Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

For

The Photoisomerization Mechanism of Methacrolein Oxide (MACR-OO): Cyclic Dioxole Formation Pathway Revealed

Jiawei Yang[#], Yazhen Li[#], Lily Makroni, Fengyi Liu[*]

Key Laboratory of Applied Surface and Colloid Chemistry of Ministry of Education, Key Laboratory for Macromolecular Science of Shaanxi Province, School of Chemistry & Chemical Engineering, Shaanxi Normal University, Xi'an, Shaanxi 710119, People's Republic of China

*** Corresponding author. Electronic mail: fengyiliu@snnu.edu.cn**

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Figure S3. The hydrogen bond energies in SA and SS predicted basing on ρ_{BCP}. The ρ_{BCP} of SA and SS configurations calculated at CCSD(T)/def2-TZVP level are 0.013434 a.u. and 0.022214 a.u., respectively. According to the prediction formula of hydrogen bond energy: E_HB = -223.08*ρ_{BCP} + 0.7423, the hydrogen bond energies of SA and SS configurations are estimated to be -2.25 kcal mol^{-1} and -4.21 kcal mol^{-1}, respectively.

Figure S4. The dihedral angle (ϕ) of (a) SA/AA and (b) SS/AS energy profiles for ground state S_0 and the lowest excited singlet state S_1 are computed at CASSCF(12*e*,9*o*)/def2-TZVP level. Geometries are optimized on S_1 state. All energies are relative to the ground-state energy of AA-MACR-OO.

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Additional Computational Details

The concept of odd electron density

The odd electron density (OED)[1][2] is a function of measuring the distribution of odd electrons based on the density matrix. When calculation cannot obtain the spin density of the excited state to investigate the distribution of odd electrons, the OED method can be used to reflect the distribution of odd electrons to some extent. The OED calculation is based on the spin-free natural orbits, and Head-Gordon defined the odd electron density that associated with the kth (k = 1, …, M) $\phi_k(r)$ of occupation number n_k in 2003[3], and the main formula was as follows:

$$D_k^{\mathrm{odd}}(r) = \min(2 - n_k, n_k)\phi_k^*(r)\phi_k(r)$$

D^{odd} is the odd electron density and n_k is the occupation number. As can be seen from the formula, the OED of the system is the sum of the effective odd electron contributions of the natural orbitals. The OED reflects the overall electron density change that cannot distinguish the direction of spin. But it is more general, as long as you get the probability density of the wave function, you can get the OED.

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[1] T. Lu and F. W. Chen. Multiwfn: A Multifunctional Wavefunction Analyzer. J. Comput. Chem., 2012, 33, 580-592.

[2] N. Masayoshi, F. Hitoshi, M. Takuya, et al. (Hyper) Polarizability Density Analysis for Open-shell Molecular Systems Based on Natural Orbitals and Occupation Numbers. Theor. Chem. Acc., 2011, 130, 711-724.

[3] H. Martin. Characterizing Unpaired Electrons from the One-particle Density Matrix. Chem. Phys. Lett., 2003, 372, 508-511.

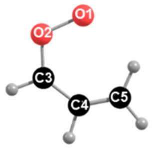
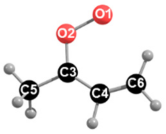
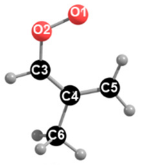
Table S1. Relative energy (in kcal/mol) of important structures are calculated at PBE0/def2-SVP, CASSCF/def2-SVP, CASSCF/def2-TZVP, CASPT2/def2-TZVP levels.

	Electronic state	PBE0/ def2-SVP	CASSCF/ def2-SVP	CASSCF/ def2-TZVP	MS-CASPT2/ def2-TZVP
AA	S_0	—	0.0	0.0	0.0
	S_1	—	37.4	39.2	45.8
AS	S_0	—	2.0	2.4	3.7
	S_1	—	37.8	39.7	46.3
SA	S_0	—	3.4	4.0	3.0
	S_1	—	40.2	41.8	46.7
SS	S_0	—	2.1	2.4	2.3
	S_1	—	40.5	41.7	46.9
anti-Dioxirane	S_0	—	-24.0	-23.2	-20.4
syn-Dioxirane	S_0	—	-21.5	-22.7	-17.1
1, 2-Dioxole	S_0	—	-25.4	-25.5	-27.8
$\mathrm{TS}_{\mathrm{AA}/\textit{anti}\text{-}\mathrm{Dioxirane}}$	S_0	22.2	21.5	27.7	18.6
$\mathrm{TS}_{\mathrm{AS}/\textit{syn}\text{-}\mathrm{Dioxirane}}$	S_0	20.5	20.0	23.7	17.2
$\mathrm{TS}_{\mathrm{SA}/\textit{anti}\text{-}\mathrm{Dioxirane}}$	S_0	22.2	20.4	23.7	18.6
$\mathrm{TS}_{\mathrm{SS}/\textit{syn}\text{-}\mathrm{Dioxirane}}$	S_0	20.5	25.0	27.7	17.2
$\mathrm{TS}_{\mathrm{SS/Dioxole}}$	S_0	10.8	22.2	22.9	15.3
$\mathrm{ConInt}_{\mathrm{CO\text{-}A}}$	S_1/S_0	—	—	29.2	32.6
$\mathrm{ConInt}_{\mathrm{CO\text{-}S}}$	S_1/S_0	—	—	30.1	32.2
$\mathrm{ConInt}_{\mathrm{CC}}$	S_1/S_0	—	—	38.9	40.1

Table S2. Excitation energy (in kcal mol^{-1}) is calculated at CASSCF/def2-TZVP, CASPT2/def2-TZVP levels. And the energy windows in the dynamic simulation used to generate the dynamic trajectory for S_1 and S_2 states.

