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## **Electronic Supplementary Information**

Interconversion between a planar 1,3-dichlorobicyclo[1.1.0]tetrasilane

and a (chloro)(chlorosilyl)cyclotrisilene

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## 1. NMR spectra



Figure S1. <sup>1</sup>H NMR spectrum of 4 in C<sub>6</sub>D<sub>6</sub> at 302 K ( $\bullet = C_6HD_5$ ,  $\mathbf{v} = 6$ ).



Figure S2. <sup>1</sup>H NMR spectrum of 4 in C<sub>6</sub>D<sub>6</sub> at 302 K after 1 day ( $\bullet = C_6HD_5$ ,  $\bullet = 4$ ,  $\forall = 6$ ).



Figure S3. <sup>1</sup>H NMR spectrum of 4 in C<sub>6</sub>D<sub>6</sub> at 333 K ( $\bullet = C_6HD_5$ ,  $\bullet = 4$ ,  $\lor = 6$ ).



Figure S4. <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of 4 in C<sub>6</sub>D<sub>6</sub> in 333 K ( $\bullet = C_6D_6$ ,  $\bullet = 4$ ,  $\mathbf{v} = 6$ ).



Figure S5. <sup>13</sup>C (DEPT135) NMR spectrum of 4 in C<sub>6</sub>D<sub>6</sub> at 333 K ( $\bullet = C_6D_6$ ,  $\bullet = 4$ ,  $\forall = 6$ ).



Figure S6. <sup>1</sup>H-<sup>13</sup>C HMBC NMR spectrum of 4 in C<sub>6</sub>D<sub>6</sub> at 333 K.



**Figure S7.** <sup>29</sup>Si{<sup>1</sup>H} NMR spectrum of **4** in C<sub>6</sub>D<sub>6</sub> at 333 K. ( $\blacklozenge = 4$ ,  $\blacktriangledown = 6$ ).



Figure S8. <sup>1</sup>H-<sup>29</sup>Si HMBC NMR spectrum of 4 in  $C_6D_6$  at 333 K.



Figure S9. <sup>1</sup>H NMR spectrum of 7·(benzene)<sub>2</sub> in THF- $d_8$  at 296 K ( $\bullet$  = THF- $d_8$ , × = benzene).



Figure S10. <sup>13</sup>C{<sup>1</sup>H} NMR spectrum of 7·(benzene)<sub>2</sub> in THF- $d_8$  in 301 K ( $\bullet$  = THF- $d_8$ , × = benzene).



Figure S11. <sup>13</sup>C (DEPT135) NMR spectrum of  $7 \cdot (\text{benzene})_2$  in THF- $d_8$  at 301 K (x = benzene).



Figure S12. <sup>1</sup>H-<sup>13</sup>C HSQC NMR spectrum of 7·(benzene)<sub>2</sub> in THF-*d*<sub>8</sub> at 300 K.



Figure S13. <sup>29</sup>Si{<sup>1</sup>H} NMR spectrum of 7·(benzene)<sub>2</sub> in THF- $d_8$  at 301 K.



Figure S14. <sup>1</sup>H-<sup>29</sup>Si HMBC NMR spectrum of 7·(benzene)<sub>2</sub> in THF-*d*<sub>8</sub> at 301 K.



**Figure S15.** <sup>1</sup>H NMR spectrum of the reaction mixture of 7 with CCl<sub>4</sub> in the presence of BPh<sub>3</sub> in C<sub>6</sub>D<sub>6</sub> at 302 K ( $\bullet$  = C<sub>6</sub>HD<sub>5</sub>,  $\checkmark$  = BPh<sub>3</sub>•DMAP,  $\blacklozenge$  = 3, × = ferrocene,  $\blacksquare$  = toluene).



**Figure S16.** <sup>1</sup>H NMR spectra (TMS region) of the reaction mixture of **4**+**6** with DMAP in C<sub>6</sub>D<sub>6</sub> at room temperature ( $\bullet = 4$ ,  $\bullet = 6$ ,  $\blacksquare = 7$ ,  $\times =$  by products).



**Figure S17.** <sup>1</sup>H NMR spectra (TMS region) of a) the equilibrium mixture of **4**+**6** and b) the reaction mixture of **7** with BPh<sub>3</sub> in toluene-*d*<sub>8</sub> at variable temperature. c) <sup>1</sup>H NMR spectra (TMS region) of the reaction mixture of **7** with BPh<sub>3</sub> (left: just after warming up, right: after 1 hour) in toluene-*d*<sub>8</sub> at room temperature ( $\bullet = 4$ ,  $\bullet = 6$ ).



**Figure S18.** <sup>1</sup>H NMR spectrum of the reaction mixture of 7 with BPh<sub>3</sub> in C<sub>6</sub>D<sub>6</sub> at 300 K ( $\bullet = C_6HD_5$ ,  $\checkmark = BPh_3 \bullet DMAP$ ,  $\bullet = 4+6$ ,  $\times =$  ferrocene,  $\blacksquare =$  toluene).

# 2. X-Ray diffraction analysis



**Figure S19.** ORTEP drawings of **4**. Thermal ellipsoids are shown at the 50% probability level. Hydrogen atoms were omitted for clarity.



**Figure S20.** ORTEP drawings of 7. Thermal ellipsoids are shown at the 50% probability level. Hydrogen atoms were omitted for clarity.

## 3. UV-vis absorption spectrum



Figure S21. UV-Vis absorption spectrum of the equilibrium mixture of 4 and 6 in hexane at room temperature.



Figure S22. UV-Vis absorption spectrum of  $7 \cdot (benzene)_2$  dissolved in hexane at room temperature. Table S1. UV-vis Absorption Bands of  $7 \cdot (benzene)_2$ 

Absorption maximum / nm	$\epsilon$ / 10 <sup>4</sup> cm <sup>-1</sup> mol <sup>-1</sup> dm <sup>3</sup>
519	1,100
362	5,400
315 sh <sup>a)</sup>	7,600
275 <sup>b)</sup>	28,000
236 <sup>b)</sup>	31,000

a) sh = shoulder, b) the absorption bands of benzene involved the crystals of **7** should be overlapped.

#### 4. Computational study

The atomic coordinates and energies of all equilibrium and transition structures are summarized in the file named "optimized\_structures.xyz". The selected structural parameters of  $4_{opt}$ ,  $4'_{opt}$ ,  $4''_{opt}$ , are summarized in Table S2 and S3. Frontier Kohn-Sham orbitals and their energy levels of  $4_{opt}$  were shown in Figure S23. Isotropic chemical shielding tensors were calculated at the GIAO/M06L/6-311+G(2df,p) level of theory (Table S4 and S5). Absolute isotropic shielding tensors of  $2^{9}$ Si nucleus in tetramethylsilane were calculated to be 361.4 (GIAO/M06L/6-311+G(2df,p)). Excitation energies and oscillator strengths of  $4_{opt}$  and  $6_{opt}$  were calculated at the B3LYP/6-311G(d) level of theory (Tables S6 and S7). A possible reaction route between  $4_{opt}$  and  $6_{opt}$  calculated at the B3LYP-D3/B1 (basis B1: 6-311G(d) [core Si4Cl2], 6-31G(d) [carbon atoms in silacyclopentane rings], 3-21G\* [others]) were shown in Figure S25.

C, ç Si Cl1-

Cl <sup>1</sup> —S		C) <sup>2</sup>												
Cpd	-			distance/Å	L					angle/°			$E^{ m b,c}$	$\Delta E^{c,e}$
	Si <sup>1</sup> –Si <sup>2</sup>	Si <sup>1</sup> -Si <sup>3</sup>	Si <sup>1</sup> -Si <sup>4</sup>	Si <sup>2</sup> -Si <sup>3</sup>	Si <sup>2</sup> –Si <sup>4</sup>	Si <sup>1</sup> -Cl <sup>1</sup>	Si <sup>2</sup> -Cl <sup>2</sup>	Cl1-Si1-Si2	Cl <sup>2</sup> -Si <sup>2</sup> -Si <sup>1</sup>	Si1-Si3-Si2	Si1-Si4-Si2	Si <sup>3</sup> -Si <sup>1</sup> -Si <sup>2</sup> -Si <sup>4</sup>	$[\Delta G]^{ m b,d}$	$[\Delta \Delta G]$
XRD														
4	2.581(2)	2.3249(17)	2.3361(17)	2.3361(17)	2.3249(17)	2.0690(18)	2.0690(18)	178.27(11)	178.27(11)	67.26(6)	67.26(6)	180.00	-	
DFT <sup>a</sup>														
4 <sub>opt</sub>	2.58285	2.31823	2.33167	2.33167	2.31823	2.10926	2.10926	178.572	178.572	67.485	67.485	180.000	-5662.014735	0.0
													[-5662.116181]	[0.0]
4′ <sub>opt</sub>	2.89287	2.39590	2.41124	2.45983	2.43874	2.14902	2.14000	109.187	113.787	73.121	73.233	-174.450	-5662.015099	-1.0
													[-5662.115585]	[1.6]
4″ <sub>opt</sub>	2.44338	2.32745	2.33875	2.33875	2.32745	2.10637	2.10637	160.679	160.679	63.152	63.152	-149.598	-5662.009600	13.5

note (job name)

tn08a

TN74a

TN84a

TN77\_120

[-5662.114172]

[5.3]

## Table S2. Selected Structural Parameters of 4, $4_{opt}$ , $4'_{opt}$ and $4''_{opt}$

a. optimized at the B3LYP-D3/6-311G(d) level of theory. b. in hartree. c. Zero-point vibrational energy corrections were included. d. at 298.15 K. e. in kJ mol<sup>-1</sup>.

Table S3. Selected Structural Parameters of 7<sub>opt</sub>





Figure S23. Frontier Kohn-Sham orbitals of 4<sub>opt</sub> at the B3LYP-D3/6-311G(d) level of theory.

