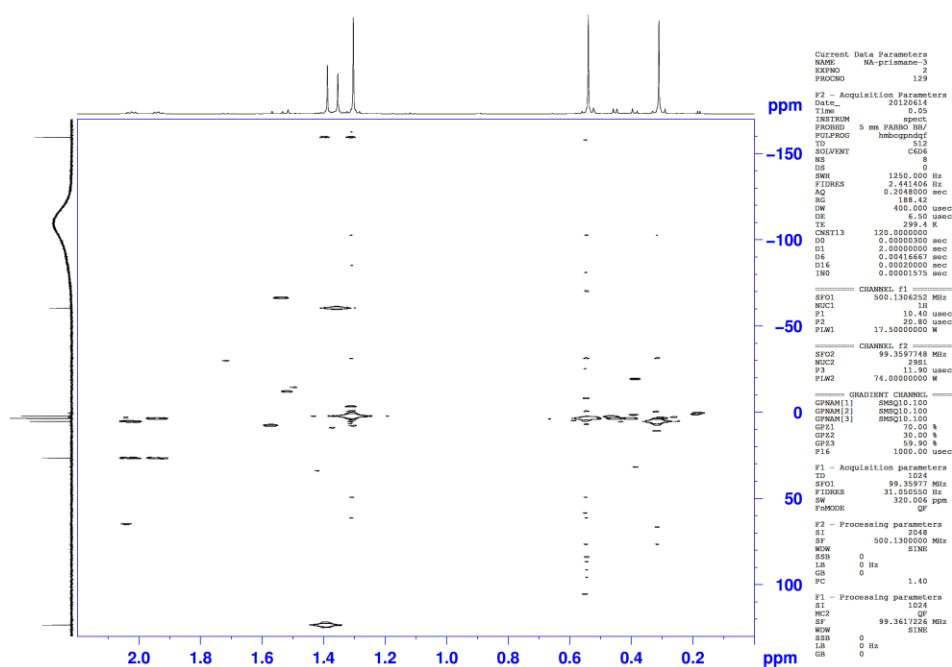


Figure S12. $^{29}\text{Si}\{^1\text{H}\}$ NMR spectrum of **9** using the inverse-gated pulse sequence in C_6D_6 at rt.

Figure S13. ^1H - ^{29}Si HMBC 2D NMR spectrum of **9** in C_6D_6 at rt.Figure S14. ^1H - ^{29}Si HMBC 2D NMR spectrum of **9** in C_6D_6 at rt.

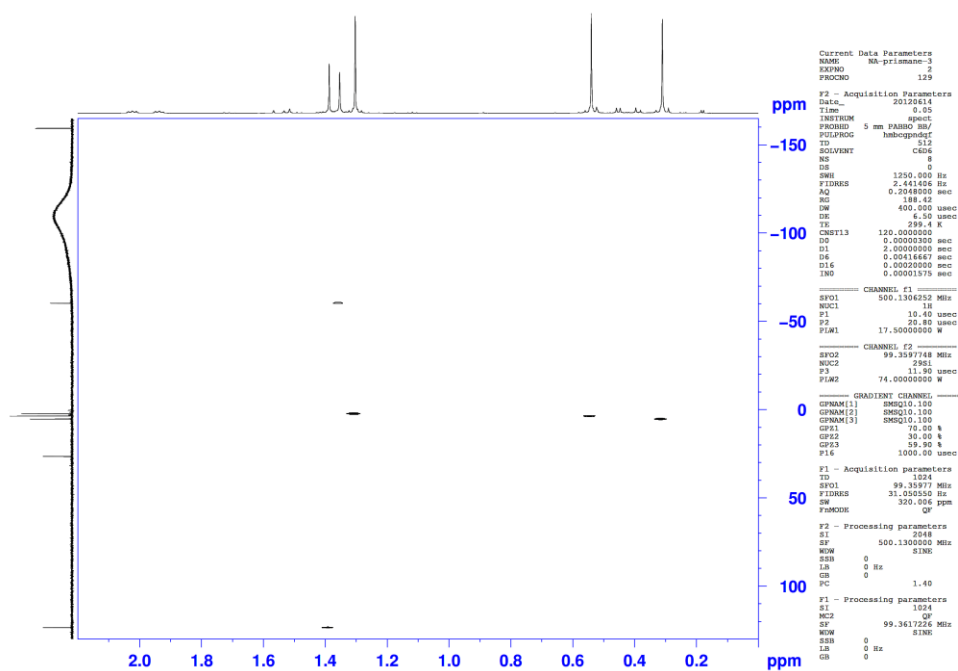


Figure S15. ^1H - ^{29}Si HMBC 2D NMR spectrum of **9** in C_6D_6 at rt.

2. Time Course of The Product Yields during Thermal Reaction of 7

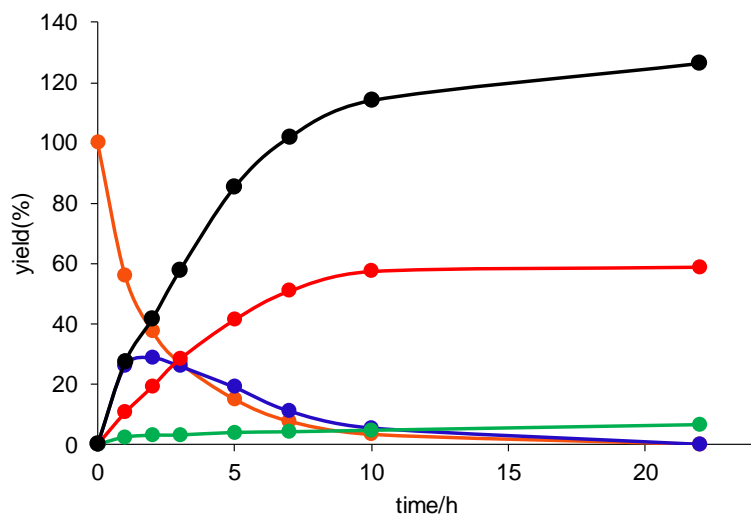
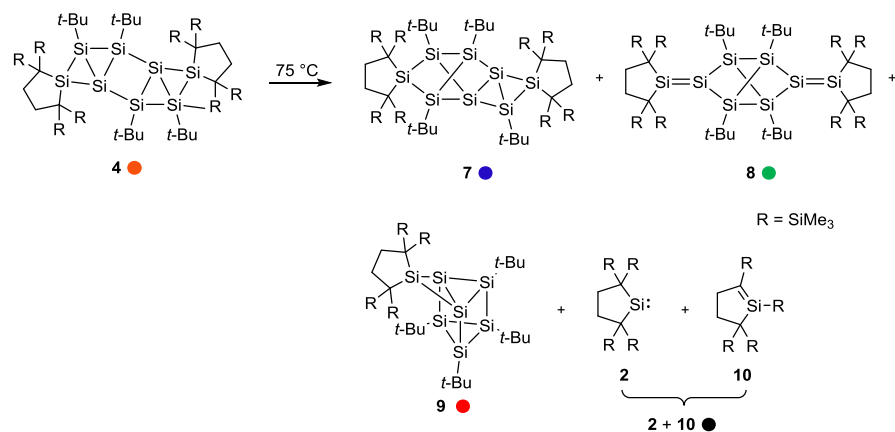
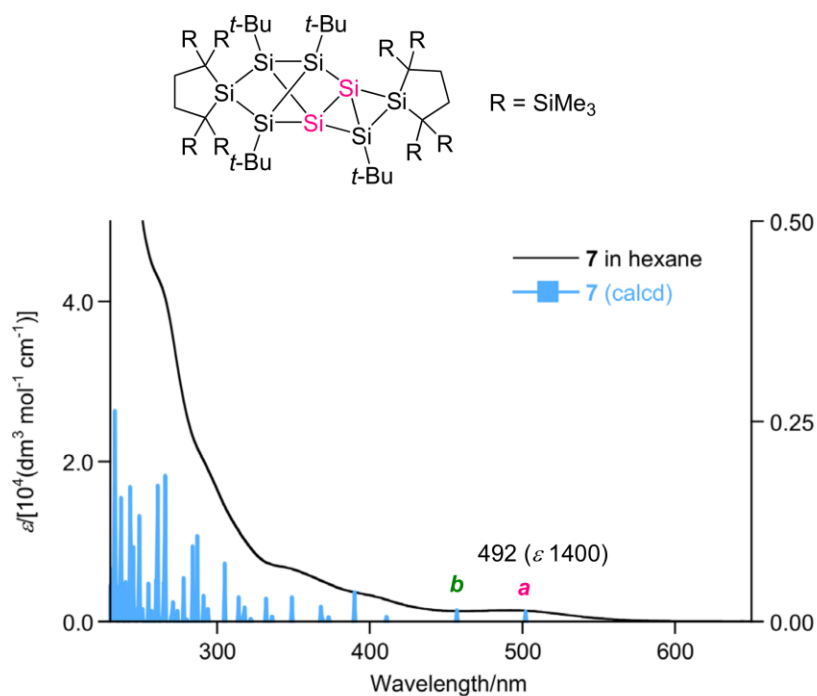


Figure S16. The time course of the product yields during thermolysis of **7** monitored by ^1H NMR spectrum.

3. UV-vis Spectra

Compound 7

(a)



(b)

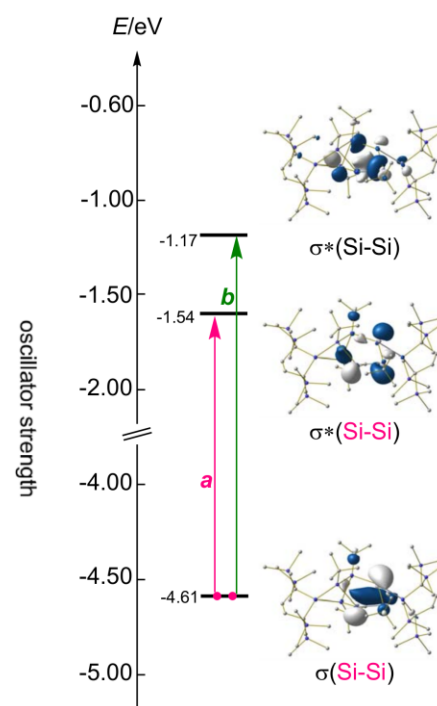


Figure S17. (a) UV-vis absorption spectra of **7** at room temperature in hexane (black line) as well as band positions and oscillator strengths (vertical blue bars) of **7**_{opt} calculated at the TD-B3LYP-D3/6-311G(d)[hexane]/B3PW91-D3/6-31G(d) level of theory. (b) Selected frontier Kohn-Sham orbitals (isosurface value = 0.05) and major transitions.

Compound 8

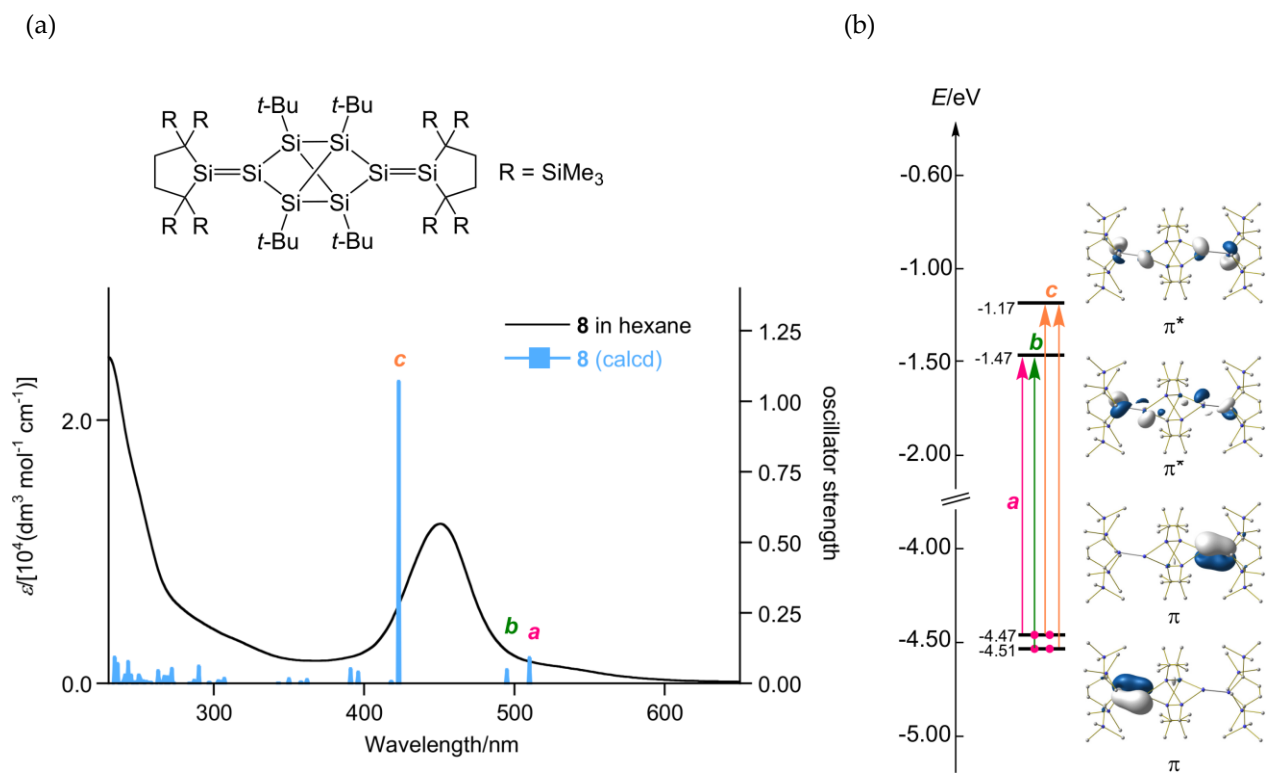
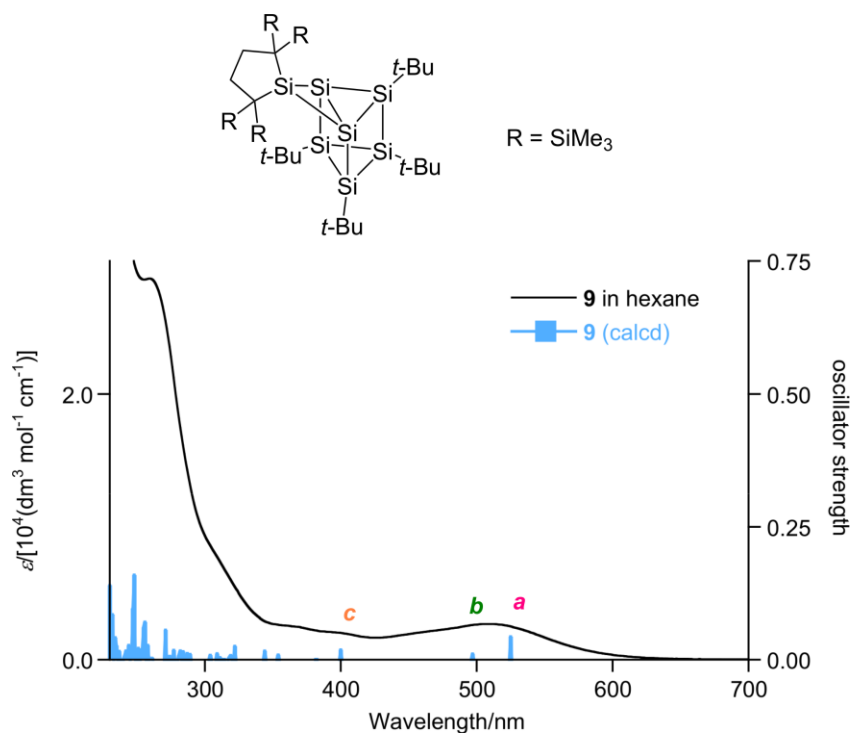