		CASSCF/ def2-TZVP	MS-CASPT2/ def2-TZVP	Energy windows (kcal mol^{-1})	Energy windows (eV)	Absorption intensity
AA	S_1	45.0	48.5	23.1~62.3	1.0~2.7	0.018
	S_2	91.4	71.9	62.3~124.5	2.7~5.4	10.161
AS	S_1	44.8	48.9	20.8~57.7	0.9~2.5	0.018
	S_2	92.7	75.6	57.7~129.1	2.5~5.6	7.737
SA	S_1	48.3	50.5	20.8~60.0	0.9~2.6	0.019
	S_2	93.2	77.5	60.0~122.2	2.6~5.3	9.234
SS	S_1	47.3	49.4	23.1~60.0	1.0~2.6	0.017
	S_2	97.0	83.1	60.0~126.8	2.6~5.5	6.053

Table S3. The RESP charges (e) of C and O atoms of VCI, MVK-OO and MACR-OO on the S_0 and S_1 (red) state at CASSCF/def2-TZVP levels.

		RESP/e					
		O1	O2	C3	C4	C5	C6
 VCI	AA	-0.28(-0.07)	-0.04(0.00)	0.31(-0.13)	-0.22(-0.10)	-0.47(-0.52)	
	AS	-0.30(-0.06)	0.03(0.00)	0.34(-0.15)	-0.40(-0.14)	-0.25(-0.39)	
	SA	-0.27(-0.04)	-0.07(-0.07)	0.27(-0.11)	-0.07(-0.04)	-0.57(-0.58)	
	SS	-0.23(0.00)	-0.09(-0.09)	0.37(-0.02)	-0.31(-0.15)	-0.25(-0.39)	
 MVK-OO	AA	-0.26(-0.04)	-0.15(-0.19)	0.66(0.24)	-0.41(-0.24)	-0.52(-0.15)	-0.27(-0.37)
	AS	-0.33(-0.06)	-0.02(-0.08)	0.62(0.22)	-0.48(-0.26)	-0.48(-0.21)	-0.29(-0.51)
	SA	-0.29(-0.08)	-0.08(-0.10)	0.51(0.21)	-0.23(-0.27)	-0.47(-0.25)	-0.38(-0.32)
	SS	-0.29(-0.02)	-0.10(-0.13)	0.62(0.30)	-0.37(-0.25)	-0.44(-0.31)	-0.33(-0.50)
 MACR-OO	AA	-0.28(-0.03)	-0.02(0.05)	0.14(-0.28)	0.15(0.17)	-0.61(-0.59)	-0.17(-0.17)
	AS	-0.27(-0.05)	-0.01(-0.02)	0.16(-0.28)	0.09(0.30)	-0.53(-0.61)	-0.29(-0.40)
	SA	-0.26(-0.05)	-0.04(-0.07)	0.12(-0.22)	0.32(0.31)	-0.75(-0.69)	-0.16(-0.11)
	SS	-0.24(-0.05)	-0.06(-0.07)	0.15(-0.21)	0.17(0.31)	-0.41(-0.47)	-0.39(-0.44)

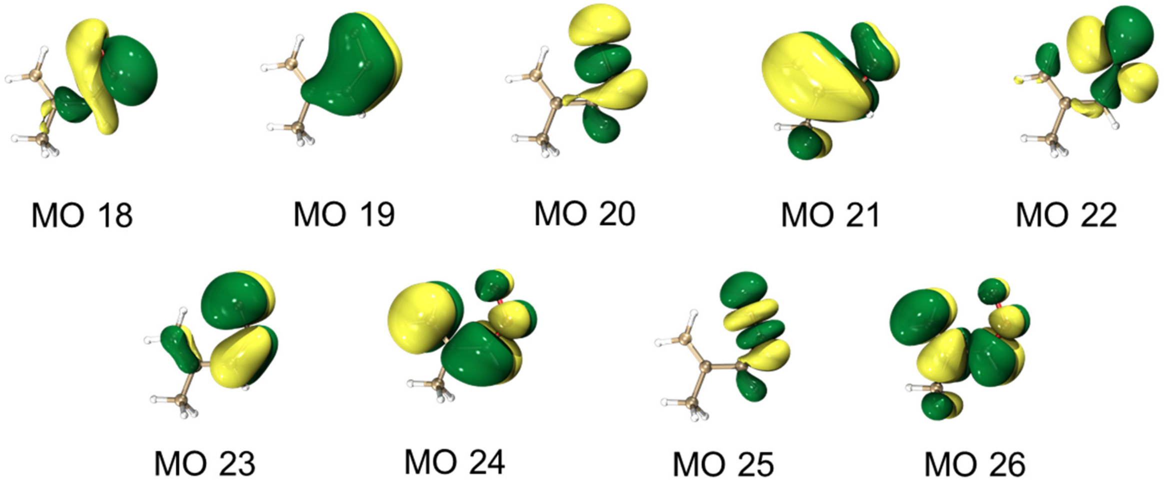
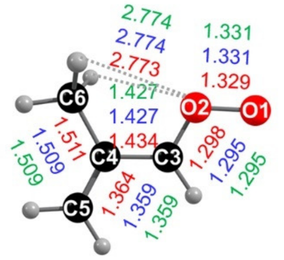
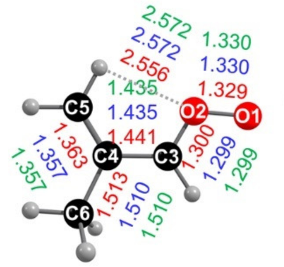


Figure S1. The active orbitals used in the CASSCF(12*e*,9*o*)/def2-TZVP and CASPT2(12*e*,9*o*)/def2-TZVP calculations of MACR-OO. The CASSCF(12*e*,9*o*) active orbitals include: the 2s orbital of the middle oxygen atom (MO 18), a lone-pair orbital of terminal oxygen (MO 22), the σ/σ* orbitals of O-O bond (MO 20 and MO 25), and the all π/π* orbitals are selected (MO 19, MO 21, MO 23, MO 24 and MO 26), which includes the key structures related to O-O dissociation and isomerization.