Table S4. Experimental and Theoretical Isotropic <sup>29</sup>Si Chemical Shifts of 4, 4<sub>opt</sub>, 4'<sub>opt</sub> and 4''<sub>opt</sub>

Compound	SiMe <sub>3</sub>	Si (bridge)	Si (bridgehead)	note
<b>4</b> <sup>a</sup>	4.6	-7.9	126.4	TN420_7
4 <sub>opt</sub> <sup>b,c</sup>	5.0 (356.4) <sup>d</sup>	-17.1 (378.5)	150.2 (211.2)	nmr2_TN74a
4′ opt <sup>b,c</sup>	5.3 (356.1) <sup>d</sup>	139.5 (221.9)	-37.1 (398.3)	nmr2_TN77_120
		137.1 (224.3)	-49.9 (411.3)	
4″opt <sup>b,c</sup>	4.8 (356.6) <sup>d</sup>	-25.1 (386.5)	86.5 (274.8)	nmr_TN84a

a. Experimental <sup>29</sup>Si Chemical Shifts of **4** in benzene- $d_6$  at 333 K. b. GIAO/M06L/6-311+G(2df,p) level of theory. Absolute chemical shift for tetramethylsilane = 361.4. c. the absolute chemical shift is shown in the parentheses. d. average values.

Table S5. Experimental and Theoretical Isotropic <sup>29</sup>Si Chemical Shifts of 6<sub>opt</sub>



	SiMe <sub>3</sub>	Si <sup>2</sup> =Si <sup>1</sup> -Cl	Si <sup>2</sup> =Si <sup>1</sup> -Cl	Si <sup>4</sup> (Si <sub>3</sub> ring)	Si <sup>3</sup> (chlorosilyl)	Note
Experimental <sup>a</sup>	2.9, 3.3,	104.1	48.7	78.2	32.9	TN420_7
	6.1					
Theoretical <sup>b,c</sup>	4.2	97.0	49.4	75.4	38.1	nmr2_TN82a
	(357.2) <sup>d</sup>	(264.4)	(311.9)	(286.0)	(323.3)	

a. Experimental <sup>29</sup>Si Chemical Shifts of **6** in benzene- $d_6$  at 333 K. b. GIAO/M06L/6-311+G(2df,p) level of theory. Absolute chemical shift for tetramethylsilane = 361.4. c. the absolute chemical shift is shown in the parentheses. d. average values.



Figure S24. Experimental UV-vis absorption spectrum of the equilibrium mixture of 4 and 6 in hexane (black) and calculated band positions of  $4_{opt}$  and  $6_{opt}$  at the TD-B3LYP-D3/6-311G(d) level (red and blue).

# Table S6. Transition Energy, Wavelength, and Oscillator Strengths of the Electronic Transition of $4_{opt}$

(The 237<sup>th</sup> orbital is highest occupied orbital shown in Figure S23)

Excited State	1:	Singlet-AU	2.6596 eV	466.17 nm	f=0.0332						
<s**2>=0.000</s**2>		onigiot rio	2.0070 01	100.17 1811	1 010002	Excited State	16:	Singlet-AU	4.9319 eV	251.39 nm	f=0.0005
237 -> 238		0.67896				<s**2>=0.000</s**2>		5			
237 -> 239 This state for ont	imizatio	-0.17174 n and/or second-order	correction			228 -> 238		0.68938			
Total Energy, E(T	D-HF/T	D-KS = -5662.9743	1013 as the 1-particle Pt	noCl density		Excited State	17:	Singlet-AG	4.9464 eV	250.65 nm	f=0.0000
copying the exer	icu sidi		13 the 1-particle ru	loor acrisity.		226 -> 238		-0 10228			
Excited State	2:	Singlet-AG	2.8801 eV	430.48 nm	f=0.0000	227 -> 238		0.68694			
236 -> 238		0.70504				Excited State	18:	Singlet-AU	5.0255 eV	246.71 nm	f=0.0202
Excited State	3:	Singlet-AU	3.0056 eV	412.51 nm	f=0.0162	223 -> 238		0.40022			
237 -> 238		0 16949				223 > 230		0 11984			
237 -> 239		0.67597				Evolted State	10.	Singlet AC	E 02E1 oV	246.24 nm	f 0.0000
Excited State	4:	Singlet-AU	3.6254 eV	341.99 nm	f=0.0096	<s**2>=0.000</s**2>	19:	Singlet-AG	5.0351 eV	240.24 1111	1=0.0000
<s**2>=0.000</s**2>		0 ( 07 ( 0				224 -> 238		-0.18600			
237 -> 240		0.00709				220 -> 230		0.00705			
Excited State <s**2>=0.000</s**2>	5:	Singlet-AG	3.7152 eV	333.72 nm	f=0.0000	Excited State <s**2>=0.000</s**2>	20:	Singlet-AU	5.0715 eV	244.47 nm	f=0.4028
237 -> 241		0.70481				225 -> 238		-0.25689			
E 1 1 01 1	,	01 1 1 1 0	0.0744 14		(	230 -> 240		-0.16019			
<pre>Excited State <s**2>=0.000</s**2></pre>	6:	Singlet-AG	3.8/46 eV	319.99 nm	t=0.0000	236 -> 241 237 -> 242		0.36213			
236 -> 239		0.69880				201 7 242		0.10010			
						Excited State	21:	Singlet-AU	5.0853 eV	243.81 nm	f=0.0392
Excited State	7:	Singlet-AG	4.1861 eV	296.18 nm	f=0.0000	<s**2>=0.000</s**2>		0.4500/			
<s-2>=0.000</s-2>		0 11200				219 -> 238		0.15226			
235 -> 238		0.69584				225 -> 238		-0.37875			
						236 -> 241		-0.11926			
Excited State	8:	Singlet-AU	4.1991 eV	295.26 nm	f=0.0026	237 -> 242		-0.16915			
234 -> 238		0.70535				Excited State	22:	Singlet-AG	5.1078 eV	242.74 nm	f=0.0000
Excited State	0.	Singlet AC	4 272E oV	200.12 nm	f 0.0000	<s**2>=0.000</s**2>		0 10510			
<s**2>=0.000</s**2>	9:	Singlet-AG	4.2/35 eV	290.12 1111	1=0.0000	218 -> 238 221 -> 238		-0.10510			
233 -> 238		0.68739				224 -> 238		0.66031			
235 -> 238		0.11840				226 -> 238		0.16395			
236 -> 240		-0.10203									
Excited State	10.	Singlet ALL	4 2106 oV	207.02 nm	f_0.0012	Excited State	23:	Singlet-AG	5.1488 eV	240.80 nm	f=0.0000
<s**2>=0.000</s**2>	10.	Sillylet-AU	4.3190 80	207.03 1111	1=0.0013	235 -> 239		0.69109			
230 -> 238		-0.35899				Evolted State	24.	Singlet ALL	E 140E	240.24 nm	f 0.000E
231 -> 238		0.19538				<pre><s**2>=0 000</s**2></pre>	24:	Singlet-AU	5.1005 eV	240.20 1111	I=0.0005
						219 -> 238		-0.10107			
Excited State <s**2>=0.000</s**2>	11:	Singlet-AU	4.4516 eV	278.52 nm	f=0.0074	234 -> 239		0.69475			
230 -> 238		-0.30886				Excited State	25:	Singlet-AG	5.1750 eV	239.58 nm	f=0.0000
231 -> 238		0.49899				<s**2>=0.000</s**2>					
232 -> 238		-0.3/3/1				218 -> 238		-0.19/45			
Excited State	12:	Singlet-AU	4.4717 eV	277.27 nm	f=0.0059	220 -> 238		0.64258			
<s**2>=0.000</s**2>						226 -> 238		0.12372			
230 -> 238		0.50949									
231 -> 238		0.44481				Excited State	26:	Singlet-AU	5.1898 eV	238.90 nm	f=0.0031
232 -> 238		0.17234				<5~2>=0.000		0.56210			
Excited State	13:	Singlet-AG	4.5559 eV	272.14 nm	f=0.0000	222 -> 238		-0.37669			
<s**2>=0.000</s**2>											
229 -> 238		0.10870				Excited State	27:	Singlet-AU	5.1938 eV	238.72 nm	f=0.0022
235 -> 236 -> 240		0.67874				<3 2>=0.000 219 -> 238		0.33384			
						222 -> 238		0.56757			
Excited State	14:	Singlet-AU	4.6516 eV	266.54 nm	f=0.0240	223 -> 238		-0.20751			
<5***2>=0.000		0 55002				Excited State	20.	Singlet AC	5 0111 AV	227.02 pm	f_0.0000
230 -> 241 237 -> 242		-0.42495				<s**2>=0.000</s**2>	20.	Sillylet-AG	J.ZITI UV	231.73 1111	1-0.0000
-57 - 272						218 -> 238		0.35523			
Excited State	15:	Singlet-AG	4.6548 eV	266.36 nm	f=0.0000	220 -> 238		0.52265			
<s**2>=0.000</s**2>		0.40440				221 -> 238		0.23219			
229 -> 238 236 -> 210		-0.11101				233 -> 239		0.10324			
200 / 240											

