Supporting Information

Theoretical Exploration of Siloxy Carbenes: Photogeneration and [2+1] Photocyclization Mechanisms

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1. Selected Orbitals in Active Space

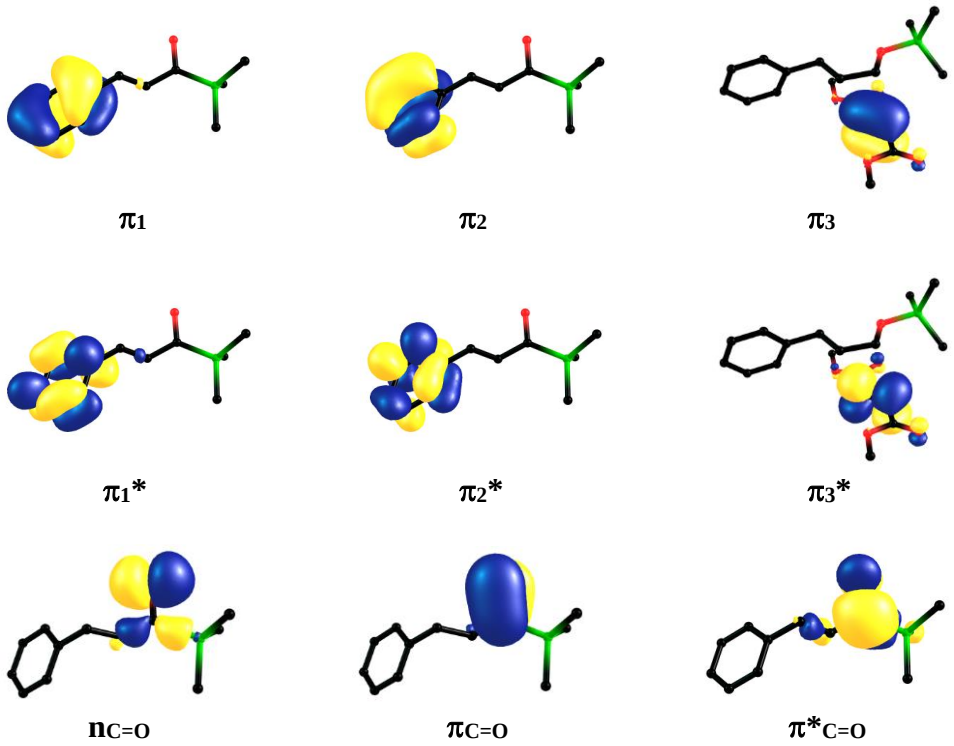


Fig. S1 Molecular orbitals of **1** with a fumarate in defining the active spaces for the CASPT2//CASSCF(10e/9o) calculations.

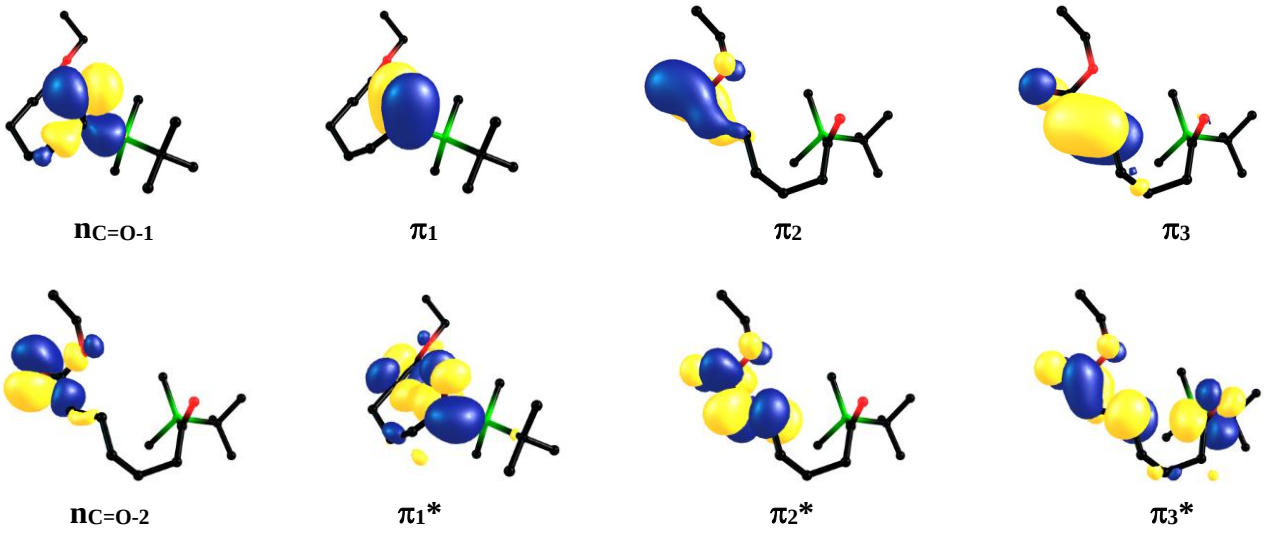


Fig. S2 Molecular orbitals of **2** used in defining the active spaces for the CASPT2//CASSCF(10e/8o) calculations.

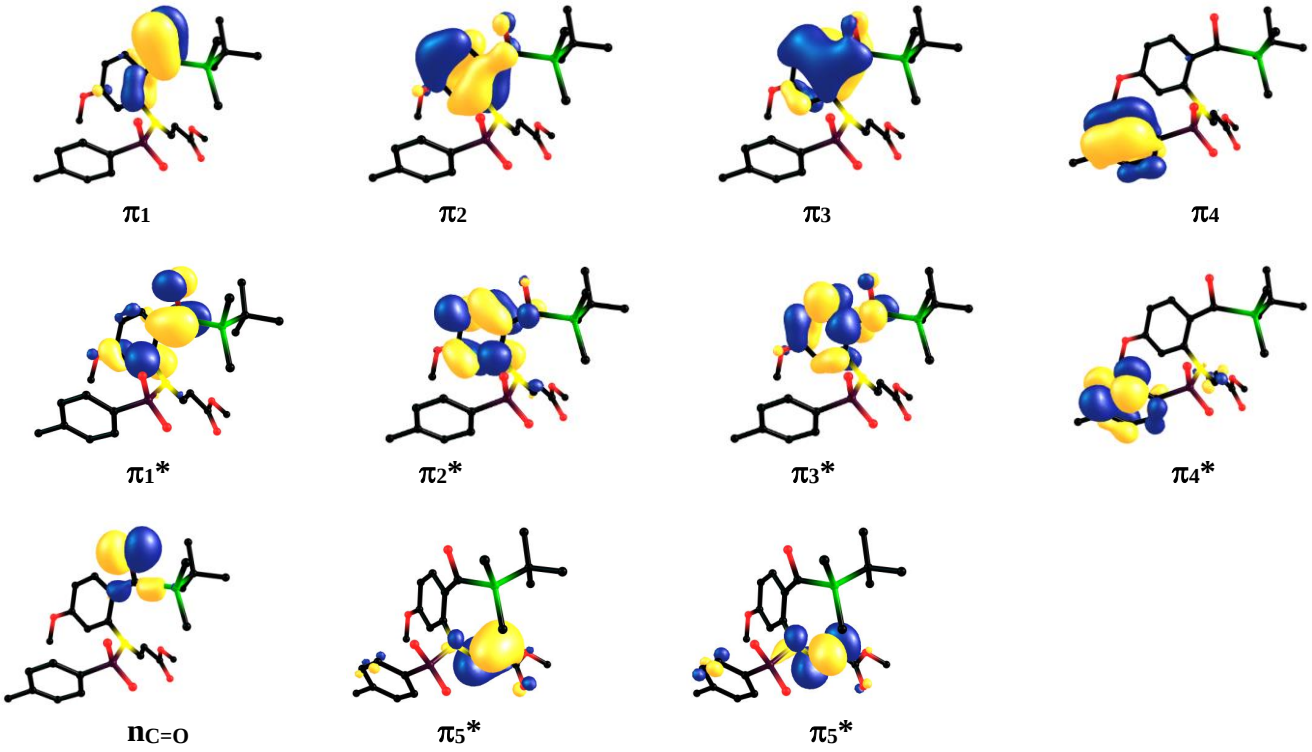


Fig. S3 Molecular orbitals of **3** used in defining the active spaces for the CASPT2//CASSCF(12e/11o) calculations.

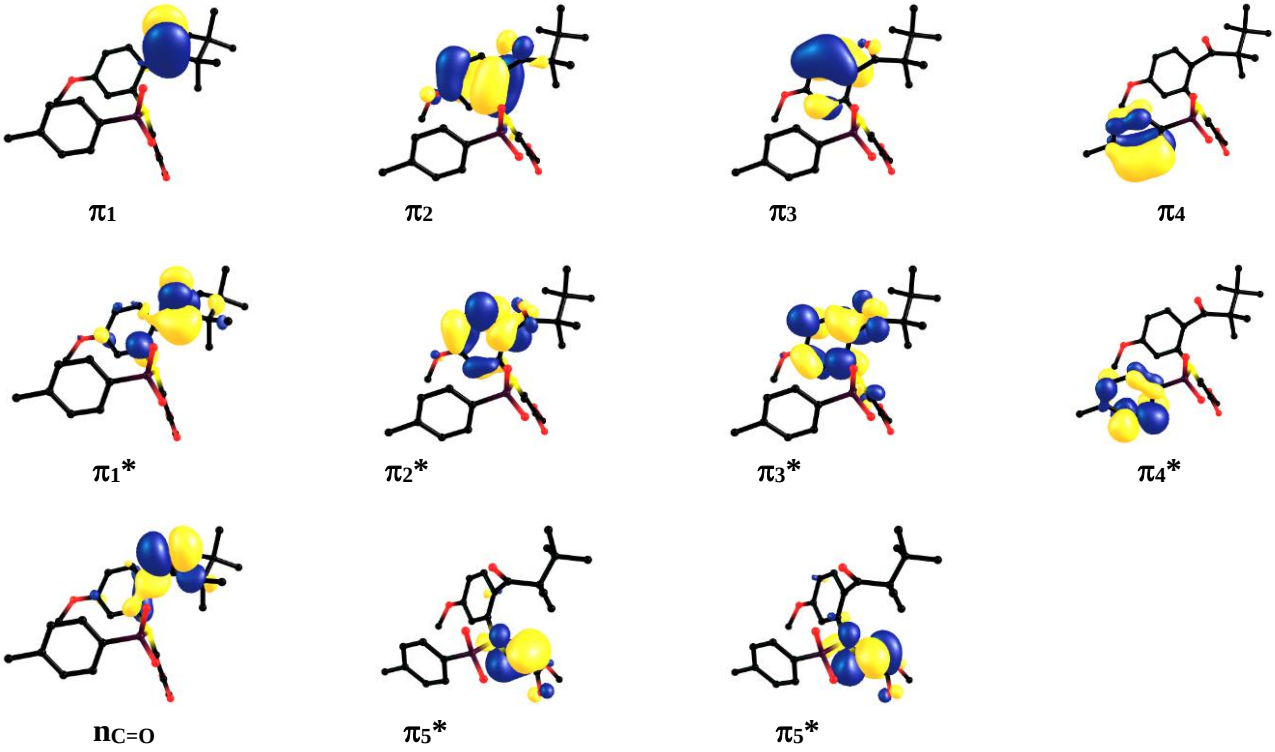
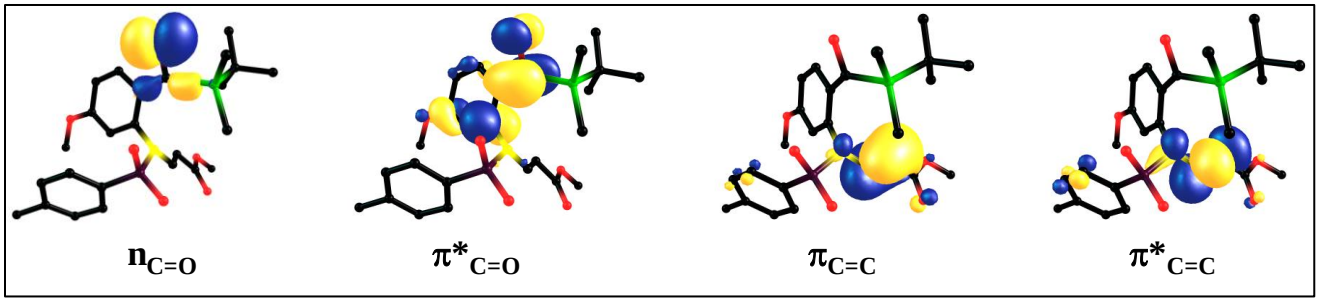
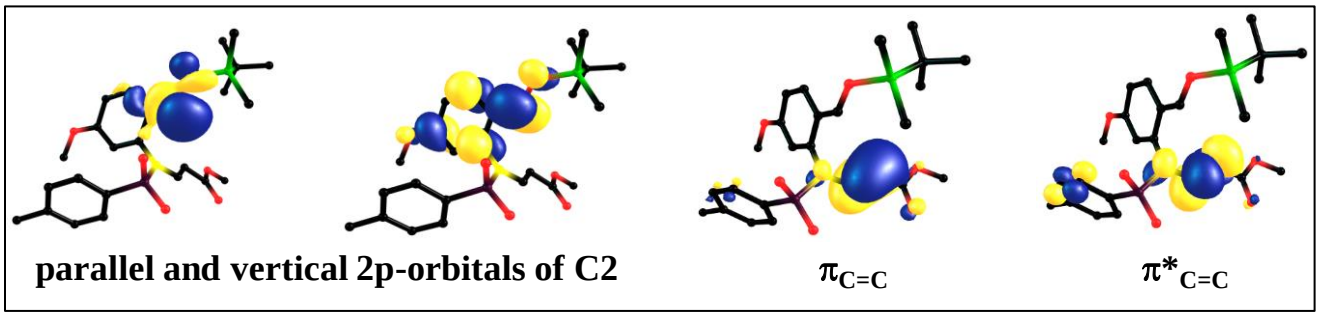


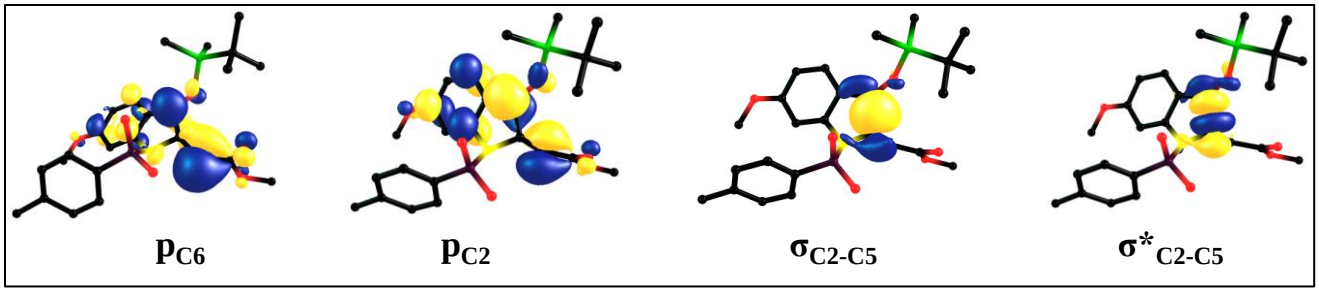
Fig. S4 Molecular orbitals of **4** used in defining the active spaces for the CASPT2//CASSCF(12e/11o) calculations.



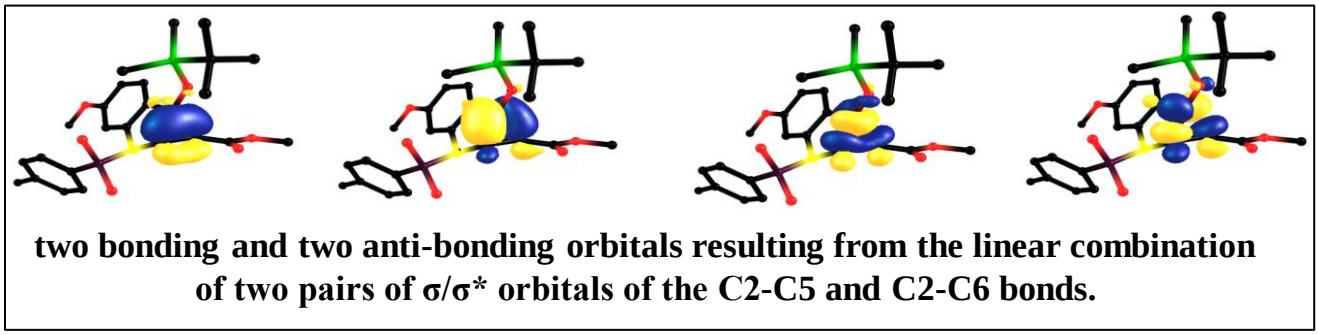
$S_{NP}(^1n\pi^*)$



$S_{\Sigma P}(\sigma^1\pi^1)$



STC(T_1/S_0)



***exo*-P3**

Fig. S5 Orbital evolutions of **3** in some key electronic configurations are schematically shown along the photogeneration of for siloxy carbene and [2+1] photocyclization pathways.

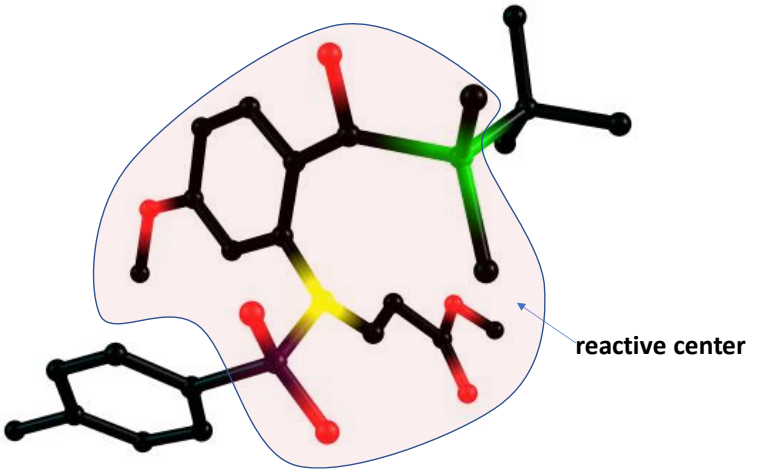


Fig. S6 Schematic illustration of the mixed basis sets for calculations on **3** and **4**. The 6-31G(d) was used to the atoms in shadow, the STO-3G was applied to the remaining atoms.

2. Charge Population and Molecular Orbital Composition Analyses

To further explore the excited-state properties of different transitions for **1**-**4**, charge translocation calculations were performed based on the CASPT2 computations and an appropriate fragment partitioning strategy, as summarized in Table S1. As shown in Table S2 and S3, the contributions of different fragments for n, π* and σ orbital compositions were obtained based on the Hirshfeld orbital composition analysis carried out using the Multiwfn program.[S1]

Table S1. Charge populations (*e*) of **1-4** in the ground (S_0) and $S_{NP}(^1n\pi^*)$ states in the Franck-Condon (FC) region.

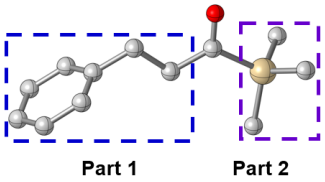
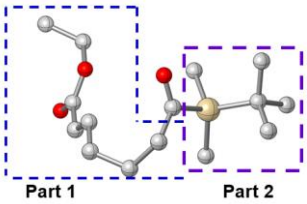
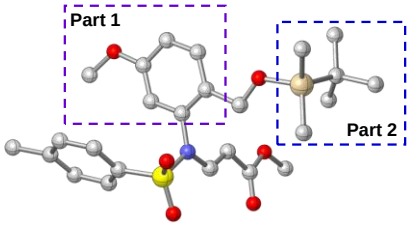
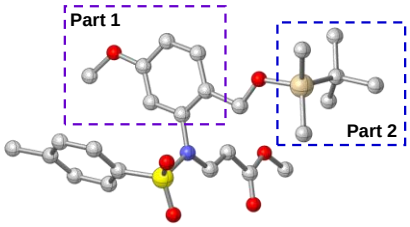
Species	Fragment Partition	Part	S_0	S_{NP}
1		C	0.14	0.29
		O	-0.32	-0.51
		Part 1	0.04	0.06
		Part 2	0.15	0.16
2		C	0.14	0.33
		O	-0.32	-0.52
		Part 1	0.06	0.06
		Part 2	0.12	0.13
3		C	0.07	0.36
		O	-0.30	-0.61
		Part 1	0.09	0.13
		Part 2	-0.74	-0.76
4		C	0.22	0.37
		O	-0.32	-0.51
		Part 1	0.06	0.09
		Part 2	-0.73	-0.71

Table S2. The fragment contributions (%) to n and π* orbital components in $S_{NP}(^1n\pi^*)$ state of **1-4** in the Franck-Condon (FC) region.