Figure S18. (a) UV-vis absorption spectra of **8** at room temperature in hexane (black line) and calculated band positions and oscillator strengths (vertical blue bars) of **8_{opt}** calculated at the TD-B3LYP-D3/6-311G(d) [hexane]/B3PW91-D3/6-31G(d) level of theory. (b) Selected frontier Kohn-Sham orbitals (isosurface value = 0.05) and major transitions.

Compound 9

(a)



(b)

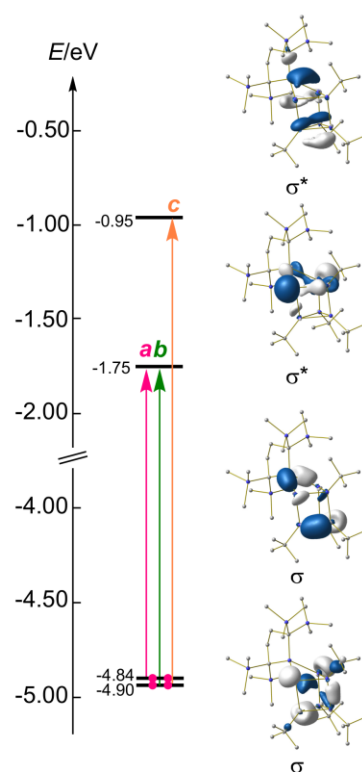


Figure S19. (a) UV-vis absorption spectra of 9 at room temperature in hexane (black line) and calculated band positions and oscillator strengths (vertical blue bars) of 9_{opt} calculated at the TD-B3LYP-D3/6-311G(d) [hexane]//B3PW91-D3/6-31G(d) level of theory. (b) Selected frontier Kohn-Sham orbitals (isosurface value = 0.05) and major transitions.

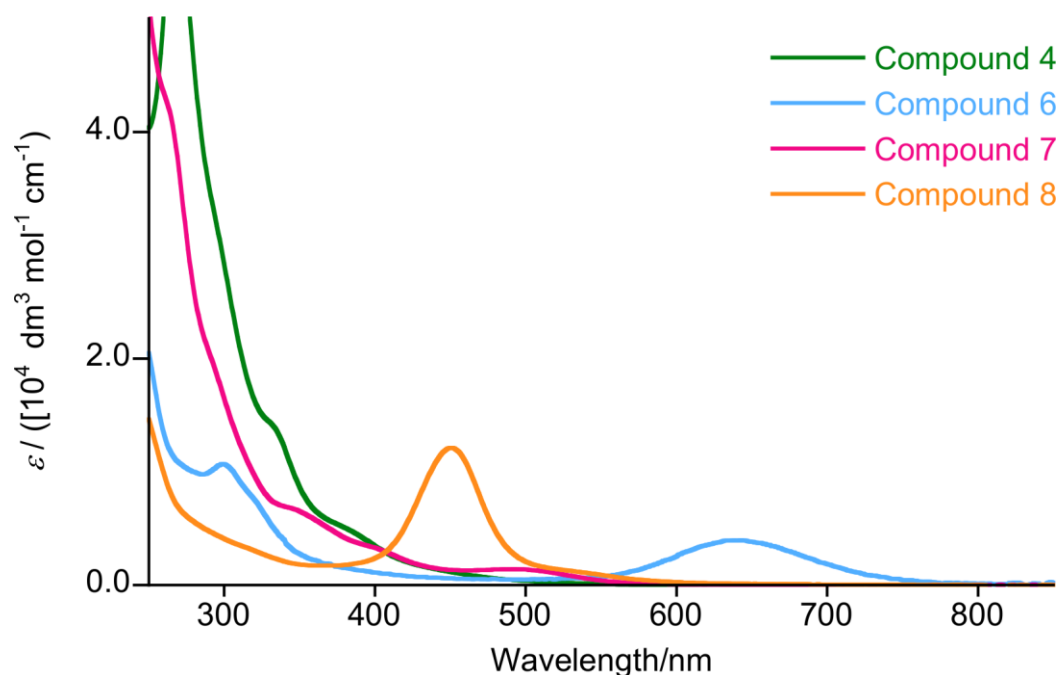
Si₈R₈ isomers

Figure S20. UV-vis absorption spectra of Si₈R₈ isomers **4**, **6**, **7**, and **8** at room temperature in hexane.

4. DFT Calculations

All theoretical calculations were performed using the Gaussian 09^{S1} and GRRM14^{S2} programs. Geometry optimizations and frequency analyses of **2**, **4**, **6**, **7**, **8**, and **9** (**2**_{opt}, **4**_{opt}, **6**_{opt}, **7**_{opt}, **8**_{opt}, and **9**_{opt}) were carried out at the B3PW91-D3/6-31G(d) level of theory for all compounds. Imaginary frequencies were not found in any of the optimized structures. Atomic coordinates for these compounds are summarized in a .xyz file (optimized_structures.xyz). The transition energies and oscillator strengths of the electron transitions of **4**, **6**, **7**, **8**, and **9** were calculated using a time-dependent hybrid DFT method (TD DFT) at the B3LYP/6-311G(d) level of theory (Tables S1-S5). Selected Kohn-Sham orbitals of **7**, **8**, and **9** are shown in Figures S17-S19, respectively.

Calculated Transition Energies and Oscillator Strengths of the Electron Transitions

Table S1. Transition Energy, Wavelength, and Oscillator Strengths of the Electronic Transition of **4_{opt}**

Excited State 314 -> 315	1:	Singlet-A 0.70076	2.6945 eV	460.14 nm	f=0.0001	<S**2>=0.000
Excited State 313 -> 315	2:	Singlet-A 0.69537	2.9123 eV	425.73 nm	f=0.0050	<S**2>=0.000
Excited State 312 -> 315 314 -> 316 314 -> 318	3:	Singlet-A -0.47889 0.49944 0.10191	3.0658 eV	404.41 nm	f=0.0028	<S**2>=0.000
Excited State 312 -> 315 314 -> 316	4:	Singlet-A 0.49918 0.49162	3.1398 eV	394.88 nm	f=0.0007	<S**2>=0.000
Excited State 312 -> 315 314 -> 317 314 -> 318	5:	Singlet-A 0.11921 0.30617 0.60991	3.1669 eV	391.50 nm	f=0.0002	<S**2>=0.000
Excited State 313 -> 317 314 -> 317 314 -> 318	6:	Singlet-A -0.16022 0.59881 -0.30441	3.2524 eV	381.21 nm	f=0.0003	<S**2>=0.000
Excited State 312 -> 317 313 -> 316 313 -> 317	7:	Singlet-A 0.11773 0.66382 -0.15202	3.3451 eV	370.64 nm	f=0.0175	<S**2>=0.000
Excited State 313 -> 316 313 -> 317 313 -> 318 314 -> 317	8:	Singlet-A 0.12947 0.62323 -0.22202 0.15461	3.3579 eV	369.23 nm	f=0.0019	<S**2>=0.000
Excited State 312 -> 317 313 -> 317 313 -> 318	9:	Singlet-A 0.25062 0.19832 0.60887	3.4987 eV	354.37 nm	f=0.0089	<S**2>=0.000
Excited State 312 -> 316 312 -> 317 312 -> 318	10:	Singlet-A 0.63327 0.10933 0.26268	3.5504 eV	349.21 nm	f=0.0030	<S**2>=0.000
Excited State 311 -> 315 312 -> 316 312 -> 317 313 -> 316 313 -> 318	11:	Singlet-A -0.30713 -0.12010 0.57420 -0.10077 -0.17504	3.6245 eV	342.07 nm	f=0.0651	<S**2>=0.000
Excited State 311 -> 315 312 -> 316 312 -> 318	12:	Singlet-A 0.13168 -0.25991 0.61902	3.6422 eV	340.41 nm	f=0.0183	<S**2>=0.000
Excited State 310 -> 316 310 -> 318	13:	Singlet-A -0.10080 0.10531	3.8036 eV	325.96 nm	f=0.1101	<S**2>=0.000

311 -> 315	0.57190								
311 -> 317	-0.14155								
312 -> 317	0.22610								
313 -> 316	-0.12301								
313 -> 318	-0.10156								
314 -> 319	-0.14720								
Excited State 14:	Singlet-A	3.9675 eV	312.50 nm	f=0.0021	<S**2>=0.000				
310 -> 315	0.65301								
311 -> 316	0.11570								
314 -> 320	0.20575								
Excited State 15:	Singlet-A	4.0091 eV	309.26 nm	f=0.1379	<S**2>=0.000				
311 -> 317	-0.15976								
313 -> 319	0.16290								
314 -> 319	0.63852								
Excited State 16:	Singlet-A	4.0689 eV	304.71 nm	f=0.0008	<S**2>=0.000				
310 -> 315	-0.17156								
311 -> 316	0.57102								
311 -> 318	-0.14119								
312 -> 319	0.10201								
313 -> 319	-0.10183								
314 -> 320	0.25862								
Excited State 17:	Singlet-A	4.0797 eV	303.91 nm	f=0.0024	<S**2>=0.000				
311 -> 317	0.19162								
312 -> 320	-0.12428								
313 -> 319	0.62872								
314 -> 319	-0.12197								
Excited State 18:	Singlet-A	4.1184 eV	301.05 nm	f=0.0102	<S**2>=0.000				
310 -> 315	-0.14542								
311 -> 316	-0.23191								
312 -> 319	-0.14941								
313 -> 320	0.20086								
314 -> 320	0.57118								
Excited State 19:	Singlet-A	4.1959 eV	295.49 nm	f=0.0012	<S**2>=0.000				
311 -> 316	0.16126								
311 -> 317	-0.11073								
311 -> 318	-0.19916								
312 -> 319	-0.39007								
313 -> 320	0.47109								
314 -> 320	-0.16905								
Excited State 20:	Singlet-A	4.2445 eV	292.11 nm	f=0.1994	<S**2>=0.000				
310 -> 316	-0.10759								
310 -> 318	0.12700								
311 -> 317	0.58879								
312 -> 320	0.16073								
313 -> 319	-0.13279								
314 -> 319	0.15617								
Excited State 21:	Singlet-A	4.2648 eV	290.72 nm	f=0.0293	<S**2>=0.000				
310 -> 317	-0.14021								
311 -> 316	0.21071								
311 -> 318	0.59735								
313 -> 320	0.21422								
Excited State 22:	Singlet-A	4.3050 eV	288.00 nm	f=0.0679	<S**2>=0.000				
309 -> 315	0.54548								
310 -> 316	-0.33328								
310 -> 318	-0.19460								
313 -> 321	-0.11150								
Excited State 23:	Singlet-A	4.3878 eV	282.56 nm	f=0.0372	<S**2>=0.000				
309 -> 315	0.28995								
310 -> 316	0.32995								
310 -> 317	0.14051								

310 -> 318	0.22035						
311 -> 317	-0.11504						
312 -> 319	0.10095						
312 -> 320	0.41670						
313 -> 319	0.13517						
Excited State 24:	Singlet-A	4.4164 eV	280.74 nm	f=0.0098	<S**2>=0.000		
310 -> 317	0.23662						
310 -> 318	-0.13896						
312 -> 319	0.50986						
313 -> 320	0.34430						
Excited State 25:	Singlet-A	4.4789 eV	276.82 nm	f=0.0464	<S**2>=0.000		
310 -> 317	0.56469						
310 -> 318	0.10574						
311 -> 318	0.15989						
312 -> 319	-0.13551						
312 -> 320	-0.17255						
313 -> 320	-0.15556						
Excited State 26:	Singlet-A	4.4915 eV	276.04 nm	f=0.0624	<S**2>=0.000		
310 -> 317	-0.12813						
310 -> 318	0.55452						
312 -> 320	-0.26936						
314 -> 321	0.15268						
Excited State 27:	Singlet-A	4.5327 eV	273.53 nm	f=0.0740	<S**2>=0.000		
309 -> 315	-0.21234						
310 -> 316	-0.26703						
312 -> 320	0.33206						
313 -> 319	0.10501						
314 -> 321	0.45966						
314 -> 323	-0.13682						
Excited State 28:	Singlet-A	4.5875 eV	270.27 nm	f=0.0035	<S**2>=0.000		
309 -> 316	0.34012						
314 -> 321	0.13887						
314 -> 322	0.56805						
314 -> 324	0.10357						
Excited State 29:	Singlet-A	4.6455 eV	266.89 nm	f=0.4909	<S**2>=0.000		
309 -> 317	0.23145						
310 -> 316	0.35006						
310 -> 318	-0.15502						
312 -> 320	-0.18786						
313 -> 321	-0.13596						
314 -> 321	0.38142						
314 -> 322	-0.10531						
Excited State 30:	Singlet-A	4.6844 eV	264.67 nm	f=0.0038	<S**2>=0.000		
309 -> 316	0.47846						
309 -> 317	0.13895						
309 -> 318	0.29919						
313 -> 322	-0.18003						
314 -> 322	-0.27933						
Excited State 31:	Singlet-A	4.7427 eV	261.42 nm	f=0.0186	<S**2>=0.000		
309 -> 317	0.20633						
309 -> 318	0.32804						
311 -> 319	-0.13675						
313 -> 321	0.35403						
313 -> 322	0.36383						
314 -> 322	0.10739						
314 -> 324	-0.14909						
Excited State 32:	Singlet-A	4.7501 eV	261.01 nm	f=0.0661	<S**2>=0.000		
309 -> 318	-0.20990						
312 -> 322	0.11412						
313 -> 321	0.50105						
313 -> 322	-0.29820						