Excited State <s**2>=0.000</s**2>	29:	Singlet-AG	5.2177 eV	237.62 nm	f=0.0000	232 -> 239 237 -> 243		0.24274 -0.32682			
220 -> 238		-0.12864									
233 -> 239		0.42332				Excited State	39:	Singlet-AU	5.5349 eV	224.00 nm	t=0.0018
235 -> 239		0.13669				<s**2>=0.000</s**2>					
237 -> 244		-0.39387				214 -> 238		0.63465			
237 -> 245		-0.29668				219 -> 238		-0.10541			
237 -> 246		-0.16483				237 -> 247		-0.22362			
Excited State	30:	Singlet-AU	5.2547 eV	235.95 nm	f=0.0003	Excited State	40:	Singlet-AG	5.5714 eV	222.54 nm	f=0.0000
<5 2>=0.000		0 50000				<5 2>=0.000		0.44/05			
216 -> 238		0.50300				237 -> 244		-0.44605			
217 -> 238		-0.45883				237 -> 245		0.46699			
						237 -> 246		0.22863			
<pre>Excited State <s**2>=0.000</s**2></pre>	31:	Singlet-AG	5.2555 eV	235.91 nm	t=0.0000	237 -> 251		-0.11452			
218 -> 238		0.48456				Excited State	41:	Singlet-AG	5.5938 eV	221.65 nm	f=0.0000
220 -> 238		-0.35848				<s**2>=0.000</s**2>		5			
233 -> 239		0.26227				229 -> 239		-0.20244			
237 -> 244		0.17618				235 -> 240		0.40339			
237 -> 245		0.12631				235 -> 240		0.52537			
237 -> 243		0.12031				230 -> 242		0.32337			
Excited State	32:	Singlet-AG	5.2592 eV	235.75 nm	f=0.0000	Excited State	42:	Singlet-AU	5.6071 eV	221.12 nm	f=0.0073
<s**2>=0.000</s**2>						<s**2>=0.000</s**2>					
218 -> 238		-0.2/1/1				214 -> 238		0.20388			
220 -> 238		0.20680				234 -> 240		0.39/18			
233 -> 239		0.47753				237 -> 247		0.49449			
237 -> 244		0.29746				237 -> 250		0.12358			
237 -> 245		0.20868									
237 -> 246		0.11740				Excited State <s**2>=0.000</s**2>	43:	Singlet-AG	5.6117 eV	220.94 nm	f=0.0000
Excited State	33:	Singlet-AU	5.3132 eV	233.35 nm	f=0.0009	229 -> 239		0.66507			
<\$**2>=0.000		J				235 -> 240		0 16996			
216 -> 238		0 45422				236 -> 242		0 12094			
217 -> 238		0.51970				200 / 212		0.12071			
217 7 200		0.01770				Excited State	44.	Singlet-ALL	5.6269 eV	220.34 nm	f=0.0124
Excited State	34.	Singlet-ALL	5.3368 eV	232.32 nm	f=0.0165	<s**2>=0.000</s**2>		Singlet No	5.0207 04	220.34 1111	1-0.0124
<pre><s**2>=0.000</s**2></pre>	011	olligiot rio	0.0000 01	LULIUL IIII	1 0.0100	214 -> 238		-0 11033			
22/=0.000		-0 28832				214 -> 230		0.57325			
230 -> 237		0.20037				234 -> 240		-0.36564			
232 -> 237		0.02000				237 -> 247		-0.30304			
Excited State	35:	Singlet-AU	5.3509 eV	231.71 nm	f=0.0007	Excited State	45:	Singlet-AG	5.6392 eV	219.86 nm	f=0.0000
<5 2>=0.000		0.40700				<5 2>=0.000		0.54500			
230 -> 239		-0.13/89				235 -> 240		0.54533			
231 -> 239		0.67966				236 -> 242		-0.43265			
Excited State	36:	Singlet-AU	5.4520 eV	227.41 nm	f=0.0120	Excited State	46:	Singlet-AG	5.6920 eV	217.82 nm	f=0.0000
<s**2>=0.000</s**2>						<s**2>=0.000</s**2>					
230 -> 239		0.30533				213 -> 238		0.69754			
232 -> 239		0.13337									
237 -> 243		0.60911				Excited State	47:	Singlet-AU	5.7024 eV	217.43 nm	f=0.0012
						<s**2>=0.000</s**2>		-			
Excited State	37:	Singlet-AG	5.4572 eV	227.19 nm	f=0.0000	212 -> 238		0.69660			
<s**2>=0.000</s**2>		J									
215 -> 238		0.69902				Excited State	48:	Singlet-AG	5.7406 eV	215.98 nm	f=0.0000
						<s**2>=0.000</s**2>					
Excited State	38:	Sinalet-AU	5.4674 eV	226.77 nm	f=0.0147	233 -> 240		-0.45825			
<s**2>=0.000</s**2>	50.	olingiot no	0.1071 01			234 -> 241		0.52326			
230 -> 230		0.53689				201 / 211		1.02020			
231 -> 239		0.15871									

# Table S7. Transition Energy, Wavelength, and Oscillator Strengths of the Electronic Transition of $6_{opt}$

(The 237<sup>th</sup> orbital is highest occupied orbital)

Excited State 1:	Singlet-A	2.8294 eV	438.21 nm	f=0.0119	Excited State	12:	Singlet-A	4.7404 eV	261.55 nm	f=0.0779
<s**2>=0.000</s**2>					<s**2>=0.000</s**2>					
235 -> 238	-0.10313				232 -> 238		0.58426			
237 -> 238	0.55576				233 -> 238		-0.22881			
237 -> 239	0.41018				235 -> 239		-0.20115			
Total Energy E(TD LE)	on and/or second-order corr	rection.			236 -> 240		-0.11054			
Conving the excited sta	1D-N3 = -3002.9003376 te density for this state as the	9 ne 1₌narticle R	hoCl density		230 -> 241		-0.13764			
Copying the excited sta	te density for this state as th	ic r-particic r	anoor density.		Excited State	13.	Singlet-A	4.8290 eV	256 75 nm	f=0.0029
Excited State 2:	Singlet-A	3.1085 eV	398.86 nm	f=0.0270	<s**2>=0.000</s**2>	10.	Singlet H	4.0270 61	200.75 1111	1-0.0027
<s**2>=0.000</s**2>					231 -> 238		0.66840			
235 -> 239	0.10704				235 -> 239		-0.11868			
236 -> 238	-0.11310				236 -> 241		-0.12109			
237 -> 238	-0.37316									
237 -> 239	0.55405				Excited State	14:	Singlet-A	4.9788 eV	249.02 nm	f=0.0933
					<s**2>=0.000</s**2>					
Excited State 3:	Singlet-A	3.4281 eV	361.67 nm	f=0.0118	229 -> 238		0.11948			
<s**2>=0.000</s**2>	0.40740				230 -> 238		-0.31436			
235 -> 238	-0.12/10				234 -> 239		-0.14263			
230 -> 230	0.00975				233 -> 240		0.33190			
237 -> 240	0.11911				230 -> 240		0.11/93			
Excited State 4:	Singlet-A	3.6728 eV	337.57 nm	f=0.0041	237 -> 243		0.10112			
<s**2>=0.000</s**2>	oingiotri	0.0720 01	007107 1111	1 0.0011	Excited State	15:	Singlet-A	4.9925 eV	248.34 nm	f=0.0229
236 -> 238	-0.11450				<s**2>=0.000</s**2>		5.0			
236 -> 239	-0.21754				230 -> 238		0.58306			
237 -> 240	0.64817				234 -> 239		0.14760			
					235 -> 240		0.31559			
Excited State 5:	Singlet-A	3.8813 eV	319.44 nm	f=0.0282						
<s**2>=0.000</s**2>					Excited State	16:	Singlet-A	4.9980 eV	248.07 nm	f=0.0014
235 -> 238	-0.47416				<s**2>=0.000</s**2>					
236 -> 238	-0.10104				230 -> 238		-0.19593			
236 -> 239	0.49811				234 -> 239		0.67251			
Evolted State /	Cinglet A	2.071/ aV	212.17	6 0 0 2 / 2	Evolted State	17.	Cinglet A	E 0004 a)/	3/3/1 mm	£ 0.0020
EXCILED SIBLE 0:	Singlet-A	3.9/10 eV	312.17 1111	1=0.0262	EXCILED SIBLE	17:	Singlet-A	5.0894 eV	243.01 1111	1=0.0030
235 -> 238	0 44981				22 -0.000		0 11075			
235 -> 239	-0 25459				227 > 230		0.68518			
236 -> 239	0.39936				200 / 207		0.00010			
237 -> 238	0.11617				Excited State	18:	Singlet-A	5.1050 eV	242.87 nm	f=0.0006
237 -> 240	0.17884				<s**2>=0.000</s**2>					
					229 -> 238		0.59390			
Excited State 7:	Singlet-A	4.3211 eV	286.92 nm	f=0.0086	230 -> 238		0.11099			
<s**2>=0.000</s**2>					232 -> 239		-0.32523			
235 -> 239	0.13699									
237 -> 241	0.68537				Excited State	19:	Singlet-A	5.1132 eV	242.48 nm	f=0.0027
Evolted State 0	Cinglet A	4 4000	07/10 mm	6 0 0000	<5~2>=0.000		0 21220			
EXCILED STATE 8:	Singlet-A	4.4902 eV	276.12 nm	T=0.0230	229 -> 238		0.31238			
<3 2>=0.000	0 11710				232 -> 239		0.01292			
232 -> 230	-0.43612				Excited State	20.	Singlet-A	51707 eV	239.78 nm	f=0.0312
236 -> 240	0.48258				<s**2>=0.000</s**2>	20.	olingiot i t	0.1707 00	207.70 1111	1 0.0012
237 -> 241	0.10130				231 -> 239		0.67103			
					236 -> 241		0.15682			
Excited State 9:	Singlet-A	4.5790 eV	270.77 nm	f=0.0479						
<s**2>=0.000</s**2>					Excited State	21:	Singlet-A	5.2568 eV	235.85 nm	f=0.0182
232 -> 238	0.12873				<s**2>=0.000</s**2>					
234 -> 238	0.59681				236 -> 241		-0.17062			
235 -> 239	0.13107				237 -> 242		0.42620			
236 -> 240	0.28444				237 -> 243		0.40154			
Excited State 10:	Singlet A	4.6100 oV	260.42 nm	f_0 1294	237 -> 244		-0.14040			
EXCILCU SIZIE 10.	Sillylet-A	4.0190 81	200.42 1111	1=0.1204	237 -> 243		0.16943			
231 -> 238	-0 15323				237 -> 240		-0.10027			
232 -> 238	-0.29016				Excited State	22:	Singlet-A	5.3215 eV	232.99 nm	f=0.0294
234 -> 238	0.36315				<s**2>=0.000</s**2>		5.0			
235 -> 239	-0.27410				224 -> 238		0.11823			
235 -> 240	0.15939				226 -> 238		-0.19520			
236 -> 240	-0.32784				227 -> 238		0.20345			
236 -> 241	-0.11324				228 -> 238		0.54467			
	<b>a</b>				236 -> 241		-0.25899			
Excited State 11:	Singlet-A	4.7169 eV	262.85 nm	t=0.0219	Europa de Cristi	22	<u> </u>	F 0570	001.40	6 0 0 105
<5 2>=0.000	0 14710				Excited State	23:	Singlet-A	5.3579 eV	231.40 nm	1=0.0493
232 -> 238 232 -> 238	U. 10 / 18 0.650/7				<> 2>=0.000 22>=0.000 222 220 222 222 222 222 222 222 222		-0 13009			
233 -> 230	-0 10812				222 -> 238		0.17550			
200 / 207					227 -> 238		-0.33953			
							· · · · · · · · · · · · · · · · · · ·			