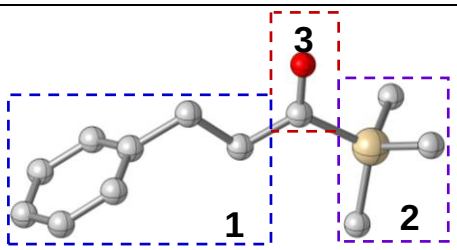
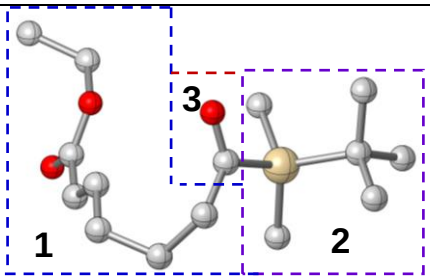
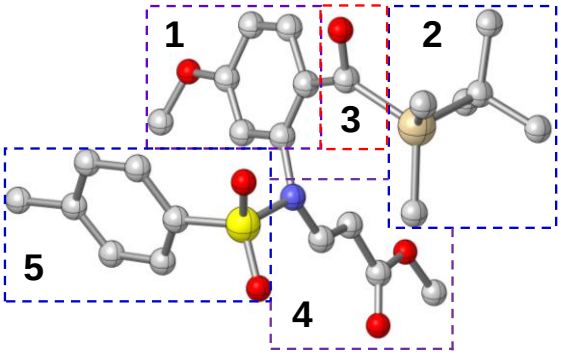
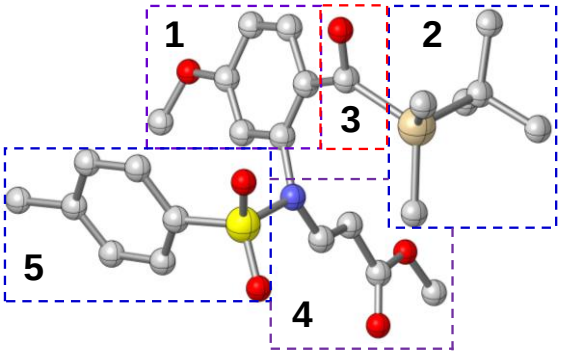
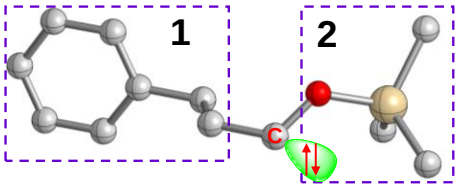
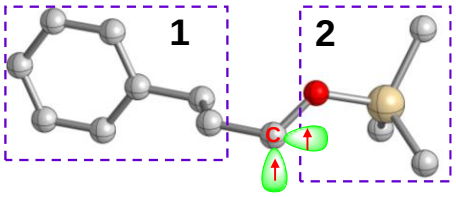
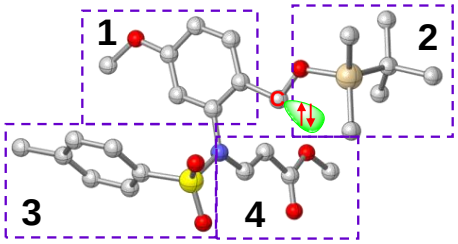
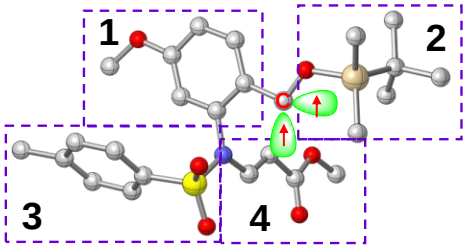
Species	Fragment Partition	Part	n	π*
1		1	7.62	10.31
		2	10.53	10.31
		3	81.85	78.49
2		1	7.45	43.44
		2	8.07	7.23
		3	84.48	49.33
3		1	8.05	39.13
		2	7.74	5.77
		3	84.10	51.26
		4	0.08	2.36
		5	0.04	1.48
4		1	16.18	35.69
		2	9.32	7.00
		3	72.64	52.79
		4	1.07	1.57
		5	1.15	4.10

Table S3. The fragment contributions (%) to σ and π* orbital components in $S_0(\sigma^2\pi^0)$ and $T_{\Sigma P}(\sigma^1\pi^1)$ carbenes of **1** and **3**.

Species	Fragment Partition	Part	σ	π*
1 **$^1A_1$-$\sigma^2\pi^0$**		C	65.99	67.61
		1	17.20	17.60
		2	16.82	14.80
1 **$^3B_1$-$\sigma^1\pi^1$**		C	73.97	70.47
		1	13.53	14.69
		2	12.50	14.84
3 **$^1A_1$-$\sigma^2\pi^0$**		C	69.60	29.19
		1	12.47	62.57
		2	16.30	6.07
		3	0.32	0.71
		4	1.32	1.46
3 **$^3B_1$-$\sigma^1\pi^1$**		C	71.47	37.43
		1	11.75	48.49
		2	14.80	9.53
		3	0.43	1.45
		4	1.55	3.11

3. Rate Constant Calculations

3.1 Intersystem Crossing Rate Constant Calculations

The intersystem crossing (ISC) rates between singlet and triplet states in this work were estimated in the Condon approximation as[S2]

$$k_{\mathrm{ISC}} = \frac{2\pi}{\hbar} \cdot \left| \left\langle {}^{1}\psi_0 \middle| \widehat{H}_{SO} \middle| {}^{3}\psi_0 \right\rangle \right|^2 \cdot |\langle \chi_0 | \chi_n \rangle|^2 \cdot \rho \qquad \text{(eq. 1)}$$

where the electronic coupling between the singlet state ${}^{1}\psi_0$ and the triplet state ${}^{3}\psi_0$ can be calculated as the SOC, the Franck–Condon factor of $\langle \chi_0 | \chi_n \rangle$ is taken equal to 1 at the STC point, and $\rho = 1/\Delta E_{S/T}$ is the reciprocal of the energy difference between the singlet and triplet states.

Table S4. The computed spin–orbit coupling values (SOC, cm^{-1}) and the singlet−triplet energy gaps ($\Delta E_{S/T,}$ kcal/mol) of the involved singlet–triplet crossings (STCs) between singlet and triplet states. The rate of intersystem crossing (k_{ISC}, s^{-1}) is estimated in the Condon approximation.

species	Critial points	$\Delta E_{S/T}$	SOC	k_{ISC}
1	STC(S_{NP}/T_{NP})	7.4	1.07	5.2×10^{8}
1	STC($T_{\Sigma P}/S_0$)	1.7	12.93	3.3×10^{11}
3	STC(S_{NP}/T_{NP})	5.7	2.14	2.7×10^{9}

3.2 Rate Constant Calculations with the transition state theory

The rates via an energy barrier in an adiabatic potential energy surface can be estimated using the transition state theory (TST) as follows[S3,S4]

$$k_{\mathrm{TST}} = \frac{k_{\mathrm{B}}T}{h} \cdot exp\left(-\frac{\Delta G^{\neq}}{k_{\mathrm{B}}T}\right) \qquad \text{(eq. 2)}$$

where k_{TST} is the rate constant, $\Delta G^{\neq}$ is the Gibbs free energy barrier, k_B is the Boltzmann constant (8.62×10^{-5} eV/K), h is the Planck constant (6.626×10^{-34} Js) and T is the absolute temperature (298 K). $\Delta G^{\neq}$ is

obtained by consideration the Gibbs correction through frequency analyses for potential energy barrier ($\Delta E^{\neq}$). Firstly, the minima and transition states are reoptimized at the TD-B3LYP-D3/PCM level, followed by frequency analyses to obtain the Gibbs free energy corrections, because the frequency analysis at the CASSCF level is extremely expensive, if not impossible. Secondly, if the geometries optimized at the DFT level are similar to the CASSCF results, the correction terms would be added to the potential energy barriers at the CASPT2//CASSCF level. Finally, the TST rate can be calculated using $\Delta G^{\neq}$.

Table S4. The computed thermal correction to Gibbs free energy ($G_{\text{Corr.}}$, Hatree) for the S_{NP}-Min and S_{NP}-TS of **3**, as well as the Gibbs free energy barrier ($\Delta G^{\neq}$, kcal/mol) of the 1,2-silyl transfer process in $S_{NP}(^1n\pi^*)$ state.

species	$G_{\text{Corr.}}$ of S_{NP}-Min	$G_{\text{Corr.}}$ of S_{NP}-TS	$\Delta G^{\neq}$	k_{TST}
3	0.495754	0.494125	3.0	3.9×10^{10}

4. Geometric Parameters of Critical Structures

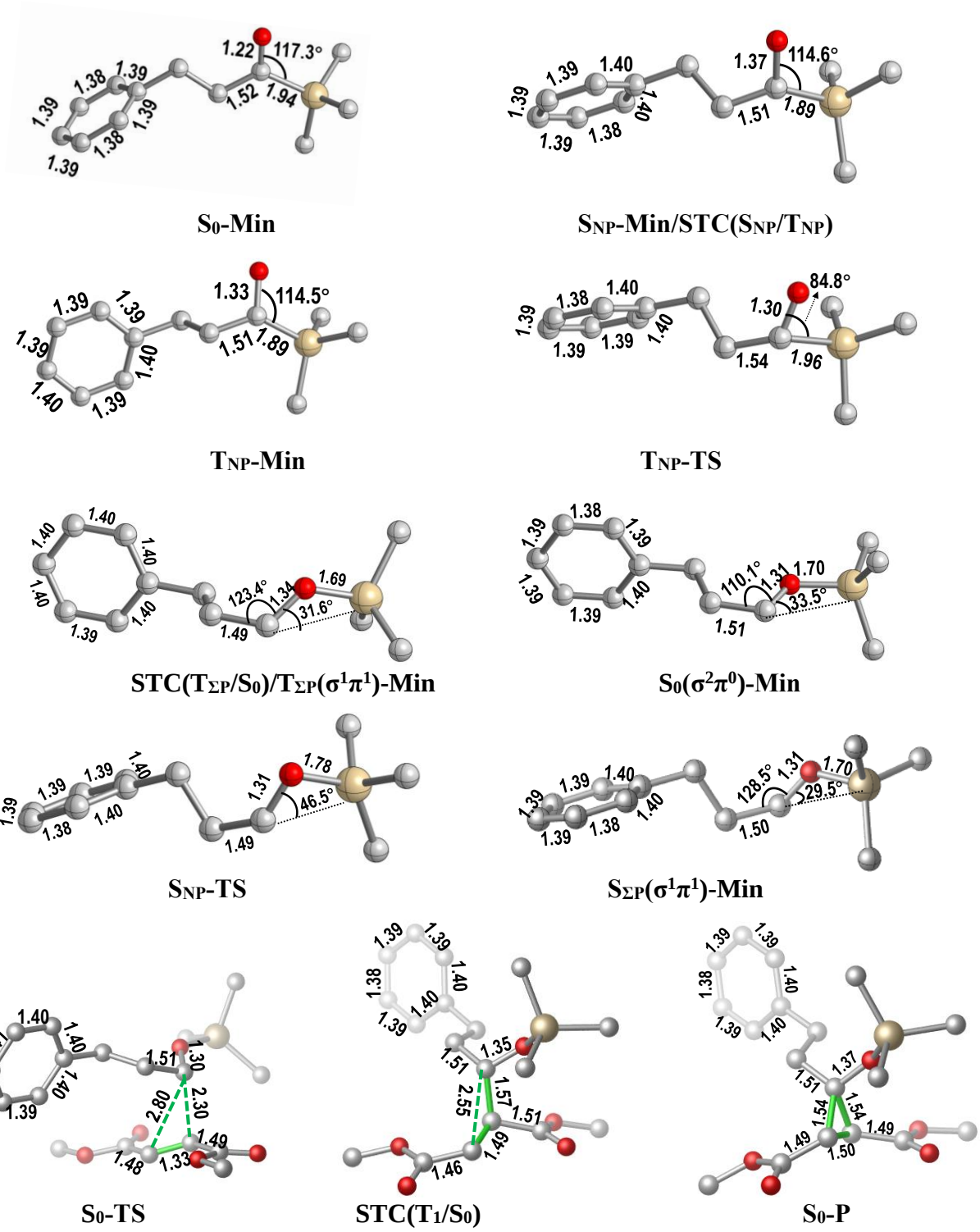
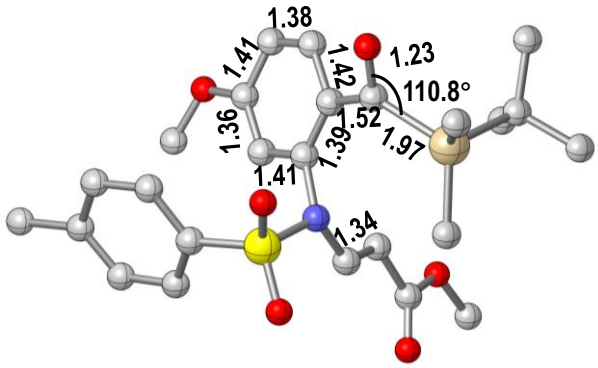
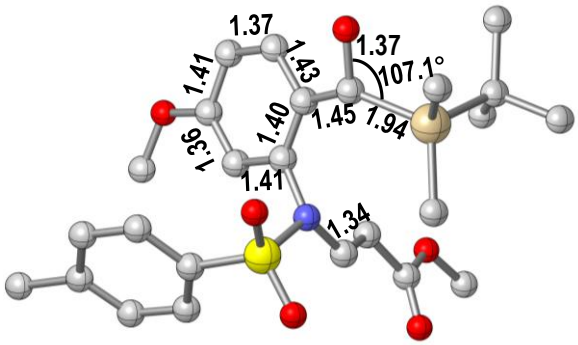


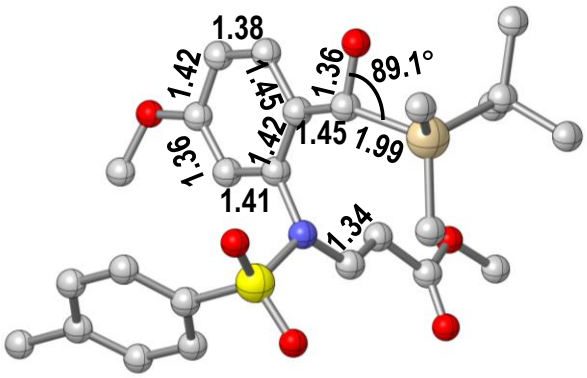
Fig. S7 The critical structures for **1** along the photogeneration of carbenes and [2+1] cycloaddition reaction pathways in Fig. 1 and Fig. 2. Selected key bond distances are given in Å and angels are given in degree.



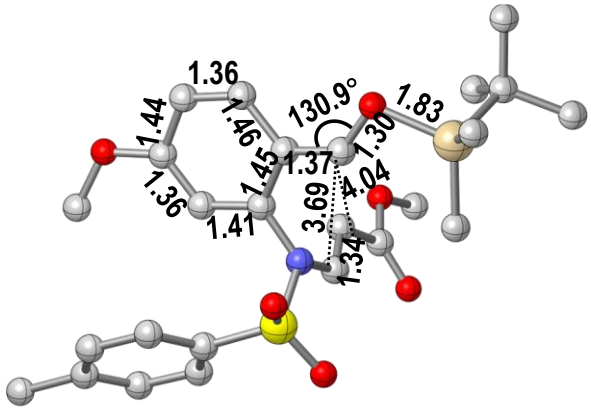
S_0-Min



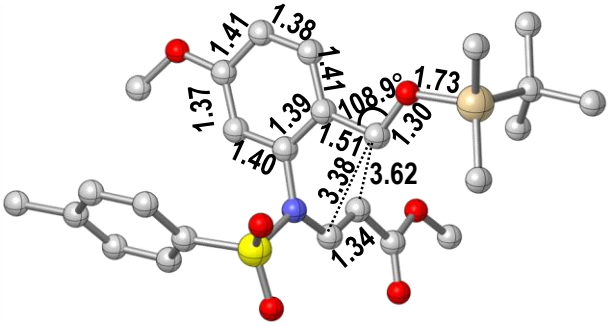
S_{NP}-Min/STC(S_{NP}/T_{NP})



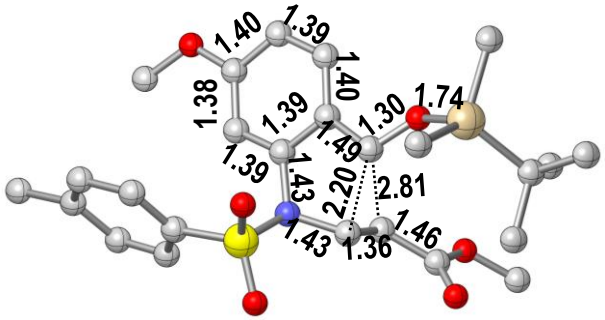
S_{NP}-TS



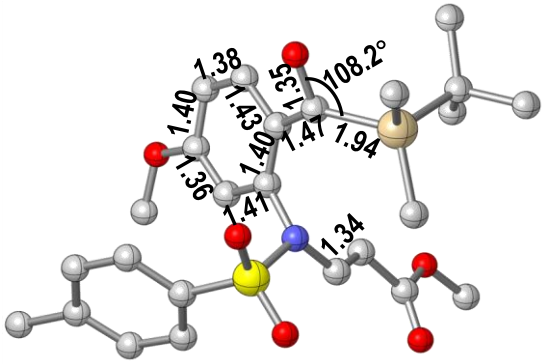
CI($S_{\Sigma P}$/S_0)



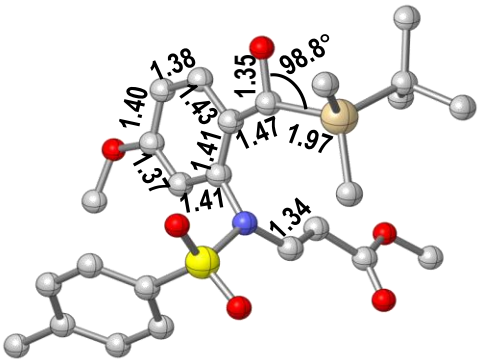
$S_0(\sigma^2\pi^0)$-Min



S_0-TS



T_{NP}-Min



T_{NP}-TS

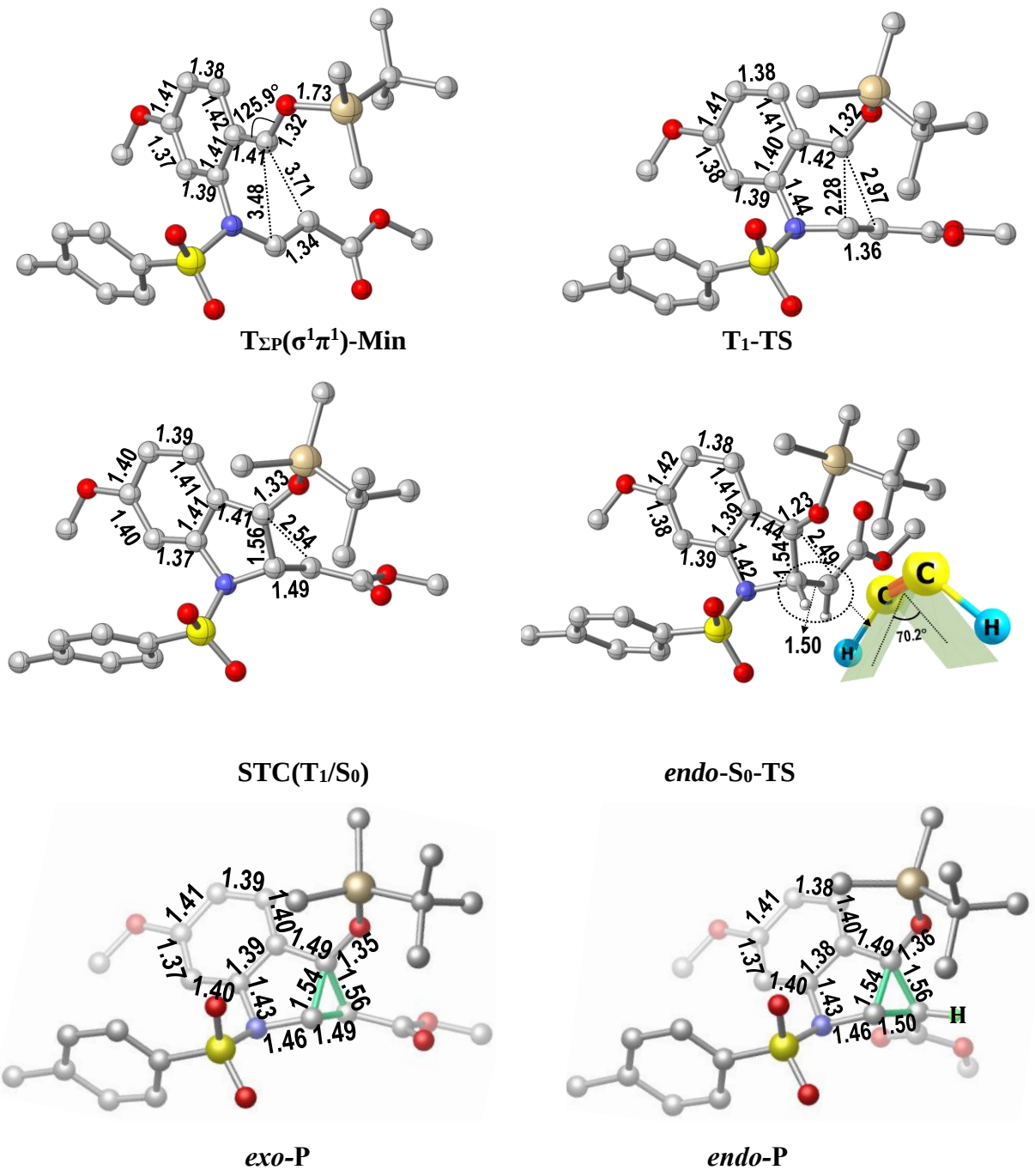


Fig. S8. The critical structures for **3** along the photogeneration of carbene and [2+1] cycloaddition reaction pathways in Fig. 3. Selected key bond distances are given in Å and angels are given in degree.

5. References

(1) T. Lu, and F. Chen, Multiwfn: A multifunctional wavefunction analyzer. *J. Comput. Chem*., 2012, **33**, 580–592.

(2) C. M. Marian, Spin–orbit coupling and intersystem crossing in molecules. *WIREs Comput. Mol. Sci.*, 2012, **2**, 187–203.

(3) S. Ruccolo, Y. Qin, C. Schnedermann, D. G. Nocera, General strategy for improving the quantum efficiency of photoredox hydroamidation catalysis, *J. Am. Chem. Soc*., 2018, **140**, 14926–14937.

(4) D. G. Truhlar, W. L. Hase and J. T. Hynes, Current status of transition-state theory, *J. Phys. Chem.* 1983, **87**, 2664–2682.

6. Tables for the Absolute and Relative Energies

Table S6. Absolute energies (A.E., Hartree) and relative energies (R.E., kcal/mol) for the ground-state minima of **1-4** upon irradiation at the Franck Condon region obtained by CASPT2//CASSCF/PCM calculations.

Species	States	CASSCF	RASSCF	CASPT2	
		A.E.	A.E.	A.E.	R.E.
1	Root1[S_0]	-828.75867	-828.77721	-830.48507	0.0
	Root2[$S_{NP}(^1n\pi^*)$]		-828.63471	-830.35755	80.0
	Root3		-828.54403	-830.29419	
	Root4		-828.48922	-830.22898	
2	Root1[S_0]	-1898.98428	-1097.92068	-1100.37611	0.0
	Root2[$S_{NP}(^1n\pi^*)$]		-1097.78774	-1100.25698	74.8
	Root3		-1097.72008	-1100.18945	
	Root4		-1097.65575	-1100.13089	
3	Root1[S_0]	-2149.92701	-2150.05847	-2153.61137	0.0
	Root2[$S_{NP}(^1n\pi^*)$]		-2149.92975	-2153.50001	69.9
	Root3[$S_{PP}(^1\pi\pi^*)$]		-2149.83928	-2153.45876	95.8
	Root4		-2149.81428	-2153.42890	
	Root5		-2149.77968	-2153.40464	
4	Root1[S_0]	-1097.93863	-1898.97416	-1902.58464	0.0
	Root2[$S_{NP}(^1n\pi^*)$]		-1898.81048	-1902.43397	94.5
	Root3[$S_{PP}(^1\pi\pi^*)$]		-1898.75056	-1902.41957	103.6
	Root4		-1898.69086	-1902.37632	
	Root5		-1898.67482	-1902.39195	

Table S7. Absolute energies (A.E., Hartree) and relative energies (R.E., kcal/mol) for the optimized structures of **1** along the pathways for photogeneration of siloxy carbene and intermolecular [2+1] cycloaddition with a fumarate obtained by CASPT2//CASSCF/PCM calculations. The corresponding energy profile is plotted in Fig. 1.