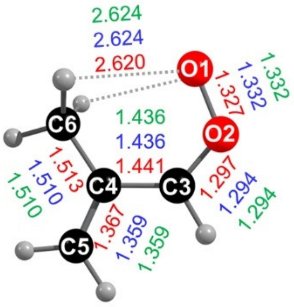
C5C4C3O2 = 180.0° -180.0° -180.0°
C6C4C3O2 = 0.0° 0.0° 0.0°
C4C3O2O1 = 180.0° 180.0° 180.0°
∠C3O2O1 = 118.1° 117.9° 117.9°
∠O2C3C4 = 118.6° 118.6° 118.6°
∠C3C4C5 = 119.1° 118.9° 118.9°
∠C3C4C6 = 118.5° 118.9° 118.9°
ΔE = **0.0** **0.0** **0.0**

S_0-AA-**MACR-OO**



C5C4C3O2 = 0.0° 0.0° 0.0°
C6C4C3O2 = 180.0° 180.0° 180.0°
C4C3O2O1 = -180.0° -180.0° -180.0°
∠C3O2O1 = 117.9° 118.6° 118.6°
∠O2C3C4 = 119.8° 119.7° 119.7°
∠C3C4C5 = 122.6° 123.3° 123.3°
∠C3C4C6 = 115.3° 114.9° 114.9°
ΔE = **2.0** **2.4** **3.7**

S_0-AS-**MACR-OO**



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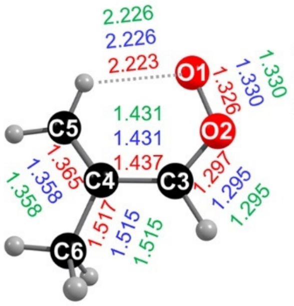
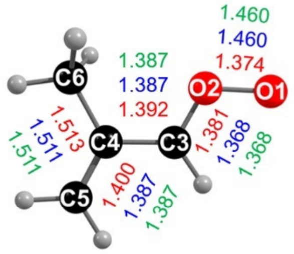
C6C4C3O2 = 0.0° 0.0° 0.0°
C4C3O2O1 = 0.0° 0.0° 0.0°
∠C3O2O1 = 121.7° 121.4° 121.4°
∠O2C3C4 = 129.2° 129.6° 129.6°
∠C3C4C5 = 116.2° 116.0° 116.0°
∠C3C4C6 = 123.1° 123.3° 123.3°
ΔE = **3.4** **4.0** **3.0**

S_0-SA-**MACR-OO**



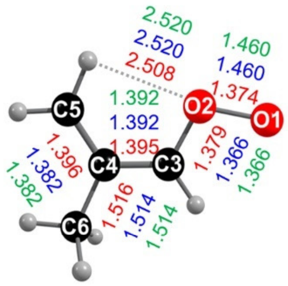
C5C4C3O2 = 0.0° 0.0° 0.0°
C6C4C3O2 = -180.0° -180.0° -180.0°
C4C3O2O1 = 0.0° 0.0° 0.0°
∠C3O2O1 = 121.1° 120.6° 120.6°
∠O2C3C4 = 129.2° 129.5° 129.5°
∠C3C4C5 = 125.7° 126.0° 126.0°
∠C3C4C6 = 113.5° 113.3° 113.3°
ΔE = **2.1** **2.4** **2.3**

S_0-SS-**MACR-OO**



C5C4C3O2 = -180.0° -180.0° -180.0°
C6C4C3O2 = 0.1° 0.0° 0.0°
C4C3O2O1 = 180.0° -180.0° -180.0°
∠C3O2O1 = 112.2° 107.6° 107.6°
∠O2C3C4 = 117.8° 118.5° 118.5°
∠C3C4C5 = 120.0° 120.0° 120.0°
∠C3C4C6 = 119.0° 119.1° 119.1°
ΔE = **37.4** **39.2** **45.8**

S_1-AA-**MACR-OO**



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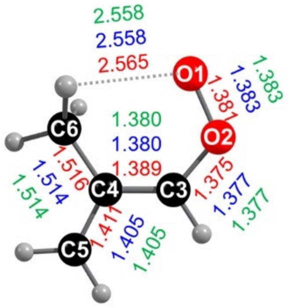
C6C4C3O2 = -180.0° 180.0° 180.0°
C4C3O2O1 = -180.0° -180.0° -180.0°
∠C3O2O1 = 112.4° 107.6° 107.6°
∠O2C3C4 = 118.5° 119.1° 119.1°
∠C3C4C5 = 122.4° 122.7° 122.7°
∠C3C4C6 = 116.6° 116.5° 116.5°
ΔE = **37.8** **39.7** **46.3**

S_1-AS-**MACR-OO**



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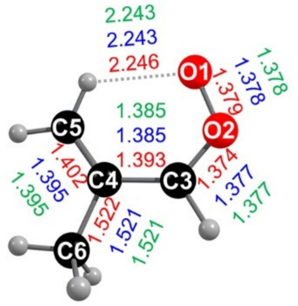
C4C3O2O1 = -2.7° 0.0° 0.0°
∠C3O2O1 = 116.7° 116.2° 116.2°
∠O2C3C4 = 129.5° 129.7° 129.7°
∠C3C4C5 = 117.4° 117.3° 117.3°
∠C3C4C6 = 123.7° 124.1° 124.1°
ΔE = **40.2** **41.8** **46.7**