228 -> 238		0.39113				229 -> 239		-0.21542			
230 -> 239		0.16730				234 -> 240		0.62294			
236 -> 241		0.30798									
						Excited State	33:	Singlet-A	5.5728 eV	222.48 nm	f=0.0008
Excited State	24.	Singlet-A	5.3723 eV	230 78 nm	f=0.0327	<\$**2>=0.000					
<s**2>-0.000</s**2>	2.11	oingiotri	0.0720 01	2001/0 1111	1 010021	220 -> 238		-0 24675			
22 = 0.000		0.24705				220 > 230		0.50277			
223 -> 230		0.24703				221 -2 230		0.30277			
227 -> 238		0.43905				222 -> 238		-0.34434			
230 -> 239		0.34197				224 -> 238		-0.13/20			
236 -> 241		0.20959									
237 -> 242		0.15964				Excited State	34:	Singlet-A	5.5845 eV	222.02 nm	f=0.0096
						<s**2>=0.000</s**2>					
Excited State	25:	Singlet-A	5.3798 eV	230.46 nm	f=0.0175	232 -> 240		-0.12341			
<s**2>=0.000</s**2>		° .				235 -> 241		-0.11700			
225 -> 238		-0 24750				237 -> 243		0 31238			
226 -> 238		-0.10062				237 -> 244		0.44435			
220 -> 230		0.10002				237 -> 244		0.11133			
227 -> 230		-0.10094				237 -> 240		0.29062			
229 -> 239		-0.11187				237 -> 248		0.17765			
230 -> 239		0.52/51									
236 -> 241		-0.21771				Excited State	35:	Singlet-A	5.5998 eV	221.41 nm	f=0.0016
						<s**2>=0.000</s**2>					
Excited State	26:	Singlet-A	5.4182 eV	228.83 nm	f=0.0225	220 -> 238		-0.19042			
<s**2>=0.000</s**2>		-				221 -> 238		0.29492			
225 -> 238		0 44183				222 -> 238		0 53253			
226 -> 238		0 15/61				222 - 200		0 15381			
220 > 230		0.10270				223 > 230		0.16101			
227 -> 230		-0.10270				224 -> 230		0.10171			
230 -> 239		0.17462									
236 -> 241		-0.150/1				Excited State	36:	Singlet-A	5.6259 eV	220.38 nm	t=0.0035
237 -> 242		-0.29685				<s**2>=0.000</s**2>					
237 -> 243		0.20069				219 -> 238		0.22338			
237 -> 245		-0.13121				220 -> 238		0.25045			
						231 -> 240		0.15327			
Excited State	27.	Singlet-A	5.4355 eV	228.10 nm	f=0.0282	232 -> 240		0 50023			
<s**2>=0.000</s**2>	27.	Singlet M	0.4000 0.4	220.10 1111	1-0.0202	232 -> 240		0.12024			
175 . 120		0 22742				233 -> 240		0.12724			
220 -> 230		-0.33703				237 -> 244		0.13903			
226 -> 238		0.43156									
227 -> 238		0.28293				Excited State	37:	Singlet-A	5.6441 eV	219.67 nm	t=0.0082
230 -> 239		0.10945				<s**2>=0.000</s**2>					
237 -> 242		-0.15740				219 -> 238		0.61858			
237 -> 243		0.18101				232 -> 240		-0.24289			
237 -> 244		-0.10193									
						Excited State	38:	Singlet-A	5.6499 eV	219.45 nm	f=0.0113
Excited State	28·	Singlet-A	54482 eV	227.57 nm	f=0 1172	Excited State	38:	Singlet-A	5.6499 eV	219.45 nm	f=0.0113
Excited State	28:	Singlet-A	5.4482 eV	227.57 nm	f=0.1172	Excited State <s**2>=0.000</s**2>	38:	Singlet-A	5.6499 eV	219.45 nm	f=0.0113
Excited State <s**2>=0.000</s**2>	28:	Singlet-A	5.4482 eV	227.57 nm	f=0.1172	Excited State <s**2>=0.000 218 -&gt; 238 210 -&gt; 238</s**2>	38:	Singlet-A	5.6499 eV	219.45 nm	f=0.0113
Excited State <s**2>=0.000 225 -&gt; 238</s**2>	28:	Singlet-A 0.12299	5.4482 eV	227.57 nm	f=0.1172	Excited State <s**2>=0.000 218 -&gt; 238 219 -&gt; 238</s**2>	38:	Singlet-A -0.31698 -0.13618	5.6499 eV	219.45 nm	f=0.0113
Excited State <s**2>=0.000 225 -&gt; 238 226 -&gt; 238</s**2>	28:	Singlet-A 0.12299 0.40380	5.4482 eV	227.57 nm	f=0.1172	Excited State <s**2>=0.000 218 -&gt; 238 219 -&gt; 238 220 -&gt; 238</s**2>	38:	Singlet-A -0.31698 -0.13618 0.46518	5.6499 eV	219.45 nm	f=0.0113
Excited State <s**2>=0.000 225 -&gt; 238 226 -&gt; 238 229 -&gt; 239</s**2>	28:	Singlet-A 0.12299 0.40380 -0.21172	5.4482 eV	227.57 nm	f=0.1172	Excited State <s**2>=0.000 218 -&gt; 238 219 -&gt; 238 220 -&gt; 238 221 -&gt; 238</s**2>	38:	Singlet-A -0.31698 -0.13618 0.46518 0.27141	5.6499 eV	219.45 nm	f=0.0113
Excited State <s**2>=0.000 225 -&gt; 238 226 -&gt; 238 229 -&gt; 239 236 -&gt; 241</s**2>	28:	Singlet-A 0.12299 0.40380 -0.21172 -0.17410	5.4482 eV	227.57 nm	f=0.1172	Excited State <s**2>=0.000 218 -&gt; 238 219 -&gt; 238 220 -&gt; 238 221 -&gt; 238 232 -&gt; 240</s**2>	38:	Singlet-A -0.31698 -0.13618 0.46518 0.27141 -0.21428	5.6499 eV	219.45 nm	f=0.0113
Excited State <s**2>=0.000 225 -&gt; 238 226 -&gt; 238 229 -&gt; 239 236 -&gt; 241 237 -&gt; 242</s**2>	28:	Singlet-A 0.12299 0.40380 -0.21172 -0.17410 0.20221	5.4482 eV	227.57 nm	f=0.1172	Excited State <s**2>=0.000 218 -&gt; 238 219 -&gt; 238 220 -&gt; 238 221 -&gt; 238 232 -&gt; 240</s**2>	38:	Singlet-A -0.31698 -0.13618 0.46518 0.27141 -0.21428	5.6499 eV	219.45 nm	f=0.0113
Excited State <s**2>=0.000 225 -&gt; 238 226 -&gt; 238 229 -&gt; 239 236 -&gt; 241 237 -&gt; 242 237 -&gt; 243</s**2>	28:	Singlet-A 0.12299 0.40380 -0.21172 -0.17410 0.20221 -0.30213	5.4482 eV	227.57 nm	f=0.1172	Excited State <s**2>=0.000 218 -&gt; 238 219 -&gt; 238 220 -&gt; 238 232 -&gt; 240 Excited State</s**2>	38: 39:	Singlet-A -0.31698 -0.13618 0.46518 0.27141 -0.21428 Singlet-A	5.6499 eV 5.6580 eV	219.45 nm 219.13 nm	f=0.0113 f=0.0023
Excited State <s**2>=0.000 225 -&gt; 238 226 -&gt; 238 229 -&gt; 239 236 -&gt; 241 237 -&gt; 242 237 -&gt; 243 237 -&gt; 244</s**2>	28:	Singlet-A 0.12299 0.40380 -0.21172 -0.121172 -0.20221 -0.30213 0.19641	5.4482 eV	227.57 nm	f=0.1172	Excited State <\$**2>=0.000 218 -> 238 219 -> 238 220 -> 238 221 -> 238 232 -> 240 Excited State <\$**2>=0.000	38: 39:	Singlet-A -0.31698 -0.13618 0.46518 0.27141 -0.21428 Singlet-A	5.6499 eV 5.6580 eV	219.45 nm 219.13 nm	f=0.0113 f=0.0023
Excited State <\$**2>=0.000 225 -> 238 226 -> 238 229 -> 239 236 -> 241 237 -> 242 237 -> 243 237 -> 244	28:	Singlet-A 0.12299 0.40380 -0.21172 -0.17410 0.20221 -0.30213 0.19641	5.4482 eV	227.57 nm	f=0.1172	Excited State <\$**2>=0.000 218 -> 238 219 -> 238 220 -> 238 232 -> 240 Excited State <\$**2>=0.000 219 -> 238	38: 39:	Singlet-A -0.31698 -0.13618 0.46518 0.27141 -0.21428 Singlet-A -0.12110	5.6499 eV 5.6580 eV	219.45 nm 219.13 nm	f=0.0113 f=0.0023
Excited State <s**2>=0.000 225 -&gt; 238 226 -&gt; 238 229 -&gt; 239 236 -&gt; 241 237 -&gt; 242 237 -&gt; 243 237 -&gt; 244 Excited State</s**2>	28:	Singlet-A 0.12299 0.40380 -0.21172 -0.17410 0.20221 -0.30213 0.19641 Singlet-A	5.4482 eV	227.57 nm	f=0.1172	Excited State <\$**2>=0.000 218 -> 238 219 -> 238 220 -> 238 232 -> 240 Excited State <\$**2>=0.000 219 -> 238 235 -> 241	38: 39:	Singlet-A -0.31698 -0.13618 0.46518 0.27141 -0.21428 Singlet-A -0.12110 -0.21434	5.6499 eV 5.6580 eV	219.45 nm 219.13 nm	f=0.0113 f=0.0023
Excited State <s**2>=0.000 225 -&gt; 238 226 -&gt; 238 229 -&gt; 239 236 -&gt; 241 237 -&gt; 242 237 -&gt; 243 Excited State</s**2>	28: 29:	Singlet-A 0.12299 0.40380 -0.21172 -0.17410 0.20221 0.30213 0.30213 0.19641	5.4482 eV 5.4948 eV	227.57 nm 225.64 nm	f=0.1172 f=0.0120	Excited State <\$**2>=0.000 218 -> 238 219 -> 238 220 -> 238 232 -> 240 Excited State <\$**2>=0.000 219 -> 238 235 -> 241 237 -> 242	38: 39:	Singlet-A -0.31698 -0.13618 0.46518 0.27141 -0.21428 Singlet-A -0.12110 -0.21434 -0.2724	5.6499 eV 5.6580 eV	219.45 nm 219.13 nm	f=0.0113 f=0.0023
Excited State <\$**2>=0.000 225 -> 238 226 -> 238 229 -> 239 236 -> 241 237 -> 242 237 -> 243 237 -> 244 Excited State <\$**2>=0.000 222 -> 220	28: 29:	Singlet-A 0.12299 0.40380 -0.21172 -0.17410 0.20221 -0.30213 0.19641 Singlet-A 0.26757	5.4482 eV 5.4948 eV	227.57 nm 225.64 nm	f=0.1172 f=0.0120	Excited State <\$**2>=0.000 218 -> 238 219 -> 238 220 -> 238 232 -> 240 Excited State <\$**2>=0.000 219 -> 238 235 -> 241 237 -> 242 237 -> 244	38: 39:	Singlet-A -0.31698 -0.13618 0.46518 0.27141 -0.21428 Singlet-A -0.12110 -0.21434 -0.27924 0.11001	5.6499 eV 5.6580 eV	219.45 nm 219.13 nm	f=0.0113 f=0.0023
Excited State <s**2>=0.000 225 -&gt; 238 226 -&gt; 238 229 -&gt; 239 236 -&gt; 241 237 -&gt; 242 237 -&gt; 244 Excited State <s**2>=0.000 223 -&gt; 239 223 -&gt; 238</s**2></s**2>	28: 29:	Singlet-A 0.12299 0.40380 -0.21172 -0.17410 0.20221 -0.30213 0.19641 Singlet-A 0.26757 0.5707	5.4482 eV 5.4948 eV	227.57 nm 225.64 nm	f=0.1172 f=0.0120	Excited State <s**2>=0.000 218 -&gt; 238 220 -&gt; 238 221 -&gt; 238 232 -&gt; 240 Excited State <s**2>=0.000 219 -&gt; 238 235 -&gt; 241 237 -&gt; 242 237 -&gt; 2</s**2></s**2>	38:	Singlet-A -0.31698 -0.13618 0.46518 0.27141 -0.21428 Singlet-A -0.12110 -0.21434 -0.27924 0.11091 0.2037	5.6499 eV 5.6580 eV	219.45 nm 219.13 nm	f=0.0113 f=0.0023
Excited State <s**2>=0.000 225 -&gt; 238 226 -&gt; 238 229 -&gt; 239 236 -&gt; 241 237 -&gt; 242 237 -&gt; 243 237 -&gt; 244 Excited State <s**2>=0.000 223 -&gt; 238 229 -&gt; 239 229 -&gt; 239</s**2></s**2>	28: 29:	Singlet-A 0.12299 0.40380 -0.21172 -0.17410 0.20221 -0.30213 0.19641 Singlet-A 0.26757 0.57807 0.2025	5.4482 eV 5.4948 eV	227.57 nm 225.64 nm	f=0.1172 f=0.0120	Excited State <\$**2>=0.000 218 -> 238 219 -> 238 220 -> 238 232 -> 240 Excited State <\$**2>=0.000 219 -> 238 235 -> 241 237 -> 244 237 -> 244 237 -> 244 237 -> 244	38:	Singlet-A -0.31698 -0.13618 0.46518 0.27141 -0.21428 Singlet-A -0.12110 -0.21434 -0.27924 0.11091 0.38376 0.2727	5.6499 eV 5.6580 eV	219.45 nm 219.13 nm	f=0.0113 f=0.0023