1	CASSCF	RASSCF	CASPT2	
	A.E.	A.E.	A.E.	R.E.

S_0-Min	Root1[S_0]	-828.75867	-828.77721	-830.48507	0.0
	Root2[$S_{NP}(^1n\pi^*)$]		-828.63471	-830.35755	80.0
	Root3		-828.54403	-830.29419	
	Root4		-828.48922	-830.22898	
S_{NP}-1	Root1[S_0]		-828.77563		
	Root2[$S_{NP}(^1n\pi^*)$]	-828.61538	-828.63751	-830.36235	77.0
	Root3		-828.54730		
	Root4		-828.49375		
S_{NP}-2	Root1[S_0]		-828.77352		
	Root2[$S_{NP}(^1n\pi^*)$]	-828.62476	-828.64692	-830.36559	75.0
	Root3		-828.54516		
	Root4		-828.50111		
S_{NP}-3	Root1[S_0]		-828.76011		
	Root2[$S_{NP}(^1n\pi^*)$]	-828.63389	-828.65560	-830.36691	74.2
	Root3		-828.53089		
	Root4		-828.50597		
S_{NP}-4	Root1[S_0]		-828.74599		
	Root2[$S_{NP}(^1n\pi^*)$]	828.63745	-828.65916	-830.36690	73.4
	Root3		-828.51627		
	Root4		-828.50791		
S_{NP}-Min STC(S_{NP}/T_{NP})	Root1[S_0]		-828.74662		
	Root2[$S_{NP}(^1n\pi^*)$]	-828.66336	-828.66142	-830.37009	72.2
	Root3		-828.51645		
	Root4		-828.50979		
	Root1[$T_{NP}(^3n\pi^*)$]		-828.67013	-830.38184	64.8
	Root2		-828.63112		
	Root3		-828.58478		
	Root4		-828.53514		
T_{NP}-1	Root1[$T_{NP}(^3n\pi^*)$]	-828.67685	-828.67055	-830.38374	63.6
	Root2		-828.62991		
	Root3		-828.58954		
	Root4		-828.54066		

T_{NP}-2	Root1[$T_{NP}(^3n\pi^*)$]	-828.67708	-828.67058	-830.38461	63.0
	Root2		-828.62481		
	Root3		-828.59365		
	Root4		-828.54405		
T_{NP}-3 T_{NP}-Min	Root1[$T_{NP}(^3n\pi^*)$]	-828.67684	-828.67045	-830.38539	62.5
	Root2		-828.62429		
	Root3		-828.59513		
	Root4		-828.54628		
T_{NP}-4	Root1[$T_{NP}(^3n\pi^*)$]	-828.67661	-828.67027	-830.38479	62.9
	Root2		-828.62472	-830.36235	
	Root3		-828.59431		
	Root4		-828.54468		
T_{NP}-5	Root1[$T_{NP}(^3n\pi^*)$]	-828.67531	-828.66903	-830.38375	63.6
	Root2		-828.62319		
	Root3		-828.59126		
	Root4		-828.54168		
T_{NP}-6	Root1[$T_{NP}(^3n\pi^*)$]	-828.67155	-828.66527	-830.48761	64.5
	Root2		-828.61606		
	Root3		-828.58562		
	Root4		-828.53609		
T_{NP}-7 T_{NP}-TS	Root1[$T_{NP}(^3n\pi^*)$]	-828.66006	-828.65402	-830.37976	66.1
	Root2		-828.59334		
	Root3		-828.57040		
	Root4		-828.52082		
T_{NP}-8	Root1[$T_{NP}(^3n\pi^*)$]	-828.64728	-828.64094	-830.38172	64.9
	Root2		-828.55713		
	Root3		-828.55136		
	Root4		-828.50181		
T_{NP}-9	Root1[$T_{NP}(^3n\pi^*)$]	-828.64019	-828.63472	-830.38437	63.2
	Root2		-828.53228		
	Root3		-828.52079		

	Root4		-828.48089		
T_{NP}-10	Root1[$T_{NP}(^3n\pi^*)$]	-828.63833	-828.63085	-830.38689	61.6
	Root2		-828.52067		
	Root3		-828.47950		
	Root4		-828.46502		
T_{NP}-11	Root1[$T_{NP}(^3n\pi^*)$]	-828.63893	-828.63110	-830.37881	62.0
	Root2		-828.51770		
	Root3		-828.47995		
	Root4		-828.46210		
T_{NP}-12	Root1[$T_{NP}(^3n\pi^*)$]	-828.66659	-828.66078	-830.38865	60.5
	Root2		-828.50929		
	Root3		-828.48990		
	Root4		-828.45311		
T_{NP}-13	Root1[$T_{NP}(^3n\pi^*)$]	-828.67899	-828.67265	-830.39422	57.0
	Root2		-828.52113		
	Root3		-828.50149		
	Root4		-828.46482		
T_{NP}-14	Root1[$T_{NP}(^3n\pi^*)$]	-828.68872	-828.68819	-830.40176	52.3
	Root2		-828.53197		
	Root3		-828.51245		
	Root4		-828.48372		
T_{NP}-15	Root1[$T_{NP}(^3n\pi^*)$]	-828.69597	-828.69550	-830.40660	49.2
	Root2		-828.53919		
	Root3		-828.52339		
	Root4		-828.49083		
T_{NP}-16	Root1[$T_{NP}(^3n\pi^*)$]	-828.70050	-828.70007	-830.40952	47.4
	Root2		-828.54373		
	Root3		-828.52797		
	Root4		-828.49546		
	Root1[$T_{\Sigma P}(\sigma^1\pi^1)$]	-828.70429	-828.69900	-830.40999	47.1

STC($T_{\Sigma P}/S_0$)/ $T_{\Sigma P}(\sigma^1\pi^1)$-Min	Root2		-828.62450		
	Root3		-828.53483		
	Root4		-828.52436		
	Root1[$S_0(\sigma^2\pi^0)$]		-828.70386	-830.41272	45.4
	Root2		-828.54569		
	Root3		-828.53785		
	Root4		-828.49858		
The Stepwise [2+1] cycloaddition driven by the $T_{\Sigma P}(\sigma^1\pi^1)$ carbene in Fig. 1a					
CYC-T_1-1	Root1[T_1]	-1360.05451	-1360.05633	-1363.18180	45.1
	Root2		-1359.93353		
	Root3		-1359.92046		
	Root4		-1359.89293		
CYC-T_1-2	Root1[T_1]	-1360.05346	-1360.05490	-1363.18168	45.2
	Root2		-1359.93496		
	Root3		-1359.91869		
	Root4		-1359.89169		
CYC-T_1-3	Root1[T_1]	-1360.05161	-1360.05291	-1363.18142	45.3
	Root2		-1359.93670		
	Root3		-1359.91584		
	Root4		-1359.88983		
T_1-TS	Root1[T_1]	-1360.04917	-1360.05088	-1363.18119	45.5
	Root2		-1359.93856		
	Root3		-1359.91266		
	Root4		-1359.88794		
CYC-T_1-5	Root1[T_1]	-1360.04437	-1360.04687	-1363.18168	45.2
	Root2		-1359.94260		
	Root3		-1359.90558		
	Root4		-1359.88412		
CYC-T_1-6	Root1[T_1]	-1360.04167	-1360.04487	-1363.18274	44.5
	Root2		-1359.94397		
	Root3		-1359.90163		
	Root4		-1359.88220		

CYC-T_1-7	Root1[T_1]	-1360.03933	-1360.03822	-1363.18538	42.8
	Root2		-1359.93582		
	Root3		-1359.88806		
	Root4		-1359.87687		
CYC-T_1-8	Root1[T_1]	-1360.04234	-1360.04185	-1363.18971	40.1
	Root2		-1359.93652		
	Root3		-1359.88882		
	Root4		-1359.87754		
CYC-T_1-9	Root1[T_1]	-1360.05270	-1360.04788	-1363.19365	37.7
	Root2		-1359.96193		
	Root3		-1359.92611		
	Root4		-1359.89320		
CYC-T_1-10	Root1[T_1]	-1360.06015	-1360.05653	-1363.20213	32.3
	Root2		-1359.95877		
	Root3		-1359.90834		
	Root4		-1359.90048		
CYC-T_1-11	Root1[T_1]	-1360.06736	-1360.06561	-1363.20841	28.4
	Root2		-1359.95843		
	Root3		-1359.90878		
	Root4		-1359.87134		
CYC-T_1-12	Root1[T_1]	-1360.07448	-1360.07358	-1363.21739	22.8
	Root2		-1359.95776		
	Root3		-1359.91493		
	Root4		-1359.87742		
CYC-T_1-13	Root1[T_1]	-1360.08005	-1360.08076	-1363.22590	17.4
	Root2		-1359.96005		
	Root3		-1359.92013		
	Root4		-1359.88250		
STC(T_1/S_0)	Root1[T_1]	-1360.08406	-1360.08928	-1363.22902	15.5
	Root2		-1359.93110		

	Root3		-1359.93047		
	Root4		-1359.88841		
	Root1[S_0]		-1360.08283	-1363.23086	14.3
	Root2		-1359.95745		
	Root3		-1359.92112		
	Root4		-1359.87559		
CYC-S_0-1	Root1[S_0]	-1360.09070	-1360.08891	-1363.23739	10.2
	Root2		-1359.95158		
	Root3		-1359.91930		
	Root4		-1359.87387		
CYC-S_0-2	Root1[S_0]	-1360.09654	-1360.09501	-1363.24465	5.7
	Root2		-1359.94105		
	Root3		-1359.91162		
	Root4		-1359.86723		
CYC-S_0-3	Root1[S_0]	-1360.10267	-1360.10092	-1363.25402	-0.2
	Root2		-1359.90672		
	Root3		-1359.89563		
	Root4		-1359.88339		
CYC-S_0-4	Root1[S_0]	-1360.11012	-1360.10798	-1363.26108	-4.7
	Root2		-1359.89059		
	Root3		-1359.87657		
	Root4		-1359.87410		
CYC-S_0-5	Root1[S_0]	-1360.11929	-1360.12149	-1363.26840	-9.2
	Root2		-1359.90611		
	Root3		-1359.83838		
	Root4		-1359.83782		
CYC-S_0-6	Root1[S_0]	-1360.12916	-1360.13290	-1363.27722	-14.8
	Root2		-1359.91849		
	Root3		-1359.84937		
	Root4		-1359.80148		

CYC-S_0-7	Root1[S_0]	-1360.13865	-1360.14227	-1363.28714	-21.0
	Root2		-1359.92789		
	Root3		-1359.85866		
	Root4		-1359.81070		
CYC-S_0-8	Root1[S_0]	-1360.14572	-1360.14953	-1363.29480	-25.8
	Root2		-1359.93507		
	Root3		-1359.86568		
	Root4		-1359.81795		
CYC-S_0-9	Root1[S_0]	-1360.14906	-1360.15273	-1363.29808	-27.9
	Root2		-1359.93817		
	Root3		-1359.86888		
	Root4		-1359.82105		
P1	Root1[S_0]	-1360.16063	-1360.16665	-1363.30890	-34.7
	Root2		-1359.95128		
	Root3		-1359.88276		
	Root4		-1359.83466		
The [2+1] cycloaddition in a concerted asynchronous manner driven by the $S_0(\sigma^2\pi^0)$ carbene in Fig. 1b					
$T_{\Sigma P}(\sigma^1\pi^1)$-Min //STC($T_{\Sigma P}$/$S_0$)	Root1[$T_{\Sigma P}(\sigma^1\pi^1)$]	-828.70429	-828.69900	-830.40999	47.1
	Root2		-828.62450		
	Root3		-828.53483		
	Root4		-828.52436		
	Root1[$S_0(\sigma^2\pi^0)$]		-828.70386	-830.41272	45.4
	Root2		-828.54569		
	Root3		-828.53785		
	Root4		-828.49858		
S_0-1	Root1[$S_0(\sigma^2\pi^0)$]	-828.71655	-828.70602	-830.41746	42.4
	Root2		-828.24533		
	Root3		-828.53122		
	Root4		-828.51607		
S_0-2	Root1[$S_0(\sigma^2\pi^0)$]	-828.71928	-828.70958	-830.42146	39.9
	Root2		-828.61943		

	Root3		-828.52835		
	Root4		-828.50826		
S_0-3	Root1[$S_0(\sigma^2\pi^0)$]	-828.72148	-828.71209	-830.42431	38.1
	Root2		-828.61694		
	Root3		-828.52627		
	Root4		-828.50198		
S_0-4	Root1[$S_0(\sigma^2\pi^0)$]	-828.72419	-828.71883	-830.43283	32.8
	Root2		-828.61050		
	Root3		-828.52471		
	Root4		-828.49046		
S_0-5	Root1[$S_0(\sigma^2\pi^0)$]	-828.72621	-828.72069	-830.43478	31.6
	Root2		-828.60819		
	Root3		-828.52275		
	Root4		-828.49230		
S_0-6	Root1[$S_0(\sigma^2\pi^0)$]	-828.72781	-828.72185	-830.43611	30.7
	Root2		-828.60617		
	Root3		-828.52072		
	Root4		-828.49327		
S_0-7	Root1[$S_0(\sigma^2\pi^0)$]	-828.73376	-828.72376	-830.43794	29.6
	Root2		-828.60250		
	Root3		-828.51690		
	Root4		-828.49471		
$S_0(\sigma^2\pi^0)$-Min	Root1[$S_0(\sigma^2\pi^0)$]	-828.73304	-828.72560	-830.43970	28.5
	Root2		-828.60040		
	Root3		-828.51900		
	Root4		-828.49560		
CYC-S_0-1	Root1[S_0]	-1360.10144	-1360.10115	-1363.20880	28.2
	Root2		-1359.92109		
	Root3		-1359.82191		
	Root4		-1359.80648		

CYC-S_0-2	Root1[S_0]	-1360.09927	-1360.09872	-1363.20858	28.3
	Root2		-1359.91863		
	Root3		-1359.81939		
	Root4		-1359.80395		
CYC-S_0-3	Root1[S_0]	-1360.09287	-1360.09413	-1363.20429	31.0
	Root2		-1359.91367		
	Root3		-1359.79974		
	Root4		-1359.79721		
CYC-S_0-4	Root1[S_0]	-1360.08929	-1360.09019	-1363.20315	31.7
	Root2		-1359.90971		
	Root3		-1359.79579		
	Root4		-1359.79313		
CYC-S_0-5	Root1[S_0]	-1360.08685	-1360.08768	-1363.20251	32.1
	Root2		-1359.90718		
	Root3		-1359.79324		
	Root4		-1359.79055		
CYC-S_0-6	Root1[S_0]	-1360.08366	-1360.08447	-1363.20187	32.5
	Root2		-1359.90395		
	Root3		-1359.79001		
	Root4		-1359.78731		
CYC-S_0-TS	Root1[S_0]	-1360.08053	-1360.08126	-1363.20159	33.0
	Root2		-1359.90067		
	Root3		-1359.78675		
	Root4		-1359.78401		
CYC-S_0-8	Root1[S_0]	-1360.07642	-1360.07702	-1363.20239	32.2
	Root2		-1359.89633		
	Root3		-1359.78241		
	Root4		-1359.77969		
CYC-S_0-9	Root1[S_0]	-1360.07132	-1360.07178	-1363.20485	30.6
	Root2		-1359.88860		
	Root3		-1359.77505		

	Root4		-1359.77133		
CYC-S_0-10	Root1[S_0]	-1360.06371	-1360.05853	-1363.20943	27.8
	Root2		-1359.93209		
	Root3		-1359.91556		
	Root4		-1359.85465		
CYC-S_0-11	Root1[S_0]	-1360.06383	-1360.05980	-1363.21516	24.2
	Root2		-1359.92539		
	Root3		-1359.91576		
	Root4		-1359.85978		
CYC-S_0-12	Root1[S_0]	-1360.06877	-1360.06475	-1363.22309	19.2
	Root2		-1359.92311		
	Root3		-1359.89741		
	Root4		-1359.86940		
CYC-S_0-13	Root1[S_0]	-1360.08479	-1360.08259	-1363.23142	14.0
	Root2		-1359.90595		
	Root3		-1359.90196		
	Root4		-1359.86349		
CYC-S_0-14	Root1[S_0]	-1360.09053	-1360.08923	-1363.23653	10.8
	Root2		-1359.91661		
	Root3		-1359.90898		
	Root4		-1359.87418		
CYC-S_0-15	Root1[S_0]	-1360.09904	-1360.10269	-1363.24232	7.1
	Root2		-1359.93952		
	Root3		-1359.92798		
	Root4		-1359.92084		
CYC-S_0-16	Root1[S_0]	-1360.10623	-1360.09830	-1363.25078	1.8
	Root2		-1359.92919		
	Root3		-1359.91826		
	Root4		-1359.88677		
CYC-S_0-17	Root1[S_0]	-1360.11249	-1360.10907	-1363.25802	-2.7

	Root2		-1359.93678		
	Root3		-1359.92716		
	Root4		-1359.91527		
CYC-S_0-18	Root1[S_0]	-1360.11888	-1360.11545	-1363.26519	-7.2
	Root2		-1359.93344		
	Root3		-1359.90884		
	Root4		-1359.89011		
CYC-S_0-19	Root1[S_0]	-1360.13144	-1360.13270	-1363.27623	-14.2
	Root2		-1359.95351		
	Root3		-1359.83776		
	Root4		-1359.83595		
CYC-S_0-20	Root1[S_0]	-1360.14981	-1360.15205	-1363.29240	-24.3
	Root2		-1359.97282		
	Root3		-1359.85633		
	Root4		-1359.85513		
CYC-S_0-21	Root1[S_0]	-1360.14557	-1360.15077	-1363.29674	-27.0
	Root2		-1359.93552		
	Root3		-1359.86679		
	Root4		-1359.81794		
P1	Root1[S_0]	-1360.16063	-1360.16665	-1363.30890	-34.7
	Root2		-1359.95128		
	Root3		-1359.88276		
	Root4		-1359.83466		

Table S8. Absolute energies (A.E., Hartree) and relative energies (R.E., kcal/mol) for the optimized structures of **1** along the pathways for photogeneration of siloxy carbene in $S_{NP}(^1n\pi^*)$ state obtained by CASPT2//CASSCF/PCM calculations. The corresponding energy profile is plotted in Fig. 2.

1		**CASSCF**	**RASSCF**	**CASPT2**	
		A.E.	**A.E.**	**A.E.**	**R.E.**
S_0-Min	Root1[S_0]	-828.75867	-828.77721	-830.48507	0.0
	Root2[$S_{NP}(^1n\pi^*)$]		-828.63471	-830.35755	80.0

	Root3		-828.54403		
	Root4		-828.48922		
S_{NP}-1	Root1[S_0]		-828.77563	-830.48761	-9.0
	Root2[$S_{NP}(^1n\pi^*)$]	-828.61538	-828.63751	-830.36235	77.0
	Root3		-828.54730		
	Root4		-828.49375		
S_{NP}-2	Root1[S_0]		-828.77352	-830.48498	0.06
	Root2[$S_{NP}(^1n\pi^*)$]	-828.62476	-828.64692	-830.36559	75.0
	Root3		-828.54516	-830.29915	
	Root4		-828.50111	-830.23675	
S_{NP}-3	Root1[S_0]		-828.76011	-830.47266	7.8
	Root2[$S_{NP}(^1n\pi^*)$]	-828.63389	-828.65560	-830.36691	74.2
	Root3		-828.53089	-830.28734	
	Root4		-828.50597	-830.23376	
S_{NP}-4	Root1[S_0]		-828.74599	-830.46306	17.2
	Root2[$S_{NP}(^1n\pi^*)$]	828.63745	-828.65916	-830.36690	73.4
	Root3		-828.51627	-830.27798	
	Root4		-828.50791	-830.23231	
S_{NP}-Min STC(S_{NP}/T_{NP})	Root1[S_0]		-828.74662	-830.45775	17.1
	Root2[$S_{NP}(^1n\pi^*)$]	-828.66336	-828.66142	-830.37009	72.2
	Root3		-828.51645		
	Root4		-828.50979		
	Root1[$T_{NP}(^3n\pi^*)$]		-828.67013	-830.38184	64.8
	Root2		-828.63112		
	Root3		-828.58478		
	Root4		-828.53514		
S_{NP}-6	Root1		-830.45849	-830.45849	16.68
	Root2[$S_{NP}(^1n\pi^*)$]	-828.66155	-830.36903	-830.36903	72.82
	Root3		-830.45849		
	Root4		-830.36903		
S_{NP}-7	Root1		-828.74030	-830.45301	20.1
	Root2[$S_{NP}(^1n\pi^*)$]	-828.65674	-828.65498	-830.36475	75.5

	Root3		-828.51105		
	Root4		-828.50491		
S_{NP}-8	Root1		-828.73667	-830.44996	22.0
	Root2[$S_{NP}(^1n\pi^*)$]	-828.65303	-828.65118	-830.36226	77.1
	Root3		-828.50752		
	Root4		-828.50185		
S_{NP}-9	Root1		-828.73138	-830.44564	24.7
	Root2[$S_{NP}(^1n\pi^*)$]	-828.64732	-828.64540	-830.35867	79.3
	Root3		-828.50225		
	Root4		-828.49708		
S_{NP}-10	Root1		-828.72417	-830.44018	28.2
	Root2[$S_{NP}(^1n\pi^*)$]	-828.63901	-828.63693	-830.35403	82.2
	Root3		-828.49496		
	Root4		-828.49011		
S_{NP}-11	Root1		-828.65914	-830.40270	51.7
	Root2[$S_{NP}(^1n\pi^*)$]	-828.58858	-828.58886	-830.34982	84.9
	Root3		-828.48329		
	Root4		-828.47409		
S_{NP}-12	Root1		-828.65248	-830.39089	59.1
	Root2[$S_{NP}(^1n\pi^*)$]	-828.59020	-828.58864	-830.34751	86.3
	Root3		-828.49705		
	Root4		-828.48169		
S_{NP}-13	Root1		-828.64898	-830.38429	63.2
	Root2[$S_{NP}(^1n\pi^*)$]	-828.59194	-828.58949	-830.34647	87.0
	Root3		-828.50341		
	Root4		-828.48563		
S_{NP}-TS	Root1		-828.64701	-830.37389	69.8
	Root2[$S_{NP}(^1n\pi^*)$]	-828.59439	-828.59140	-830.34572	87.4
	Root3		-828.50888		
	Root4		-828.48992		
S_{NP}-15	Root1		-828.65108	-830.37312	70.2

	Root2[$S_{NP}(^1n\pi^*)$]	-828.60463	-828.60086	-830.34671	86.8
	Root3		-828.51879		
	Root4		-828.50417		
S_{NP}-16	Root1		-828.65701	-830.37612	68.4
	Root2[$S_{NP}(^1n\pi^*)$]	-828.61019	-828.60776	-830.34886	85.5
	Root3		-828.52622		
	Root4		-828.51387		
S_{NP}-17	Root1		-828.67160	-830.38620	62.0
	Root2[$S_{NP}(^1n\pi^*)$]	-828.61882	-828.61659	-830.35401	82.2
	Root3		-828.53206		
	Root4		-828.52626		
S_{NP}-18	Root1		-828.67704	-830.39042	59.4
	Root2[$S_{NP}(^1n\pi^*)$]	-828.62167	-828.61959	-830.35611	80.9
	Root3		-828.53399		
	Root4		-828.53001		
S_{NP}-19	Root1		-828.67995	-830.39258	58.0
	Root2[$S_{NP}(^1n\pi^*)$]	-828.62478	-828.62241	-830.35779	79.9
	Root3		-828.53632		
	Root4		-828.53287		
$S_{\Sigma P}(\sigma^1\pi^1)$-Min	Root1		-828.68231	-830.39423	57.0
	Root2[$S_{NP}(^1\sigma\pi^*)$]	-828.62610	-828.62359	-830.35826	79.6
	Root3		-828.53605		
	Root4		-828.53371		

Table S9. Absolute energies (A.E., Hartree) and relative energies (R.E., kcal/mol) for the optimized structures of **3** along the pathways for photogeneration of siloxy carbene mediated by $S_{NP}(^1n\pi^*)$ state and the intramolecular [2+1] cycloaddition obtained by CASPT2//CASSCF/PCM calculations. The corresponding energy profile is plotted in Fig. 3a.