S_1-SA-**MACR-OO**



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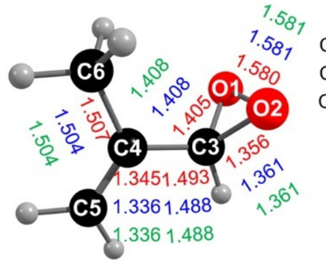
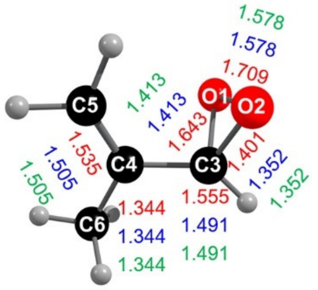
C6C4C3O2 = -180.0° -180.0° -180.0°
C4C3O2O1 = 0.0° 0.0° 0.0°
∠C3O2O1 = 117.0° 116.4° 116.4°
∠O2C3C4 = 130.1° 130.1° 130.1°
∠C3C4C5 = 127.3° 127.7° 127.7°
∠C3C4C6 = 114.0° 113.7° 113.7°
ΔE = **40.5** **41.7** **46.9**

S_1-SS-**MACR-OO**



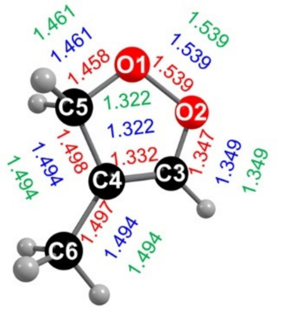
C5C4C3O2 = -143.4° -143.9° -143.9°
C6C4C3O2 = 37.2° 36.4° 36.4°
C4C3O2O1 = -111.1° -110.0° -110.0°
∠C3O2O1 = 56.6° 57.2° 57.2°
∠O2C3C4 = 118.2° 118.2° 118.2°
∠C3C4C5 = 118.7° 117.9° 117.9°
∠C3C4C6 = 117.3° 117.4° 117.4°
ΔE = **-24.0** **-23.2** **-20.4**

S_0-*anti*-Dioxirane



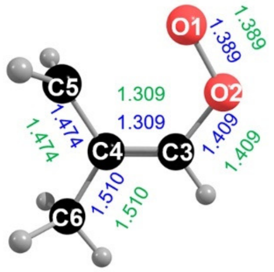
C5C4C3O2 = 9.0° -9.7° -9.7°
C6C4C3O2 = -165.0° 170.8° 170.8°
C4C3O2O1 = -88.1° -111.2° -111.2°
∠C3O2O1 = 62.9° 57.0° 57.0°
∠O2C3C4 = 114.9° 119.5° 119.5°
∠C3C4C5 = 117.8° 120.9° 120.9°
∠C3C4C6 = 118.0° 115.0° 115.0°
ΔE = **-21.5** **-22.7** **-17.1**

S_0-*syn*-Dioxirane



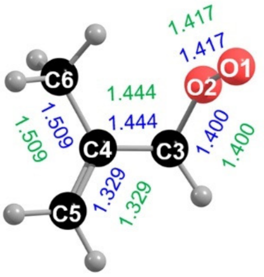
C5C4C3O2 = -0.3° -0.3° -0.3°
C6C4C3O2 = -179.6° 179.7° -179.7°
C4C3O2O1 = -1.6° -1.6° -1.6°
∠C3O2O1 = 104.5° 104.3° 104.3°
∠O2C3C4 = 116.6° 116.8° 116.8°
∠C3C4C5 = 107.5° 107.8° 107.8°
∠C3C4C6 = 128.7° 128.6° 128.6°
ΔE = **-25.4** **-25.5** **-27.8**

S_0-Heterocyclopentane Dioxole



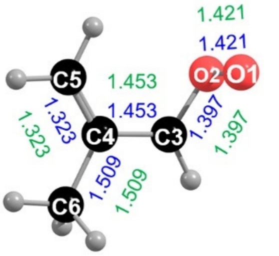
C5C4C3O2 = 0.4° 0.4°
C6C4C3O2 = -179.2° -179.2°
C4C3O2O1 = 2.9° 2.9°
∠C3O2O1 = 111.7° 111.7°
∠O2C3C4 = 126.0° 126.0°
∠C3C4C5 = 122.0° 122.0°
∠C3C4C6 = 120.0° 120.0°
ΔE = **38.9** **40.1**

ConInt_{CC}



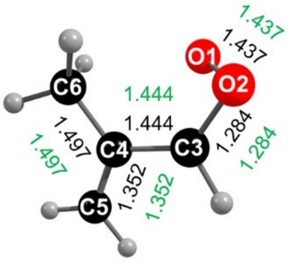
C5C4C3O2 = 177.7° 177.7°
C6C4C3O2 = 0.2° 0.2°
C4C3O2O1 = 88.2° 88.2°
∠C3O2O1 = 98.0° 98.0°
∠O2C3C4 = 121.3° 121.3°
∠C3C4C5 = 118.5° 118.5°
∠C3C4C6 = 118.8° 118.8°
ΔE = **29.2** **32.6**

ConInt$_{\text{CO-A}}$



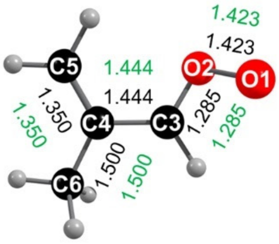
C5C4C3O2 = -3.2° -3.2°
C6C4C3O2 = 175.0° 175.0°
C4C3O2O1 = 89.6° 89.6°
∠C3O2O1 = 96.7° 96.7°
∠O2C3C4 = 122.7° 122.7°
∠C3C4C5 = 123.7° 123.7°
∠C3C4C6 = 113.6° 113.6°
ΔE = **30.1** **32.2**

ConInt$_{\text{CO-S}}$



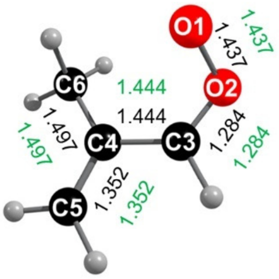
C5C4C3O2 = 178.3° 178.3°
C6C4C3O2 = 1.5° 1.5°
C4C3O2O1 = 58.6° 58.6°
∠C3O2O1 = 93.1° 93.1°
∠O2C3C4 = 126.4° 126.4°
∠C3C4C5 = 115.5° 115.5°
∠C3C4C6 = 121.2° 121.2°
ΔE = **22.2** **18.6**