314 -> 321	0.12096								
314 -> 323	0.13425								
Excited State 33:	Singlet-A	4.7805 eV	259.35 nm	f=0.0018	<S**2>=0.000				
309 -> 317	-0.15148								
313 -> 321	-0.12561								
314 -> 321	0.12711								
314 -> 323	0.58465								
314 -> 325	0.25608								
Excited State 34:	Singlet-A	4.7936 eV	258.64 nm	f=0.0036	<S**2>=0.000				
309 -> 316	0.20182								
313 -> 322	0.35267								
314 -> 322	-0.16048								
314 -> 324	0.48647								
314 -> 326	0.17860								
Excited State 35:	Singlet-A	4.8414 eV	256.09 nm	f=0.0532	<S**2>=0.000				
309 -> 316	-0.13979								
309 -> 317	0.49980								
312 -> 321	-0.16799								
312 -> 322	-0.23524								
314 -> 324	0.18546								
Excited State 36:	Singlet-A	4.8519 eV	255.54 nm	f=0.0242	<S**2>=0.000				
309 -> 316	-0.22599								
309 -> 317	-0.14372								
309 -> 318	0.41757								
311 -> 319	0.12677								
312 -> 321	-0.12173								
312 -> 322	0.20668								
313 -> 322	-0.18904								
314 -> 324	0.25584								
Excited State 37:	Singlet-A	4.9026 eV	252.90 nm	f=0.0224	<S**2>=0.000				
309 -> 316	-0.12408								
309 -> 318	0.12264								
311 -> 319	-0.14039								
312 -> 321	0.52358								
312 -> 322	-0.12907								
313 -> 322	-0.12150								
313 -> 324	0.22899								
314 -> 324	0.17889								
Excited State 38:	Singlet-A	4.9609 eV	249.92 nm	f=0.2126	<S**2>=0.000				
311 -> 320	0.15107								
312 -> 322	0.13557								
313 -> 323	0.57665								
313 -> 325	0.21157								
313 -> 329	0.11134								
Excited State 39:	Singlet-A	4.9719 eV	249.37 nm	f=0.0330	<S**2>=0.000				
311 -> 319	0.62122								
312 -> 321	0.12426								
313 -> 322	0.13660								
313 -> 324	0.13467								
Excited State 40:	Singlet-A	5.0452 eV	245.75 nm	f=0.1792	<S**2>=0.000				
305 -> 315	-0.11351								
307 -> 315	-0.12346								
309 -> 317	0.14006								
311 -> 320	0.30882								
312 -> 321	0.13702								
312 -> 322	0.45352								
313 -> 321	-0.13638								
313 -> 323	-0.17273								
Excited State 41:	Singlet-A	5.0546 eV	245.29 nm	f=0.0013	<S**2>=0.000				
306 -> 315	0.16589								
308 -> 315	0.32509								

311 -> 319	-0.11319						
312 -> 321	-0.25959						
312 -> 322	0.10779						
313 -> 324	0.47420						
313 -> 326	0.13686						
Excited State 42:	Singlet-A	5.0714 eV	244.48 nm	f=0.0116	<S**2>=0.000		
304 -> 315	-0.11533						
306 -> 315	0.22780						
308 -> 315	0.49253						
312 -> 321	0.12564						
312 -> 323	-0.12325						
313 -> 324	-0.33572						
313 -> 326	-0.10520						
Excited State 43:	Singlet-A	5.1410 eV	241.17 nm	f=0.0395	<S**2>=0.000		
305 -> 315	0.10318						
307 -> 315	0.19093						
310 -> 319	0.23748						
311 -> 320	0.49267						
312 -> 322	-0.16594						
312 -> 324	0.18269						
314 -> 325	-0.15527						
Excited State 44:	Singlet-A	5.1530 eV	240.61 nm	f=0.0000	<S**2>=0.000		
308 -> 315	0.11841						
312 -> 321	0.10908						
312 -> 323	0.60503						
312 -> 325	0.22893						
Excited State 45:	Singlet-A	5.1546 eV	240.53 nm	f=0.0118	<S**2>=0.000		
307 -> 315	0.22614						
314 -> 323	-0.26464						
314 -> 325	0.54543						
314 -> 326	0.11034						
314 -> 331	-0.14962						
Excited State 46:	Singlet-A	5.1818 eV	239.27 nm	f=0.1447	<S**2>=0.000		
307 -> 315	0.46639						
310 -> 319	-0.39145						
312 -> 322	0.12434						
312 -> 324	0.11740						
313 -> 323	-0.11668						
314 -> 325	-0.15620						
Excited State 47:	Singlet-A	5.2052 eV	238.19 nm	f=0.0254	<S**2>=0.000		
307 -> 315	-0.29067						
310 -> 319	-0.17260						
312 -> 324	0.50697						
312 -> 326	0.14981						
313 -> 325	0.14812						
314 -> 325	0.10475						
314 -> 327	0.10474						
Excited State 48:	Singlet-A	5.2237 eV	237.35 nm	f=0.0020	<S**2>=0.000		
306 -> 315	0.60780						
308 -> 315	-0.31397						
Excited State 49:	Singlet-A	5.2484 eV	236.23 nm	f=0.2035	<S**2>=0.000		
305 -> 315	-0.19315						
307 -> 315	0.22529						
308 -> 316	0.10714						
310 -> 319	0.35482						
311 -> 320	-0.20461						
312 -> 324	0.16990						
313 -> 325	0.10217						
314 -> 324	0.10146						
314 -> 326	-0.24203						
314 -> 327	0.20490						
314 -> 334	0.10447						

Excited State	50:	Singlet-A	5.2487 eV	236.22 nm	f=0.0383	<S**2>=0.000
	310 -> 319	0.14993				
	314 -> 324	-0.23558				
	314 -> 325	-0.10312				
	314 -> 326	0.58801				
Excited State	51:	Singlet-A	5.2714 eV	235.20 nm	f=0.0064	<S**2>=0.000
	310 -> 319	-0.12731				
	311 -> 320	0.11985				
	312 -> 324	-0.10749				
	313 -> 325	-0.24624				
	314 -> 327	0.49777				
	314 -> 330	-0.18535				
	314 -> 331	0.14769				
	314 -> 334	0.18229				
Excited State	52:	Singlet-A	5.2985 eV	234.00 nm	f=0.0159	<S**2>=0.000
	305 -> 315	0.23404				
	310 -> 320	0.57268				
	313 -> 325	0.17737				
Excited State	53:	Singlet-A	5.2991 eV	233.97 nm	f=0.0422	<S**2>=0.000
	305 -> 315	0.37761				
	310 -> 320	-0.32556				
	312 -> 324	-0.11109				
	313 -> 323	-0.12851				
	313 -> 325	0.35470				
Excited State	54:	Singlet-A	5.3279 eV	232.71 nm	f=0.0460	<S**2>=0.000
	302 -> 315	-0.20918				
	305 -> 315	0.32401				
	310 -> 319	0.14648				
	311 -> 320	-0.13928				
	312 -> 324	0.20683				
	313 -> 323	0.13937				
	313 -> 325	-0.30442				
	314 -> 327	-0.16922				
	314 -> 331	-0.13986				
Excited State	55:	Singlet-A	5.3396 eV	232.20 nm	f=0.0030	<S**2>=0.000
	301 -> 315	-0.12694				
	303 -> 315	0.64927				
Excited State	56:	Singlet-A	5.3737 eV	230.72 nm	f=0.0131	<S**2>=0.000
	305 -> 315	-0.12545				
	314 -> 329	0.57330				
	314 -> 330	-0.25862				
Excited State	57:	Singlet-A	5.3774 eV	230.57 nm	f=0.0020	<S**2>=0.000
	304 -> 315	-0.11653				
	312 -> 325	-0.21043				
	313 -> 324	-0.19197				
	313 -> 325	-0.10787				
	313 -> 326	0.59920				
Excited State	58:	Singlet-A	5.3923 eV	229.93 nm	f=0.0041	<S**2>=0.000
	304 -> 315	0.62710				
	306 -> 315	0.14917				
	314 -> 328	-0.12361				
Excited State	59:	Singlet-A	5.4069 eV	229.31 nm	f=0.0017	<S**2>=0.000
	304 -> 315	0.14214				
	309 -> 319	0.13716				
	311 -> 321	0.10915				
	314 -> 328	0.55778				
	314 -> 333	-0.24805				
Excited State	60:	Singlet-A	5.4159 eV	228.93 nm	f=0.0104	<S**2>=0.000
	302 -> 315	0.18221				

308 -> 316	0.17580						
311 -> 322	0.10621						
313 -> 327	0.48988						
313 -> 329	-0.22118						
313 -> 331	0.17907						
313 -> 334	0.14832						
314 -> 327	-0.11959						
Excited State 61:	Singlet-A	5.4179 eV	228.84 nm	f=0.0392	<S**2>=0.000		
300 -> 315	0.18787						
302 -> 315	0.51567						
305 -> 315	0.21606						
313 -> 325	-0.12275						
313 -> 327	-0.22927						
Excited State 62:	Singlet-A	5.4779 eV	226.33 nm	f=0.0532	<S**2>=0.000		
308 -> 316	0.28035						
311 -> 322	-0.19174						
313 -> 327	0.13085						
313 -> 329	0.39610						
313 -> 330	-0.23459						
314 -> 330	0.15643						
314 -> 331	0.14293						
314 -> 334	-0.14799						
Excited State 63:	Singlet-A	5.4832 eV	226.12 nm	f=0.0379	<S**2>=0.000		
302 -> 315	-0.17235						
307 -> 317	0.12897						
308 -> 316	0.37093						
311 -> 322	0.10481						
313 -> 327	-0.13724						
313 -> 329	-0.27839						
313 -> 330	0.18565						
314 -> 327	0.11888						
314 -> 329	0.18500						
314 -> 330	0.19463						
314 -> 334	-0.20597						
Excited State 64:	Singlet-A	5.4989 eV	225.47 nm	f=0.0045	<S**2>=0.000		
307 -> 316	0.52271						
308 -> 317	0.31043						
308 -> 318	-0.10743						
312 -> 325	0.15595						
314 -> 331	-0.12394						

JOB name: na92ATD2

Method/Basis: TD-B3LYP-D3/6-311G(d) [hexane]//B3PW91-D3/6-31G(d)

Table S2. Transition Energy, Wavelength, and Oscillator Strengths of the Electronic Transition of **6_{opt}**

Excited State 1:	Singlet-A	2.0528 eV	603.98 nm	f=0.4077	<S**2>=0.000		
314 -> 315	0.70275						
Excited State 2:	Singlet-A	2.0911 eV	592.92 nm	f=0.0000	<S**2>=0.000		
313 -> 315	0.70490						
Excited State 3:	Singlet-A	2.7307 eV	454.04 nm	f=0.0000	<S**2>=0.000		
314 -> 316	0.69919						
Excited State 4:	Singlet-A	2.8777 eV	430.85 nm	f=0.0002	<S**2>=0.000		
312 -> 315	0.69931						
Excited State 5:	Singlet-A	2.9647 eV	418.21 nm	f=0.0148	<S**2>=0.000		
314 -> 317	0.70261						

Excited State 311 -> 315	6:	Singlet-A 0.68955	3.2861 eV	377.30 nm	f=0.0000	<S**2>=0.000
Excited State 314 -> 318	7:	Singlet-A 0.68943	3.3469 eV	370.45 nm	f=0.0000	<S**2>=0.000
Excited State 312 -> 317 313 -> 316	8:	Singlet-A 0.10179 0.68685	3.3675 eV	368.18 nm	f=0.0093	<S**2>=0.000
Excited State 310 -> 315 312 -> 316 313 -> 317	9:	Singlet-A -0.25987 0.13096 0.63180	3.4830 eV	355.97 nm	f=0.0000	<S**2>=0.000
Excited State 310 -> 315 313 -> 317	10:	Singlet-A 0.64573 0.25038	3.5283 eV	351.40 nm	f=0.0000	<S**2>=0.000
Excited State 314 -> 319 314 -> 321	11:	Singlet-A 0.67666 -0.14868	3.6179 eV	342.69 nm	f=0.0000	<S**2>=0.000
Excited State 308 -> 315 309 -> 315 314 -> 320	12:	Singlet-A 0.49966 0.44465 0.19976	3.7133 eV	333.89 nm	f=0.0001	<S**2>=0.000
Excited State 308 -> 315 313 -> 318 313 -> 319 314 -> 320	13:	Singlet-A -0.17977 0.30884 0.12733 0.57399	3.8569 eV	321.46 nm	f=0.0533	<S**2>=0.000
Excited State 309 -> 315 312 -> 317 313 -> 318 313 -> 319 314 -> 320	14:	Singlet-A 0.11454 0.18481 0.56583 0.11037 -0.31446	3.8632 eV	320.94 nm	f=0.1376	<S**2>=0.000
Excited State 307 -> 315	15:	Singlet-A 0.68658	3.8733 eV	320.10 nm	f=0.0000	<S**2>=0.000
Excited State 312 -> 316 314 -> 319 314 -> 321	16:	Singlet-A -0.13599 0.12740 0.65764	3.8972 eV	318.13 nm	f=0.0000	<S**2>=0.000
Excited State 308 -> 315 309 -> 315 313 -> 319	17:	Singlet-A -0.41651 0.47827 -0.25729	4.0169 eV	308.66 nm	f=0.0959	<S**2>=0.000
Excited State 308 -> 315 309 -> 315 311 -> 316 312 -> 317 313 -> 318 313 -> 319 314 -> 323	18:	Singlet-A -0.14780 0.19190 -0.10621 0.16651 -0.20709 0.55270 -0.15430	4.1693 eV	297.38 nm	f=0.2024	<S**2>=0.000
Excited State 312 -> 316 313 -> 317 314 -> 321	19:	Singlet-A 0.66140 -0.11202 0.14322	4.2137 eV	294.24 nm	f=0.0000	<S**2>=0.000
Excited State	20:	Singlet-A	4.2495 eV	291.76 nm	f=0.0501	<S**2>=0.000