3		**CASSCF**	**RASSCF**	**CASPT2**	
		A.E.	**A.E.**	**A.E.**	**R.E.**
S_0-Min	Root1[S_0]	-2149.94818	-2150.05847	-2153.61137	0.0

	Root2[$S_{NP}(^1n\pi^*)$]		-2149.92975	-2153.50001	69.9
	Root3[$S_{PP}(^1\pi\pi^*)$]		-2149.83928	-2153.45876	95.8
	Root4		-2149.81428		
	Root5		-2149.77968		
S_{NP}-1	Root1[S_0]		-2150.05639	-2153.61037	0.6
	Root2[$S_{NP}(^1n\pi^*)$]	-2149.93547	-2149.93860	-2153.50363	67.6
	Root3		-2149.84001		
	Root4		-2149.82056		
	Root5		-2149.78589		
S_{NP}-2	Root1[S_0]		-2150.03278	-2153.59376	11.0
	Root2[$S_{NP}(^1n\pi^*)$]	-2149.94808	-2149.95098	-2153.50812	64.8
	Root3		-2149.83730		
	Root4		-2149.82403		
	Root5		-2149.80345		
S_{NP}-3	Root1[S_0]		-2150.03148	-2153.59236	11.9
	Root2[$S_{NP}(^1n\pi^*)$]	-2149.94862	-2149.95152	-2153.50846	64.6
	Root3		-2149.83768		
	Root4		-2149.82471		
	Root5		-2149.80388		
S_{NP}-4	Root1[S_0]		-2150.03066	-2153.59274	11.7
	Root2[$S_{NP}(^1n\pi^*)$]	-2149.94916	-2149.95207	-2153.51012	63.5
	Root3		-2149.83860		
	Root4		-2149.82654		
	Root5		-2149.80405		
S_{NP}-Min/ STC(S_{NP}/T_{NP})	Root1[S_0]		-2150.03287	-2153.59320	11.4
	Root2[$S_{NP}(^1n\pi^*)$]	-2149.94819	-2149.95309	-2153.51076	63.1
	Root3		-2149.83894		
	Root4		-2149.83197		
	Root5		-2149.79791		
	Root1[$T_{NP}(^3n\pi^*)$]		-2149.96020	-2153.51991	57.4
	Root2		-2149.92818		
	Root3		-2149.87926		
	Root4		-2149.84867		
	Root5		-2149.83902		

S_{NP}-6	Root1[S_0]		-2150.02578	-2153.58837	14.4
	Root2[$S_{NP}(^1n\pi^*)$]	-2149.94601	-2149.95023	-2153.50907	64.2
	Root3		-2149.83799		
	Root4		-2149.83138		
	Root5		-2149.80104		
S_{NP}-7	Root1[S_0]		-2150.02469	-2153.58690	15.4
	Root2[$S_{NP}(^1n\pi^*)$]	-2149.94529	-2149.94887	-2153.50767	65.1
	Root3		-2149.83663		
	Root4		-2149.83053		
	Root5		-2149.79987		
S_{NP}-8	Root1[S_0]		-2150.02483	-2153.58585	16.0
	Root2[$S_{NP}(^1n\pi^*)$]	-2149.93910	-2149.94311	-2153.50472	66.9
	Root3		-2149.83252		
	Root4		-2149.83035		
	Root5		-2149.79015		
S_{NP}-TS	Root1[S_0]		-2150.01953	-2153.58241	18.2
	Root2[$S_{NP}(^1n\pi^*)$]	-2149.93334	-2149.93829	-2153.50440	67.1
	Root3		-2149.82710		
	Root4		-2149.82391		
	Root5		-2149.78913		
S_{NP}-10	Root1[S_0]		-2150.01330	-2153.57835	20.7
	Root2[$S_{NP}(^1n\pi^*)$]	-2149.92467	-2149.92920	-2153.50524	66.6
	Root3		-2149.82198		
	Root4		-2149.81553		
	Root5		-2149.78313		
S_{NP}-11	Root1[S_0]		-2150.00103	-2153.56961	26.2
	Root2[$S_{NP}(^1n\pi^*)$]	-2149.91322	-2149.91722	-2153.51167	62.6
	Root3		-2149.81545		
	Root4		-2149.80046		
	Root5		-2149.77546		
S_{NP}-12	Root1[S_0]		-2149.98858	-2153.56049	31.9
	Root2[$S_{NP}(^1n\pi^*)$]	-2149.90745	-2149.91130	-2153.51810	58.5

	Root3		-2149.81258		
	Root4		-2149.78747		
	Root5		-2149.77131		
S_{NP}-13	Root1[S_0]		-2149.94756	-2153.53962	45.0
	Root2[$S_{NP}(^1n\pi^*)$]	-2149.90578	-2149.90675	-2153.52237	55.9
	Root3		-2149.81370		
	Root4		-2149.78740		
	Root5		-2149.78188		
CI($S_{\Sigma P}$/S_0)	Root1[$S_0(\sigma^2\pi^0)$]		-2149.96418	-2153.53243	49.5
	Root2[$S_{\Sigma P}(\delta^1\pi^1)$]	-2149.97398	-2149.94810	-2153.52985	51.2
	Root3		-2149.84216		
	Root4		-2149.83092		
	Root5		-2149.81613		
S_0-1	Root1[$S_0(\sigma^2\pi^0)$]	-2149.98203	-2149.96583	-2153.53625	47.1
	Root2		-2149.94483	-2153.52995	51.1
	Root3		-2149.85661		
	Root4		-2149.83467		
	Root5		-2149.82967		
S_0-2	Root1[$S_0(\sigma^2\pi^0)$]	-2149.98849	-2149.97210	-2153.54193	43.6
	Root2		-2149.94055		
	Root3		-2149.85627		
	Root4		-2149.83053		
	Root5		-2149.82966		
S_0-3	Root1[$S_0(\sigma^2\pi^0)$]	-2149.99545	-2149.97957	-2153.54771	39.9
	Root2		-2149.93040		
	Root3		-2149.85143		
	Root4		-2149.82648		
	Root5		-2149.81919		
S_0-4	Root1[$S_0(\sigma^2\pi^0)$]	-2150.00266	-2149.98698	-2153.55497	35.4
	Root2		-2149.92243		
	Root3		-2149.84528		
	Root4		-2149.82363		
	Root5		-2149.80717		

S_0-5	Root1[$S_0(\sigma^2\pi^0)$]	-2150.00646	-2149.99028	-2153.557485	33.8
	Root2		-2149.92288		
	Root3		-2149.84639		
	Root4		-2149.82535		
	Root5		-2149.80810		
S_0-6	Root1[$S_0(\sigma^2\pi^0)$]	-2150.01700	-2153.57611	-2153.56655	30.5
	Root2		-2153.51036		
	Root3		-2153.54692		
	Root4		-2153.44084		
	Root5		-2149.79662		
S_0-7	Root1[$S_0(\sigma^2\pi^0)$]	-2150.01700	-2150.00432	-2153.56655	28.1
	Root2		-2149.92218		
	Root3		-2149.84788		
	Root4		-2149.81784		
	Root5		-2149.79662		
S_0-8	Root1[$S_0(\sigma^2\pi^0)$]	-2150.01935	-2150.01165	-2153.57081	25.5
	Root2		-2149.91743		
	Root3		-2149.84672		
	Root4		-2149.81642		
	Root5		-2149.78852		
S_0-9	Root1[$S_0(\sigma^2\pi^0)$]	-2150.02301	-2150.01322	-2153.57342	23.8
	Root2		-2149.91645		
	Root3		-2149.83928		
	Root4		-2149.82100		
	Root5		-2149.79817		
$S_0(\sigma^2\pi^0)$-Min	Root1[$S_0(\sigma^2\pi^0)$]	-2150.03139	-2150.02382	-2153.57706	21.5
	Root2		-2149.92726		
	Root3		-2149.84962		
	Root4		-2149.81382		
	Root5		-2149.80968		
***exo*-S_0-1**	Root1[S_0]	-2150.02913	-2150.01408	-2153.57478	23.0
	Root2		-2149.92327		
	Root3		-2149.84473		

	Root4		-2149.83571		
	Root5		-2149.81374		
***exo*-S_0-2**	Root1[S_0]	-2150.02754	-2150.01270	-2153.57391	23.5
	Root2		-2149.92100		
	Root3		-2149.84368		
	Root4		-2149.83664		
	Root5		-2149.81261		
***exo*-S_0-3**	Root1[S_0]	-2150.02113	-2150.00795	-2153.57191	24.8
	Root2		-2149.91235		
	Root3		-2149.84029		
	Root4		-2149.83831		
	Root5		-2149.81030		
***exo*-S_0-4**	Root1[S_0]	-2150.01520	-2150.00645	-2153.57118	25.2
	Root2		-2149.90954		
	Root3		-2149.83889		
	Root4		-2149.83822		
	Root5		-2149.80947		
***exo*-S_0-5**	Root1[S_0]	-2150.01944	-2150.00267	-2153.56943	26.3
	Root2		-2149.90330		
	Root3		-2149.84008		
	Root4		-2149.83508		
	Root5		-2149.80627		
***exo*-S_0-6**	Root1[S_0]	-2150.01173	-2149.99989	-2153.56833	27.0
	Root2		-2149.90009		
	Root3		-2149.84392		
	Root4		-2149.83216		
	Root5		-2149.80317		
***exo*-S_0-7**	Root1[S_0]	-2150.00574	-2149.99512	-2153.56694	27.9
	Root2		-2149.89663		
	Root3		-2149.85278		
	Root4		-2149.82764		
	Root5		-2149.79900		

***exo*-S_0-TS**	Root1[S_0]	-2149.99828	-2149.98992	-2153.56629	28.3
	Root2		-2149.89132		
	Root3		-2149.85690		
	Root4		-2149.82242		
	Root5		-2149.79585		
***exo*-S_0-9**	Root1[S_0]	-2149.99657	-2149.99019	-2153.57034	25.7
	Root2		-2149.89268		
	Root3		-2149.85788		
	Root4		-2149.82701		
	Root5		-2149.80177		
***exo*-S_0-10**	Root1[S_0]	-2149.99854	-2149.99466	-2153.57756	21.2
	Root2		-2149.89605		
	Root3		-2149.85233		
	Root4		-2149.83914		
	Root5		-2149.81695		
***exo*-S_0-11**	Root1[S_0]	-2150.00108	-2149.99895	-2153.58219	18.3
	Root2		-2149.89906		
	Root3		-2149.84911		
	Root4		-2149.83780		
	Root5		-2149.82189		
***exo*-S_0-12**	Root1[S_0]	-2150.00363	-2150.00132	-2153.58453	16.8
	Root2		-2149.89874		
	Root3		-2149.85072		
	Root4		-2149.83367		
	Root5		-2149.82387		
***exo*-S_0-13**	Root1[S_0]	-2150.00595	-2150.00423	-2153.58654	15.6
	Root2		-2149.89872		
	Root3		-2149.85341		
	Root4		-2149.83202		
	Root5		-2149.82413		
***exo*-S_0-14**	Root1[S_0]	-2150.01012	-2150.00770	-2153.59144	12.5
	Root2		-2149.89243	-2153.51008	
	Root3		-2149.85408		

	Root4		-2149.83004		
	Root5		-2149.81628		
***exo*-S_0-15**	Root1[S_0]	-2150.01644	-2150.01558	-2153.59863	8.0
	Root2		-2149.89455		
	Root3		-2149.86242		
	Root4		-2149.83667		
	Root5		-2149.80027		
***exo*-S_0-16**	Root1[S_0]	-2150.02439	-2150.02312	-2153.60644	3.1
	Root2		-2149.89553		
	Root3		-2149.86771		
	Root4		-2149.84239		
	Root5		-2149.80562		
***exo*-S_0-17**	Root1[S_0]	-2150.03521	-2150.03259	-2153.61668	-3.3
	Root2		-2149.89117		
	Root3		-2149.86686		
	Root4		-2149.83838		
	Root5		-2149.80369		
***exo*-S_0-18**	Root1[S_0]	-2150.04401	-2150.04104	-2153.62328	-7.5
	Root2		-2149.86228		
	Root3		-2149.85065		
	Root4		-2149.81485		
	Root5		-2149.78701		
***exo*-S_0-19**	Root1[S_0]	-2150.05504	-2150.05118	-2153.63040	-11.9
	Root2		-2149.84152		
	Root3		-2149.81514		
	Root4		-2149.77986		
	Root5		-2149.75945		
***exo*-S_0-20**	Root1[S_0]	-2150.06576	-2150.06541	-2153.63930	-17.5
	Root2		-2149.84639		
	Root3		-2149.78918		
	Root4		-2149.74154		
	Root5		-2149.70691		

***exo*-S_0-21**	Root1[S_0]	-2150.07307	-2150.07297	-2153.64709	-22.4
	Root2		-2149.85131		
	Root3		-2149.79125		
	Root4		-2149.73864		
	Root5		-2149.71316		
***exo*-S_0-22**	Root1[S_0]	-2150.083917	-2150.08436	-2153.65534	-27.6
	Root2		-2149.86013		
	Root3		-2149.79801		
	Root4		-2149.74614		
	Root5		-2149.72269		
***exo*-P3**	Root1[S_0]	-2150.087062	-2150.08718	-2153.66133	-31.4
	Root2		-2149.86285		
	Root3		-2149.80094		
	Root4		-2149.74898		
	Root5		-2149.72479		

Table S7. Absolute energies (A.E., Hartree) and relative energies (R.E., kcal/mol) for the optimized structures of **3** along the pathways for photogeneration of siloxy carbene mediated by $T_{NP}(^3n\pi^*)$ state and the intramolecular [2+1] cycloaddition obtained by CASPT2//CASSCF/PCM calculations. The corresponding energy profile is plotted in Fig. 3b.

3		**CASSCF**	**RASSCF**	**CASPT2**	
		A.E.	**A.E.**	**A.E.**	**R.E.**
S_0-Min	Root1[S_0]	-2149.94818	-2150.05847	-2153.61137	0.0
	Root2[$S_{NP}(^1n\pi^*)$]		-2149.92975	-2153.50001	69.9
	Root3[$S_{PP}(^1\pi\pi^*)$]		-2149.83928	-2153.45876	95.8
	Root4		-2149.81428	-2153.42890	
	Root5		-2149.77968	-2153.40464	
S_{NP}-1	Root1[S_0]		-2150.05639	-2153.61037	0.6
	Root2[$S_{NP}(^1n\pi^*)$]	-2149.93547	-2149.93860	-2153.50363	67.6
	Root3		-2149.84001		
	Root4		-2149.82056		
	Root5		-2149.78589		
S_{NP}-2	Root1[S_0]		-2150.03278	-2153.59376	11.0

	Root2[$S_{NP}(^1n\pi^*)$]	-2149.94808	-2149.95098	-2153.50812	64.8
	Root3		-2149.83730		
	Root4		-2149.82403		
	Root5		-2149.80345		
S_{NP}-3	Root1[S_0]		-2150.03148	-2153.59236	11.9
	Root2[$S_{NP}(^1n\pi^*)$]	-2149.94862	-2149.95152	-2153.50846	64.6
	Root3		-2149.83768		
	Root4		-2149.82471		
	Root5		-2149.80388		
S_{NP}-4	Root1[S_0]		-2150.03066	-2153.59274	11.7
	Root2[$S_{NP}(^1n\pi^*)$]	-2149.94916	-2149.95207	-2153.51012	63.5
	Root3		-2149.83860		
	Root4		-2149.82654		
	Root5		-2149.80405		
S_{NP}-Min/ STC(S_{NP}/T_{NP})	Root1[S_0]		-2150.03287	-2153.59320	11.4
	Root2[$S_{NP}(^1n\pi^*)$]	-2149.94819	-2149.95309	-2153.51076	63.1
	Root3		-2149.83894		
	Root4		-2149.83197		
	Root5		-2149.79791		
	Root1[$T_{NP}(^3n\pi^*)$]		-2149.96020	-2153.51991	57.4
	Root2		-2149.92818		
	Root3		-2149.87926		
	Root4		-2149.84867		
	Root5		-2149.83902		
T_{NP}-1	Root1[$T_{NP}(^3n\pi^*)$]	-2149.96340	-2149.95594	-2153.52232	55.9
	Root2		-2149.92320		
	Root3		-2149.88201		
	Root4		-2149.88027		
	Root5		-2149.85030		
T_{NP}-Min	Root1[$T_{NP}(^3n\pi^*)$]	-2149.96489	-2149.95666	-2153.52270	55.6
	Root2		-2149.92063		
	Root3		-2149.88657		
	Root4		-2149.88469		
	Root5		-2149.85321		

T_{NP}-3	Root1[$T_{NP}(^3n\pi^*)$]	-2149.95418	-2149.94628	-2153.51926	57.8
	Root2		-2149.90987		
	Root3		-2149.87364		
	Root4		-2149.87062		
	Root5		-2149.84246		
T_{NP}-TS	Root1[$T_{NP}(^3n\pi^*)$]	-2149.95731	-2149.94978	-2153.51886	58.0
	Root2		-2149.91607		
	Root3		-2149.87629		
	Root4		-2149.87371		
	Root5		-2149.84563		
T_{NP}-5	Root1[$T_{NP}(^3n\pi^*)$]	-2149.94803	-2149.94026	-2153.52198	56.1
	Root2		-2149.89817		
	Root3		-2149.86833		
	Root4		-2149.86268		
	Root5		-2149.83530		
T_{NP}-6	Root1[$T_{NP}(^3n\pi^*)$]	-2149.94319	-2149.93548	-2153.52687	53.0
	Root2		-2149.88700		
	Root3		-2149.86285		
	Root4		-2149.85289		
	Root5		-2149.82771		
T_{NP}-7	Root1[$T_{NP}(^3n\pi^*)$]	2149.94010	-2149.93229	-2153.53186	49.9
	Root2		-2149.87774		
	Root3		-2149.85754		
	Root4		-2149.84297		
	Root5		-2149.82040		
T_{NP}-8	Root1[$T_{NP}(^3n\pi^*)$]	-2149.93733	-2149.93210	-2153.53830	45.8
	Root2		-2149.85894		
	Root3		-2149.84067		
	Root4		-2149.81862		
	Root5		-2149.81130		
T_{NP}-9	Root1[$T_{NP}(^3n\pi^*)$]	-2149.96941	-2149.93221	-2153.54003	44.8
	Root2		-2149.83788		

	Root3		-2149.82153		
	Root4		-2149.80997		
	Root5		-2149.79302		
T_{NP}-10	Root1[$T_{NP}(^3n\pi^*)$]	-2149.93967	-2149.97501	-2153.54537	41.4
	Root2		-2149.85199		
	Root3		-2149.82653		
	Root4		-2149.80828		
	Root5		-2149.80633		
T_{NP}-11	Root1[$T_{NP}(^3n\pi^*)$]	-2149.98421	-2149.98126	-2153.54818	39.6
	Root2		-2149.85716		
	Root3		-2149.83278		
	Root4		-2149.81404		
	Root5		-2149.81197		
T_{NP}-12	Root1[$T_{NP}(^3n\pi^*)$]	-2149.99544	-2149.99477	-2153.55688	34.2
	Root2		-2149.86573		
	Root3		-2149.84613		
	Root4		-2149.84216		
	Root5		-2149.81812		
$T_{\Sigma P}(\sigma^1\pi^1)$-Min	Root1[$T_{\Sigma P}(\sigma^1\pi^1)$]	-2150.00620	-2150.00243	-2153.56417	29.6
	Root2		-2149.87761		
	Root3		-2149.85319		
	Root4		-2149.84899		
	Root5		-2149.84265		
CYC-T_1-1	Root1[T_1]	-2150.00367	-2150.00421	-2153.56340	30.1
	Root2		-2149.87787		
	Root3		-2149.85692		
	Root4		-2149.83711		
	Root5		-2149.83529		
CYC-T_1-2	Root1[T_1]	-2149.99946	-2149.99929	-2153.55992	32.3
	Root2		-2149.87052		
	Root3		-2149.86157		
	Root4		-2149.83368		
	Root5		-2149.83234		