S$_0$-TS$_{\text{AA/}anti\text{-Dioxirane}}$



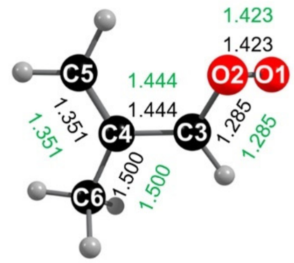
C5C4C3O2 = 13.8° 13.8°
C6C4C3O2 = -166.6° -166.6°
C4C3O2O1 = -133.0° -133.0°
∠C3O2O1 = 93.6° 93.6°
∠O2C3C4 = 120.8° 120.8°
∠C3C4C5 = 118.0° 118.0°
∠C3C4C6 = 118.0° 118.0°
ΔE = **20.5** **17.2**

S$_0$-TS$_{\text{AS/}syn\text{-Dioxirane}}$



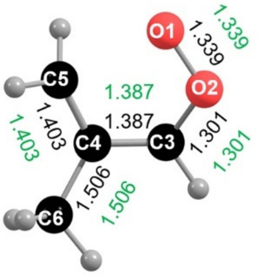
C5C4C3O2 = -178.3° -178.3°
C6C4C3O2 = -1.4° -1.4°
C4C3O2O1 = -58.6° -58.6°
∠C3O2O1 = 93.1° 93.1°
∠O2C3C4 = 126.4° 126.4°
∠C3C4C5 = 115.5° 115.5°
∠C3C4C6 = 121.2° 121.2°
ΔE = **22.2** **18.6**

S$_0$-TS$_{\text{SA/}anti\text{-Dioxirane}}$



C5C4C3O2 = -13.7° -13.7°
C6C4C3O2 = 166.6° 166.6°
C4C3O2O1 = 133.0° 133.0°
∠C3O2O1 = 93.6° 93.6°
∠O2C3C4 = 120.8° 120.8°
∠C3C4C5 = 118.0° 118.0°
∠C3C4C6 = 117.7° 117.7°
ΔE = **20.5** **17.2**

S$_0$-TS$_{\text{SS/}syn\text{-Dioxirane}}$



C5C4C3O2 = 13.3° - 13.3°
C6C4C3O2 = -152.2° -152.2°
C4C3O2O1 = -18.6° -18.6°
∠C3O2O1 = 113.3° 113.3°
∠O2C3C4 = 119.9° 119.9°
∠C3C4C5 = 118.1° 118.1°
∠C3C4C6 = 119.1° 119.1°
ΔE = **10.8** **15.3**

S$_0$-TS$_{\text{SS/Dioxole}}$

Figure S2. The geometric structure (bond lengths in Angstrom) and relative energy (in kcal mol^{-1}) of key configurations obtained by PBE0/def2-SVP (black), SA3-CASSCF/def2-SVP (red), SA3-CASSCF/def2-TZVP (blue) and MS3-CASPT2 (green) levels.

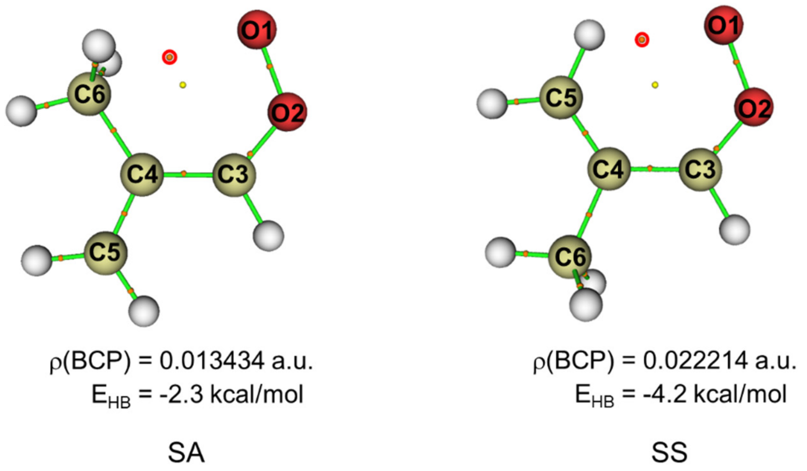


Figure S3. The hydrogen bond energies in SA and SS are predicted based on ρ_{BCP}. The ρ_{BCP} of SA and SS configurations calculated at the CCSD(T)/def2-TZVP level are 0.013434 a.u. and 0.022214 a.u., respectively. According to the prediction formula of hydrogen bond energy: E_HB = $-223.08*\rho_{(BCP)} + 0.7423$, the hydrogen bond energies of SA and SS configurations are estimated to be -2.25 kcal mol^{-1} and -4.21 kcal mol^{-1}, respectively.[1][2]