311 -> 316	0.48512						
312 -> 317	-0.12252						
313 -> 319	0.12705						
314 -> 322	0.45162						
Excited State 21:	Singlet-A	4.2836 eV	289.44 nm	f=0.0447	<S**2>=0.000		
311 -> 316	-0.47160						
312 -> 317	-0.11432						
314 -> 322	0.48708						
Excited State 22:	Singlet-A	4.3395 eV	285.71 nm	f=0.0000	<S**2>=0.000		
312 -> 319	0.12718						
313 -> 320	0.66021						
Excited State 23:	Singlet-A	4.3469 eV	285.22 nm	f=0.0610	<S**2>=0.000		
312 -> 317	-0.18404						
313 -> 319	0.18721						
313 -> 321	0.12356						
314 -> 323	0.59012						
314 -> 327	-0.18260						
Excited State 24:	Singlet-A	4.3875 eV	282.59 nm	f=0.0815	<S**2>=0.000		
312 -> 317	0.57471						
313 -> 318	-0.14533						
313 -> 319	-0.13401						
314 -> 322	0.17962						
314 -> 323	0.24951						
Excited State 25:	Singlet-A	4.4079 eV	281.28 nm	f=0.0000	<S**2>=0.000		
314 -> 324	0.68365						
Excited State 26:	Singlet-A	4.4596 eV	278.01 nm	f=0.0000	<S**2>=0.000		
308 -> 316	0.13205						
309 -> 316	-0.15154						
311 -> 317	0.65864						
Excited State 27:	Singlet-A	4.4821 eV	276.62 nm	f=0.2879	<S**2>=0.000		
312 -> 317	0.10595						
312 -> 320	0.11493						
313 -> 321	0.66628						
Excited State 28:	Singlet-A	4.5136 eV	274.69 nm	f=0.0207	<S**2>=0.000		
306 -> 315	0.69678						
Excited State 29:	Singlet-A	4.5155 eV	274.58 nm	f=0.0000	<S**2>=0.000		
314 -> 325	0.67235						
Excited State 30:	Singlet-A	4.5445 eV	272.82 nm	f=0.0000	<S**2>=0.000		
303 -> 315	0.13891						
305 -> 315	0.68327						
Excited State 31:	Singlet-A	4.6132 eV	268.76 nm	f=0.0088	<S**2>=0.000		
304 -> 315	0.69937						
Excited State 32:	Singlet-A	4.6546 eV	266.37 nm	f=0.0000	<S**2>=0.000		
303 -> 315	0.65953						
305 -> 315	-0.15273						
312 -> 318	-0.15373						
Excited State 33:	Singlet-A	4.6902 eV	264.35 nm	f=0.0000	<S**2>=0.000		
303 -> 315	0.16444						
312 -> 318	0.57595						
312 -> 319	0.10672						
313 -> 322	-0.15721						
314 -> 326	-0.19717						
Excited State 34:	Singlet-A	4.7218 eV	262.58 nm	f=0.0000	<S**2>=0.000		
312 -> 318	0.20607						
314 -> 326	0.65178						

Excited State 35:	Singlet-A	4.7378 eV	261.69 nm	f=0.0452	<S**2>=0.000
309 -> 317	-0.11903				
310 -> 316	0.49036				
311 -> 318	0.16051				
314 -> 323	-0.13021				
314 -> 327	-0.37784				
314 -> 333	-0.11939				
Excited State 36:	Singlet-A	4.7545 eV	260.77 nm	f=0.0292	<S**2>=0.000
310 -> 316	0.39117				
314 -> 323	0.17577				
314 -> 327	0.52153				
Excited State 37:	Singlet-A	4.8515 eV	255.56 nm	f=0.0376	<S**2>=0.000
310 -> 316	-0.16083				
311 -> 318	0.59711				
314 -> 327	0.13466				
314 -> 328	-0.12839				
314 -> 329	0.12420				
314 -> 332	-0.10725				
Excited State 38:	Singlet-A	4.8623 eV	254.99 nm	f=0.0000	<S**2>=0.000
308 -> 316	0.15784				
310 -> 317	-0.13372				
312 -> 319	0.31533				
313 -> 320	-0.13343				
313 -> 322	0.38014				
313 -> 323	0.29266				
314 -> 330	-0.18478				
314 -> 331	0.15126				
Excited State 39:	Singlet-A	4.8764 eV	254.25 nm	f=0.0000	<S**2>=0.000
308 -> 316	-0.25477				
309 -> 316	-0.27380				
310 -> 317	0.45286				
311 -> 320	-0.11320				
312 -> 319	0.11204				
313 -> 322	0.18357				
313 -> 323	-0.16679				
314 -> 330	-0.14200				
Excited State 40:	Singlet-A	4.9151 eV	252.25 nm	f=0.0351	<S**2>=0.000
311 -> 318	0.21360				
314 -> 328	0.54425				
314 -> 329	-0.24775				
314 -> 332	0.16348				
314 -> 333	0.15266				
Excited State 41:	Singlet-A	4.9414 eV	250.91 nm	f=0.0000	<S**2>=0.000
309 -> 316	-0.19162				
310 -> 317	0.17743				
311 -> 320	-0.13726				
312 -> 318	-0.12911				
313 -> 322	-0.26368				
313 -> 323	0.49178				
313 -> 327	-0.14733				
314 -> 330	0.12700				
Excited State 42:	Singlet-A	4.9555 eV	250.20 nm	f=0.0000	<S**2>=0.000
312 -> 318	0.10326				
312 -> 319	-0.37983				
313 -> 322	0.41024				
313 -> 323	0.18532				
314 -> 330	0.18778				
314 -> 331	-0.24694				
Excited State 43:	Singlet-A	4.9703 eV	249.45 nm	f=0.0000	<S**2>=0.000
307 -> 317	0.10959				
308 -> 316	-0.38471				
309 -> 316	0.41885				

311 -> 317	0.17028						
312 -> 319	-0.10669						
313 -> 323	0.17090						
314 -> 330	-0.18160						
314 -> 331	0.17065						
Excited State 44:	Singlet-A	4.9827 eV	248.83 nm	f=0.0178	<S**2>=0.000		
314 -> 328	0.38920						
314 -> 329	0.47344						
314 -> 332	-0.10368						
314 -> 333	-0.19866						
314 -> 335	0.16171						
Excited State 45:	Singlet-A	4.9915 eV	248.39 nm	f=0.0112	<S**2>=0.000		
300 -> 315	0.22307						
302 -> 315	-0.18795						
311 -> 319	0.15141						
313 -> 324	0.54050						
313 -> 325	0.14962						
314 -> 332	-0.12554						
Excited State 46:	Singlet-A	5.0181 eV	247.07 nm	f=0.0060	<S**2>=0.000		
302 -> 315	0.65208						
313 -> 324	0.17335						
313 -> 325	0.10601						
Excited State 47:	Singlet-A	5.0231 eV	246.83 nm	f=0.0000	<S**2>=0.000		
301 -> 315	0.43786						
308 -> 316	-0.11576						
309 -> 316	0.14723						
312 -> 319	0.22051						
314 -> 330	0.38395						
Excited State 48:	Singlet-A	5.0339 eV	246.30 nm	f=0.0000	<S**2>=0.000		
301 -> 315	0.54119						
309 -> 316	-0.11370						
312 -> 319	-0.20027						
314 -> 330	-0.30962						
Excited State 49:	Singlet-A	5.0465 eV	245.68 nm	f=0.0326	<S**2>=0.000		
300 -> 315	0.62511						
302 -> 315	0.16220						
311 -> 319	-0.12894						
313 -> 325	-0.15469						
Excited State 50:	Singlet-A	5.0613 eV	244.97 nm	f=0.0149	<S**2>=0.000		
308 -> 317	-0.16554						
310 -> 316	-0.12245						
311 -> 319	-0.25928						
311 -> 321	0.11427						
313 -> 324	0.17387						
313 -> 325	0.19234						
314 -> 329	0.17334						
314 -> 332	0.42041						
314 -> 333	-0.15855						
314 -> 335	-0.16144						
Excited State 51:	Singlet-A	5.0761 eV	244.25 nm	f=0.0642	<S**2>=0.000		
300 -> 315	0.11271						
307 -> 316	0.30949						
309 -> 317	0.13939						
313 -> 324	-0.18406						
313 -> 325	0.49114						
314 -> 329	-0.11070						
314 -> 335	0.10606						
Excited State 52:	Singlet-A	5.0918 eV	243.50 nm	f=0.0000	<S**2>=0.000		
308 -> 316	0.31165						
310 -> 317	0.20725						
312 -> 319	-0.20987						

314 -> 330	0.13624								
314 -> 331	0.47627								
314 -> 336	0.12759								
Excited State 53:	Singlet-A	5.1028 eV	242.97 nm	f=0.0183	<S**2>=0.000				
308 -> 317	-0.10586								
311 -> 319	-0.24776								
312 -> 320	0.13278								
314 -> 329	0.24871								
314 -> 332	-0.15328								
314 -> 333	0.52469								
Excited State 54:	Singlet-A	5.1061 eV	242.82 nm	f=0.0000	<S**2>=0.000				
308 -> 316	0.31854								
309 -> 316	0.33185								
310 -> 317	0.35186								
314 -> 330	-0.13696								
314 -> 331	-0.27248								
314 -> 334	0.10725								
Excited State 55:	Singlet-A	5.1194 eV	242.18 nm	f=0.3424	<S**2>=0.000				
307 -> 316	0.40340								
308 -> 317	-0.11620								
309 -> 317	0.33296								
313 -> 324	0.13345								
313 -> 325	-0.32121								
314 -> 332	0.10259								
Excited State 56:	Singlet-A	5.1394 eV	241.24 nm	f=0.0245	<S**2>=0.000				
308 -> 317	0.25470								
310 -> 319	-0.10353								
311 -> 319	0.30968								
312 -> 320	-0.19987								
313 -> 324	-0.15515								
314 -> 329	0.21762								
314 -> 332	0.34019								
314 -> 333	0.22336								
Excited State 57:	Singlet-A	5.1766 eV	239.51 nm	f=0.0585	<S**2>=0.000				
299 -> 315	-0.15016								
308 -> 317	0.11960								
310 -> 318	-0.16187								
311 -> 319	0.15236								
312 -> 320	0.55927								
314 -> 332	0.11469								
Excited State 58:	Singlet-A	5.1801 eV	239.35 nm	f=0.0000	<S**2>=0.000				
310 -> 317	-0.10888								
314 -> 330	-0.11979								
314 -> 334	0.57267								
314 -> 337	-0.20971								
314 -> 340	-0.19510								
Excited State 59:	Singlet-A	5.2016 eV	238.36 nm	f=0.0384	<S**2>=0.000				
311 -> 319	-0.17822								
314 -> 332	0.17884								
314 -> 335	0.51503								
314 -> 338	0.28327								
314 -> 341	-0.10536								
Excited State 60:	Singlet-A	5.2238 eV	237.34 nm	f=0.0031	<S**2>=0.000				
299 -> 315	0.65191								
312 -> 320	0.15433								
Excited State 61:	Singlet-A	5.2314 eV	237.00 nm	f=0.0005	<S**2>=0.000				
297 -> 315	0.13628								
298 -> 315	0.67630								
Excited State 62:	Singlet-A	5.2323 eV	236.96 nm	f=0.3561	<S**2>=0.000				
299 -> 315	0.12787								

307 -> 316	-0.42196						
308 -> 317	-0.13242						
309 -> 317	0.44674						
311 -> 321	0.14238						
Excited State 63:	Singlet-A	5.2544 eV	235.96 nm	f=0.0997	<S**2>=0.000		
308 -> 317	0.45264						
310 -> 318	-0.18666						
311 -> 319	-0.30452						
311 -> 321	0.22987						
312 -> 320	-0.10913						
313 -> 326	0.10676						
314 -> 332	-0.12037						
314 -> 338	0.13582						
Excited State 64:	Singlet-A	5.2663 eV	235.43 nm	f=0.0000	<S**2>=0.000		
286 -> 315	-0.11222						
293 -> 315	0.25971						
297 -> 315	0.55334						
307 -> 317	-0.22199						
312 -> 321	0.13920						

JOB name: na92BTD2

Method/Basis: TD-B3LYP-D3/6-311G(d) [hexane]//B3PW91-D3/6-31G(d)

Table S3. Transition Energy, Wavelength, and Oscillator Strengths of the Electronic Transition of 7_{opt}