Excited State <s**2>=0.000 225 -&gt; 238 226 -&gt; 238 229 -&gt; 239 236 -&gt; 241 237 -&gt; 242 237 -&gt; 243 Excited State <s**2>=0.000 223 -&gt; 238 229 -&gt; 239 234 -&gt; 240</s**2></s**2>	28: 29:	Singlet-A 0.12299 0.40380 -0.21172 -0.17410 0.20221 -0.30213 0.19641 Singlet-A 0.26757 0.57807 0.18565 0.40741	5.4482 eV 5.4948 eV	227.57 nm 225.64 nm	f=0.1172 f=0.0120	Excited State <\$**2>=0.000 218 -> 238 219 -> 238 220 -> 238 232 -> 240 Excited State <\$**2>=0.000 219 -> 238 235 -> 241 237 -> 244 237 -> 245 237 -> 245 237 -> 245	38:	Singlet-A -0.31698 -0.13618 0.27141 -0.21428 Singlet-A -0.12110 -0.21434 -0.27924 0.11091 0.38376 -0.33587 -0.33587	5.6499 eV 5.6580 eV	219.45 nm 219.13 nm	f=0.0113 f=0.0023
Excited State <s**2>=0.000 225 -&gt; 238 226 -&gt; 238 229 -&gt; 239 236 -&gt; 241 237 -&gt; 242 237 -&gt; 243 237 -&gt; 244 Excited State <s**2>=0.000 223 -&gt; 238 229 -&gt; 239 234 -&gt; 243 237 -&gt; 243</s**2></s**2>	28: 29:	Singlet-A 0.12299 0.40380 -0.21172 -0.17410 0.20221 -0.30213 0.19641 Singlet-A 0.26757 0.57807 0.18565 -0.10711	5.4482 eV 5.4948 eV	227.57 nm 225.64 nm	f=0.1172 f=0.0120	Excited State <\$**2>=0.000 218 -> 238 220 -> 238 221 -> 238 232 -> 240 Excited State <\$**2>=0.000 219 -> 238 235 -> 241 237 -> 242 237 -> 245 237 -> 246 237 -> 246 237 -> 247	38: 39:	Singlet-A -0.31698 -0.13618 0.46518 0.27141 -0.21428 Singlet-A -0.12110 -0.21434 -0.27924 0.11091 0.38376 -0.33587 0.11529	5.6499 eV 5.6580 eV	219.45 nm 219.13 nm	f=0.0113 f=0.0023
Excited State <s**2>=0.000 225 -&gt; 238 226 -&gt; 238 229 -&gt; 239 236 -&gt; 241 237 -&gt; 242 237 -&gt; 243 237 -&gt; 244 Excited State <s**2>=0.000 223 -&gt; 238 229 -&gt; 239 234 -&gt; 240 237 -&gt; 243</s**2></s**2>	28: 29:	Singlet-A 0.12299 0.40380 -0.21172 -0.17410 0.20221 -0.30213 0.19641 Singlet-A 0.26757 0.57807 0.18565 -0.10711	5.4482 eV 5.4948 eV	227.57 nm 225.64 nm	f=0.1172 f=0.0120	Excited State <s**2>=0.000 218 -&gt; 238 220 -&gt; 238 221 -&gt; 238 232 -&gt; 240 Excited State <s**2>=0.000 219 -&gt; 238 235 -&gt; 241 237 -&gt; 244 237 -&gt; 244 237 -&gt; 244 237 -&gt; 244 237 -&gt; 244 237 -&gt; 244</s**2></s**2>	38: 39:	Singlet-A -0.31698 -0.13618 0.46518 0.27141 -0.21428 Singlet-A -0.12110 -0.21434 -0.27924 0.11091 0.38376 -0.33587 0.11529 0.11496	5.6499 eV 5.6580 eV	219.45 nm 219.13 nm	f=0.0113 f=0.0023
Excited State <s**2>=0.000 225 -&gt; 238 226 -&gt; 238 229 -&gt; 239 236 -&gt; 241 237 -&gt; 242 237 -&gt; 243 237 -&gt; 244 Excited State <s**2>=0.000 223 -&gt; 238 229 -&gt; 239 234 -&gt; 240 237 -&gt; 243 Excited State</s**2></s**2>	28: 29: 30:	Singlet-A 0.12299 0.40380 -0.21172 -0.17410 0.20221 -0.30213 0.19641 Singlet-A 0.26757 0.57807 0.18565 -0.10711 Singlet-A	5.4482 eV 5.4948 eV 5.5149 eV	227.57 nm 225.64 nm 2224.82 nm	f=0.1172 f=0.0120 f=0.0159	Excited State <\$**2>=0.000 218 -> 238 219 -> 238 220 -> 238 232 -> 240 Excited State <\$**2>=0.000 219 -> 238 235 -> 241 237 -> 245 237 -> 245 237 -> 248 237 -> 250	38: 39:	Singlet-A -0.31698 -0.13618 0.27141 -0.21428 Singlet-A -0.12110 -0.21434 -0.27924 0.11091 0.38376 -0.33587 0.11529 0.11496 0.11578	5.6499 eV 5.6580 eV	219.45 nm 219.13 nm	f=0.0113 f=0.0023
Excited State <s**2>=0.000 225 -&gt; 238 226 -&gt; 238 229 -&gt; 239 236 -&gt; 241 237 -&gt; 242 237 -&gt; 243 237 -&gt; 244 Excited State <s**2>=0.000 233 -&gt; 238 229 -&gt; 239 234 -&gt; 243 Excited State <s**2>=0.000</s**2></s**2></s**2>	28: 29: 30:	Singlet-A 0.12299 0.40380 -0.21172 -0.17410 0.20221 -0.30213 0.19641 Singlet-A 0.26757 0.57807 0.18565 -0.10711	5.4482 eV 5.4948 eV 5.5149 eV	227.57 nm 225.64 nm 224.82 nm	f=0.1172 f=0.0120 f=0.0159	Excited State <\$**2>=0.000 218 -> 238 219 -> 238 220 -> 238 232 -> 240 Excited State <\$**2>=0.000 219 -> 238 235 -> 241 237 -> 242 237 -> 245 237 -> 245 237 -> 247 237 -> 248 237 -> 248 237 -> 248 237 -> 250	38: 39:	Singlet-A -0.31698 -0.13618 0.27141 -0.21428 Singlet-A -0.12110 -0.21434 -0.27924 0.11091 0.38376 -0.33587 0.11529 0.11496 0.11578	5.6499 eV 5.6580 eV	219.45 nm 219.13 nm	f=0.0113 f=0.0023
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Excited State <\$**2>=0.000 225 -> 238 226 -> 238 229 -> 239 236 -> 241 237 -> 242 237 -> 243 237 -> 244 Excited State <\$**2>=0.000 223 -> 238 229 -> 239 234 -> 240 237 -> 243 Excited State <\$**2>=0.000 223 -> 243	28: 29: 30:	Singlet-A 0.12299 0.40380 -0.21172 -0.17410 0.20221 -0.30213 0.19641 Singlet-A 0.26757 0.57807 0.18565 -0.10711 Singlet-A -0.18300 0.44787	5.4482 eV 5.4948 eV 5.5149 eV	227.57 nm 225.64 nm 2224.82 nm	f=0.1172 f=0.0120 f=0.0159	Excited State <\$**2>=0.000 218 -> 238 219 -> 238 220 -> 238 232 -> 240 Excited State <\$**2>=0.000 219 -> 238 235 -> 241 237 -> 242 237 -> 245 237 -> 244 237 -> 245 237 -> 248 237 -> 2	<ul><li>38:</li><li>39:</li><li>40:</li></ul>	Singlet-A -0.31698 -0.13618 0.27141 -0.21428 Singlet-A -0.12110 -0.21434 -0.27924 0.11091 0.38376 -0.33587 0.11529 0.11496 0.11578 Singlet-A	5.6499 eV 5.6580 eV 5.7148 eV	219.45 nm 219.13 nm 216.95 nm	f=0.0113 f=0.0023 f=0.0042
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Excited State <\$**2>=0.000 225 -> 238 226 -> 238 229 -> 239 236 -> 241 237 -> 242 237 -> 243 237 -> 244 Excited State <\$**2>=0.000 223 -> 238 229 -> 239 234 -> 240 237 -> 243 Excited State <\$**2>=0.000 222 -> 238 223 -> 238 224 -> 238 224 -> 238 226 -> 238 227 -> 238 228 -> 238 238 -> 238 238 -> 238 -> 238 238 -> 23	28: 29: 30:	Singlet-A 0.12299 0.40380 -0.21172 -0.17410 0.20221 -0.30213 0.19641 Singlet-A 0.26757 0.57807 0.18565 -0.10711 Singlet-A -0.18300 0.44787 0.38222 -0.11551 0.11551	5.4482 eV 5.4948 eV 5.5149 eV	227.57 nm 225.64 nm 224.82 nm	f=0.1172 f=0.0120 f=0.0159	Excited State <\$**2>=0.000 218 -> 238 220 -> 238 221 -> 238 232 -> 240 Excited State <\$**2>=0.000 219 -> 238 235 -> 241 237 -> 244 237 -> 244 237 -> 244 237 -> 244 237 -> 248 237 -> 248 238 -> 248 -> 248 248 ->	<ul><li>38:</li><li>39:</li><li>40:</li></ul>	Singlet-A -0.31698 -0.13618 0.46518 0.27141 -0.21428 Singlet-A -0.12110 -0.21434 -0.27924 0.11091 0.38376 -0.33587 0.11529 0.11496 0.11578 Singlet-A 0.14424 0.23376 0.52346	5.6499 eV 5.6580 eV 5.7148 eV	219.45 nm 219.13 nm 216.95 nm	f=0.0113 f=0.0023 f=0.0042
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Excited State <s**2>=0.000 225 -&gt; 238 226 -&gt; 238 229 -&gt; 239 236 -&gt; 241 237 -&gt; 242 237 -&gt; 243 Excited State <s**2>=0.000 223 -&gt; 238 229 -&gt; 239 234 -&gt; 243 Excited State <s**2>=0.000 222 -&gt; 238 223 -&gt; 238 224 -&gt; 243 Excited State <s**2>=0.000 222 -&gt; 238 224 -&gt; 238 226 -&gt; 238 227 -&gt; 238 228 -&gt; 238 226 -&gt; 238 228 -&gt; 238 229 -&gt; 239 237 -&gt; 244</s**2></s**2></s**2></s**2>	28: 29: 30:	Singlet-A 0.12299 0.40380 -0.21172 -0.17410 0.20221 -0.30213 0.19641 Singlet-A 0.26757 0.57807 0.57807 0.18565 -0.10711 Singlet-A -0.18300 0.44787 0.38222 -0.11551 -0.11574 -0.11574 -0.1239	5.4482 eV 5.4948 eV 5.5149 eV	227.57 nm 225.64 nm 224.82 nm	f=0.1172 f=0.0120	Excited State <\$**2>=0.000 218 -> 238 219 -> 238 220 -> 238 232 -> 240 Excited State <\$**2>=0.000 219 -> 238 235 -> 241 237 -> 242 237 -> 244 237 -> 245 237 -> 244 237 -> 248 237 -> 248 238 -> 248 249 -> 248 -> 248 249 -> 248 -> 248 -> 248 -> 248 -> 248 -> 248 -> 248 -> 248 -> 248 -> 248 -> 248 -> 2	<ul><li>38:</li><li>39:</li><li>40:</li></ul>	Singlet-A -0.31698 -0.13618 0.27141 -0.21428 Singlet-A -0.12110 -0.21434 -0.27924 0.11091 0.38376 -0.33587 0.11529 0.11496 0.11578 Singlet-A 0.14424 0.23376 0.52346 -0.52346 -0.12278 0.20051	5.6499 eV 5.6580 eV 5.7148 eV	219.45 nm 219.13 nm 216.95 nm	f=0.0113 f=0.0023 f=0.0042
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Excited State <\$**2>=0.000 225 -> 238 229 -> 239 236 -> 241 237 -> 242 237 -> 243 237 -> 244 Excited State <\$**2>=0.000 223 -> 238 229 -> 239 234 -> 240 237 -> 243 Excited State <\$**2>=0.000 222 -> 238 226 -> 238 227 -> 238 226 -> 238 226 -> 238 227 -> 238 227 -> 238 228 -> 238 229 -> 239 234 -> 240	28: 29: 30: 31:	Singlet-A 0.12299 0.40380 -0.21172 -0.17410 0.20211 -0.30213 0.19641 Singlet-A 0.26757 0.57807 0.18565 -0.10711 Singlet-A -0.18300 0.44787 0.38222 -0.11551 -0.11574 -0.15239 -0.11574 -0.15239 -0.11574 -0.15239 -0.11574 -0.15239 -0.11574 -0.15239 -0.17387 Singlet-A	5.4482 eV 5.4948 eV 5.5149 eV 5.5304 eV	227.57 nm 225.64 nm 2224.82 nm 2224.19 nm	f=0.1172 f=0.0120 f=0.0159	Excited State <\$**2>=0.000 218 -> 238 220 -> 238 221 -> 238 232 -> 240 Excited State <\$**2>=0.000 219 -> 238 235 -> 241 237 -> 242 237 -> 242 237 -> 244 237 -> 248 237 -> 248 219 -> 238 216 -> 238 218 -> 238 219 -> 238 233 -> 240 237 -> 248 219 -> 238 219 -> 238 233 -> 240 237 -> 248 237 -> 248 218 -> 238 219 -> 238 233 -> 240 237 -> 244 237 -> 248 237 -> 248 218 -> 238 219 -> 238 233 -> 240 237 -> 244 237 -> 248 237 -> 248 238 -> 238 237 -> 248 238 -> 238 237 -> 248 237 -> 248 238 -> 238 237 -> 248 237 -> 248 237 -> 248 237 -> 2	<ul><li>38:</li><li>39:</li><li>40:</li><li>41:</li></ul>	Singlet-A -0.31698 -0.13618 0.46518 0.27141 -0.21428 Singlet-A -0.12110 -0.21434 -0.27924 0.11091 0.38376 -0.33587 0.11529 0.11496 0.11578 Singlet-A 0.14424 0.23376 0.52346 -0.12278 0.23051 -0.12144 0.0391 -0.12245 Singlet-A	5.6499 eV 5.6580 eV 5.7148 eV	219.45 nm 219.13 nm 216.95 nm	f=0.0113 f=0.0023 f=0.0042