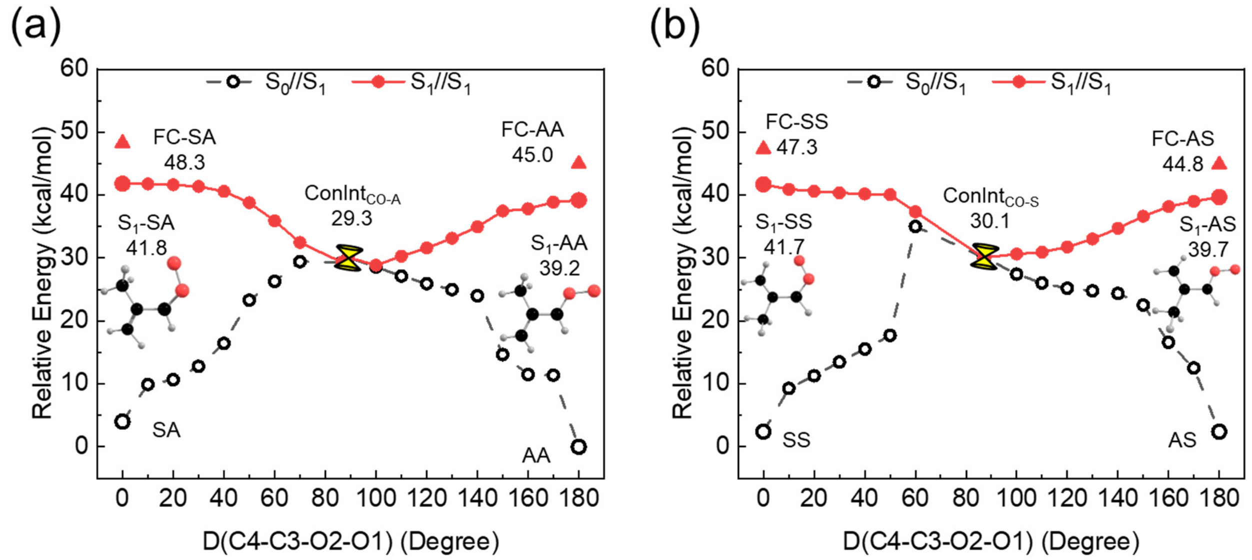


Figure S4. The dihedral angle (ϕ) of (a) SA/AA and (b) SS/AS energy profiles for ground state S_0 and the lowest excited singlet state S_1 are computed at CASSCF(12*e*,9*o*)/def2-TZVP level. Geometries are optimized on S_1 state. All energies are relative to the ground-state energy of AA-MACR-OO.

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[1] T. Lu and F. W. Chen. Multiwfn: A Multifunctional Wavefunction Analyzer. J. Comput. Chem., 2012, 33, 580-592.

[2] S. Emamian, T. Lu, H. Kruse and H. Emamian. Exploring Nature and Predicting Strength of Hydrogen Bonds: A Correlation Analysis Between Atoms-in-Molecules Descriptors, Binding Energies, and Energy Components of Symmetry-Adapted Perturbation Theory. J. Comput. Chem., 2019, 40, 2868-2881.

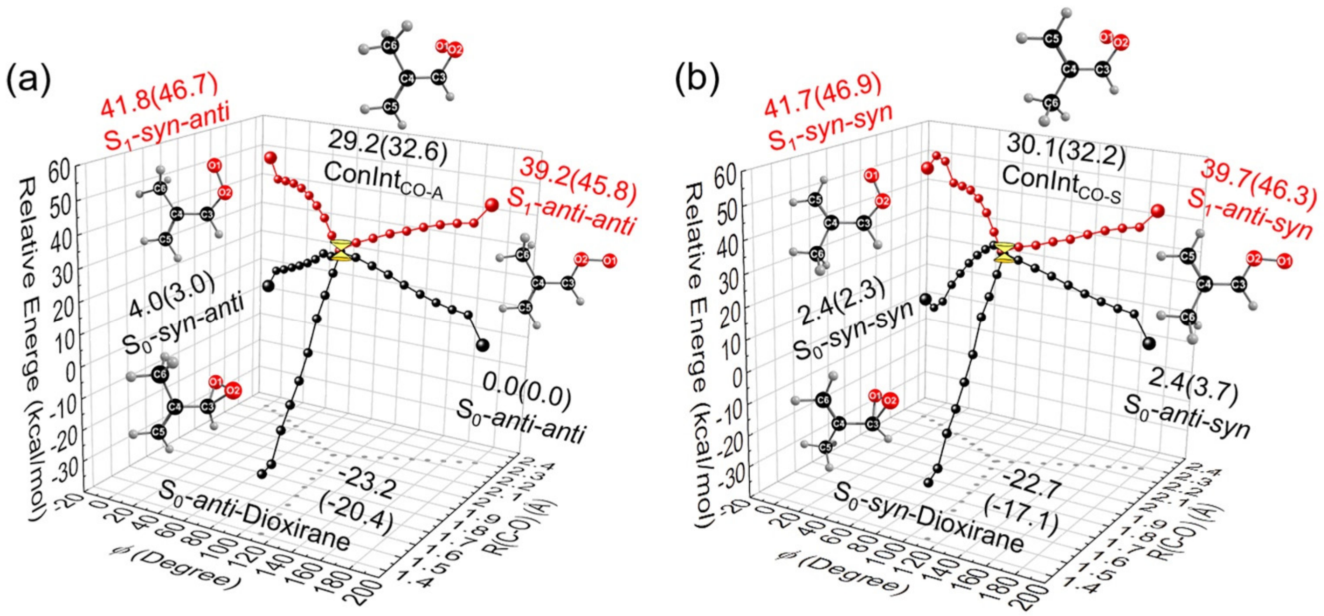

Figure S5. The interpolated S_1 and S_0 energy profiles of MACR-OO on MS3-CASPT2(12*e*, 9*o*)/def2-TZVP level. The relative energy calculated by CASPT2 is in parenthesis, and the relative energy calculated by CASSCF is outside the parenthesis.

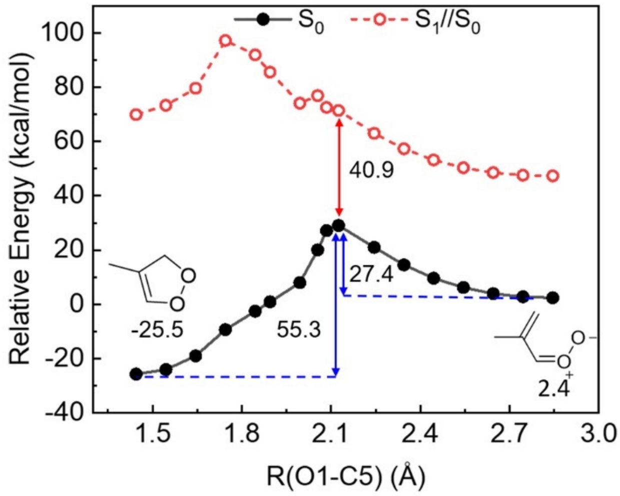

Figure S6. The S_0-state potential energy surface (PES) of the SS configuration by SA3-CASSCF(12*e*, 9*o*)/def2-TZVP to heterocyclopentane dioxole was obtained by the restricted optimization of the O1-C5 bond length.