Excited State 1:	Singlet-A	2.4657 eV	502.83 nm	f=0.0131	<S**2>=0.000		
314 -> 315	0.68157						
314 -> 316	0.14239						
Excited State 2:	Singlet-A	2.7108 eV	457.37 nm	f=0.0146	<S**2>=0.000		
314 -> 315	-0.13603						
314 -> 316	0.68790						
Excited State 3:	Singlet-A	3.0149 eV	411.23 nm	f=0.0065	<S**2>=0.000		
311 -> 315	-0.10574						
313 -> 315	0.66578						
314 -> 317	-0.18393						
Excited State 4:	Singlet-A	3.1799 eV	389.90 nm	f=0.0372	<S**2>=0.000		
311 -> 315	-0.10628						
312 -> 315	0.13020						
313 -> 315	0.15095						
314 -> 317	0.65822						
Excited State 5:	Singlet-A	3.3261 eV	372.76 nm	f=0.0062	<S**2>=0.000		
314 -> 318	0.69068						
Excited State 6:	Singlet-A	3.3633 eV	368.64 nm	f=0.0041	<S**2>=0.000		
313 -> 316	0.68947						
Excited State 7:	Singlet-A	3.3698 eV	367.93 nm	f=0.0191	<S**2>=0.000		
311 -> 315	0.13769						
312 -> 315	0.66380						
Excited State 8:	Singlet-A	3.5502 eV	349.23 nm	f=0.0309	<S**2>=0.000		
311 -> 315	0.65584						
313 -> 315	0.12025						

Excited State 9:	Singlet-A	3.6953 eV	335.52 nm	f=0.0069	<S**2>=0.000
314 -> 319	0.68213				
Excited State 10:	Singlet-A	3.7322 eV	332.20 nm	f=0.0293	<S**2>=0.000
311 -> 316	-0.23009				
312 -> 316	0.64985				
Excited State 11:	Singlet-A	3.8476 eV	322.24 nm	f=0.0037	<S**2>=0.000
311 -> 316	0.45035				
312 -> 316	0.17004				
313 -> 317	-0.10416				
314 -> 320	0.49503				
Excited State 12:	Singlet-A	3.8935 eV	318.44 nm	f=0.0181	<S**2>=0.000
310 -> 315	0.33556				
311 -> 316	0.34483				
313 -> 317	0.35327				
313 -> 318	-0.17848				
314 -> 320	-0.28176				
Excited State 13:	Singlet-A	3.9161 eV	316.60 nm	f=0.0063	<S**2>=0.000
310 -> 315	0.58859				
312 -> 316	-0.12042				
313 -> 317	-0.27261				
313 -> 318	0.17876				
Excited State 14:	Singlet-A	3.9540 eV	313.57 nm	f=0.0312	<S**2>=0.000
311 -> 316	-0.23146				
313 -> 317	0.51518				
313 -> 318	0.19308				
314 -> 320	0.32690				
Excited State 15:	Singlet-A	4.0677 eV	304.80 nm	f=0.0730	<S**2>=0.000
309 -> 315	-0.12822				
310 -> 316	-0.10884				
311 -> 316	0.17680				
312 -> 316	0.10367				
312 -> 317	0.18480				
313 -> 318	0.57722				
314 -> 320	-0.15639				
314 -> 321	-0.10220				
Excited State 16:	Singlet-A	4.2206 eV	293.76 nm	f=0.0164	<S**2>=0.000
309 -> 315	-0.27369				
310 -> 316	0.51328				
312 -> 318	-0.12011				
313 -> 319	0.17671				
314 -> 321	-0.27168				
Excited State 17:	Singlet-A	4.2360 eV	292.69 nm	f=0.0063	<S**2>=0.000
309 -> 315	0.50102				
310 -> 316	0.20899				
312 -> 317	0.33858				
313 -> 319	0.14624				
314 -> 321	-0.18072				
Excited State 18:	Singlet-A	4.2591 eV	291.10 nm	f=0.0328	<S**2>=0.000
310 -> 316	0.34037				
312 -> 317	0.13702				
312 -> 318	0.13129				
314 -> 321	0.55705				
Excited State 19:	Singlet-A	4.3216 eV	286.89 nm	f=0.1076	<S**2>=0.000

309 -> 315	-0.20885						
310 -> 316	-0.16482						
311 -> 317	0.10639						
312 -> 317	0.38989						
313 -> 318	-0.15009						
313 -> 319	0.28179						
313 -> 320	0.10539						
314 -> 322	-0.33839						
Excited State 20:	Singlet-A	4.3591 eV	284.42 nm	f=0.0093	<S**2>=0.000		
309 -> 315	-0.21595						
312 -> 317	0.12469						
313 -> 319	0.25420						
314 -> 322	0.55854						
Excited State 21:	Singlet-A	4.3724 eV	283.56 nm	f=0.0855	<S**2>=0.000		
310 -> 316	-0.11539						
311 -> 317	-0.25463						
312 -> 317	-0.26695						
312 -> 318	0.18440						
313 -> 319	0.46275						
313 -> 320	-0.14711						
314 -> 322	-0.12751						
Excited State 22:	Singlet-A	4.4343 eV	279.60 nm	f=0.0032	<S**2>=0.000		
311 -> 317	0.52879						
312 -> 317	-0.18851						
312 -> 318	0.36407						
Excited State 23:	Singlet-A	4.4634 eV	277.78 nm	f=0.0547	<S**2>=0.000		
309 -> 315	-0.10919						
309 -> 316	0.12726						
311 -> 317	-0.32642						
311 -> 318	-0.21101						
312 -> 318	0.48039						
313 -> 319	-0.18027						
313 -> 320	0.11770						
314 -> 321	-0.10970						
Excited State 24:	Singlet-A	4.5278 eV	273.83 nm	f=0.0138	<S**2>=0.000		
309 -> 316	0.13096						
314 -> 323	0.61245						
314 -> 324	-0.20173						
Excited State 25:	Singlet-A	4.5690 eV	271.36 nm	f=0.0250	<S**2>=0.000		
311 -> 318	0.47527						
313 -> 320	0.45563						
314 -> 323	-0.10981						
Excited State 26:	Singlet-A	4.6007 eV	269.49 nm	f=0.0078	<S**2>=0.000		
308 -> 315	-0.12694						
309 -> 316	0.48308						
311 -> 318	0.26150						
313 -> 320	-0.36558						
Excited State 27:	Singlet-A	4.6632 eV	265.88 nm	f=0.1828	<S**2>=0.000		
305 -> 315	-0.10017						
308 -> 315	-0.15987						
309 -> 316	-0.33135						
311 -> 318	0.29102						
311 -> 319	-0.10242						
312 -> 319	0.34614						
313 -> 319	-0.12111						

313 -> 320	-0.13694								
314 -> 325	-0.17292								
Excited State 28:	Singlet-A	4.6808 eV	264.88 nm	f=0.0495	<S**2>=0.000				
308 -> 315	0.19147								
312 -> 319	0.13948								
314 -> 325	0.56721								
314 -> 327	0.16634								
Excited State 29:	Singlet-A	4.7040 eV	263.57 nm	f=0.0063	<S**2>=0.000				
305 -> 315	0.19044								
307 -> 315	-0.10431								
308 -> 315	0.51471								
309 -> 316	0.12602								
312 -> 319	0.21865								
314 -> 323	-0.10755								
314 -> 325	-0.22059								
Excited State 30:	Singlet-A	4.7523 eV	260.90 nm	f=0.1704	<S**2>=0.000				
308 -> 315	-0.17237								
309 -> 316	0.22643								
311 -> 318	-0.12563								
311 -> 319	-0.15532								
312 -> 318	-0.12384								
312 -> 319	0.44773								
313 -> 320	0.19383								
314 -> 326	0.14269								
Excited State 31:	Singlet-A	4.7813 eV	259.31 nm	f=0.0527	<S**2>=0.000				
313 -> 320	-0.11032								
314 -> 324	0.14108								
314 -> 325	-0.12495								
314 -> 326	0.59057								
314 -> 327	0.14373								
Excited State 32:	Singlet-A	4.8332 eV	256.53 nm	f=0.0139	<S**2>=0.000				
305 -> 315	-0.10198								
307 -> 315	-0.27470								
310 -> 317	0.56070								
310 -> 318	-0.12472								
Excited State 33:	Singlet-A	4.8635 eV	254.93 nm	f=0.0101	<S**2>=0.000				
311 -> 319	-0.20180								
312 -> 319	-0.11970								
313 -> 321	0.11936								
314 -> 323	0.15934								
314 -> 324	0.43876								
314 -> 325	-0.17664								
314 -> 326	-0.25723								
314 -> 327	0.19462								
314 -> 328	-0.14024								
Excited State 34:	Singlet-A	4.8687 eV	254.66 nm	f=0.0380	<S**2>=0.000				
307 -> 315	0.54078								
308 -> 315	0.10789								
310 -> 317	0.25564								
310 -> 318	-0.14587								
311 -> 319	0.15964								
314 -> 324	0.16372								
314 -> 326	-0.10729								
Excited State 35:	Singlet-A	4.8954 eV	253.27 nm	f=0.0005	<S**2>=0.000				
307 -> 315	-0.24025								

311 -> 319	0.50220						
312 -> 319	0.20924						
313 -> 321	-0.18767						
314 -> 324	0.19735						
Excited State 36:	Singlet-A	4.9333 eV	251.32 nm	f=0.0038	<S**2>=0.000		
305 -> 315	0.15797						
306 -> 315	0.18603						
308 -> 315	-0.15597						
311 -> 319	0.17166						
311 -> 320	0.15170						
313 -> 321	0.45258						
313 -> 322	0.13196						
314 -> 328	-0.23196						
Excited State 37:	Singlet-A	4.9396 eV	251.00 nm	f=0.0128	<S**2>=0.000		
306 -> 315	0.13619						
310 -> 318	-0.27824						
313 -> 321	0.13585						
314 -> 324	0.21185						
314 -> 327	-0.11152						
314 -> 328	0.46445						
314 -> 329	-0.17703						
Excited State 38:	Singlet-A	4.9518 eV	250.38 nm	f=0.0011	<S**2>=0.000		
304 -> 315	-0.13437						
305 -> 315	-0.20934						
306 -> 315	-0.29821						
308 -> 315	0.14312						
310 -> 318	0.26565						
311 -> 319	0.18177						
312 -> 320	-0.15783						
313 -> 321	0.32164						
314 -> 328	0.22791						
Excited State 39:	Singlet-A	4.9876 eV	248.58 nm	f=0.1324	<S**2>=0.000		
305 -> 315	0.21355						
306 -> 315	0.22908						
310 -> 317	0.20416						
310 -> 318	0.46373						
311 -> 320	0.12253						
313 -> 321	-0.12416						
314 -> 328	0.15405						
314 -> 329	-0.11219						
Excited State 40:	Singlet-A	4.9935 eV	248.29 nm	f=0.0039	<S**2>=0.000		
312 -> 320	0.37361						
313 -> 321	0.16739						
313 -> 322	-0.15160						
314 -> 324	-0.22788						
314 -> 327	0.41385						
314 -> 328	0.14154						
Excited State 41:	Singlet-A	5.0029 eV	247.83 nm	f=0.0135	<S**2>=0.000		
310 -> 318	0.19055						
312 -> 320	0.41951						
313 -> 321	0.10920						
313 -> 322	-0.12503						
314 -> 324	0.13025						
314 -> 327	-0.39561						
314 -> 328	-0.11671						
314 -> 329	-0.10324						

Excited State 42:	Singlet-A	5.0306 eV	246.46 nm	f=0.0059	<S**2>=0.000
304 -> 315	-0.34165				
305 -> 315	0.47761				
306 -> 315	-0.29493				
Excited State 43:	Singlet-A	5.0571 eV	245.17 nm	f=0.0939	<S**2>=0.000
304 -> 315	0.11333				
306 -> 315	-0.17730				
308 -> 316	-0.12969				
311 -> 319	-0.12338				
312 -> 320	0.21739				
313 -> 322	0.53669				
314 -> 329	-0.11125				
Excited State 44:	Singlet-A	5.0779 eV	244.17 nm	f=0.0024	<S**2>=0.000
304 -> 315	0.47943				
305 -> 315	0.12929				
306 -> 315	-0.36507				
308 -> 316	-0.15872				
311 -> 320	0.15124				
313 -> 322	-0.20170				
Excited State 45:	Singlet-A	5.0893 eV	243.62 nm	f=0.0796	<S**2>=0.000
304 -> 315	-0.10829				
308 -> 316	-0.17474				
309 -> 318	-0.13397				
310 -> 319	0.11093				
311 -> 320	0.22464				
312 -> 320	0.16966				
313 -> 323	0.13953				
314 -> 328	0.13683				
314 -> 329	0.37383				
314 -> 330	-0.18736				
314 -> 332	0.17879				
314 -> 333	-0.11299				
Excited State 46:	Singlet-A	5.1113 eV	242.57 nm	f=0.1688	<S**2>=0.000
304 -> 315	0.16944				
305 -> 315	0.12984				
305 -> 316	0.14102				
308 -> 316	0.29889				
309 -> 317	0.16448				
309 -> 318	0.14291				
311 -> 320	-0.24898				
313 -> 322	0.14798				
313 -> 323	-0.14313				
314 -> 329	0.28500				
Excited State 47:	Singlet-A	5.1422 eV	241.11 nm	f=0.0240	<S**2>=0.000
303 -> 315	-0.10340				
305 -> 315	-0.12127				
308 -> 316	0.37004				
309 -> 317	0.10638				
311 -> 320	0.44795				
313 -> 322	0.15032				
Excited State 48:	Singlet-A	5.1756 eV	239.56 nm	f=0.0498	<S**2>=0.000
307 -> 316	0.10076				
308 -> 316	-0.14623				
309 -> 317	0.55487				
310 -> 319	-0.30169				
Excited State 49:	Singlet-A	5.2118 eV	237.89 nm	f=0.0101	<S**2>=0.000