CYC-T_1-3	Root1[T_1]	-2149.99558	-2149.99556	-2153.55723	34.0
	Root2		-2149.86744		
	Root3		-2149.86161		
	Root4		-2149.83013		
	Root5		-2149.82783		
CYC-T_1-4	Root1[T_1]	-2149.99286	-2149.99299	-2153.55593	34.8
	Root2		-2149.86535		
	Root3		-2149.86254		
	Root4		-2149.82784		
	Root5		-2149.82425		
CYC-T_1-5	Root1[T_1]	-2149.98731	-2149.98772	-2153.55469	35.6
	Root2		-2149.86979		
	Root3		-2149.86013		
	Root4		-2149.82362		
	Root5		-2149.82267		
CYC-T_1-6 T_1-TS	Root1[T_1]	-2149.98344	-2149.98424	-2153.55372	36.2
	Root2		-2149.87448		
	Root3		-2149.85746		
	Root4		-2149.82416		
	Root5		-2149.82119		
CYC-T_1-7	Root1[T_1]	-2149.98473	-2149.98752	-2153.55669	34.3
	Root2		-2149.87021		
	Root3		-2149.86124		
	Root4		-2149.82922		
	Root5		-2149.82235		
CYC-T_1-8	Root1[T_1]	-2149.98692	-2149.98972	-2153.55894	32.9
	Root2		-2149.87274		
	Root3		-2149.85505		
	Root4		-2149.83186		
	Root5		-2149.82534		
CYC-T_1-9	Root1[T_1]	-2149.98934	-2149.99488	-2153.56380	29.8
	Root2		-2149.87812		

	Root3		-2149.84106		
	Root4		-2149.83728		
	Root5		-2149.82892		
CYC-T_1-10	Root1[T_1]	-2149.99208	-2150.00009	-2153.56886	26.7
	Root2		-2149.88325		
	Root3		-2149.84439		
	Root4		-2149.84025		
	Root5		-2149.81253		
CYC-T_1-11	Root1[T_1]	-2150.00293	-2150.00619	-2153.57194	24.7
	Root2		-2149.88970		
	Root3		-2149.85020		
	Root4		-2149.84518		
	Root5		-2149.80417		
CYC-T_1-12	Root1[T_1]	-2150.00970	-2150.01300	-2153.57870	20.5
	Root2		-2149.89551		
	Root3		-2149.85766		
	Root4		-2149.85166		
	Root5		-2149.81091		
CYC-T_1-13	Root1[T_1]	-2150.01534	-2150.01835	-2153.58482	16.7
	Root2		-2149.89987		
	Root3		-2149.86395		
	Root4		-2149.85660		
	Root5		-2149.81619		
CYC-T_1-14	Root1[T_1]	-2150.02271	-2150.02565	-2153.59410	10.8
	Root2		-2149.90539		
	Root3		-2149.87270		
	Root4		-2149.86247		
	Root5		-2149.82425		
CYC-T_1-15	Root1[T_1]	-2150.02607	-2150.02855	-2153.59774	8.5
	Root2		-2149.90826		
	Root3		-2149.87557		
	Root4		-2149.86438		
	Root5		-2149.82727		

CYC-T_1-16	Root1[T_1]	-2150.02719	-2150.02967	-2153.59926	7.6
	Root2		-2149.90948		
	Root3		-2149.87689		
	Root4		-2149.86501		
	Root5		-2149.82850		
CYC-T_1-17	Root1[T_1]	-2150.02853	-2150.03028	-2153.59993	7.2
	Root2		-2149.91017		
	Root3		-2149.87759		
	Root4		-2149.86568		
	Root5		-2149.82918		
STC(T_1/S_0)	Root1[T_1]	-2150.02860	-2150.03141	-2153.60108	6.5
	Root2		-2149.91141		
	Root3		-2149.87863		
	Root4		-2149.86710		
	Root5		-2149.83040		
	Root1[S_0]		-2150.02936	-2153.60656	3.0
	Root2		-2149.92713		
	Root3		-2149.89364		
	Root4		-2149.87739		
	Root5		-2149.82593		
The pathway of *exo*-cyclopropane formation after STC(T_1/S_0) in Fig. 3b					
***exo*-S_0-1**	Root1[S_0]	-2150.03209	-2150.03064	-2153.60794	2.1
	Root2		-2149.92719		
	Root3		-2149.89252		
	Root4		-2149.87737		
	Root5		-2149.82487		
***exo*-S_0-2**	Root1[S_0]	-2150.03440	-2150.03233	-2153.61132	0.0
	Root2		-2149.92480		
	Root3		-2149.88803		
	Root4		-2149.87106		
	Root5		-2149.81899		
***exo*-S_0-3**	Root1[S_0]	2150.03904	-2150.03503	-2153.61648	-3.2
	Root2		-2149.89666		
	Root3		-2149.86887		

	Root4		-2149.83968		
	Root5		-2149.81022		
***exo*-S_0-4**	Root1[S_0]	-2150.04971	-2150.04363	-2153.62186	-6.6
	Root2		-2149.83948		
	Root3		-2149.82518		
	Root4		-2149.78745		
	Root5		-2149.76456		
***exo*-S_0-5**	Root1[S_0]	-2150.06039	-2150.05852	-2153.63208	-13.0
	Root2		-2149.84128		
	Root3		-2149.78581		
	Root4		-2149.73673		
	Root5		-2149.70235		
***exo*-S_0-6**	Root1[S_0]	-2150.06837	-2150.06661	-2153.64052	-18.3
	Root2		-2149.84692		
	Root3		-2149.78866		
	Root4		-2149.73598		
	Root5		-2149.70898		
***exo*-S_0-7**	Root1[S_0]	-2150.07301	-2150.07259	-2153.64677	-22.2
	Root2		-2149.85141		
	Root3		-2149.79254		
	Root4		-2149.73913		
	Root5		-2149.71432		
***exo*-S_0-8**	Root1[S0]	-2150.08561	-2150.08382	-2153.65926	-30.0
	Root2		-2149.85930		
	Root3		-2149.79677		
	Root4		-2149.74380		
	Root5		-2149.72129		
***exo*-P3**	Root1[S_0]	-2150.087062	-2150.08718	-2153.66133	-31.4
	Root2		-2149.86285		
	Root3		-2149.80094		
	Root4		-2149.74898		
	Root5		-2149.72479		
The pathway of *endo*-cyclopropane formation after the STC(T_1/S_0) in Fig. 3b					

STC(T_1/S_0)	Root1[T_1]	-2150.02860	-2150.03141	-2153.60108	6.5
	Root2		-2149.91141		
	Root3		-2149.87863		
	Root4		-2149.86710		
	Root5		-2149.83040		
	Root1[S_0]		-2150.02936	-2153.60656	3.0
	Root2		-2149.92713		
	Root3		-2149.89364		
	Root4		-2149.87739		
	Root5		-2149.82593		
***endo*-S_0-1**	Root1[S_0]	-2150.03229	-2150.00735	-2153.60389	4.7
	Root2		-2149.94293		
	Root3		-2149.86896		
	Root4		-2149.83431		
	Root5		-2149.79909		
***endo*-S_0-2**	Root1[S_0]	-2150.02225	-2150.00229	-2153.60312	5.2
	Root2		-2149.94162	-2153.56268	
	Root3		-2149.86517		
	Root4		-2149.82965		
	Root5		-2149.79364		
***endo*-S_0-3**	Root1[S_0]	-2150.02043	-2149.98994	-2153.59434	10.7
	Root2		-2149.94953		
	Root3		-2149.84708		
	Root4		-2149.81060		
	Root5		-2149.79727		
***endo*-S_0-4**	Root1[S_0]	-2150.02259	-2149.98826	-2153.59200	12.2
	Root2		-2149.95162		
	Root3		-2149.84341		
	Root4		-2149.80625		
	Root5		-2149.80047		
***endo*-S_0-5**	Root1[S_0]	-2150.02536	-2149.98437	-2153.58842	14.4
	Root2		-2149.94545		
	Root3		-2149.83533		
	Root4		-2149.79825		

	Root5		-2149.79714		
***endo*-S_0-TS**	Root1[S_0]	-2150.02740	-2149.99126	-2153.58574	16.1
	Root2		-2149.94873		
	Root3		-2149.83836		
	Root4		-2149.80408		
	Root5		-2149.8002		
***endo*-S_0-7**	Root1[S_0]	-2150.03084	-2149.99440	-2153.59253	11.8
	Root2		-2149.94829		
	Root3		-2149.83755		
	Root4		-2149.80587		
	Root5		-2149.79845		
***endo*-S_0-8**	Root1[S_0]	-2150.02250	-2149.99803	-2153.59651	9.3
	Root2		-2149.95715		
	Root3		-2149.84496		
	Root4		-2149.81182		
	Root5		-2149.80552		
***endo*-S_0-9**	Root1[S_0]	-2150.02250	-2149.99902	-2153.60331	5.1
	Root2		-2149.96134		
	Root3		-2149.85173		
	Root4		-2149.81554		
	Root5		-2149.81372		
***endo*-S_0-10**	Root1[S_0]	-2150.02713	-2150.02538	-2153.60564	3.6
	Root2		-2149.92126		
	Root3		-2149.88378		
	Root4		-2149.86577		
	Root5		-2149.81485		
***endo*-S_0-11**	Root1[S_0]	-2150.03576	-2150.03197	-2153.61328	-1.2
	Root2		-2149.85301		
	Root3		-2149.84187		
	Root4		-2149.80328		
	Root5		-2149.78191		
***endo*-S_0-12**	Root1[S_0]	-2150.05083	-2150.04553	-2153.62564	-9.0

	Root2		-2149.82959		
	Root3		-2149.78637		
	Root4		-2149.74524		
	Root5		-2149.73137		
***endo*-S_0-13**	Root1[S_0]	-2150.06236	-2150.06199	-2153.63492	-14.8
	Root2		-2149.84160		
	Root3		-2149.78210		
	Root4		-2149.73135		
	Root5		-2149.70338		
***endo*-S_0-14**	Root1[S0]	-2150.06756	-2150.06728	-2153.64031	-18.2
	Root2		-2149.84497		
	Root3		-2149.78507		
	Root4		-2149.73330		
	Root5		-2149.70754		
***endo*-S_0-15**	Root1[S0]	-2150.074189	-2150.07301	-2153.64460	-20.9
	Root2		-2149.84911		
	Root3		-2149.78710		
	Root4		-2149.73393		
	Root5		-2149.71236		
***endo*-S_0-16**	Root1[S0]	-2150.07917	-2150.08043	-2153.65652	-28.3
	Root2		-2149.85637		
	Root3		-2149.79259		
	Root4		-2149.74054		
	Root5		-2149.71665		
***endo*-S_0-17**	Root1[S0]	-2150.08098	-2150.08074	-2153.65803	-29.3
	Root2		-2149.85690		
	Root3		-2149.79354		
	Root4		-2149.74153		
	Root5		-2149.71846		
***endo*-P3**	Root1[S_0]	-2150.081645	-2150.08078	-2153.65908	-29.9
	Root2		-2149.85621		
	Root3		-2149.79241		
	Root4		-2149.74057		

	Root5		-2149.71796		

7. Cartesian Coordinates

7.1 The minima of **1–4** in the ground-state obtained at the CASPT2//CASSCF/PCM level of theory.

1

6	-3.221651750	-0.146581420	0.532267830
6	-1.891899130	0.224089390	0.546688840
6	-2.500845010	2.466092390	-0.003773030
6	-3.833636040	2.106563010	-0.015281150
6	-4.206847520	0.792732700	0.245149070
1	-3.493704340	-1.163631610	0.747572940
1	-1.139561410	-0.509852860	0.775301530
1	-2.225270170	3.486119370	-0.205311480
1	-4.583012920	2.846733080	-0.228365810
1	-5.243384480	0.510050670	0.239390350
6	-1.508353800	1.532722000	0.273294250
6	-0.048408890	1.924849500	0.249584040
6	0.584251750	1.731719040	-1.132846360
6	2.051923210	2.119718730	-1.208558940
14	3.100263280	1.928202060	-2.830283980
8	2.617070890	2.572003820	-0.227195360
1	0.061443310	2.961109280	0.548081180
1	0.504881230	1.338328170	0.973997390
1	0.491847250	0.692930230	-1.444127420
1	0.041155440	2.303569130	-1.883351640
6	3.590704590	3.670208030	-3.371464040
6	4.627256850	0.917172380	-2.371354180
6	2.090020130	1.064103520	-4.172522320
1	4.259862910	3.642543830	-4.227318050
1	2.724843250	4.263043590	-3.652643300
1	1.780392320	0.068748510	-3.866852680
1	1.194926730	1.623551970	-4.428627230
1	5.329887580	0.862961410	-3.198449510
1	5.141769250	1.366353090	-1.527800260
1	4.366773970	-0.100729770	-2.095343390
1	2.675261460	0.955782420	-5.081534860
1	4.102187160	4.192129580	-2.568712690

2

6	-0.033127004	2.179046166	2.526477192
6	-0.744077056	0.818538063	2.615778203
6	-1.791534138	0.523406042	1.525774116
6	0.885136067	2.425011186	1.334921102
8	0.556325042	3.270882253	0.516956038
14	2.665277204	1.662805126	1.102042086
6	2.899594223	1.453060114	-0.758319057
6	3.888013302	4.244879326	1.019510078
6	3.928377302	2.930238227	1.820802138
1	4.172023319	4.094592315	-0.017253999
1	2.902920224	4.699672362	1.028432080
1	4.585149351	4.964425381	1.445376111
6	3.621315276	3.244246249	3.296719253
6	5.352126425	2.345410179	1.732236134
1	3.611011280	2.350720182	3.914775303
1	4.379601339	3.909142301	3.705647286
1	2.664161207	3.743517289	3.415113265
1	6.078722455	3.068837236	2.097498163
1	5.462503433	1.447967111	2.333202182
1	5.630264422	2.098983162	0.711525056
1	2.216722173	0.706659054	-1.151551089
1	2.700640210	2.382529185	-1.280766098
6	-1.260218097	0.262957023	0.140051014
6	-1.211638091	-0.963747073	-0.406022029
6	-0.725579057	-1.267551097	-1.769097134
8	-0.325713026	-0.201117015	-2.449086189
6	0.133701008	-0.380162031	-3.791212294
6	-1.022531077	-0.423691030	-4.771371365
1	0.560739042	2.302185177	3.429843263
1	-0.781157061	2.966784229	2.520334196
1	-1.271302096	0.807956063	3.565005276

1	-2.363502183	-0.341423028	1.846982140
1	-1.555961122	-1.829935139	0.130521013
1	0.764066060	0.477156035	-3.972756307
1	0.733018056	-1.275886099	-3.843205297
1	-0.639661050	-0.483089038	-5.785327432
1	-1.650148127	-1.287975100	-4.593540356
1	-1.627638128	0.472158035	-4.686537362
6	2.842118218	-0.010475000	1.969251152
1	3.837620297	-0.412629029	1.802417139
1	2.692734206	0.052633006	3.043133235
8	-0.714275053	-2.378493182	-2.213546168
1	-0.023074001	0.009840003	2.657484207
1	-2.485592191	1.359565104	1.479526115
1	-0.914824070	1.103354086	-0.433447031
1	2.135123163	-0.735672054	1.577927122
1	3.910527301	1.137670087	-1.001442078

3

16	6.438206954	10.557082043	7.024422895
14	5.099578065	9.797700837	2.789924921
8	1.840450547	8.425746746	9.209078091
8	7.841020650	10.275593138	6.949473087
8	7.890714680	5.601860674	6.416546565
8	6.019362103	4.471421117	6.057916846
8	5.907800796	11.668572869	6.299671631
7	5.672114351	9.196542147	6.403323748
6	4.237065547	9.180210361	6.523599122
6	1.509030149	9.185260194	7.019553406
1	0.453020065	9.184920938	7.217791300
6	3.733590252	8.752806174	7.773838000
1	4.441422508	8.487075267	8.528279178
6	6.705970430	5.581722569	6.262886933
6	2.007725000	9.623152198	5.814067048
1	1.329001117	9.977205698	5.062787101
6	3.395460627	9.645900258	5.526689723
6	3.785525078	10.253976935	4.183858294
6	5.820736428	6.764047633	6.273097408
1	4.771536760	6.598016789	6.138955050
6	2.394666114	8.762285908	8.031007877
6	6.501101998	9.826502367	9.607036422
1	7.312247640	9.158272472	9.331112821
6	5.944042664	10.676718859	8.675572649
6	6.369714696	7.979274081	6.425284339
1	7.429180307	8.077338562	6.527483653
6	4.998617703	10.689130129	11.310360300
6	4.886970130	11.569083948	9.031854249
1	4.467401587	12.228002440	8.281379943
6	6.009627517	9.829666582	10.931235229
1	6.458509050	9.162595691	11.656808888
6	6.814129603	9.308199552	3.341487537
1	7.227599336	10.020215319	4.047189389
1	7.464870084	9.310064425	2.468824162
1	6.863854431	8.319293006	3.781760114
6	4.430565490	11.572654995	10.332787885
1	3.638366251	12.249115925	10.629282669
6	2.681533260	8.083869880	10.284296198
1	3.214714576	7.161638450	10.078933250
1	2.033167445	7.933478552	11.134284879
1	3.394797563	8.867071153	10.499920211
6	4.276518124	8.398435168	1.810132210
6	6.749063132	3.255367068	6.015894669
1	7.479281116	3.280499770	5.220290608
1	6.020237732	2.482422604	5.831255360
1	7.248878876	3.082356244	6.957907802
6	4.517736228	10.753955030	12.758654401
1	4.666982919	9.801206954	13.256995750
1	3.465945486	11.019966877	12.801961102
1	5.083410213	11.514006598	13.295843076
8	2.985948044	11.089371383	3.772389941
6	5.247108120	11.377311489	1.808598215
1	5.720189522	12.150952592	2.406778886
1	5.866929103	11.215225555	0.930138079

1	4.285777879	11.753414111	1.478743663	6	6.838580079	9.815393508	9.434757530
6	5.253742971	7.911899921	0.705213167	1	7.715392014	9.260079612	9.122024412
1	6.155180630	7.482793900	1.132221191	6	6.131277534	10.633097402	8.486795756
1	4.777437880	7.144178300	0.098860867	6	6.894960898	8.008323160	6.347576407
1	5.541229344	8.723010055	0.041440971	1	7.927505199	8.254617121	6.473132970
6	3.945979975	7.205382940	2.745357709	6	5.246343078	10.549282711	11.144689880
1	3.183184920	7.470605149	3.471564100	6	5.031959145	11.359256120	8.861506272
1	3.570151504	6.366480999	2.163128350	1	4.504499653	11.970005142	8.134647559
1	4.826324602	6.863354041	3.283246803	6	6.392219493	9.772764470	10.734179782
6	2.967755962	8.885927220	1.134973103	1	6.915367032	9.175880686	11.471429208
1	2.256126500	9.259361149	1.864903606	6	5.752950886	8.188934107	3.105460096
1	3.164819242	9.676689166	0.417281529	1	6.474173967	8.480415678	3.855159718
1	2.496519151	8.063079352	0.601119118	1	6.305801937	7.826648461	2.246962303
				1	5.146195014	7.378179156	3.490998811
4				6	4.589420621	11.314346963	10.211632965
16	6.610029854	10.584372613	6.830916322	1	3.734053023	11.913106893	10.498754909
6	4.907216293	9.417265152	2.694911025	6	2.945325853	8.064947507	10.032083707
8	2.159330794	8.058467784	8.865520558	1	3.668845696	7.256735624	10.021596260
8	8.038355239	10.500917445	6.748654449	1	2.263206399	7.913378125	10.855295278
8	8.712204150	5.856111239	6.534061697	1	3.457869437	9.010537720	10.144048722
8	7.009768443	4.467788013	6.246176044	6	3.873543643	9.036281187	1.526325794
8	5.930928911	11.606293258	6.099617918	6	7.890028655	3.356824713	6.310751914
7	6.043458030	9.120186527	6.238465138	1	8.629417756	3.414842098	5.525342438
6	4.615525242	8.931052122	6.260608031	1	7.270975677	2.483769366	6.178710496
6	1.874078370	8.664343931	6.626486208	1	8.385568593	3.323290058	7.270259648
1	0.813837440	8.579852316	6.777857360	6	4.830115178	10.557921688	12.614646750
6	4.085574378	8.504661733	7.505527090	1	5.098567363	9.622824743	13.096355318
1	4.776831993	8.353284442	8.307889078	1	3.760220637	10.715219414	12.710306121
6	7.543921069	5.669987112	6.369082964	1	5.342020674	11.367384176	13.133219657
6	2.389851109	9.112244582	5.433289409	8	3.664948247	11.136093448	3.835575699
1	1.705687491	9.399949150	4.660145335	6	5.894076849	10.534856863	2.246114826
6	3.782738774	9.256133908	5.197531589	1	6.589929638	10.742457966	3.052742622
6	4.121021432	10.016659672	3.895119861	1	6.462269913	10.209513716	1.381254862
6	6.512000668	6.724253239	6.279754352	1	5.371284018	11.449824700	2.002309299
1	5.496197948	6.411585157	6.149467526	6	4.602527098	8.266479053	0.386995800
6	2.744501209	8.381041482	7.697976790	1	4.882684625	7.267146921	0.697530334

1	3.929365127	8.175324250	-0.460483538
1	5.491074136	8.788481399	0.051419481
6	2.733542064	8.120652620	2.046222909
1	2.032925611	8.673694810	2.660748611
1	2.178363464	7.724890163	1.200788905
1	3.113749668	7.282930532	2.619744878
6	3.225694914	10.298172549	0.894120026
1	2.767560769	10.934784950	1.641957701
1	3.957632813	10.881869025	0.348308630
1	2.454881627	9.987976942	0.194821287

7.2 Critical structures of **1** along the pathways for photogeneration of siloxy carbene and the intermolecular [2+1] cycloaddition with a fumarate as shown in Fig.1 and Fig. 2 of the main article.