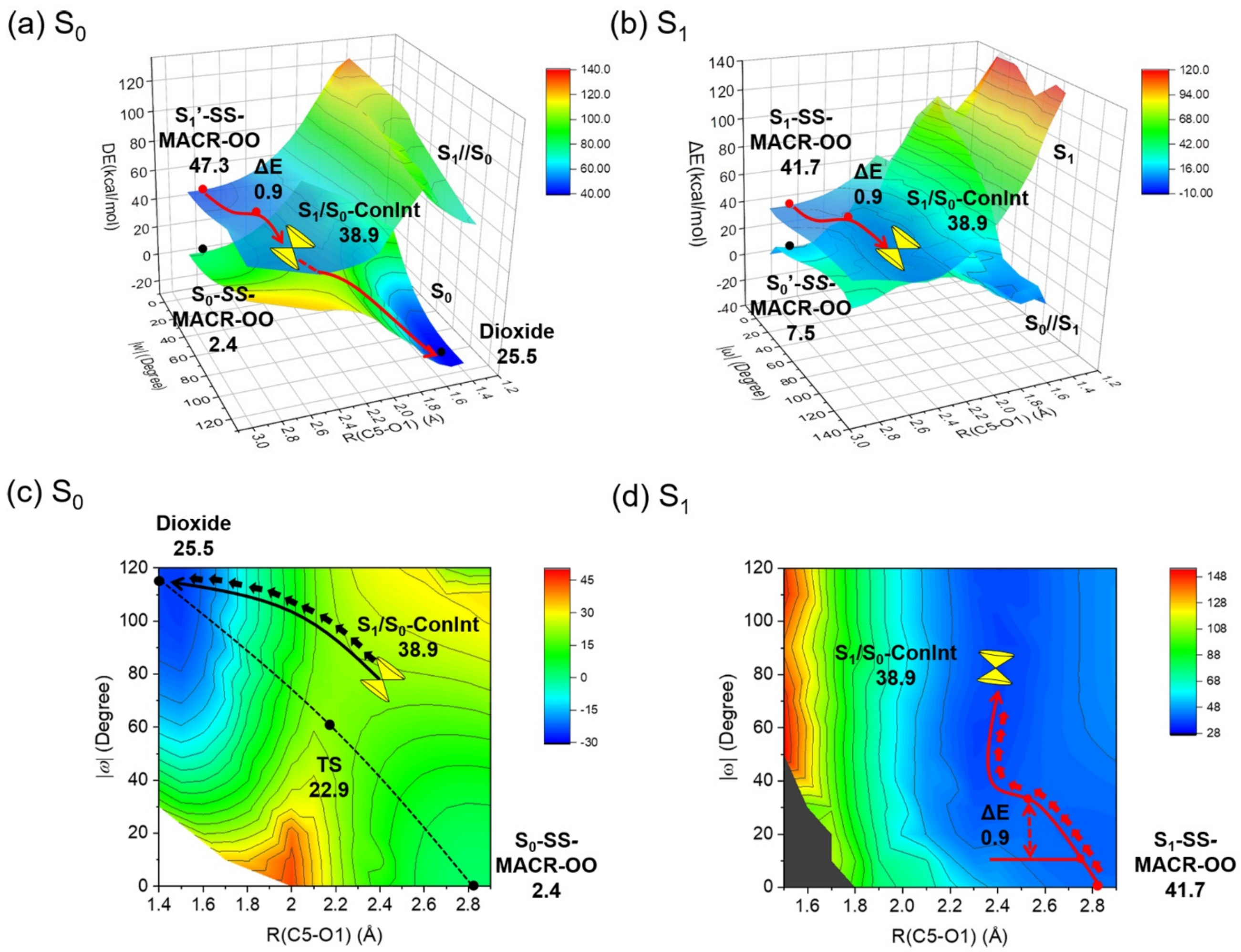

Figure S7. The PESs of S_0 (a) and S_1 (b) states and the 2-D contour plots of S_0 (c) and S_1 (d) are calculated by the SA3-CASSCF (12*e*,9*o*)/def2-TZVP. The red route represents the process from S_1-min through ConInt to the S_0-heterocyclopentane dioxole, and the black route represents the isomerization route in the ground state.