304 -> 316	0.10584						
305 -> 316	0.13165						
306 -> 316	0.14406						
307 -> 316	0.36949						
309 -> 317	-0.12498						
310 -> 319	-0.11791						
312 -> 321	-0.13996						
313 -> 323	0.33317						
313 -> 324	-0.10388						
314 -> 329	0.13009						
314 -> 330	0.24601						
Excited State 50:	Singlet-A	5.2221 eV	237.42 nm	f=0.1324	<S**2>=0.000		
303 -> 315	-0.12443						
307 -> 316	-0.26195						
309 -> 317	0.25322						
310 -> 319	0.25381						
311 -> 320	-0.17161						
312 -> 321	-0.15091						
313 -> 323	0.37105						
313 -> 324	-0.10924						
Excited State 51:	Singlet-A	5.2300 eV	237.07 nm	f=0.0227	<S**2>=0.000		
307 -> 316	0.38222						
309 -> 317	0.13518						
310 -> 319	0.23960						
314 -> 329	-0.30238						
314 -> 330	-0.28793						
314 -> 334	-0.10472						
Excited State 52:	Singlet-A	5.2675 eV	235.37 nm	f=0.0447	<S**2>=0.000		
303 -> 315	-0.14932						
307 -> 316	0.15275						
310 -> 319	0.35710						
312 -> 321	0.18221						
313 -> 323	-0.21748						
314 -> 329	0.13390						
314 -> 330	0.35784						
Excited State 53:	Singlet-A	5.2935 eV	234.22 nm	f=0.0011	<S**2>=0.000		
303 -> 315	0.51738						
304 -> 316	-0.14477						
305 -> 316	-0.12506						
306 -> 316	-0.27895						
307 -> 316	0.12369						
308 -> 316	0.15660						
Excited State 54:	Singlet-A	5.3067 eV	233.64 nm	f=0.0430	<S**2>=0.000		
303 -> 315	0.27732						
304 -> 316	0.10569						
305 -> 316	0.31246						
306 -> 316	0.32152						
307 -> 316	-0.20993						
308 -> 316	-0.18832						
309 -> 318	-0.11424						
310 -> 319	0.13763						
313 -> 325	0.10092						
313 -> 326	0.11139						
314 -> 330	0.10218						
Excited State 55:	Singlet-A	5.3307 eV	232.59 nm	f=0.2639	<S**2>=0.000		
309 -> 318	0.53599						
311 -> 321	0.13924						

312 -> 321	0.13620								
313 -> 325	-0.10421								
314 -> 331	0.16499								
314 -> 336	0.16057								
Excited State 56:	Singlet-A	5.3403 eV	232.17 nm	f=0.0285	<S**2>=0.000				
309 -> 318	0.10568								
312 -> 321	-0.20108								
314 -> 330	0.11364								
314 -> 331	-0.41053								
314 -> 332	0.41162								
314 -> 333	-0.13678								
314 -> 335	0.11137								
Excited State 57:	Singlet-A	5.3474 eV	231.86 nm	f=0.0398	<S**2>=0.000				
302 -> 315	0.14104								
305 -> 316	-0.13921								
306 -> 316	0.11468								
310 -> 319	-0.12488								
312 -> 321	0.38881								
312 -> 322	-0.21160								
313 -> 323	0.14158								
314 -> 330	0.11952								
314 -> 332	0.11774								
314 -> 333	-0.19001								
314 -> 335	0.11494								
314 -> 336	0.19398								
Excited State 58:	Singlet-A	5.3640 eV	231.14 nm	f=0.0192	<S**2>=0.000				
312 -> 321	-0.19528								
313 -> 326	-0.11780								
314 -> 330	0.23753								
314 -> 331	0.33661								
314 -> 333	-0.25286								
314 -> 334	-0.30033								
314 -> 335	0.16779								
314 -> 336	0.16047								
Excited State 59:	Singlet-A	5.3754 eV	230.65 nm	f=0.0098	<S**2>=0.000				
302 -> 315	0.55799								
305 -> 316	-0.21635								
306 -> 316	0.12014								
312 -> 321	-0.10156								
312 -> 322	0.19317								
Excited State 60:	Singlet-A	5.3779 eV	230.54 nm	f=0.0038	<S**2>=0.000				
302 -> 315	0.28799								
305 -> 316	0.43329								
306 -> 316	-0.39070								
312 -> 321	0.12511								
Excited State 61:	Singlet-A	5.3827 eV	230.34 nm	f=0.0038	<S**2>=0.000				
313 -> 325	0.18913								
314 -> 329	-0.13300								
314 -> 331	0.26907								
314 -> 332	0.32590								
314 -> 333	0.22882								
314 -> 334	0.29789								
314 -> 335	-0.13676								
Excited State 62:	Singlet-A	5.3876 eV	230.13 nm	f=0.0256	<S**2>=0.000				
306 -> 316	-0.10019								
312 -> 321	-0.11372								

313 -> 325	0.10034						
314 -> 332	-0.26238						
314 -> 333	-0.32405						
314 -> 334	0.39280						
314 -> 336	0.20403						
Excited State 63:	Singlet-A	5.3997 eV	229.61 nm	f=0.0164	<S**2>=0.000		
300 -> 315	0.16116						
302 -> 315	-0.14900						
304 -> 316	0.31266						
306 -> 316	-0.13463						
311 -> 321	-0.11523						
311 -> 322	-0.13009						
312 -> 322	0.43082						
313 -> 323	0.12968						
Excited State 64:	Singlet-A	5.4092 eV	229.21 nm	f=0.0250	<S**2>=0.000		
300 -> 315	-0.22081						
304 -> 316	0.49694						
305 -> 316	-0.10411						
306 -> 316	-0.18059						
309 -> 318	0.10547						
312 -> 321	-0.15117						
312 -> 322	-0.24846						
313 -> 325	0.11259						

JOB name: na92CTD2

Method/Basis: TD-B3LYP-D3/6-311G(d) [hexane]//B3PW91-D3/6-31G(d)

Table S4. Transition Energy, Wavelength, and Oscillator Strengths of the Electronic Transition of **8_{opt}**

Excited State 1:	Singlet-A	2.4354 eV	509.08 nm	f=0.0918	<S**2>=0.000		
314 -> 315	0.63974						
314 -> 316	0.22220						
Excited State 2:	Singlet-A	2.5068 eV	494.59 nm	f=0.0486	<S**2>=0.000		
313 -> 315	0.60992						
313 -> 316	-0.29928						
314 -> 315	-0.11794						
Excited State 3:	Singlet-A	2.9340 eV	422.58 nm	f=1.0708	<S**2>=0.000		
313 -> 315	0.21618						
313 -> 316	0.46108						
314 -> 315	0.18552						
314 -> 316	-0.43639						
Excited State 4:	Singlet-A	2.9690 eV	417.60 nm	f=0.0076	<S**2>=0.000		
313 -> 315	0.23378						
313 -> 316	0.40347						
314 -> 315	-0.14904						
314 -> 316	0.47970						
Excited State 5:	Singlet-A	3.1341 eV	395.60 nm	f=0.0406	<S**2>=0.000		
314 -> 317	0.69202						
Excited State 6:	Singlet-A	3.1685 eV	391.31 nm	f=0.0524	<S**2>=0.000		
313 -> 317	0.69284						
Excited State 7:	Singlet-A	3.4225 eV	362.26 nm	f=0.0140	<S**2>=0.000		
312 -> 315	-0.12237						
313 -> 319	0.11237						

314 -> 316	0.10315						
314 -> 318	0.62918						
314 -> 319	0.14615						
314 -> 321	0.12558						
Excited State 8:	Singlet-A	3.4598 eV	358.36 nm	f=0.0055	<S**2>=0.000		
312 -> 315	0.69006						
Excited State 9:	Singlet-A	3.5404 eV	350.20 nm	f=0.0171	<S**2>=0.000		
313 -> 316	0.10302						
313 -> 318	-0.18392						
313 -> 319	0.61809						
313 -> 321	-0.13668						
314 -> 318	-0.16163						
Excited State 10:	Singlet-A	3.6199 eV	342.50 nm	f=0.0023	<S**2>=0.000		
313 -> 318	0.58326						
313 -> 321	-0.17494						
314 -> 319	0.29056						
Excited State 11:	Singlet-A	3.6405 eV	340.57 nm	f=0.0010	<S**2>=0.000		
313 -> 318	-0.27946						
313 -> 319	-0.13460						
314 -> 318	-0.17510						
314 -> 319	0.54973						
314 -> 320	0.12042						
314 -> 321	0.17134						
Excited State 12:	Singlet-A	3.7621 eV	329.56 nm	f=0.0012	<S**2>=0.000		
312 -> 316	0.69469						
Excited State 13:	Singlet-A	3.9025 eV	317.70 nm	f=0.0009	<S**2>=0.000		
314 -> 320	0.58295						
314 -> 321	-0.36570						
Excited State 14:	Singlet-A	3.9367 eV	314.95 nm	f=0.0008	<S**2>=0.000		
313 -> 320	0.59741						
313 -> 321	-0.33799						
Excited State 15:	Singlet-A	4.0412 eV	306.80 nm	f=0.0186	<S**2>=0.000		
311 -> 315	0.68098						
Excited State 16:	Singlet-A	4.0629 eV	305.16 nm	f=0.0073	<S**2>=0.000		
310 -> 315	0.22208						
312 -> 317	-0.10934						
313 -> 319	-0.10782						
313 -> 320	-0.15835						
313 -> 321	-0.31071						
314 -> 319	-0.20732						
314 -> 320	0.23252						
314 -> 321	0.39639						
Excited State 17:	Singlet-A	4.0910 eV	303.07 nm	f=0.0102	<S**2>=0.000		
309 -> 315	-0.11042						
313 -> 318	0.13515						
313 -> 319	0.18361						
313 -> 320	0.22165						
313 -> 321	0.42654						
314 -> 319	-0.12362						
314 -> 320	0.19926						
314 -> 321	0.33072						
Excited State 18:	Singlet-A	4.1789 eV	296.69 nm	f=0.0045	<S**2>=0.000		
309 -> 316	-0.12177						
310 -> 315	0.44697						
311 -> 316	0.14444						
312 -> 317	-0.39980						
313 -> 320	0.14348						
313 -> 321	0.15351						
314 -> 320	-0.11814						

314 -> 321	-0.13145								
Excited State 19:	Singlet-A	4.2722 eV	290.21 nm	f=0.0199	<S**2>=0.000				
309 -> 315	-0.35547								
310 -> 315	0.12350								
310 -> 316	0.19470								
311 -> 316	-0.12138								
312 -> 317	0.18777								
314 -> 322	0.48404								
314 -> 324	0.11704								
Excited State 20:	Singlet-A	4.2805 eV	289.65 nm	f=0.0416	<S**2>=0.000				
309 -> 315	0.42065								
310 -> 316	-0.21273								
311 -> 316	0.13634								
312 -> 317	-0.10860								
314 -> 322	0.45909								
314 -> 324	0.11596								
Excited State 21:	Singlet-A	4.3014 eV	288.24 nm	f=0.0014	<S**2>=0.000				
310 -> 315	-0.18240								
312 -> 317	-0.16861								
313 -> 322	0.61907								
313 -> 324	0.10416								
313 -> 325	0.10575								
Excited State 22:	Singlet-A	4.3192 eV	287.06 nm	f=0.0118	<S**2>=0.000				
309 -> 315	-0.24550								
310 -> 315	-0.35869								
310 -> 316	0.12865								
311 -> 316	0.35924								
312 -> 317	-0.27753								
313 -> 322	-0.24086								
Excited State 23:	Singlet-A	4.3615 eV	284.27 nm	f=0.0015	<S**2>=0.000				
310 -> 315	0.15541								
311 -> 316	0.53815								
312 -> 317	0.38617								
Excited State 24:	Singlet-A	4.5389 eV	273.16 nm	f=0.0035	<S**2>=0.000				
314 -> 323	0.44280								
314 -> 325	0.51995								
Excited State 25:	Singlet-A	4.5577 eV	272.03 nm	f=0.0334	<S**2>=0.000				
309 -> 315	0.12339								
310 -> 316	0.20773								
313 -> 323	-0.21142								
313 -> 324	0.12429								
313 -> 325	-0.11713								
314 -> 323	0.28646								
314 -> 324	0.38643								
314 -> 325	-0.29791								
Excited State 26:	Singlet-A	4.5664 eV	271.51 nm	f=0.0196	<S**2>=0.000				
308 -> 315	-0.10182								
310 -> 316	0.12549								
313 -> 323	0.34024								
313 -> 324	-0.30301								
313 -> 325	0.43020								
314 -> 323	0.16000								
314 -> 324	0.11336								
Excited State 27:	Singlet-A	4.5825 eV	270.56 nm	f=0.0189	<S**2>=0.000				
308 -> 315	-0.20781								
309 -> 315	0.24058								
309 -> 316	0.11506								
310 -> 316	0.41417								
312 -> 318	0.23099								
313 -> 323	-0.11551								
314 -> 323	-0.17336								

314 -> 324	-0.22372								
314 -> 325	0.16893								
Excited State 28:	Singlet-A	4.6104 eV	268.92 nm	f=0.0237	<S**2>=0.000				
312 -> 318	-0.29047								
313 -> 323	-0.36212								
313 -> 324	0.18349								
313 -> 325	0.46610								
Excited State 29:	Singlet-A	4.6148 eV	268.66 nm	f=0.0200	<S**2>=0.000				
308 -> 315	0.20326								
309 -> 315	-0.10018								
309 -> 316	-0.12302								
310 -> 316	-0.19744								
312 -> 318	0.54509								
312 -> 319	-0.13348								
313 -> 323	-0.15204								
313 -> 325	0.18104								
Excited State 30:	Singlet-A	4.6361 eV	267.43 nm	f=0.0048	<S**2>=0.000				
307 -> 315	0.10850								
308 -> 315	0.10561								
309 -> 316	0.63069								
310 -> 315	0.14684								
310 -> 316	-0.13566								
313 -> 325	0.10460								
Excited State 31:	Singlet-A	4.6608 eV	266.02 nm	f=0.0054	<S**2>=0.000				
314 -> 323	-0.15199								
314 -> 324	0.18767								
314 -> 325	0.13089								
314 -> 326	0.61350								
Excited State 32:	Singlet-A	4.6892 eV	264.40 nm	f=0.0075	<S**2>=0.000				
308 -> 315	-0.21055								
312 -> 319	0.28826								
313 -> 323	0.11779								
313 -> 324	0.18900								
313 -> 326	0.52590								
Excited State 33:	Singlet-A	4.6982 eV	263.90 nm	f=0.0007	<S**2>=0.000				
308 -> 315	-0.13902								
312 -> 318	0.16867								
312 -> 319	0.54959								
313 -> 324	-0.12292								
313 -> 326	-0.31047								
Excited State 34:	Singlet-A	4.7200 eV	262.68 nm	f=0.0453	<S**2>=0.000				
308 -> 315	0.51681								
310 -> 316	0.27471								
312 -> 319	0.26124								
Excited State 35:	Singlet-A	4.7864 eV	259.03 nm	f=0.0005	<S**2>=0.000				
307 -> 315	0.58221								
313 -> 324	0.12515								
313 -> 327	-0.10989								
314 -> 323	0.13050								
314 -> 324	-0.15487								
314 -> 325	-0.10127								
314 -> 327	-0.14308								
Excited State 36:	Singlet-A	4.8054 eV	258.01 nm	f=0.0045	<S**2>=0.000				
307 -> 315	0.24295								
314 -> 322	-0.11779								
314 -> 323	-0.29172								
314 -> 324	0.39070								
314 -> 325	0.23288								
314 -> 326	-0.27731								
314 -> 328	-0.11513								