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Excited State <\$**2>=0.000 225 -> 238 229 -> 239 236 -> 241 237 -> 242 237 -> 243 237 -> 244 Excited State <\$**2>=0.000 223 -> 238 229 -> 239 234 -> 240 237 -> 243 Excited State <\$**2>=0.000 222 -> 238 224	28: 29: 30: 31:	Singlet-A 0.12299 0.40380 -0.21172 -0.17410 0.20221 -0.30213 0.19641 Singlet-A 0.26757 0.57807 0.57807 0.18565 -0.10711 Singlet-A -0.18300 0.44787 0.38222 -0.11551 -0.11574 -0.15239 -0.11574 -0.15239 -0.11574 -0.15239 -0.11574 -0.15239 -0.11574 -0.15239 -0.17387 Singlet-A	5.4482 eV 5.4948 eV 5.5149 eV 5.5304 eV	227.57 nm 225.64 nm 2224.82 nm 2224.19 nm	f=0.1172 f=0.0120 f=0.0159	Excited State <\$**2>=0.000 218 -> 238 219 -> 238 220 -> 238 232 -> 240 Excited State <\$**2>=0.000 219 -> 238 235 -> 240 237 -> 244 237 -> 245 237 -> 245 237 -> 244 237 -> 245 237 -> 248 237 -> 248 237 -> 248 237 -> 248 237 -> 248 237 -> 248 237 -> 248 216 -> 238 216 -> 238 218 -> 238 219 -> 238 220 -> 238 233 -> 240 237 -> 244 237 -> 246 Excited State <\$**2>=0.000 215 -> 238 233 -> 240 237 -> 246 Excited State <\$**2>=0.000 217 -> 238 232 -> 240 232 -> 240 233 -> 240 234 -> 240 237 -> 240 240 -> 240 241 -> 240	<ul><li>38:</li><li>39:</li><li>40:</li><li>41:</li></ul>	Singlet-A -0.31698 -0.13618 0.27141 -0.21428 Singlet-A -0.12110 -0.21434 -0.27924 0.11091 0.38376 -0.33587 0.11529 0.11496 0.11578 Singlet-A 0.14424 0.23376 0.52346 -0.52346 -0.52346 -0.52346 -0.12278 0.23051 -0.12144 0.10391 -0.12245 Singlet-A 0.13852 -0.13915 0.41491	5.6499 eV 5.6580 eV 5.7148 eV 5.7232 eV	219.45 nm 219.13 nm 216.95 nm	f=0.0113 f=0.0023 f=0.0042
Excited State <\$**2>=0.000 225 -> 238 226 -> 238 229 -> 239 236 -> 241 237 -> 242 237 -> 244 Excited State <\$**2>=0.000 223 -> 238 229 -> 239 234 -> 243 Excited State <\$**2>=0.000 222 -> 238 224 -> 238 226 -> 238 227 -> 238 226 -> 238 226 -> 238 227 -> 238 226 -> 238 226 -> 238 227 -> 238 226 -> 238 227 -> 238 226 -> 238 227 -> 238 228 -> 238 229 -> 239 234 -> 240	28: 29: 30: 31:	Singlet-A 0.12299 0.40380 -0.21172 -0.30213 0.19641 Singlet-A 0.26757 0.57807 0.18565 -0.10711 Singlet-A -0.18300 0.44787 0.38222 -0.11551 -0.15239 -0.17387 Singlet-A -0.17387 -0.1736 -0.10745 -0.36817 0.51736 -0.10285 0.10218 -0.10245 -0.	5.4482 eV 5.4948 eV 5.5149 eV	227.57 nm 225.64 nm 224.82 nm 2224.19 nm	f=0.1172 f=0.0120 f=0.0159	Excited State <\$**2>=0.000 218 -> 238 220 -> 238 221 -> 238 232 -> 240 Excited State <\$**2>=0.000 219 -> 238 235 -> 241 237 -> 242 237 -> 242 237 -> 245 237 -> 248 237 -> 248 218 -> 238 218 -> 238 219 -> 238 233 -> 240 237 -> 246 Excited State <\$**2>=0.000 217 -> 238 232 -> 240 233 -> 240 237 -> 248 237 -> 240 237 -> 248 248 -> 240 237 -> 248 249 -> 248 240 -> 248 240 -> 248 241	<ul><li>38:</li><li>39:</li><li>40:</li><li>41:</li></ul>	Singlet-A -0.31698 -0.13618 0.46518 0.27141 -0.21428 Singlet-A -0.12110 -0.21434 -0.27924 0.11091 0.33587 0.11529 0.11529 0.11529 0.11578 Singlet-A 0.14424 0.23376 0.52346 -0.12278 0.23051 -0.12144 0.13931 -0.12245 Singlet-A	5.6499 eV 5.6580 eV 5.7148 eV 5.7232 eV	219.45 nm 219.13 nm 216.95 nm	f=0.0113 f=0.0023 f=0.0042
Excited State <\$**2>=0.000 225 -> 238 226 -> 238 229 -> 239 236 -> 241 237 -> 242 237 -> 243 237 -> 244 Excited State <\$**2>=0.000 223 -> 239 234 -> 240 Excited State <\$**2>=0.000 222 -> 238 224 -> 238 226 -> 238 228 -> 238 229 -> 239 234 -> 240 Excited State <\$**2>=0.000 222 -> 238 228 -> 238 229 -> 239 234 -> 240 Excited State <\$**2>=0.000 222 -> 238 229 -> 239 234 -> 240 Excited State <\$**2>=0.000 222 -> 238 229 -> 239 234 -> 240 Excited State <\$**2>=0.000 222 -> 238 229 -> 239 234 -> 248 229 -> 239 234 -> 248 229 -> 239 234 -> 248 229 -> 239 234 -> 240 Excited State <\$**2>=0.000 222 -> 238 229 -> 239 234 -> 248 229 -> 239 234 -> 240 Excited State <\$**2>=0.000 222 -> 238 229 -> 239 234 -> 240 Excited State <\$**2>=0.000 222 -> 238 229 -> 239 234 -> 248 229 -> 239 234 -> 248 229 -> 238 229 -> 239 234 -> 240 Excited State <\$**2>=0.000 222 -> 238 229 -> 239 234 -> 248 229 -> 238 229 -> 238 239 -> 238 -> 238 239 -> 238 239 -> 238 239	<ul> <li>28:</li> <li>29:</li> <li>30:</li> <li>31:</li> </ul>	Singlet-A 0.12299 0.40380 -0.21172 -0.17410 0.20221 -0.30213 0.19641 Singlet-A 0.26757 0.57807 0.18565 -0.10711 Singlet-A -0.18300 0.44787 0.38222 -0.1551 -0.11551 -0.11551 -0.15239 -0.17387 Singlet-A -0.10745 -0.36817 0.51736 -0.10285 0.10611 0.13521	5.4482 eV 5.4948 eV 5.5149 eV 5.5304 eV	227.57 nm 225.64 nm 2224.82 nm 2224.19 nm	f=0.1172 f=0.0120 f=0.0159	Excited State <\$**2>=0.000 218 -> 238 220 -> 238 221 -> 238 232 -> 240 Excited State <\$**2>=0.000 219 -> 238 235 -> 241 237 -> 244 237 -> 244 237 -> 244 237 -> 244 237 -> 248 237 -> 248 218 -> 238 218 -> 238 219 -> 238 219 -> 238 219 -> 238 233 -> 240 237 -> 246 Excited State <\$**2>=0.000 217 -> 238 233 -> 246 Excited State <\$**2>=0.000 217 -> 238 232 -> 240 237 -> 246	<ul><li>38:</li><li>39:</li><li>40:</li><li>41:</li></ul>	Singlet-A -0.31698 -0.13618 0.27141 -0.21428 Singlet-A -0.12110 -0.21434 -0.27924 0.11091 0.38376 -0.33587 0.11529 0.11496 0.11578 Singlet-A 0.14424 0.23376 0.2346 -0.122144 0.23051 -0.12144 0.10391 -0.12245 Singlet-A	5.6499 eV 5.6580 eV 5.7148 eV 5.7232 eV	219.45 nm 219.13 nm 216.95 nm	f=0.0113 f=0.0023 f=0.0042
Excited State <\$**2>=0.000 225 -> 238 226 -> 238 227 -> 239 236 -> 241 237 -> 242 237 -> 243 Excited State <\$**2>=0.000 223 -> 238 229 -> 239 234 -> 240 237 -> 243 Excited State <\$**2>=0.000 222 -> 238 224 -> 238 224 -> 238 224 -> 238 226 -> 238 227 -> 238 228 -> 238 229 -> 239 234 -> 240 Excited State <\$**2>=0.000 Excited State <\$**2>=0.000 222 -> 238 223 -> 238 224 -> 238 226 -> 238 227 -> 238 227 -> 238 227 -> 238 223 -> 238 223 -> 238 224 -> 238 227 -> 238 223 -> 238 223 -> 238 224 -> 238 225 -> 238 226 -> 238 227 -> 238 227 -> 238 228 -> 238 229 -> 239 234 -> 240 Excited State	<ul> <li>28:</li> <li>29:</li> <li>30:</li> <li>31:</li> <li>32:</li> </ul>	Singlet-A 0.12299 0.40380 -0.21172 -0.17410 0.20221 -0.30213 0.19641 Singlet-A 0.26757 0.57807 0.57807 0.18565 -0.10711 Singlet-A -0.18300 0.44787 0.38222 -0.11551 -0.11574 -0.15239 -0.11574 -0.15239 -0.11574 -0.15239 -0.11574 -0.15239 -0.11574 -0.15239 -0.11574 -0.15239 -0.11574 -0.15239 -0.11574 -0.15239 -0.11574 -0.15239 -0.11574 -0.15239 -0.11574 -0.1285 -0.10285 0.10611 0.51736 -0.10285 0.10611 0.13521	5.4482 eV 5.4948 eV 5.5149 eV 5.5304 eV	227.57 nm 2225.64 nm 2224.82 nm 2224.19 nm	f=0.1172 f=0.0120 f=0.0152 f=0.0529	Excited State <\$**2>=0.000 218 -> 238 220 -> 238 221 -> 238 232 -> 240 Excited State <\$**2>=0.000 219 -> 238 235 -> 241 237 -> 242 237 -> 244 237 -> 245 237 -> 244 237 -> 245 237 -> 248 237 -> 248 216 -> 238 216 -> 238 219 -> 238 220 -> 238 233 -> 240 237 -> 246 Excited State <\$**2>=0.000 215 -> 238 219 -> 238 220 -> 238 233 -> 240 237 -> 246 Excited State	<ul> <li>38:</li> <li>39:</li> <li>40:</li> <li>41:</li> </ul>	Singlet-A -0.31698 -0.13618 0.46518 0.27141 -0.21428 Singlet-A -0.12110 -0.21434 -0.27924 0.11091 0.38376 -0.3587 0.11529 0.11496 0.11578 Singlet-A 0.1424 0.23376 0.52346 -0.12278 0.23051 -0.12245 Singlet-A 0.13852 -0.138	5.6499 eV 5.6580 eV 5.7148 eV 5.7232 eV	219.45 nm 219.13 nm 216.95 nm 216.63 nm	f=0.0113 f=0.0023 f=0.0042
Excited State <\$**2>=0.000 225 -> 238 226 -> 238 227 -> 239 236 -> 241 237 -> 242 237 -> 243 237 -> 244 Excited State <\$**2>=0.000 223 -> 238 229 -> 239 234 -> 240 Excited State <\$**2>=0.000 222 -> 238 226 -> 238 226 -> 238 228 -> 238 228 -> 238 229 -> 239 234 -> 240 Excited State <\$**2>=0.000 222 -> 238 226 -> 238 227 -> 238 228 -> 238 229 -> 239 234 -> 240 Excited State <\$**2>=0.000 222 -> 238 224 -> 238 225 -> 238 224 -> 238 234 -> 240 Excited State <\$**2>=0.000	<ul> <li>28:</li> <li>29:</li> <li>30:</li> <li>31:</li> <li>32:</li> </ul>	Singlet-A 0.12299 0.40380 -0.21172 -0.17410 0.20221 -0.30213 0.19641 Singlet-A 0.26757 0.57807 0.18565 -0.10711 Singlet-A -0.18300 0.44787 0.38222 -0.11551 -0.11574 -0.15239 -0.11574 -0.15239 -0.11574 -0.15239 -0.11574 -0.15736 -0.17387 Singlet-A -0.0745 -0.36817 0.51736 -0.10285 0.10611 0.51736 -0.10285 0.10611 0.13521	5.4482 eV 5.4948 eV 5.5149 eV 5.5304 eV	227.57 nm 225.64 nm 2224.82 nm 2224.19 nm	f=0.1172 f=0.0120 f=0.0159 f=0.0152	Excited State <s**2>=0.000 218 -&gt; 238 220 -&gt; 238 221 -&gt; 238 232 -&gt; 240 Excited State <s**2>=0.000 219 -&gt; 238 235 -&gt; 241 237 -&gt; 242 237 -&gt; 242 237 -&gt; 244 237 -&gt; 248 237 -&gt; 248 219 -&gt; 238 218 -&gt; 238 218 -&gt; 238 219 -&gt; 238 233 -&gt; 240 237 -&gt; 246 Excited State <s**2>=0.000 217 -&gt; 238 233 -&gt; 240 237 -&gt; 246 Excited State</s**2></s**2></s**2>	<ul> <li>38:</li> <li>39:</li> <li>40:</li> <li>41:</li> <li>42:</li> </ul>	Singlet-A -0.31698 -0.13618 0.46518 0.27141 -0.21428 Singlet-A -0.12110 -0.21434 -0.27924 0.11091 0.38576 -0.33587 0.11529 0.11496 0.11578 Singlet-A 0.14424 0.23376 0.52346 -0.12278 0.23051 -0.12144 0.03391 -0.12144 0.10391 -0.12245 Singlet-A 0.13852 -0.19315 0.61481 -0.10804 Singlet-A	5.6499 eV 5.6580 eV 5.7148 eV 5.7232 eV	219.45 nm 219.13 nm 216.95 nm 216.63 nm	f=0.0113 f=0.0023 f=0.0042 f=0.0030