S_0

6	-3.221651750	-0.146581420	0.532267830
6	-1.891899130	0.224089390	0.546688840
6	-2.500845010	2.466092390	-0.003773030
6	-3.833636040	2.106563010	-0.015281150
6	-4.206847520	0.792732700	0.245149070
1	-3.493704340	-1.163631610	0.747572940
1	-1.139561410	-0.509852860	0.775301530
1	-2.225270170	3.486119370	-0.205311480
1	-4.583012920	2.846733080	-0.228365810
1	-5.243384480	0.510050670	0.239390350
6	-1.508353800	1.532722000	0.273294250
6	-0.048408890	1.924849500	0.249584040
6	0.584251750	1.731719040	-1.132846360
6	2.051923210	2.119718730	-1.208558940
14	3.100263280	1.928202060	-2.830283980
8	2.617070890	2.572003820	-0.227195360
1	0.061443310	2.961109280	0.548081180
1	0.504881230	1.338328170	0.973997390
1	0.491847250	0.692930230	-1.444127420
1	0.041155440	2.303569130	-1.883351640
6	3.590704590	3.670208030	-3.371464040
6	4.627256850	0.917172380	-2.371354180
6	2.090020130	1.064103520	-4.172522320
1	4.259862910	3.642543830	-4.227318050
1	2.724843250	4.263043590	-3.652643300
1	1.780392320	0.068748510	-3.866852680
1	1.194926730	1.623551970	-4.428627230
1	5.329887580	0.862961410	-3.198449510
1	5.141769250	1.366353090	-1.527800260
1	4.366773970	-0.100729770	-2.095343390
1	2.675261460	0.955782420	-5.081534860
1	4.102187160	4.192129580	-2.568712690

S_{NP}-Min/STC(S_{NP}/T_{NP})

6	-3.530101655	0.029000089	-0.288734754
6	-2.154784172	0.152445390	-0.254949350
6	-2.364058449	2.408000487	0.529922950
6	-3.752623953	2.289716465	0.498177751
6	-4.340590773	1.097773869	0.086496986
1	-3.976378123	-0.898536100	-0.603652396
1	-1.539739077	-0.684039616	-0.543387743
1	-1.916738518	3.332899298	0.853415209
1	-4.367870035	3.120999391	0.795719130
1	-5.411758880	1.000538915	0.062628023
6	-1.545393045	1.341501395	0.152129780
6	-0.038722232	1.484924712	0.146393099
6	0.489848198	1.992586503	-1.210083162
6	1.989997207	2.171133595	-1.243660475
14	3.155638741	1.877935220	-2.701639397

8	2.405252183	3.140497059	-0.368054776
1	0.267207873	2.164854045	0.934268905
1	0.425272539	0.526461508	0.363568576
1	0.202001167	1.289397730	-1.985516690
1	0.010491231	2.939950730	-1.456993557
6	3.156965637	3.404072510	-3.819712066
6	4.892713180	1.590898240	-2.018248420
6	2.553713538	0.362112200	-3.653691954
1	3.859787712	3.285807126	-4.641593206
1	2.174962484	3.584408216	-4.250422478
1	2.412744714	-0.493311099	-2.997345512
1	1.611460449	0.549143932	-4.162601857
1	5.605896180	1.446340441	-2.827055564
1	5.236017020	2.433769074	-1.424554055
1	4.927372501	0.706422348	-1.386537157
1	3.281167533	0.077802893	-4.410726878
1	3.442314129	4.295287433	-3.266845430

T_{NP}-Min

6	-3.237730728	-0.179487451	-0.200285249
6	-1.909107268	0.164749060	-0.432845579
6	-2.204705230	2.192422248	0.800011340
6	-3.535916731	1.860556341	1.040378109
6	-4.058755892	0.671582429	0.539341241
1	-3.626545278	-1.103334464	-0.588796617
1	-1.281462939	-0.501429078	-0.999057012
1	-1.810824755	3.111860670	1.197393746
1	-4.156197342	2.523367757	1.616184393
1	-5.084888803	0.410296220	0.724017111
6	-1.378799411	1.356326708	0.065975533
6	0.057907935	1.737582337	-0.216624665
6	0.204214988	2.491948880	-1.555460335
6	1.622828864	2.907355989	-1.862346738
14	2.987066968	2.003091958	-2.803977805
8	2.055654615	3.870589188	-1.050497692
1	0.437669321	2.360397665	0.585378783
1	0.675967864	0.845480339	-0.242104608
1	-0.165603321	1.870882060	-2.363269012
1	-0.425354160	3.377202017	-1.529004611
6	3.864818240	3.234519183	-3.935268195
6	4.242452540	1.294330779	-1.578077646
6	2.175450200	0.619853226	-3.800202910
1	4.732755428	2.779959995	-4.405791925
1	3.211013897	3.595742129	-4.723681319
1	1.672983924	-0.096673725	-3.156448716
1	1.443162118	1.001979505	-4.505606782
1	5.082824440	0.837530377	-2.094770482
1	4.639521779	2.072390772	-0.931947965
1	3.796088805	0.535979690	-0.940882626
1	2.923694908	0.074922741	-4.369670391
1	4.211881341	4.098819462	-3.375344838

T_{NP}-TS

6	-3.150916506	-0.746174005	0.291589317
6	-1.977234151	-0.023933909	0.203673745
6	-3.228805391	2.006655771	-0.037784139
6	-4.417850281	1.282933899	0.049741799
6	-4.381666882	-0.098834498	0.214037523
1	-3.113057250	-1.813200597	0.424219440
1	-1.033841452	-0.538974114	0.271245452
1	-3.265426605	3.075943214	-0.158811585
1	-5.361788514	1.795766006	-0.005861342
1	-5.295401958	-0.661616455	0.284861177
6	-1.990912192	1.362514119	0.034890312
6	-0.698941046	2.144177746	-0.089775666
6	-0.248006702	2.320140352	-1.553751511
6	1.077517043	3.084335684	-1.681175953
14	2.879131050	2.318779864	-1.808456036
8	1.588445874	3.829466316	-0.744461175
1	-0.821157750	3.125472706	0.356622777
1	0.083822391	1.645310473	0.470697755

1	-0.143822910	1.350759086	-2.030407193
1	-1.022301943	2.846993190	-2.105354207
6	4.314660024	3.548027270	-1.819923677
6	3.052094079	1.054070782	-0.420856232
6	2.810151314	1.489481907	-3.494984929
1	5.210321523	3.029297541	-2.157275428
1	4.134142239	4.369317509	-2.507182469
1	1.991915258	0.776902561	-3.552715378
1	2.649841120	2.234079219	-4.270570971
1	3.994060010	0.517709719	-0.511781018
1	3.027837752	1.517015905	0.560655299
1	2.255304582	0.316443936	-0.464122796
1	3.727564019	0.957480064	-3.733403034
1	4.518899556	3.969224890	-0.841490920

S_{NP}-TS

6	-3.284971000	-0.483030000	0.578484000
6	-2.217873000	0.387829000	0.680565000
6	-3.626114000	2.212212000	0.016162000
6	-4.706729000	1.338178000	-0.090180000
6	-4.538296000	-0.015018000	0.191314000
1	-3.146661000	-1.526254000	0.801821000
1	-1.254548000	0.012172000	0.983940000
1	-3.763546000	3.258458000	-0.199760000
1	-5.670948000	1.712459000	-0.386508000
1	-5.369081000	-0.692678000	0.113718000
6	-2.366913000	1.747037000	0.403724000
6	-1.183635000	2.684808000	0.467770000
6	-0.542985000	2.843557000	-0.924935000
6	0.634273000	3.760662000	-0.905262000
14	2.785168000	3.613791000	-0.376210000
8	1.252482000	4.422903000	0.036676000
1	-1.489856000	3.661036000	0.831194000
1	-0.443074000	2.305507000	1.164515000
1	-0.245986000	1.869188000	-1.306511000
1	-1.286607000	3.226065000	-1.622983000
6	3.822385000	5.174836000	-0.456174000
6	3.004666000	2.541873000	1.151194000
6	3.346626000	2.557491000	-1.861564000
1	4.888159000	4.969067000	-0.515940000
1	3.549384000	5.750812000	-1.338313000
1	2.899505000	1.567974000	-1.875287000
1	3.161035000	3.027768000	-2.821431000
1	4.057599000	2.335202000	1.326850000
1	2.603905000	3.024106000	2.036539000
1	2.504963000	1.582878000	1.038404000
1	4.425430000	2.428361000	-1.761333000
1	3.642875000	5.806294000	0.409367000

$S_{\Sigma P}(\sigma^1\pi^1)$-Min

6	-3.293470000	-0.497938000	0.608886000
6	-2.262862000	0.420774000	0.645856000
6	-3.782323000	2.168463000	0.023804000
6	-4.826721000	1.245846000	-0.016725000
6	-4.583905000	-0.093403000	0.275609000
1	-3.097331000	-1.530157000	0.840737000
1	-1.270833000	0.093520000	0.907723000
1	-3.978350000	3.203612000	-0.198435000
1	-5.819250000	1.572039000	-0.270962000
1	-5.385592000	-0.810213000	0.248010000
6	-2.484871000	1.768159000	0.354444000
6	-1.346291000	2.763211000	0.346695000
6	-0.723620000	2.907840000	-1.061205000
6	0.418472000	3.876599000	-1.098708000
14	2.991862000	3.643819000	-0.273858000
8	1.352098000	4.075065000	-0.195157000
1	-1.693207000	3.737808000	0.674423000
1	-0.574593000	2.453892000	1.042918000
1	-0.402398000	1.919890000	-1.407161000
1	-1.475219000	3.244059000	-1.767341000
6	3.982518000	5.238340000	-0.285973000
6	3.322816000	2.645501000	1.282686000

6	3.296031000	2.625289000	-1.823767000
1	5.050581000	5.033440000	-0.278618000
1	3.765126000	5.832066000	-1.169203000
1	2.676355000	1.732959000	-1.842541000
1	3.084363000	3.190499000	-2.725872000
1	4.369800000	2.360323000	1.353328000
1	3.074049000	3.215047000	2.174195000
1	2.731197000	1.733665000	1.297658000
1	4.334354000	2.304304000	-1.867220000
1	3.756985000	5.846095000	0.586636000

STC($T_{\Sigma P}/S_0$)/$T_{\Sigma P}(\sigma^1\pi^1)$-Min

6	-2.211287306	0.169809661	-1.968919681
6	-0.933057920	0.481135977	-1.517060721
6	-1.879354886	1.630165843	0.364920255
6	-3.158121593	1.318364570	-0.088794191
6	-3.321576481	0.585733623	-1.261179152
1	-2.332110251	-0.399746569	-2.872583482
1	-0.077204320	0.146160227	-2.076153704
1	-1.761694119	2.192392551	1.274452039
1	-4.017730923	1.641471805	0.469477594
1	-4.308067783	0.342642465	-1.611797239
6	-0.745661936	1.215837113	-0.343531048
6	0.644532783	1.584679905	0.129399760
6	1.104160451	2.948289495	-0.420562724
6	2.469346047	3.349566370	0.032299693
14	4.244254844	3.048377370	2.011760236
8	2.791030277	3.551897106	1.319566136
1	0.667264560	1.616567517	1.212869418
1	1.350875580	0.820783489	-0.177734847
1	1.110811664	2.920952161	-1.504774939
1	0.385277699	3.713330542	-0.132434629
6	5.654773583	3.982915981	1.186380747
6	4.077859053	3.495449097	3.827150679
6	4.455905534	1.194062268	1.766881797
1	6.619049574	3.690086252	1.593195499
1	5.680139642	3.790037235	0.117480376
1	3.664101336	0.631169507	2.251934691
1	4.452584290	0.929605467	0.713599346
1	4.981386019	3.252880384	4.380285057
1	3.890668094	4.557777033	3.950775232
1	3.254570016	2.959003048	4.289202688
1	5.401823048	0.857377323	2.183297740
1	5.550005167	5.055054906	1.323741064

$S_0(\sigma^2\pi^0)$-Min

6	-2.614837056	-0.022787198	-1.043224416
6	-1.338627756	0.230665257	-0.543342726
6	-2.000400589	2.464238143	0.016511055
6	-3.268096347	2.220376079	-0.477537291
6	-3.585706378	0.974962598	-1.012833480
1	-2.848331744	-0.991032844	-1.449909620
1	-0.594574413	-0.547414009	-0.566706076
1	-1.771954352	3.431481685	0.431630075
1	-4.012144377	2.996920577	-0.444896453
1	-4.572657709	0.784404315	-1.395436495
6	-1.012865316	1.479465360	-0.006576895
6	0.379182625	1.762438597	0.512166889
6	1.299655709	2.314835286	-0.589801763
6	2.724756140	2.651848252	-0.235497830
14	4.447632229	2.744677091	1.747800295
8	2.930974027	2.448507322	1.038550219
1	0.332451225	2.474381576	1.328154666
1	0.813754994	0.854161608	0.915341462
1	1.347278518	1.618130220	-1.425936197
1	0.872846021	3.223674161	-1.013978646
6	4.872966581	4.562587932	1.540176617
6	4.209880373	2.300146712	3.555824141
6	5.726935686	1.636046574	0.933349719
1	5.814518277	4.795640386	2.032072477

1	4.968787304	4.830881427	0.492440092
1	5.444861193	0.588537352	1.006398696
1	5.847878881	1.874860552	-0.118941017
1	5.129883803	2.450115196	4.115629656
1	3.439287679	2.912776706	4.016109984
1	3.917570015	1.260018100	3.672696937
1	6.695523624	1.748945673	1.414872382
1	4.108119789	5.199332480	1.978033113

CYC-S_0-TS

6	0.253517533	-0.841480617	-5.826898538
6	0.979639255	-0.641286328	-4.648602127
6	-0.040348067	1.523727359	-4.378656202
6	-0.770769730	1.339348131	-5.549315490
6	-0.632584400	0.158636597	-6.285561278
1	0.365213049	-1.756360562	-6.381212923
1	1.648230616	-1.410701602	-4.301166296
1	-0.160956695	2.432291400	-3.815934788
1	-1.446239686	2.106717203	-5.884634528
1	-1.195990839	0.008676343	-7.189033533
6	0.843381860	0.537564941	-3.912320217
6	1.644767654	0.770499559	-2.651219362
6	3.054474789	1.309790581	-2.938489852
6	3.830104086	1.904059420	-1.790409594
14	4.164082543	1.485055218	0.892349113
8	3.432222078	1.418168801	-0.657285806
1	1.114071687	1.475211018	-2.022221684
1	1.715797920	-0.147149535	-2.078464086
1	3.704762332	0.493596143	-3.263248988
1	3.047109515	2.013406231	-3.759263556
6	2.707246003	1.564316556	2.066780562
6	5.106628590	-0.133487035	1.038821825
6	5.318648397	2.956872506	1.087249798
1	3.036590805	1.665159986	3.098537092
1	2.076990253	2.413086319	1.826245663
1	5.879523416	3.168574326	0.183097921
1	4.783198292	3.857332314	1.373184470
1	5.525922522	-0.252478043	2.034973638
1	4.454607044	-0.982068496	0.851524845
1	5.927730194	-0.181940272	0.328279096
1	6.034788995	2.743493936	1.877892748
1	2.099811096	0.665662015	1.998980377
6	3.582520779	4.195054430	-1.787297656
6	2.305921110	4.226428111	-2.163601773
1	3.846408301	4.216282539	-0.752960084
1	2.018108622	4.287714557	-3.193533632
6	1.227657869	4.144877150	-1.160327547
8	1.386146074	4.066189276	0.021659680
8	0.032761443	4.163273558	-1.729851010
6	-1.098416232	4.115663915	-0.873685222
1	-1.097756967	4.962621902	-0.203366214
1	-1.958659495	4.152047856	-1.522551157
1	-1.099356194	3.201018283	-0.299228218
6	4.734083737	4.391393467	-2.711844405
8	5.810801866	4.735232369	-2.335653797
8	4.420138327	4.210774736	-3.978066040
6	5.433576012	4.454192502	-4.941542830
1	4.976177481	4.267969975	-5.899029683
1	5.771503417	5.477579005	-4.879065434
1	6.267550413	3.786653908	-4.786629196

STC(T_1/S_0)

6	0.678403439	-1.464307596	-5.397645723
6	0.900172882	-0.712307789	-4.247631412
6	0.526597287	1.302995453	-5.493610059
6	0.304670801	0.550895631	-6.643206569
6	0.379947601	-0.827213188	-6.599969612
1	0.734191014	-2.537932271	-5.355567506
1	1.125919002	-1.212373690	-3.320957355
1	0.459483341	2.376827761	-5.541749155

1	0.070226639	1.048746163	-7.568066951
1	0.205657779	-1.407424042	-7.489101269
6	0.828024735	0.685170230	-4.277994137
6	1.104210675	1.504339506	-3.035002347
6	2.598188679	1.860142466	-2.895404335
6	2.926848048	2.629836241	-1.642678118
14	3.659057452	1.446554504	0.759393096
8	2.662949920	1.981405967	-0.482816882
1	0.513451978	2.414136239	-3.058579305
1	0.793112408	0.954761950	-2.153584808
1	3.175192571	0.937955942	-2.894129579
1	2.922852373	2.434153077	-3.755722657
6	2.587502908	1.444475377	2.299826311
6	4.210068316	-0.303256465	0.328618572
6	5.158750988	2.564075395	0.957314013
1	3.133363724	1.053506991	3.155723732
1	2.257249049	2.450073375	2.541820364
1	5.697806754	2.694668238	0.022465983
1	4.878058272	3.546441987	1.324814621
1	4.827462725	-0.729287134	1.116642181
1	3.354468144	-0.959472178	0.188911375
1	4.793056557	-0.323245906	-0.589548488
1	5.853195525	2.128582225	1.672840364
1	1.704732797	0.824904637	2.162096799
6	3.875811850	4.999640703	-1.588953413
6	2.635169384	4.174794043	-1.636862073
1	4.250972855	5.359576236	-0.652624834
1	2.085419788	4.381286345	-2.547904563
6	1.735857796	4.485772541	-0.460339754
8	2.108855302	4.932856005	0.580618808
8	0.468972755	4.275822378	-0.753896495
6	-0.482113820	4.490967649	0.278403073
1	-0.443829534	5.515597586	0.618546883
1	-1.443269753	4.276199073	-0.160786349
1	-0.290090239	3.825733082	1.107346717
6	4.690185230	5.316019180	-2.760982784
8	5.701262440	5.953145307	-2.706832981
8	4.164996411	4.887340162	-3.900303232
6	4.876372472	5.185461871	-5.091919399
1	4.296466582	4.757630839	-5.894253541
1	4.964609778	6.254543289	-5.220739276
1	5.861590922	4.743097547	-5.063059776

P1

6	1.287682958	-1.573407054	-5.286891470
6	1.349820580	-0.790403746	-4.136539153
6	0.715165557	1.136959820	-5.415106032
6	0.650320717	0.355373710	-6.562307062
6	0.936658288	-0.995422607	-6.503739259
1	1.509788317	-2.624600318	-5.232376572
1	1.625345399	-1.244408779	-3.200327469
1	0.489845521	2.188355584	-5.476903616
1	0.374593117	0.807047402	-7.499367414
1	0.885465486	-1.598300732	-7.392897639
6	1.065673337	0.578129542	-4.183044906
6	1.185788815	1.442826175	-2.945383269
6	2.535453584	2.172996776	-2.897655720
6	2.707033951	3.013269360	-1.650163436
14	3.647467221	1.416173025	0.486916462
8	2.615154086	2.277261654	-0.495027818
1	0.378052180	2.168913295	-2.915517648
1	1.083360176	0.826065673	-2.060826418
1	3.333490129	1.435187650	-2.915412231
1	2.655793814	2.785655011	-3.779060119
6	2.741351398	1.267160077	2.124354808
6	3.935107023	-0.286595368	-0.271058022
6	5.304379768	2.283359342	0.716231548
1	3.321613005	0.703683824	2.851353917
1	2.543053199	2.250116650	2.542358124
1	5.823402370	2.453550085	-0.222979309
1	5.195682654	3.241479197	1.216530552

1	4.533524512	-0.908301167	0.391422722
1	2.995817777	-0.805321935	-0.446369801
1	4.461183421	-0.225909795	-1.220666109
1	5.952123624	1.665850176	1.335364818
1	1.787143110	0.762222348	1.999209839
6	3.631805993	4.249042305	-1.588770318
6	2.142586742	4.440956965	-1.587996857
1	4.107616917	4.380129299	-0.639052999
1	1.680181518	4.806458045	-2.487159937
6	1.497064028	4.907721361	-0.324943598
8	2.062131501	5.113676993	0.703242718
8	0.184001712	4.954518701	-0.457194049
6	-0.570400109	5.316732140	0.689476822
1	-0.306100190	6.312305155	1.015314755
1	-1.603687465	5.284748032	0.383408041
1	-0.395086628	4.615691790	1.492447787
6	4.495909937	4.740702189	-2.697584111
8	5.649839217	4.998958530	-2.545479053
8	3.868314255	4.883844677	-3.850696653
6	4.629849477	5.355658207	-4.953541109
1	3.947360075	5.387904470	-5.787475098
1	5.017589099	6.341783344	-4.745871446
1	5.446935197	4.680991209	-5.161148938

7.3 Critical Structures of **3** along the pathways for photogeneration of siloxy carbene and the intramolecular [2+1] cycloaddition as shown in Fig.3 of the main article.