Excited State	37:	Singlet-A	4.8328 eV	256.55 nm	f=0.0041	<S**2>=0.000
	307 -> 315	-0.14516				
	311 -> 317	-0.10964				
	313 -> 322	-0.13618				
	313 -> 323	0.30636				
	313 -> 324	0.47043				
	313 -> 326	-0.29353				
	313 -> 328	0.11358				
Excited State	38:	Singlet-A	4.8572 eV	255.26 nm	f=0.0042	<S**2>=0.000
	311 -> 317	0.44947				
	314 -> 327	0.48407				
Excited State	39:	Singlet-A	4.8682 eV	254.68 nm	f=0.0033	<S**2>=0.000
	307 -> 315	-0.13257				
	308 -> 316	0.13715				
	311 -> 317	0.46777				
	313 -> 327	0.13314				
	314 -> 327	-0.43030				
Excited State	40:	Singlet-A	4.8949 eV	253.30 nm	f=0.0099	<S**2>=0.000
	307 -> 315	0.10723				
	308 -> 316	-0.11660				
	311 -> 317	-0.11540				
	313 -> 327	0.63209				
	313 -> 331	0.13253				
Excited State	41:	Singlet-A	4.9127 eV	252.37 nm	f=0.0019	<S**2>=0.000
	314 -> 328	0.26696				
	314 -> 329	-0.37619				
	314 -> 330	0.41096				
	314 -> 331	-0.24263				
	314 -> 332	0.15656				
	314 -> 333	0.11752				
Excited State	42:	Singlet-A	4.9442 eV	250.77 nm	f=0.0140	<S**2>=0.000
	307 -> 316	-0.21100				
	310 -> 317	-0.19409				
	312 -> 320	0.46686				
	312 -> 321	-0.29813				
	313 -> 328	0.10859				
	313 -> 329	0.17178				
	313 -> 330	-0.12472				
	313 -> 331	0.10030				
Excited State	43:	Singlet-A	4.9455 eV	250.70 nm	f=0.0048	<S**2>=0.000
	312 -> 320	-0.25172				
	313 -> 328	0.19200				
	313 -> 329	0.45477				
	313 -> 330	-0.29137				
	313 -> 331	0.20888				
	313 -> 332	-0.11016				
Excited State	44:	Singlet-A	4.9688 eV	249.52 nm	f=0.0304	<S**2>=0.000
	310 -> 317	0.62778				
	312 -> 320	0.20003				
Excited State	45:	Singlet-A	4.9898 eV	248.47 nm	f=0.0067	<S**2>=0.000
	305 -> 315	-0.30797				
	305 -> 316	-0.13392				
	306 -> 315	0.31258				
	308 -> 316	0.46195				
Excited State	46:	Singlet-A	5.0175 eV	247.11 nm	f=0.0185	<S**2>=0.000
	305 -> 315	0.49464				
	305 -> 316	0.14272				
	306 -> 316	-0.14924				
	308 -> 316	0.38610				
Excited State	47:	Singlet-A	5.0390 eV	246.05 nm	f=0.0011	<S**2>=0.000

312 -> 320	-0.13793								
312 -> 321	-0.21378								
314 -> 324	0.12646								
314 -> 328	0.37500								
314 -> 329	0.23491								
314 -> 331	0.23261								
314 -> 333	0.29357								
314 -> 337	0.10246								
Excited State 48:	Singlet-A	5.0534 eV	245.35 nm	f=0.0116	<S**2>=0.000				
305 -> 315	0.22004								
305 -> 316	-0.14281								
306 -> 315	0.49591								
306 -> 316	-0.22123								
307 -> 316	-0.10957								
308 -> 316	-0.17439								
312 -> 320	-0.10908								
312 -> 321	-0.19523								
313 -> 328	-0.11258								
Excited State 49:	Singlet-A	5.0555 eV	245.25 nm	f=0.0136	<S**2>=0.000				
306 -> 315	0.19077								
312 -> 320	0.27958								
312 -> 321	0.48323								
313 -> 328	0.10641								
314 -> 328	0.12694								
314 -> 329	0.11923								
314 -> 331	0.13094								
314 -> 333	0.12629								
Excited State 50:	Singlet-A	5.0666 eV	244.71 nm	f=0.0051	<S**2>=0.000				
314 -> 328	-0.31430								
314 -> 329	0.12320								
314 -> 330	0.38362								
314 -> 331	0.30483								
314 -> 332	0.29867								
314 -> 334	0.13206								
Excited State 51:	Singlet-A	5.0762 eV	244.25 nm	f=0.0048	<S**2>=0.000				
309 -> 317	-0.20631								
312 -> 321	-0.16759								
313 -> 324	-0.10205								
313 -> 328	0.41979								
313 -> 330	0.20435								
313 -> 331	-0.14290								
313 -> 333	0.28553								
Excited State 52:	Singlet-A	5.0883 eV	243.67 nm	f=0.0062	<S**2>=0.000				
303 -> 315	-0.19235								
307 -> 316	0.57924								
311 -> 318	-0.11333								
312 -> 321	-0.13609								
312 -> 322	0.15758								
Excited State 53:	Singlet-A	5.0983 eV	243.19 nm	f=0.0040	<S**2>=0.000				
303 -> 315	0.14450								
313 -> 328	-0.24361								
313 -> 329	0.36020								
313 -> 330	0.24026								
313 -> 331	-0.32114								
313 -> 332	-0.26954								
313 -> 334	0.12911								
Excited State 54:	Singlet-A	5.1086 eV	242.70 nm	f=0.0381	<S**2>=0.000				
303 -> 315	0.17634								
304 -> 315	0.11428								
308 -> 316	-0.11449								
308 -> 317	0.11001								
309 -> 317	0.56612								
311 -> 317	0.11926								

311 -> 319	0.10913								
313 -> 328	0.11905								
Excited State 55:	Singlet-A	5.1101 eV	242.63 nm	f=0.0361	<S**2>=0.000				
303 -> 315	0.47496								
303 -> 316	0.19782								
304 -> 315	0.24536								
307 -> 316	0.14575								
309 -> 317	-0.16453								
311 -> 318	-0.10504								
313 -> 330	-0.14145								
313 -> 331	0.13986								
Excited State 56:	Singlet-A	5.1375 eV	241.33 nm	f=0.0057	<S**2>=0.000				
304 -> 315	0.17447								
314 -> 328	-0.27545								
314 -> 329	-0.24949								
314 -> 330	-0.17059								
314 -> 333	0.49802								
Excited State 57:	Singlet-A	5.1506 eV	240.72 nm	f=0.0247	<S**2>=0.000				
303 -> 315	-0.25610								
303 -> 316	0.13696								
304 -> 315	0.51275								
304 -> 316	-0.27232								
314 -> 333	-0.15586								
Excited State 58:	Singlet-A	5.1737 eV	239.64 nm	f=0.0027	<S**2>=0.000				
314 -> 328	-0.10735								
314 -> 329	0.28795								
314 -> 331	-0.35915								
314 -> 332	0.37493								
314 -> 334	-0.33005								
Excited State 59:	Singlet-A	5.1767 eV	239.51 nm	f=0.0083	<S**2>=0.000				
313 -> 328	-0.25728								
313 -> 330	-0.29087								
313 -> 331	-0.13048								
313 -> 332	0.18628								
313 -> 333	0.49084								
Excited State 60:	Singlet-A	5.2099 eV	237.98 nm	f=0.0021	<S**2>=0.000				
313 -> 328	-0.16474								
313 -> 330	0.23518								
313 -> 331	0.35085								
313 -> 332	-0.30823								
313 -> 333	0.23386								
313 -> 334	-0.33344								
Excited State 61:	Singlet-A	5.2504 eV	236.14 nm	f=0.0707	<S**2>=0.000				
300 -> 315	-0.13889								
302 -> 315	-0.16461								
309 -> 317	-0.14149								
311 -> 318	0.45407								
311 -> 319	0.40055								
Excited State 62:	Singlet-A	5.2698 eV	235.27 nm	f=0.0042	<S**2>=0.000				
314 -> 326	0.12627								
314 -> 328	0.13819								
314 -> 329	-0.28211								
314 -> 330	-0.29052								
314 -> 331	0.24852								
314 -> 332	0.39270								
314 -> 333	-0.21092								
314 -> 334	-0.10154								
Excited State 63:	Singlet-A	5.3009 eV	233.89 nm	f=0.0924	<S**2>=0.000				
310 -> 318	-0.15212								
310 -> 319	-0.12227								
311 -> 318	-0.20757								

311 -> 319	0.27835
312 -> 322	-0.19872
313 -> 332	-0.12519
314 -> 334	-0.15124
314 -> 335	0.36206
314 -> 336	0.15508
314 -> 337	0.19533
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Excited State 64:	Singlet-A 5.3044 eV 233.74 nm f=0.0010 <S**2>=0.000
313 -> 326	0.12480
313 -> 328	-0.14169
313 -> 329	0.23577
313 -> 330	0.29021
313 -> 331	0.23711
313 -> 332	0.42835
314 -> 335	0.11990

JOB name: na92DTD2

Method/Basis: TD-B3LYP-D3/6-311G(d) [hexane]//B3PW91-D3/6-31G(d)

Table S5. Transition Energy, Wavelength, and Oscillator Strengths of the Electronic Transition of **9_{opt}**

Excited State 1:	Singlet-A	2.3626 eV	524.78 nm	f=0.0437	<S**2>=0.000
211 -> 212	0.70004				
Excited State 2:	Singlet-A	2.4965 eV	496.63 nm	f=0.0110	<S**2>=0.000
208 -> 212	-0.11064				
210 -> 212	0.69028				
Excited State 3:	Singlet-A	2.9717 eV	417.21 nm	f=0.0005	<S**2>=0.000
211 -> 213	0.70205				
Excited State 4:	Singlet-A	3.1024 eV	399.64 nm	f=0.0188	<S**2>=0.000
209 -> 212	0.14123				
210 -> 213	0.68574				
Excited State 5:	Singlet-A	3.2431 eV	382.30 nm	f=0.0009	<S**2>=0.000
209 -> 212	0.68658				
210 -> 213	-0.14238				
Excited State 6:	Singlet-A	3.5032 eV	353.92 nm	f=0.0092	<S**2>=0.000
211 -> 214	0.69361				
Excited State 7:	Singlet-A	3.6080 eV	343.63 nm	f=0.0168	<S**2>=0.000
210 -> 214	0.68933				
Excited State 8:	Singlet-A	3.8538 eV	321.72 nm	f=0.0257	<S**2>=0.000
208 -> 212	0.54869				
209 -> 213	0.21538				
210 -> 215	-0.13387				
210 -> 216	0.10272				
210 -> 217	0.10049				
211 -> 215	-0.12850				
211 -> 216	-0.25330				
Excited State 9:	Singlet-A	3.8856 eV	319.08 nm	f=0.0082	<S**2>=0.000
210 -> 215	0.59454				
211 -> 215	0.20263				
211 -> 216	-0.27927				

Excited State 10:	Singlet-A	3.8958 eV	318.25 nm	f=0.0039	<S**2>=0.000
210 -> 215	-0.23786				
210 -> 216	-0.10450				
211 -> 215	0.63869				
Excited State 11:	Singlet-A	3.9475 eV	314.08 nm	f=0.0012	<S**2>=0.000
207 -> 212	0.59795				
209 -> 213	0.27645				
211 -> 216	0.20321				
Excited State 12:	Singlet-A	3.9827 eV	311.30 nm	f=0.0042	<S**2>=0.000
207 -> 212	-0.33798				
208 -> 212	0.16639				
209 -> 213	0.29808				
210 -> 215	0.21689				
211 -> 216	0.45155				
Excited State 13:	Singlet-A	4.0116 eV	309.06 nm	f=0.0114	<S**2>=0.000
208 -> 213	0.10051				
209 -> 213	-0.12488				
210 -> 216	0.65201				
Excited State 14:	Singlet-A	4.0836 eV	303.62 nm	f=0.0091	<S**2>=0.000
205 -> 212	-0.12471				
207 -> 212	-0.11658				
208 -> 212	-0.30245				
209 -> 213	0.49727				
210 -> 216	0.11369				
211 -> 216	-0.29226				
Excited State 15:	Singlet-A	4.2953 eV	288.65 nm	f=0.0104	<S**2>=0.000
206 -> 212	0.64543				
211 -> 217	-0.23470				
Excited State 16:	Singlet-A	4.3189 eV	287.08 nm	f=0.0122	<S**2>=0.000
206 -> 212	0.23258				
208 -> 213	0.24547				
211 -> 217	0.60315				
Excited State 17:	Singlet-A	4.3626 eV	284.20 nm	f=0.0155	<S**2>=0.000
208 -> 213	0.33700				
209 -> 214	0.20942				
210 -> 217	0.56174				
Excited State 18:	Singlet-A	4.4037 eV	281.55 nm	f=0.0170	<S**2>=0.000
208 -> 213	0.42061				
209 -> 214	-0.30707				
210 -> 217	-0.20375				
210 -> 218	0.18705				
211 -> 217	-0.18889				
211 -> 218	-0.30737				
Excited State 19:	Singlet-A	4.4173 eV	280.68 nm	f=0.0084	<S**2>=0.000
208 -> 213	0.15732				
209 -> 214	-0.24089				
210 -> 218	0.13797				
211 -> 218	0.60063				
Excited State 20:	Singlet-A	4.4790 eV	276.81 nm	f=0.0181	<S**2>=0.000
205 -> 212	-0.12750				
208 -> 213	-0.29267				
209 -> 214	-0.29193				