217 -> 238 218 -> 238		-0.28535 0.20137				217 -> 238 218 -> 238		-0.15022 -0.18423			
220 -> 238		0.14849				220 -> 238		-0.10008			
233 -> 240		0.22360				221 -> 238		-0.17573			
237 -> 244		-0.26014				228 -> 239		0.21036			
237 -> 245		0.26557									
237 -> 246		0.32409				Excited State <s**2>=0.000</s**2>	46:	Singlet-A	5.7766 eV	214.63 nm	f=0.0126
Excited State	43:	Singlet-A	5.7377 eV	216.09 nm	f=0.0006	216 -> 238		-0.14718			
<s**2>=0.000</s**2>						218 -> 238		0.10519			
215 -> 238		0.22025				228 -> 239		0.61731			
217 -> 238		0.53744				231 -> 240		-0.11223			
237 -> 244		-0.11694				235 -> 241		-0.11925			
237 -> 245		0.22823									
237 -> 246		0.21316				Excited State <s**2>=0.000</s**2>	47:	Singlet-A	5.7791 eV	214.54 nm	f=0.0131
Excited State	44:	Singlet-A	5.7490 eV	215.66 nm	f=0.1020	226 -> 239		-0.21446			
<s**2>=0.000</s**2>						227 -> 239		0.63865			
225 -> 239		-0.13323				235 -> 241		-0.11092			
226 -> 239		-0.13273									
228 -> 239		0.19045				Excited State	48:	Singlet-A	5.8101 eV	213.39 nm	f=0.0236
235 -> 241		0.47476				<s**2>=0.000</s**2>		-			
237 -> 244		0.18679				215 -> 238		-0.13203			
237 -> 245		0.25687				231 -> 240		0.61093			
237 -> 248		-0.13173				232 -> 240		-0.19066			
						237 -> 245		-0.10795			
Excited State <s**2>=0.000</s**2>	45:	Singlet-A	5.7659 eV	215.03 nm	f=0.0003						
215 -> 238		0.10807									
216 -> 238		0.56521									