S_0-Min

16	6.438206954	10.557082043	7.024422895
14	5.099578065	9.797700837	2.789924921
8	1.840450547	8.425746746	9.209078091
8	7.841020650	10.275593138	6.949473087
8	7.890714680	5.601860674	6.416546565
8	6.019362103	4.471421117	6.057916846
8	5.907800796	11.668572869	6.299671631
7	5.672114351	9.196542147	6.403323748
6	4.237065547	9.180210361	6.523599122
6	1.509030149	9.185260194	7.019553406
1	0.453020065	9.184920938	7.217791300
6	3.733590252	8.752806174	7.773838000
1	4.441422508	8.487075267	8.528279178
6	6.705970430	5.581722569	6.262886933
6	2.007725000	9.623152198	5.814067048
1	1.329001117	9.977205698	5.062787101
6	3.395460627	9.645900258	5.526689723
6	3.785525078	10.253976935	4.183858294
6	5.820736428	6.764047633	6.273097408
1	4.771536760	6.598016789	6.138955050
6	2.394666114	8.762285908	8.031007877
6	6.501101998	9.826502367	9.607036422
1	7.312247640	9.158272472	9.331112821
6	5.944042664	10.676718859	8.675572649
6	6.369714696	7.979274081	6.425284339
1	7.429180307	8.077338562	6.527483653
6	4.998617703	10.689130129	11.310360300
6	4.886970130	11.569083948	9.031854249
1	4.467401587	12.228002440	8.281379943
6	6.009627517	9.829666582	10.931235229
1	6.458509050	9.162595691	11.656808888
6	6.814129603	9.308199552	3.341487537
1	7.227599336	10.020215319	4.047189389
1	7.464870084	9.310064425	2.468824162
1	6.863854431	8.319293006	3.781760114
6	4.430565490	11.572654995	10.332787885

1	3.638366251	12.249115925	10.629282669
6	2.681533260	8.083869880	10.284296198
1	3.214714576	7.161638450	10.078933250
1	2.033167445	7.933478552	11.134284879
1	3.394797563	8.867071153	10.499920211
6	4.276518124	8.398435168	1.810132210
6	6.749063132	3.255367068	6.015894669
1	7.479281116	3.280499770	5.220290608
1	6.020237732	2.482422604	5.831255360
1	7.248878876	3.082356244	6.957907802
6	4.517736228	10.753955030	12.758654401
1	4.666982919	9.801206954	13.256995750
1	3.465945486	11.019966877	12.801961102
1	5.083410213	11.514006598	13.295843076
8	2.985948044	11.089371383	3.772389941
6	5.247108120	11.377311489	1.808598215
1	5.720189522	12.150952592	2.406778886
1	5.866929103	11.215225555	0.930138079
1	4.285777879	11.753414111	1.478743663
6	5.253742971	7.911899921	0.705213167
1	6.155180630	7.482793900	1.132221191
1	4.777437880	7.144178300	0.098860867
1	5.541229344	8.723010055	0.041440971
6	3.945979975	7.205382940	2.745357709
1	3.183184920	7.470605149	3.471564100
1	3.570151504	6.366480999	2.163128350
1	4.826324602	6.863354041	3.283246803
6	2.967755962	8.885927220	1.134973103
1	2.256126500	9.259361149	1.864903606
1	3.164819242	9.676689166	0.417281529
1	2.496519151	8.063079352	0.601119118

SNP-Min

16	6.408775067	10.574682214	7.039905087
14	5.062316388	9.804519286	2.812277649
8	1.761791995	8.606873006	9.210385847
8	7.799242794	10.246982058	6.924335210
8	7.710165171	5.604783637	6.312609644
8	5.812362515	4.543915717	5.885756066
8	5.917646668	11.743069278	6.381976738
7	5.591378890	9.259905090	6.386718801
6	4.158585894	9.283869199	6.500773961
6	1.429924865	9.353790924	7.010325243
1	0.375198856	9.372976403	7.214498495
6	3.646985241	8.882963774	7.753498596
1	4.355352760	8.600921720	8.502060932
6	6.527761207	5.626155731	6.139273032
6	1.920975407	9.746809702	5.789192701
1	1.222348946	10.056785436	5.038484620
6	3.319592792	9.736351149	5.471813142
6	3.738318361	10.201262414	4.167982145
6	5.677062476	6.832397701	6.179889238
1	4.625826650	6.703739683	6.024677159
6	2.313791823	8.922668049	8.023099535
6	6.551577411	9.767584672	9.595521948
1	7.349315395	9.106874808	9.268715468
6	5.960146375	10.640702738	8.706864434
6	6.256812772	8.026115634	6.378056011
1	7.317192060	8.092895315	6.499389316
6	5.123183212	10.589455519	11.378268770
6	4.920778587	11.524479492	9.127742543
1	4.473550515	12.204356578	8.412980716
6	6.115713426	9.739836099	10.936996435
1	6.589873545	9.053388747	11.627053622
6	6.812351250	9.591183912	3.414792091
1	7.115109006	10.393192039	4.080011846
1	7.466180804	9.629558788	2.545398803
1	6.987781393	8.645287517	3.913399315
6	4.517921805	11.497765354	10.448571285
1	3.741450561	12.169359864	10.793350953
6	2.613507773	8.252690916	10.270981781

1	3.141137607	7.329747373	10.054916647
1	1.978989670	8.103233587	11.131670849
1	3.332314340	9.035753439	10.474763124
6	4.458014824	8.264088336	1.885953091
6	6.507351264	3.309570355	5.808524446
1	7.249793718	3.342598878	5.024399155
1	5.759487971	2.565444540	5.585030615
1	6.988114139	3.087028694	6.750203139
6	4.698580738	10.610582392	12.846022464
1	4.857880452	9.639579130	13.304410879
1	3.651775052	10.883168737	12.938240066
1	5.291315043	11.346598464	13.387400106
8	2.749380398	10.936057463	3.563344999
6	5.012804204	11.323503740	1.723944095
1	5.379031490	12.189853047	2.268112655
1	5.654078932	11.186327186	0.856784994
1	4.016079165	11.554344033	1.366070417
6	5.512172380	7.870069835	0.815535448
1	6.455638793	7.587545806	1.272505847
1	5.155325697	7.018532570	0.239932007
1	5.697295515	8.683115012	0.118756683
6	4.269583505	7.072634382	2.860203946
1	3.477809116	7.272290101	3.575918911
1	4.000645250	6.174881740	2.307330251
1	5.183512546	6.859417227	3.407008095
6	3.108378789	8.545467913	1.174816277
1	2.340931017	8.841551686	1.882920313
1	3.209473626	9.329429085	0.430573885
1	2.762722835	7.647975467	0.665634927

SNP-TS

16	6.683296825	10.860375803	6.336231005
14	4.213198283	10.843678673	2.380169430
8	3.277151432	7.584026513	9.106437126
8	7.948239740	11.014174714	5.679943000
8	8.465346191	6.743648591	3.691904431
8	6.820684786	5.261043532	3.760186695
8	5.738968541	11.930667851	6.291701004
7	5.952258512	9.547339090	5.607918536
6	4.647022496	9.183736163	6.088318343
6	2.216454293	8.411342489	7.184323432
1	1.285406231	8.098792361	7.626308569
6	4.602855426	8.507106584	7.328134705
1	5.529897807	8.324167522	7.829736792
6	7.348617040	6.448956554	3.998850614
6	2.250982923	9.063087402	5.971616662
1	1.319858178	9.249235395	5.473344211
6	3.479974975	9.514104907	5.359069390
6	3.445626858	10.276718539	4.128734598
6	6.387325609	7.334030110	4.686678526
1	5.415487992	6.941128703	4.903999615
6	3.413792555	8.154115143	7.893412373
6	7.945591261	9.504375718	8.280841664
1	8.592137431	9.119870343	7.496803709
6	6.948847124	10.412184581	7.991581367
6	6.765103024	8.583991699	4.994764086
1	7.746306231	8.927012647	4.742958960
6	7.329948090	9.596020169	10.635873731
6	6.105245665	10.933252453	9.011107379
1	5.333743601	11.646671546	8.746155792
6	8.132817981	9.088344609	9.620646702
1	8.919952947	8.379853373	9.846290051
6	6.038679348	11.018822901	2.550606288
1	6.251661866	11.635002658	3.417318785
1	6.463445216	11.504448386	1.677741127
1	6.517818178	10.057210577	2.680236659
6	6.301177987	10.535304229	10.304067372
1	5.685196724	10.945216357	11.095291660
6	4.403849574	7.511678828	9.946545856
1	5.121440536	6.789756175	9.570382378
1	4.043127605	7.179414678	10.908957079

1	4.883327221	8.476315030	10.042881092
6	3.707660779	9.522076168	1.106190010
6	7.641272432	4.304360473	3.108885238
1	7.943135243	4.664784971	2.136366227
1	7.035078144	3.418241422	3.008467463
1	8.518755151	4.093024585	3.702598473
6	7.562717815	9.202039875	12.092406856
1	8.264588355	9.894145560	12.554368275
1	7.978765700	8.201390092	12.157410936
1	6.633483730	9.236888049	12.652782332
8	2.203734698	10.548594199	3.646918469
6	3.496974799	12.537553404	1.977434116
1	3.634249516	13.216889195	2.814819404
1	4.033636229	12.963612740	1.128686975
1	2.440729962	12.532414563	1.726361843
6	4.613581013	9.716899281	-0.142001587
1	5.661832543	9.573939825	0.101081078
1	4.350183762	8.991699803	-0.909052096
1	4.492393025	10.707908672	-0.573124266
6	3.952418607	8.105619329	1.686695288
1	3.304665876	7.912063966	2.536184674
1	3.748730251	7.348890095	0.931923845
1	4.983262175	7.983653128	2.007724158
6	2.226437560	9.626239524	0.648344378
1	1.540917666	9.472294612	1.473636880
1	2.013890830	10.591924555	0.200011379
1	2.020816268	8.863852168	-0.101819693

$S_{\Sigma P}(\sigma^1\pi^1)$-Min/CI($S_{\Sigma P}/S_0$)

16	6.680145522	10.837583821	6.409711500
14	3.390487260	10.926068819	2.056720156
8	3.349930259	7.622091609	9.319314708
8	7.929892636	10.997298828	5.707516415
8	8.336496664	6.781177524	3.565706272
8	6.730375503	5.268206407	3.761559291
8	5.746481429	11.910742899	6.395369473
7	5.943034476	9.517111745	5.716018441
6	4.675820359	9.138221681	6.260207496
6	2.229528173	8.359233664	7.390633554
1	1.323143104	8.040073636	7.870234621
6	4.652887357	8.498124647	7.511602574
1	5.582681438	8.340224665	8.011092609
6	7.255606571	6.464284491	3.965960306
6	2.215993168	8.950893676	6.167110454
1	1.286670096	9.112803710	5.653916422
6	3.446328266	9.409733743	5.534064443
6	3.435234266	10.116243792	4.364250336
6	6.335356487	7.330204582	4.728761362
1	5.385725423	6.923582508	5.012578383
6	3.472205267	8.151983617	8.089705646
6	7.989194619	9.463414753	8.321005635
1	8.595913639	9.054600722	7.517548568
6	7.009748546	10.398071794	8.058462598
6	6.723374540	8.578569643	5.032022387
1	7.682943605	8.935857686	4.723613362
6	7.450553564	9.577216755	10.693021804
6	6.214967498	10.946813837	9.102356693
1	5.454420409	11.678811919	8.860706685
6	8.204860648	9.045260690	9.655882763
1	8.976356679	8.311990625	9.858431758
6	5.205932399	11.146393883	2.376352184
1	5.396402421	11.773182903	3.241173248
1	5.613979415	11.651956915	1.502262115
1	5.741550450	10.212909764	2.508417193
6	6.440625505	10.546729801	10.392242801
1	5.861565469	10.976127822	11.199963872
6	4.480284343	7.608978596	10.156817769
1	5.199886401	6.869766505	9.820464772
1	4.125768316	7.336841576	11.139521882
1	4.952874383	8.580518656	10.188664767
6	3.031386235	9.589934736	0.797257062

6	7.511305600	4.330240331	3.039149234
1	7.726975598	4.701289363	2.047832158
1	6.914273540	3.434018265	2.981706228
1	8.437816645	4.130511316	3.557691274
6	7.709410617	9.175548680	12.143596923
1	8.400720631	9.878969762	12.604496971
1	8.147497623	8.183609631	12.194621940
1	6.786278528	9.184837699	12.715322986
8	2.467149189	10.385231784	3.544100272
6	2.615918202	12.562306992	1.674627131
1	2.788606217	13.252884996	2.498329191
1	3.052983234	12.992595989	0.777903060
1	1.540549121	12.485786957	1.535854117
6	3.808250293	9.907229785	-0.506626038
1	4.882732378	9.881763765	-0.348761029
1	3.562785272	9.162705707	-1.259825099
1	3.543918272	10.883247849	-0.907559070
6	3.481274269	8.208489640	1.342240105
1	2.926907225	7.940618635	2.236636171
1	3.302384254	7.438367565	0.594481045
1	4.541434352	8.198228629	1.578257122
6	1.509878118	9.539854724	0.495216040
1	0.940207073	9.317722731	1.394311110
1	1.155220087	10.481885797	0.087226006
1	1.298265100	8.762620666	-0.235827021

$S_0(\sigma^2\pi^0)$-Min

16	2.209656514	1.437090814	1.447866520
14	-1.506409785	1.920144366	-3.517064675
8	-2.070970285	-1.039955524	3.866962530
8	3.569048503	1.307317079	1.009293528
8	3.517789711	-2.688218112	-1.504577466
8	1.658381262	-3.876470803	-1.698384670
8	1.499452115	2.644179892	1.164220407
7	1.383250723	0.176410936	0.740556143
6	-0.015530336	0.048477319	1.041866049
6	-2.672285220	-0.200396921	1.772462331
1	-3.698223204	-0.296084355	2.077872921
6	-0.346063828	-0.485078649	2.298085456
1	0.446504718	-0.757781381	2.958828361
6	2.349238761	-2.823268909	-1.288996079
6	-2.333602637	0.302609237	0.532290917
1	-3.106812319	0.601319862	-0.148221949
6	-0.987860368	0.450528026	0.132834475
6	-0.549100624	0.995292805	-1.204011795
6	1.504725281	-1.901373793	-0.509972089
1	0.472590638	-2.159300076	-0.388137113
6	-1.661586732	-0.592342650	2.668566359
6	2.751526079	0.022555746	3.666542299
1	3.389267576	-0.589812532	3.035085047
6	2.101302117	1.125099090	3.147679132
6	2.056862118	-0.785774747	-0.007507956
1	3.092894915	-0.577647588	-0.168534916
6	1.780111889	0.461970040	5.846489897
6	1.268086878	1.937823532	3.966494600
1	0.767655829	2.796193756	3.535648634
6	2.573990367	-0.311702677	5.023742853
1	3.087849479	-1.178187676	5.420965824
6	0.143837467	2.735783601	-3.753876537
1	0.335911208	3.436276433	-2.946901024
1	0.158849723	3.290110306	-4.689628514
1	0.956932344	2.018987548	-3.769108327
6	1.117535395	1.605656131	5.300046335
1	0.497285901	2.216417822	5.944522681
6	-1.105904725	-1.411821251	4.819989964
1	-0.564840848	-2.294805007	4.496014994
1	-1.649964343	-1.639710698	5.724123003
1	-0.401179517	-0.613307901	5.007667274
6	-1.790711500	0.434995065	-4.636317357
6	2.356257461	-4.857225463	-2.446581218
1	2.751383318	-4.429019832	-3.356525876
1	1.631321487	-5.621811926	-2.677611458

1	3.166329318	-5.273055665	-1.864934933
6	1.642787689	0.142251295	7.333440765
1	2.430187629	0.648029046	7.890629800
1	1.735904618	-0.925395449	7.507749370
1	0.685097219	0.483814328	7.714000489
8	-1.602097504	1.320106119	-1.892009424
6	-2.887157759	3.162511436	-3.576606837
1	-2.663833334	4.005679737	-2.928016032
1	-3.022478393	3.549611515	-4.583853417
1	-3.829185514	2.733374204	-3.251284539
6	-1.591965681	0.880575771	-6.110908020
1	-0.574716386	1.217672241	-6.289205775
1	-1.786760864	0.046727028	-6.781895564
1	-2.272263903	1.684615679	-6.381835977
6	-0.783002768	-0.697452587	-4.309322822
1	-0.916032541	-1.062072915	-3.295728454
1	-0.934256051	-1.535431241	-4.986976671
1	0.244437560	-0.362870836	-4.420011557
6	-3.233297323	-0.106314720	-4.456660109
1	-3.417423023	-0.399897300	-3.426813172
1	-3.974212455	0.635381922	-4.740003167
1	-3.384516056	-0.982001561	-5.084516405

CYC-S_0-TS

16	1.888893735	1.452479675	2.086304831
14	-0.819098880	2.186614099	-3.044070503
8	-1.992991848	-2.329825941	3.353210158
8	3.241708077	1.810251497	1.803358365
8	3.584978272	0.019643372	-2.625499411
8	2.958475495	-2.096462013	-2.805304056
8	0.883272707	2.464533365	1.932118218
7	1.555962107	0.131081856	1.109545877
6	0.233657151	-0.414346929	1.213481401
6	-2.338731703	-1.375998762	1.255230120
1	-3.342147570	-1.755076524	1.306243421
6	-0.165540413	-1.179878418	2.298964933
1	0.530775285	-1.384163739	3.080890629
6	2.975467488	-0.916540308	-2.199334075
6	-1.901895509	-0.641674151	0.163487866
1	-2.567140543	-0.439964490	-0.654193284
6	-0.598629731	-0.132780372	0.141634365
6	0.001359478	0.813363022	-0.840101718
6	2.195307084	-0.939648690	-0.960136317
1	1.743485802	-1.868279772	-0.674732770
6	-1.469041616	-1.636971248	2.326223668
6	2.518610629	-0.420740422	3.949138068
1	3.264270745	-0.762778979	3.242499604
6	1.727558006	0.735227884	3.643938831
6	2.027027989	0.203181013	-0.238093683
1	2.590773128	1.072026946	-0.490540780
6	1.302949896	-0.608776848	6.057524620
6	0.779420762	1.203742534	4.511391441
1	0.180573640	2.071471284	4.250133019
6	2.290234863	-1.085495851	5.120878857
1	2.872153584	-1.964733471	5.365448780
6	-0.588910449	3.728071071	-2.036920365
1	-1.390312525	3.835678238	-1.311909549
1	-0.599272866	4.606735528	-2.676893354
1	0.350255187	3.716510215	-1.495674975
6	0.571773340	0.522137302	5.747675624
1	-0.167723925	0.906615748	6.441439274
6	-1.195818253	-2.583493115	4.480734477
1	-0.388291321	-3.265739487	4.238055559
1	-1.843313862	-3.046084874	5.209370189
1	-0.778702970	-1.672399152	4.885373099
6	0.422237025	1.997305722	-4.442983914
6	3.706100288	-2.219364329	-3.999742061
1	3.331732896	-1.540677044	-4.751313600
1	3.579467341	-3.239957696	-4.323646475
1	4.750396420	-2.012622731	-3.819037545
6	1.126023912	-1.335348027	7.391365354

1	0.164009498	-1.095752084	7.832042947
1	1.908538313	-1.030492586	8.084153730
1	1.196502558	-2.410610172	7.254696174
8	-0.678132178	0.846829498	-1.944226656
6	-2.577578411	1.998546796	-3.610680882
1	-3.248509396	1.979580263	-2.756821429
1	-2.874778461	2.829396612	-4.244503843
1	-2.724428468	1.079629720	-4.169121803
6	-0.085948291	2.809268530	-5.667107700
1	-0.223218346	3.859517128	-5.421266714
1	0.641880007	2.754109083	-6.473274154
1	-1.026040840	2.418292169	-6.043171163
6	1.810027100	2.548023194	-4.022805738
1	2.199349533	2.025864804	-3.154870741
1	2.521865720	2.416255197	-4.834274808
1	1.759074538	3.608365859	-3.795411072
6	0.553621391	0.505533382	-4.846312209
1	0.902909184	-0.096060276	-4.013765258
1	-0.397594357	0.100947461	-5.182116878
1	1.265850581	0.401081217	-5.662197887

***exo*-P3**

16	2.177631770	1.213158904	1.833723218
14	-0.474193954	1.689006686	-2.783596268
8	-2.166771751	-1.919146655	3.313630065
8	3.579824827	1.399375309	1.587199572
8	3.390194631	-0.442885399	-2.973719764
8	2.674007454	-2.535915878	-3.073777831
8	1.301518466	2.299094613	1.498187947
7	1.754783805	-0.149468817	0.954386340
6	0.418714138	-0.652583516	1.086729707
6	-2.164750263	-1.589037240	1.003334696
1	-3.181337340	-1.936234730	1.007947370
6	-0.160872661	-1.111451540	2.271953323
1	0.415662830	-1.161567943	3.165102590
6	2.756149887	-1.341004783	-2.513603268
6	-1.540163552	-1.217988303	-0.176035534
1	-2.063946283	-1.284261509	-1.111731342
6	-0.229261741	-0.736028508	-0.132895262
6	0.696080637	-0.348605607	-1.233624004
6	1.953539139	-1.278260576	-1.263147570
1	1.870001070	-2.216458341	-0.742968197
6	-1.465795886	-1.540715526	2.223918640
6	2.537516777	-0.425048581	3.992979229
1	3.300820790	-0.929332867	3.410459288
6	1.873456518	0.731983371	3.456977916
6	1.994434406	-0.005707131	-0.480017639
1	2.682401634	0.756011585	-0.783708336
6	1.149317120	-0.185307165	6.000378663
6	0.907357739	1.391049430	4.170504098
1	0.405177707	2.252942297	3.741625036
6	2.159180820	-0.880159817	5.237374582
1	2.634587834	-1.754095313	5.666738175
6	-0.466547687	2.787143269	-1.284720851
1	-1.136057890	2.407390488	-0.518884115
1	-0.804180267	3.785416798	-1.553342536
1	0.519218608	2.878601878	-0.843644729
6	0.549945355	0.926898434	5.465829788
1	-0.195971952	1.473094547	6.029188977
6	-1.519765398	-1.952703240	4.559521180
1	-0.765249887	-2.733429191	4.580843298
1	-2.283871141	-2.177140577	5.288776103
1	-1.052085319	-1.007458505	4.797849553
6	0.512081726	2.406325408	-4.217346593
6	3.388546297	-2.734574267	-4.283204353
1	3.033489313	-2.057595590	-5.046160760
1	3.198957175	-3.756297687	-4.571635365
1	4.446409882	-2.578817918	-4.128134082
6	0.808260784	-0.685026410	7.401478513
1	-0.089256256	-0.202828750	7.775040714
1	1.630927568	-0.463068810	8.079376742

1	0.659351042	-1.761653049	7.395978351
8	0.211712390	0.185403713	-2.374102741
6	-2.222485998	1.283558989	-3.279883437
1	-2.756581690	0.817729702	-2.456616572
1	-2.765163982	2.184907915	-3.552776419
1	-2.256710648	0.603729253	-4.125246844
6	-0.290238017	3.578899910	-4.845965122
1	-0.510124088	4.352148904	-4.113893875
1	0.288307622	4.038760226	-5.644092352
1	-1.227732340	3.236294091	-5.273054168
6	1.877294074	2.946621062	-3.717447727
1	2.463194695	2.164110265	-3.244328959
1	2.455695047	3.330127684	-4.555342924
1	1.743892104	3.758394954	-3.008586062
6	0.754582674	1.325556586	-5.302141771
1	1.333189989	0.497996161	-4.906596023
1	-0.183429273	0.935971056	-5.688878792
1	1.304938290	1.753112261	-6.137787473