210 -> 217	0.26113						
210 -> 218	0.44775						
Excited State 21:	Singlet-A	4.5275 eV	273.84 nm	f=0.0065	<S**2>=0.000		
205 -> 212	0.66171						
210 -> 218	0.12658						
Excited State 22:	Singlet-A	4.5677 eV	271.44 nm	f=0.0560	<S**2>=0.000		
209 -> 214	0.43925						
209 -> 216	0.13464						
210 -> 217	-0.19121						
210 -> 218	0.43989						
Excited State 23:	Singlet-A	4.7433 eV	261.39 nm	f=0.0031	<S**2>=0.000		
204 -> 212	0.69312						
Excited State 24:	Singlet-A	4.7700 eV	259.93 nm	f=0.0031	<S**2>=0.000		
207 -> 213	0.59516						
208 -> 214	0.31646						
209 -> 215	0.15049						
Excited State 25:	Singlet-A	4.8096 eV	257.78 nm	f=0.0276	<S**2>=0.000		
207 -> 213	0.21784						
208 -> 214	-0.19629						
209 -> 216	0.12610						
210 -> 219	0.34614						
210 -> 220	-0.26116						
211 -> 219	0.35832						
211 -> 220	-0.21715						
211 -> 221	-0.11719						
Excited State 26:	Singlet-A	4.8487 eV	255.71 nm	f=0.0071	<S**2>=0.000		
207 -> 213	-0.26074						
208 -> 214	0.38171						
209 -> 215	0.31232						
209 -> 216	0.21041						
210 -> 219	0.17955						
210 -> 220	-0.26386						
210 -> 221	0.12908						
Excited State 27:	Singlet-A	4.8610 eV	255.06 nm	f=0.0610	<S**2>=0.000		
206 -> 213	0.10617						
209 -> 215	0.21199						
210 -> 219	-0.30791						
210 -> 220	0.20155						
211 -> 219	0.41414						
211 -> 220	-0.14360						
211 -> 221	-0.24362						
Excited State 28:	Singlet-A	4.8799 eV	254.07 nm	f=0.0204	<S**2>=0.000		
203 -> 212	-0.15727						
206 -> 213	0.12847						
209 -> 215	-0.22160						
209 -> 216	0.49691						
210 -> 219	-0.10859						
210 -> 220	0.14106						
211 -> 220	0.16238						
211 -> 221	-0.26186						
Excited State 29:	Singlet-A	4.9018 eV	252.93 nm	f=0.0018	<S**2>=0.000		
203 -> 212	0.55922						
206 -> 213	0.11483						
209 -> 215	-0.19572						

209 -> 216	-0.10049						
211 -> 220	0.16381						
211 -> 221	-0.23495						
Excited State 30:	Singlet-A	4.9412 eV	250.92 nm	f=0.0218	<S**2>=0.000		
203 -> 212	0.33404						
206 -> 213	0.12525						
209 -> 215	0.14635						
209 -> 216	0.32917						
211 -> 220	-0.26062						
211 -> 221	0.33493						
Excited State 31:	Singlet-A	4.9930 eV	248.31 nm	f=0.1593	<S**2>=0.000		
205 -> 213	0.13206						
207 -> 213	-0.10032						
208 -> 214	0.38890						
209 -> 215	-0.31615						
210 -> 220	0.13589						
210 -> 221	-0.17705						
211 -> 219	0.18300						
211 -> 220	-0.14473						
211 -> 221	0.21330						
Excited State 32:	Singlet-A	5.0150 eV	247.23 nm	f=0.0967	<S**2>=0.000		
206 -> 213	0.16752						
209 -> 215	-0.25757						
210 -> 219	-0.16564						
210 -> 220	-0.17422						
210 -> 221	0.52850						
211 -> 221	0.10938						
Excited State 33:	Singlet-A	5.0433 eV	245.84 nm	f=0.0105	<S**2>=0.000		
206 -> 213	-0.17264						
211 -> 219	0.34147						
211 -> 220	0.45137						
211 -> 221	0.26026						
211 -> 222	-0.16115						
Excited State 34:	Singlet-A	5.0729 eV	244.41 nm	f=0.0273	<S**2>=0.000		
203 -> 212	-0.11538						
206 -> 213	0.59393						
209 -> 216	-0.10432						
210 -> 219	0.13688						
211 -> 220	0.17272						
211 -> 221	0.15196						
Excited State 35:	Singlet-A	5.0921 eV	243.48 nm	f=0.0025	<S**2>=0.000		
201 -> 212	0.62047						
202 -> 212	-0.17569						
208 -> 215	-0.18449						
Excited State 36:	Singlet-A	5.1181 eV	242.24 nm	f=0.0171	<S**2>=0.000		
208 -> 215	-0.11961						
210 -> 219	0.37290						
210 -> 220	0.43184						
210 -> 221	0.31358						
210 -> 222	-0.16914						
Excited State 37:	Singlet-A	5.1503 eV	240.73 nm	f=0.0071	<S**2>=0.000		
201 -> 212	0.16465						
208 -> 215	0.64828						
210 -> 220	0.11697						

Excited State	38:	Singlet-A	5.1954 eV	238.64 nm	f=0.0005	<S**2>=0.000
	201 -> 212	0.18092				
	202 -> 212	0.65584				
Excited State	39:	Singlet-A	5.2328 eV	236.93 nm	f=0.0159	<S**2>=0.000
	205 -> 213	-0.18527				
	207 -> 214	-0.32843				
	209 -> 217	0.56083				
Excited State	40:	Singlet-A	5.2743 eV	235.07 nm	f=0.0134	<S**2>=0.000
	207 -> 214	0.56660				
	208 -> 216	0.14874				
	209 -> 217	0.31217				
	211 -> 222	-0.12814				
Excited State	41:	Singlet-A	5.2828 eV	234.69 nm	f=0.0132	<S**2>=0.000
	207 -> 214	0.10998				
	208 -> 216	0.17487				
	211 -> 220	0.11272				
	211 -> 222	0.62207				
Excited State	42:	Singlet-A	5.3072 eV	233.61 nm	f=0.0419	<S**2>=0.000
	205 -> 213	0.21900				
	207 -> 214	-0.16646				
	208 -> 216	0.59202				
	210 -> 222	0.13313				
	211 -> 222	-0.12630				
Excited State	43:	Singlet-A	5.3367 eV	232.33 nm	f=0.0852	<S**2>=0.000
	205 -> 213	0.43645				
	206 -> 214	0.10148				
	208 -> 216	-0.16752				
	209 -> 217	0.15342				
	209 -> 218	0.41115				
	211 -> 222	0.10578				
	211 -> 224	0.10887				
Excited State	44:	Singlet-A	5.3746 eV	230.68 nm	f=0.0167	<S**2>=0.000
	208 -> 216	-0.14703				
	209 -> 218	-0.23429				
	210 -> 221	0.10031				
	210 -> 222	0.59268				
Excited State	45:	Singlet-A	5.3842 eV	230.28 nm	f=0.1400	<S**2>=0.000
	205 -> 213	-0.39220				
	208 -> 216	0.12918				
	209 -> 217	-0.12276				
	209 -> 218	0.43321				
	210 -> 222	0.20850				
Excited State	46:	Singlet-A	5.4224 eV	228.65 nm	f=0.0194	<S**2>=0.000
	199 -> 212	0.13404				
	206 -> 214	-0.13557				
	211 -> 222	0.10739				
	211 -> 223	0.31403				
	211 -> 224	0.48793				
	211 -> 225	-0.18470				
	211 -> 226	-0.14021				
Excited State	47:	Singlet-A	5.4791 eV	226.28 nm	f=0.0031	<S**2>=0.000
	199 -> 212	0.46585				
	200 -> 212	-0.40716				
	206 -> 214	0.24382				

210 -> 224	-0.12373								
Excited State 48:	Singlet-A	5.4921 eV	225.75 nm	f=0.0099	<S**2>=0.000				
204 -> 213	-0.17210								
206 -> 214	0.16371								
210 -> 222	0.13862								
210 -> 223	0.31644								
210 -> 224	0.48120								
210 -> 225	-0.17349								
210 -> 226	-0.11628								
Excited State 49:	Singlet-A	5.5164 eV	224.76 nm	f=0.0059	<S**2>=0.000				
199 -> 212	-0.12336								
200 -> 212	-0.19985								
204 -> 213	0.60517								
207 -> 215	-0.13582								
210 -> 224	0.12505								
Excited State 50:	Singlet-A	5.5168 eV	224.74 nm	f=0.0007	<S**2>=0.000				
197 -> 212	-0.19529								
198 -> 212	0.19089								
199 -> 212	0.30885								
200 -> 212	0.46536								
204 -> 213	0.27229								
206 -> 214	0.13426								
Excited State 51:	Singlet-A	5.5346 eV	224.02 nm	f=0.0144	<S**2>=0.000				
198 -> 212	-0.11713								
199 -> 212	-0.20432								
204 -> 213	0.10562								
206 -> 214	0.18976								
207 -> 215	0.55746								
209 -> 218	-0.10895								
211 -> 223	0.16559								
Excited State 52:	Singlet-A	5.5545 eV	223.21 nm	f=0.0008	<S**2>=0.000				
197 -> 212	0.10254								
198 -> 212	0.64553								
200 -> 212	-0.18695								
207 -> 215	0.10344								
Excited State 53:	Singlet-A	5.5608 eV	222.96 nm	f=0.0071	<S**2>=0.000				
207 -> 215	-0.14194								
211 -> 223	0.55254								
211 -> 224	-0.25658								
211 -> 225	0.16419								
211 -> 226	0.19740								
Excited State 54:	Singlet-A	5.5888 eV	221.84 nm	f=0.0601	<S**2>=0.000				
198 -> 212	0.10566								
199 -> 212	-0.18777								
206 -> 214	0.38050								
206 -> 216	-0.11464								
207 -> 215	-0.27303								
210 -> 223	-0.25184								
210 -> 225	-0.10714								
211 -> 224	0.12127								
211 -> 226	0.21698								
211 -> 228	0.12160								
Excited State 55:	Singlet-A	5.6103 eV	220.99 nm	f=0.0054	<S**2>=0.000				
206 -> 214	-0.15098								
208 -> 217	0.27775								

210 -> 223	0.26807								
210 -> 225	0.10797								
211 -> 224	0.16963								
211 -> 226	0.44878								
211 -> 228	0.15358								
Excited State 56:	Singlet-A	5.6279 eV	220.30 nm	f=0.0014	<S**2>=0.000				
206 -> 214	0.11717								
210 -> 223	0.21840								
210 -> 224	-0.11599								
211 -> 224	0.20646								
211 -> 225	0.50556								
211 -> 226	-0.11888								
211 -> 227	0.26650								
Excited State 57:	Singlet-A	5.6359 eV	219.99 nm	f=0.0042	<S**2>=0.000				
197 -> 212	0.45313								
199 -> 212	0.20358								
206 -> 214	-0.11978								
208 -> 217	0.15034								
210 -> 223	-0.27135								
210 -> 224	0.19258								
211 -> 225	0.19165								
Excited State 58:	Singlet-A	5.6436 eV	219.69 nm	f=0.0077	<S**2>=0.000				
197 -> 212	0.44685								
200 -> 212	0.10840								
206 -> 214	0.17392								
208 -> 217	-0.16139								
210 -> 223	0.27557								
210 -> 224	-0.21665								
211 -> 225	-0.18907								
Excited State 59:	Singlet-A	5.6671 eV	218.78 nm	f=0.0130	<S**2>=0.000				
206 -> 214	0.11867								
208 -> 217	0.48728								
208 -> 218	0.12692								
210 -> 226	0.13889								
211 -> 226	-0.30258								
211 -> 227	-0.21568								
Excited State 60:	Singlet-A	5.6797 eV	218.29 nm	f=0.0244	<S**2>=0.000				
208 -> 217	0.13920								
210 -> 225	-0.19910								
210 -> 226	0.18933								
210 -> 227	-0.10445								
211 -> 224	-0.13058								
211 -> 225	-0.22731								
211 -> 227	0.50258								
211 -> 228	-0.14635								
211 -> 230	-0.10909								
Excited State 61:	Singlet-A	5.6839 eV	218.13 nm	f=0.0008	<S**2>=0.000				
203 -> 213	0.16653								
208 -> 217	0.18004								
210 -> 225	0.40545								
210 -> 226	-0.38070								
210 -> 227	0.11930								
211 -> 227	0.20813								
Excited State 62:	Singlet-A	5.7078 eV	217.22 nm	f=0.0062	<S**2>=0.000				
203 -> 213	-0.12856								
208 -> 217	-0.15143								

210 -> 224	0.23985
210 -> 225	0.40031
210 -> 226	0.38421
210 -> 227	0.11337
210 -> 228	0.14677

Excited State 63: Singlet-A 5.7288 eV 216.42 nm f=0.0062 <S**2>=0.000

195 -> 212	0.11309
196 -> 212	0.63361
203 -> 213	0.19482
205 -> 214	0.10534
210 -> 226	0.11675

Excited State 64: Singlet-A 5.7421 eV 215.92 nm f=0.0109 <S**2>=0.000

195 -> 212	0.24661
196 -> 212	-0.29418
203 -> 213	0.49238
205 -> 214	0.19078
210 -> 226	0.16936

JOB name: na92ETD2

Method/Basis: TD-B3LYP-D3/6-311G(d) [hexane]//B3PW91-D3/6-31G(d)