Figure S25. A possible reaction route between  $4_{opt}$  and  $6_{opt}$  calculated at the B3LYP-D3/B1 (basis B1: 6-311G(d) [core Si<sub>4</sub>Cl<sub>2</sub>], 6-31G(d) [carbon atoms in silacyclopentane rings], 3-21G\* [others]).

# 5. Preliminary estimation of the thermodynamic parameters for the equilibrium between 4 and 6

In the <sup>1</sup>H NMR spectrum of a mixture of bicyclo[1.1.0]tetrasilane **4** and cyclotrisilene **6**, the signals due to four SiMe<sub>3</sub> groups (36 H) of **6** were substantially broadened and overlapped with that due to eight SiMe<sub>3</sub> groups (72H) of **4** (Figure S26). Assuming that only signals of **4** and **6** were overlapped in this region, the equilibrium constants  $K_{eq}$  (= [**6**]:[**4**]) were determined by using the integral ratio of the SiMe<sub>3</sub> signals of <sup>1</sup>H NMR spectra in C<sub>6</sub>D<sub>6</sub> (Table S8). A plot of ln $K_{eq}$  at various reciprocal temperatures are shown in Figure S27. The thermodynamic parameters for the isomerisation of **4** to **6** are calculated to be  $\Delta H = +14.6 \pm 2.9$  kJ mol<sup>-1</sup> and  $\Delta S = +49 \pm 9$  J K<sup>-1</sup> mol<sup>-1</sup>.



Figure S26. <sup>1</sup>H NMR spectra (TMS region) of a mixture of 4 and 6 in benzene- $d_6$  at (a) 333 K, (b) 323 K, (c) 313 K, and (d) 302 K ( $\bullet = 4$ ,  $\bullet = 6$ , x = 1).

Temperature/K	Integral rati	$K_{\rm eq}  (= [6]: [4])^a$	
	bicyclotetrasilane 4	cyclotrisilene 6	
333	2.11	4.00	1.90
323	2.36	4.00	1.69
313	3.24	4.00	1.23
302	3.48	4.00	1.15

**Table S8**. The Equilibrium Constants  $K_{eq}$  (= [6]:[4]) in Benzene- $d_6$  at Various Temperatures

*a*. Equilibrium constants ( $K_{eq}$ ) were calculated using the integral ratio of SiMe<sub>3</sub> proton signals in the <sup>1</sup>H NMR spectrum.



**Figure S27.** A plot of  $\ln(K_{eq})$  vs 1/T.