T_{NP}-Min

16	6.478453582	10.530273923	7.006833943
14	5.058400598	9.854681532	2.780650439
8	1.842766492	8.480035040	9.204737356
8	7.873593680	10.207793255	6.929620421
8	7.786030297	5.540733082	6.412171539
8	5.871657726	4.454504929	6.159446539
8	5.982411825	11.667882822	6.300862862
7	5.670018545	9.197783808	6.382557774
6	4.237339957	9.220137631	6.509389125
6	1.509543223	9.252019925	7.018352280
1	0.454104741	9.257214435	7.220142593
6	3.730158479	8.800212571	7.757337989
1	4.438154442	8.521983238	8.507598296
6	6.595989406	5.550857565	6.302895537
6	2.001336026	9.666125095	5.802065520
1	1.305711217	9.995800139	5.055124498
6	3.396492554	9.678646275	5.492151118
6	3.806024642	10.249396271	4.205078852
6	5.744479605	6.757245800	6.309200208
1	4.687641036	6.617464212	6.214353124
6	2.392675360	8.822091140	8.024090843
6	6.464797211	9.712906480	9.564860254
1	7.221980955	8.991569467	9.270324802
6	5.982220739	10.634917560	8.659764219
6	6.331977743	7.959776280	6.409798920
1	7.396212670	8.026745249	6.480714227
6	5.029809585	10.639299677	11.290617544
6	4.996201474	11.594501125	9.040648752
1	4.631366972	12.305359899	8.309568739
6	5.970120519	9.714398284	10.887474917
1	6.360731171	8.991263603	11.592560473
6	6.808936469	9.558749104	3.345224952
1	7.148240000	10.331100180	4.027839542
1	7.449802186	9.598245994	2.466322249
1	6.956585917	8.594234560	3.814745827
6	4.538093365	11.594334963	10.341262129
1	3.799297254	12.320527389	10.657194282
6	2.687780245	8.094091679	10.259622304
1	3.183566409	7.155280809	10.033985358
1	2.050485257	7.958349036	11.120458112
1	3.434825863	8.846004818	10.473721227
6	4.376490486	8.369315973	1.818302405
6	6.565236217	3.217363277	6.131332040
1	7.264377578	3.194776542	5.308153595
1	5.808780832	2.459995665	6.001085008
1	7.096617013	3.061042704	7.058886675
6	4.549858473	10.697703065	12.739045843
1	4.645413183	9.727349156	13.216173059
1	3.513956007	11.019661912	12.787451856
1	5.154305237	11.413460168	13.294531721
8	2.859583692	11.072192226	3.716423996

6	5.038393962	11.416917495	1.754001802
1	5.439863484	12.247044672	2.328284189
1	5.657351947	11.300304557	0.868073223
1	4.041184667	11.691688707	1.427750619
6	5.369708234	7.999833728	0.682620850
1	6.328550315	7.681753909	1.081031701
1	4.969252541	7.179082990	0.091144293
1	5.538604466	8.836858836	0.010257307
6	4.205737497	7.140279851	2.748559056
1	3.468828280	7.331497415	3.522597303
1	3.869373419	6.279731967	2.173772936
1	5.143403710	6.868345505	3.224969036
6	3.002660409	8.714241377	1.187420665
1	2.277312947	8.996279197	1.944599705
1	3.087599575	9.529268798	0.474906338
1	2.609033802	7.850057304	0.655843983

T_{NP}-TS

16	6.724666209	10.890200973	6.386606827
14	4.159161745	10.826868088	2.342445369
8	3.306364017	7.603650575	9.079470412
8	7.994883539	11.052069732	5.742949859
8	8.519444246	6.775605870	3.755450501
8	6.868097639	5.299382800	3.798179532
8	5.778561530	11.958932108	6.356480608
7	5.993175766	9.598398291	5.617401604
6	4.675010580	9.243013117	6.069422588
6	2.253428114	8.475752885	7.176010163
1	1.314114917	8.177393333	7.604996643
6	4.625426037	8.556193648	7.304597801
1	5.551035898	8.360296358	7.803051124
6	7.398176341	6.483760013	4.048256470
6	2.300036300	9.127776939	5.963813044
1	1.369788792	9.324300458	5.470264135
6	3.513608031	9.563298070	5.339825488
6	3.374195851	10.310758236	4.077413173
6	6.431691353	7.371189571	4.726453975
1	5.455628733	6.980038894	4.928416123
6	3.437473655	8.197440948	7.876758424
6	7.947545195	9.469902996	8.316275002
1	8.585766454	9.079812472	7.528417340
6	6.977187370	10.410241495	8.038184897
6	6.810105316	8.622378429	5.031500973
1	7.796619345	8.958083660	4.791120736
6	7.328049772	9.538237082	10.672035375
6	6.149329305	10.940516257	9.066521445
1	5.401097705	11.683162868	8.814765263
6	8.118038484	9.024943829	9.649163588
1	8.882839629	8.289022533	9.864010768
6	5.997923386	10.983168473	2.520824992
1	6.224116232	11.625491014	3.365415800
1	6.426120122	11.439614437	1.631554976
1	6.477194299	10.024330731	2.673817194
6	6.330946006	10.515708955	10.353704145
1	5.726779367	10.931496484	11.151422919
6	4.431064731	7.516742684	9.921581390
1	5.140214390	6.784707348	9.548692725
1	4.066972808	7.189262032	10.885101504
1	4.921703594	8.474720619	10.021044117
6	3.659223730	9.507094313	1.062907486
6	7.689297701	4.346100376	3.142537980
1	7.997266742	4.715001309	2.175018524
1	7.081062853	3.462821361	3.030201995
1	8.563129945	4.126649592	3.738609160
6	7.541369588	9.108993158	12.121993368
1	8.242932094	9.784694401	12.608033939
1	7.948884754	8.103784195	12.168709558
1	6.606195383	9.137972015	12.673017858
8	2.079748542	10.572661603	3.803616103
6	3.476369558	12.522938322	1.907688909
1	3.630976179	13.226059360	2.721544076

1	4.011127436	12.914681730	1.042735265
1	2.419129206	12.526907786	1.662461801
6	4.589665826	9.656067552	-0.173712375
1	5.630754863	9.497685436	0.089271768
1	4.324369056	8.918793995	-0.928918404
1	4.495428100	10.638958199	-0.629085009
6	3.857156283	8.096081227	1.673252767
1	3.181029703	7.933624605	2.506673708
1	3.658808823	7.329682760	0.926859503
1	4.875615325	7.958956108	2.026538971
6	2.189187255	9.635698831	0.574861597
1	1.480197831	9.521644624	1.388659184
1	2.007564775	10.590489849	0.090626636
1	1.982218201	8.855312834	-0.156149157

$T_{\Sigma P}(\sigma^1\pi^1)$-Min

16	2.097738494	1.668349596	1.549110748
14	-1.338925339	1.853032636	-3.579829452
8	-2.015131296	-1.295967624	3.772431010
8	3.453865613	1.632146945	1.086619945
8	3.574358585	-2.169159330	-1.699539473
8	1.752945062	-3.377524439	-2.044540877
8	1.327697071	2.853988050	1.345732172
7	1.325386847	0.409728445	0.762286860
6	-0.058482712	0.202333541	1.059947004
6	-2.690185932	-0.282429941	1.768348607
1	-3.704600906	-0.474008261	2.065146748
6	-0.348419350	-0.477154490	2.236865469
1	0.473802861	-0.785143618	2.846407798
6	2.412367241	-2.361627446	-1.508622725
6	-2.410381281	0.375272777	0.587689557
1	-3.211744764	0.698078551	-0.048136016
6	-1.073628855	0.660258904	0.195371320
6	-0.777751128	1.359001599	-0.997017992
6	1.526866539	-1.530545078	-0.678380081
1	0.499201115	-1.819412487	-0.599739818
6	-1.649879675	-0.705022277	2.614159582
6	2.870124316	0.264241648	3.702710066
1	3.634597419	-0.160444256	3.058478428
6	2.020124639	1.242744749	3.222141208
6	2.040218065	-0.455802505	-0.057405846
1	3.072671480	-0.208358758	-0.177135866
6	1.767445540	0.356386976	5.857727664
6	1.015382009	1.813747771	4.049155643
1	0.359753326	2.580082546	3.654232980
6	2.732016235	-0.177519366	5.027104780
1	3.398638987	-0.944480729	5.399392802
6	0.498234022	2.042481626	-3.789866533
1	0.874114300	2.845415215	-3.163648003
1	0.736848304	2.285460657	-4.821596239
1	1.034795040	1.137077028	-3.527020399
6	0.901343565	1.372266289	5.358064958
1	0.150908021	1.803972682	6.008257953
6	-1.011041882	-1.673955086	4.678665094
1	-0.380166074	-2.449862418	4.260007424
1	-1.518809403	-2.061685246	5.548049698
1	-0.397270003	-0.827571081	4.958556001
6	-2.006527133	0.263625501	-4.335537025
6	2.491947139	-4.270188466	-2.860707056
1	2.906445889	-3.750624134	-3.711318939
1	1.788920346	-5.019689589	-3.186054712
1	3.290903664	-4.725971990	-2.295628190
6	1.651145044	-0.103103911	7.309377594
1	2.320213368	0.484536835	7.935663578
1	1.929512105	-1.147919705	7.403999672
1	0.638766883	0.030582735	7.676849071
8	-1.658229055	1.781936747	-1.883763271
6	-2.255886460	3.369644535	-4.130868913
1	-1.815024311	4.261079997	-3.693743830
1	-2.216973966	3.478179942	-5.212143691
1	-3.298041186	3.332634624	-3.833574309

6	-1.526374383	0.167029031	-5.809259367
1	-0.443872035	0.112032560	-5.870430987
1	-1.929902082	-0.728532760	-6.275506593
1	-1.859855038	1.019543379	-6.395576858
6	-1.488337742	-0.968827174	-3.549369697
1	-1.841398336	-0.955206972	-2.523841726
1	-1.847261244	-1.884677785	-4.013535203
1	-0.402884929	-1.009432273	-3.538321545
6	-3.557218576	0.267041705	-4.301227278
1	-3.926191297	0.356362242	-3.283528923
1	-3.966136443	1.083610048	-4.887520543
1	-3.942768303	-0.662059906	-4.714616476

CYC-T_1-TS

16	2.224699240	0.968142255	1.557066478
14	-0.963383978	2.004147243	-2.963572319
8	-2.155246091	-1.826120078	3.490325703
8	3.615391010	1.013192448	1.228970864
8	3.200977992	-1.004431283	-3.158247432
8	2.981229090	-3.180679451	-2.792985635
8	1.418696550	2.108149337	1.218632275
7	1.624199275	-0.390912558	0.772758304
6	0.234162986	-0.694810157	0.972133961
6	-2.474915172	-1.129662545	1.281085488
1	-3.524667116	-1.302530359	1.432201767
6	-0.232346553	-1.212163167	2.172566311
1	0.465546045	-1.438323655	2.947555415
6	2.869947311	-1.907217439	-2.450834617
6	-1.999708414	-0.650898208	0.074271964
1	-2.679027579	-0.452801901	-0.733327884
6	-0.619558755	-0.407382073	-0.100838133
6	-0.004467796	0.082012181	-1.281922794
6	2.311431216	-1.763799710	-1.092789014
1	2.007295604	-2.653825163	-0.576521219
6	-1.589103970	-1.401887462	2.339083596
6	2.662463553	-0.576145508	3.755834757
1	3.369057905	-1.125243381	3.143306736
6	1.986973907	0.570845936	3.214071827
6	2.081515058	-0.528280839	-0.578653263
1	2.501201623	0.337088299	-1.046276615
6	1.446982481	-0.202864078	5.849546636
6	1.091031220	1.286422844	3.963158365
1	0.576745627	2.139881916	3.531924956
6	2.376874990	-0.959367226	5.047189258
1	2.867011648	-1.822437814	5.481629328
6	-1.327818041	3.044747728	-1.465737904
1	-2.167568010	2.635656402	-0.911959565
1	-1.589816427	4.057600407	-1.760314654
1	-0.480128762	3.100355504	-0.790313923
6	0.825206977	0.892684363	5.303576847
1	0.133397927	1.480518518	5.893698963
6	-1.335503737	-2.031676075	4.610909318
1	-0.686265336	-2.889774842	4.464846476
1	-2.000223701	-2.232138652	5.438347762
1	-0.727531477	-1.164544581	4.830031494
6	0.486447028	2.643422343	-3.975354954
6	3.525196838	-3.462217776	-4.071451912
1	2.916562011	-3.020249843	-4.846849816
1	3.523624102	-4.536866965	-4.161980556
1	4.533832938	-3.081952196	-4.145461367
6	1.213474072	-0.606496136	7.303373708
1	1.974093383	-0.148299739	7.934144310
1	1.282556844	-1.684329130	7.417992495
1	0.238697183	-0.271618633	7.644186505
8	-0.593916979	0.421899029	-2.407859889
6	-2.489364489	1.726921390	-3.988584904
1	-3.315851583	1.406854812	-3.360155016
1	-2.796841427	2.636691981	-4.498418660
1	-2.327288748	0.960162992	-4.739094532
6	0.169809264	4.090034691	-4.445439419
1	0.061558168	4.767277782	-3.602877846

1	0.980956504	4.463361192	-5.066875853
1	-0.741165835	4.130060991	-5.037504573
6	1.786518998	2.658945704	-3.129331499
1	2.092929040	1.647261740	-2.880993992
1	2.594217130	3.117140017	-3.696623924
1	1.666645344	3.225025875	-2.209229605
6	0.709119215	1.740580375	-5.216869731
1	0.905409552	0.713576983	-4.921792131
1	-0.153626728	1.752381689	-5.876846679
1	1.566467984	2.094072053	-5.786036000

STC(T_1S_0)

16	2.349871297	0.794591173	1.647431135
14	-0.815473391	1.836663781	-3.028876300
8	-2.363176163	-1.382594898	3.688096365
8	3.711466134	0.627406003	1.224389205
8	3.321041372	-0.627261554	-2.996413525
8	2.960598147	-2.816622300	-2.885854972
8	1.750109079	2.084053733	1.444037912
7	1.475964477	-0.364461279	0.815736784
6	0.093551865	-0.510758388	1.161145464
6	-2.635505856	-0.663886896	1.475052424
1	-3.695576064	-0.729232930	1.638406980
6	-0.389524097	-0.969796765	2.354215652
1	0.281076258	-1.298804327	3.115106230
6	2.814104136	-1.568907528	-2.462975023
6	-2.129226874	-0.255308242	0.247086150
1	-2.795221340	-0.016372225	-0.560759299
6	-0.734440304	-0.167164410	0.074312361
6	0.083521395	0.190157955	-1.020755015
6	1.964881624	-1.501413531	-1.276095151
1	1.589130127	-2.418978576	-0.865997097
6	-1.775985873	-1.017707071	2.525210247
6	2.615452653	-0.980657540	3.697519859
1	3.175363490	-1.596958204	3.002672818
6	2.144812203	0.313766606	3.286659551
6	1.545557598	-0.201231884	-0.663177031
1	2.242663892	0.573934865	-0.937781494
6	1.591880706	-0.567658595	5.885644568
6	1.435731146	1.116015424	4.140898859
1	1.072075651	2.083179807	3.807051834
6	2.322400055	-1.412745915	4.972087423
1	2.661954659	-2.384427397	5.310465518
6	-1.327617118	3.012868529	-1.680075397
1	-2.151747997	2.606822164	-1.102382072
1	-1.662353838	3.952078854	-2.112255832
1	-0.516431650	3.232120105	-0.993677169
6	1.164873327	0.666621170	5.463524163
1	0.630135600	1.322176996	6.138987594
6	-1.551844377	-1.725031401	4.781554413
1	-1.044985724	-2.669624718	4.606240366
1	-2.215321314	-1.834059621	5.626861283
1	-0.811422539	-0.966270640	4.993685453
6	0.596679633	2.501497084	-4.079085590
6	3.747110794	-3.019229404	-4.047611186
1	3.298281289	-2.524678762	-4.897068980
1	3.767251635	-4.085927365	-4.205398512
1	4.748548940	-2.642616723	-3.899671404
6	1.358777291	-1.052462035	7.313952279
1	2.285365675	-0.974519841	7.880787315
1	1.050036467	-2.094380007	7.317710707
1	0.600268344	-0.453062224	7.806711073
8	-0.292917192	0.381423230	-2.286517832
6	-2.279188288	1.321614369	-4.054428037
1	-3.099073133	0.995624393	-3.420267128
1	-2.642409704	2.149577407	-4.658915310
1	-2.030909705	0.503574908	-4.722509043
6	0.165997680	3.852436969	-4.713927381
1	-0.030960240	4.603870298	-3.954742341
1	0.961638857	4.230234298	-5.352365296
1	-0.723447525	3.744162832	-5.329168864

6	1.861810723	2.735760487	-3.213026215
1	2.257010003	1.794976261	-2.844273198
1	2.640394317	3.204587251	-3.811304090
1	1.658345934	3.388081039	-2.367855598
6	0.939249373	1.494788343	-5.208194701
1	1.213976690	0.526825823	-4.799020511
1	0.101332649	1.359549123	-5.886075953
1	1.781812184	1.860223732	-5.791470809

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16	-1.730456010	-0.683647000	1.618768010
14	3.895114020	1.249900000	0.540651000
8	-2.564531010	2.547797010	-2.770693010
8	-1.772930010	-1.961770010	2.261068010
8	2.613174010	-1.407677010	-1.696174010
8	2.046511010	-3.529312020	-2.138633010
8	-1.145966010	0.407365000	2.348571010
7	-0.854057000	-0.904108010	0.211980000
6	-0.775736000	0.201580000	-0.667979000
6	-0.305008000	2.415514010	-2.253402010
1	-0.167915000	3.271262010	-2.885699010
6	-1.848102010	0.760842000	-1.357635010
1	-2.813018010	0.315262000	-1.296490010
6	1.901863010	-2.374532010	-1.408409000
6	0.752634000	1.837030010	-1.592709010
1	1.741244010	2.225314010	-1.725349010
6	0.511750000	0.716774000	-0.775905010
6	1.354216010	-0.076311000	0.086088000
6	0.946287000	-2.482595010	-0.428129000
1	0.317996000	-3.349362010	-0.393428000
6	-1.611137010	1.880533010	-2.120991010
6	-4.018916020	-1.166566010	0.229761000
1	-3.625458020	-2.162443010	0.057569000
6	-3.287849020	-0.237912000	1.047976000
6	0.564150000	-1.344725010	0.464840000
1	0.705099000	-1.518717000	1.522371010
6	-5.724905030	0.566255000	-0.069870000
6	-3.762681020	1.024702010	1.288560010
1	-3.188255020	1.716115010	1.896810010
6	-5.207166020	-0.754556000	-0.332731000
1	-5.779396050	-1.432765000	-0.954289000
6	3.252769020	2.854502010	1.215091010
1	4.048123020	3.595403020	1.189011010
1	2.923516020	2.755068010	2.244309010
1	2.424121010	3.242511020	0.632092000
6	-5.004463030	1.425694010	0.723331000
1	-5.385782030	2.414291010	0.944120010
6	-3.907307020	2.132827010	-2.660365020
1	-4.058571020	1.195559010	-3.183013020
1	-4.494593020	2.904060020	-3.132466010
1	-4.204126020	2.022043010	-1.628877010
6	5.069941030	0.353022000	1.687941010
6	3.012488010	-3.514924020	-3.149076010
1	2.800554010	-2.763164010	-3.897799020
1	2.985545010	-4.494782020	-3.607938020
1	4.003269020	-3.331947020	-2.754336010
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1	-7.872241070	0.440615000	-0.087006000
1	-7.163783060	0.661561000	-1.681549010
8	2.458280010	0.158834000	0.579380000
6	4.441405020	1.325542010	-1.226459000
1	3.974010020	2.138286010	-1.774294010
1	5.516678030	1.483081010	-1.264546000
1	4.218366020	0.389807000	-1.728257010
6	6.269242010	1.293520010	1.983384010
1	5.953879010	2.192952010	2.504362010
1	6.988535020	0.780904010	2.617388010
1	6.786652010	1.585133010	1.072641010
6	4.366714020	-0.006426000	3.022556010
1	3.533958020	-0.682702000	2.859554020

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1	3.999033020	0.878782000	3.533932020
6	5.586123020	-0.943656000	1.010209010
1	4.765534020	-1.600935010	0.737574000
1	6.156776030	-0.720367010	0.114195000
1	6.237774010	-1.480785010	1.695101010

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8	1.925709162	-3.440929171	-1.085268252
8	1.177159955	1.967333165	2.690852351
7	1.164293688	-0.472513932	1.969251036
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6	-0.869057287	-0.764711000	0.877093372
6	0.079215855	-0.374224755	-0.200874878
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1	1.785236294	-1.094421838	-1.351804296
6	-2.191612951	-1.575126605	3.174969708
6	1.858775977	-1.092531130	5.013493918
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6	1.360645038	0.168258659	4.534887022
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6	0.439905792	-0.804834949	6.991552257
6	0.451915082	0.896189427	5.258225769
1	0.076294343	1.839015276	4.872187204
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1	-0.223785912	2.751845633	0.753046949
6	-0.005228527	0.401244686	6.510412290
1	-0.699544965	0.999378360	7.086690547
6	-2.306606628	-2.118426197	5.484231080
1	-1.651422221	-2.984665213	5.472928225
1	-3.097892909	-2.282587569	6.200955097
1	-1.730768328	-1.249176497	5.769420681
6	0.506500198	2.764516206	-2.525115672
6	2.093854894	-4.837457915	-0.908971809
1	2.680624848	-5.040414159	-0.024653330
1	2.611775199	-5.184457889	-1.789084349
1	1.133910690	-5.325467216	-0.822351293
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1	0.833083531	-1.323765998	9.042970570
1	-0.341802488	-2.372116226	8.257713126
1	-0.809892682	-0.739667083	8.756984134
8	-0.363140184	0.308985346	-1.284645893
6	-2.443519811	1.793096200	-2.449978319
1	-3.209324493	1.338444365	-1.827633758
1	-2.806126948	2.772726523	-2.751911251
1	-2.337928963	1.185130904	-3.342285558
6	0.148163460	4.263236273	-2.716353641
1	0.113030906	4.787079696	-1.765561748
1	0.898990034	4.750770511	-3.334516257
1	-0.812045947	4.384616474	-3.210823647
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1	2.641241730	3.187319260	-2.375891054
1	1.845278501	3.101728290	-0.812757690

6	0.623033544	2.087186790	-3.915529413	1	1.432605894	2.537832431	-4.486042337
1	0.834072241	1.026039146	-3.817892178				
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