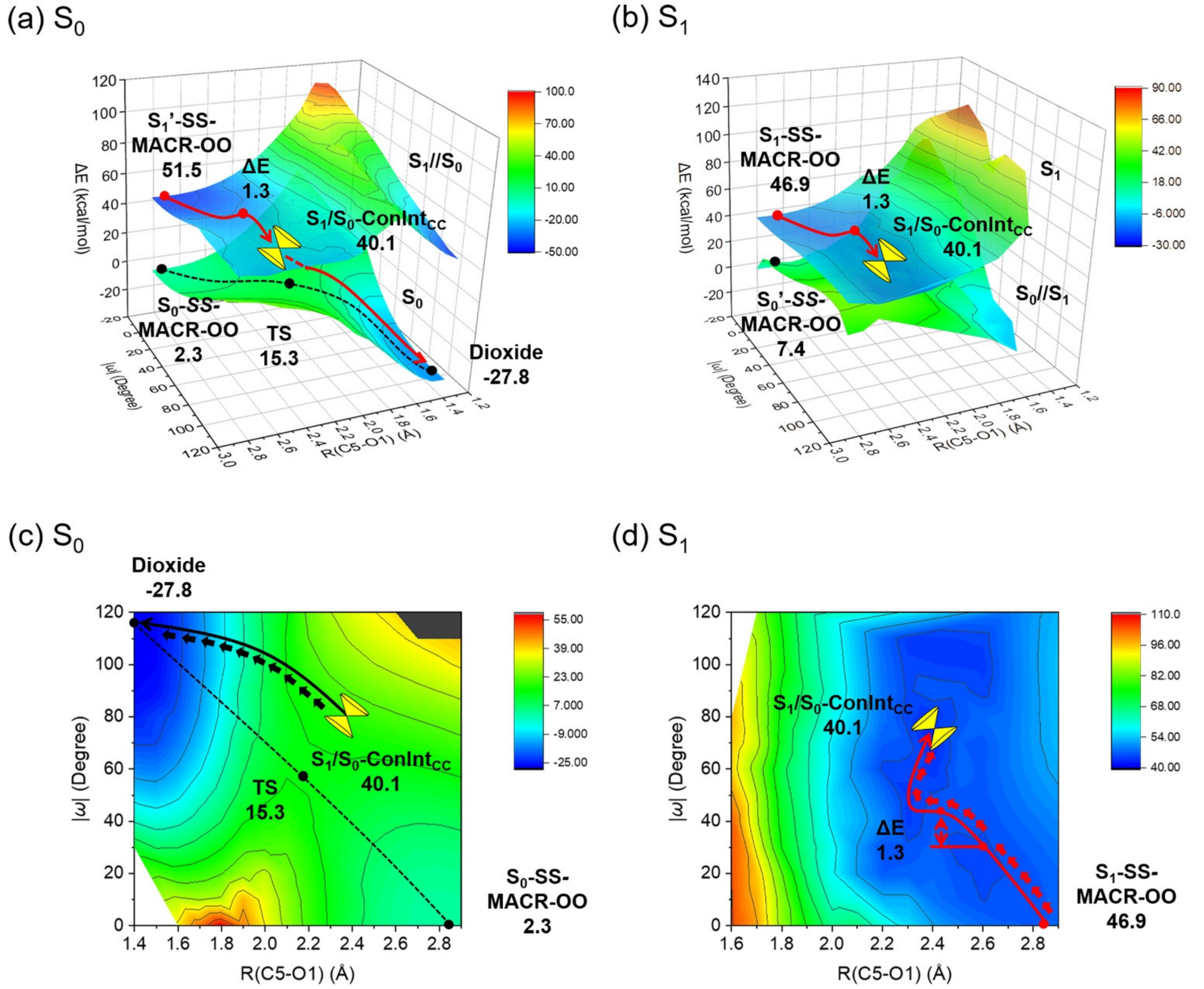

Figure S8. The PESs of S_0 (a) and S_1 (b) states and the 2-D contour plots of S_0 (c) and S_1 (d) are calculated by the MS-CASPT2(12*e*,9*o*)/def2-TZVP//SA3-CASSCF (12*e*,9*o*)/def2-TZVP. The red route represents the process from S_1-min through ConInt to the S_0-heterocyclopentane dioxole, and the black route represents the isomerization route in the ground state.

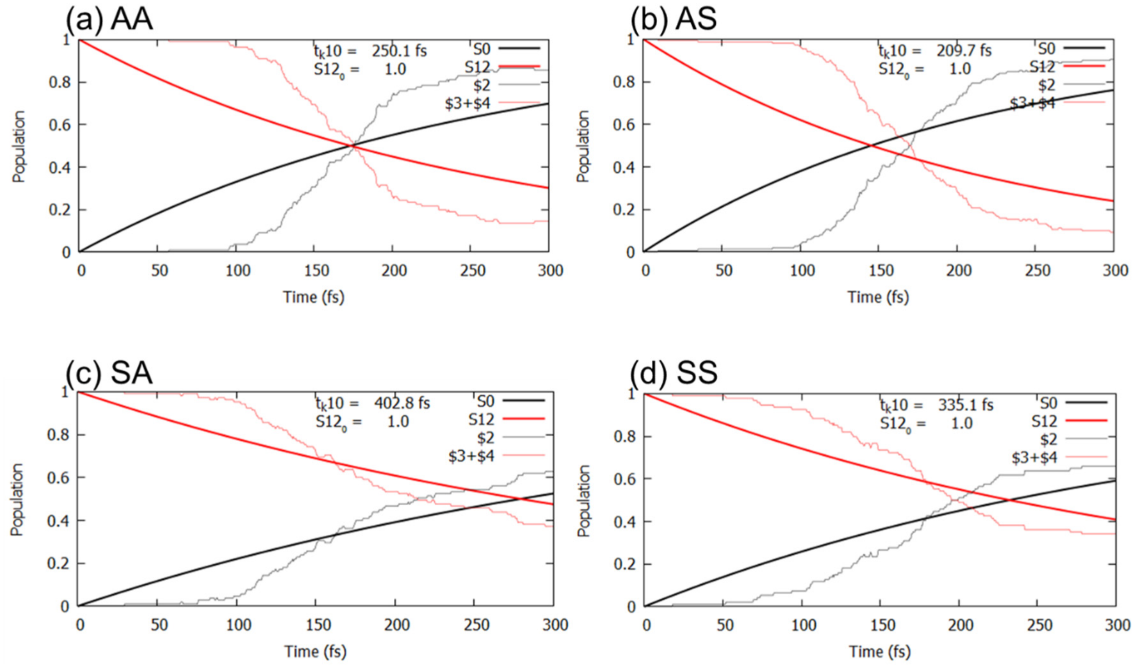

Figure S9. The state population and lifetime of S_1-state trajectories obtained by a kinetic model in SHARC2.1 program.

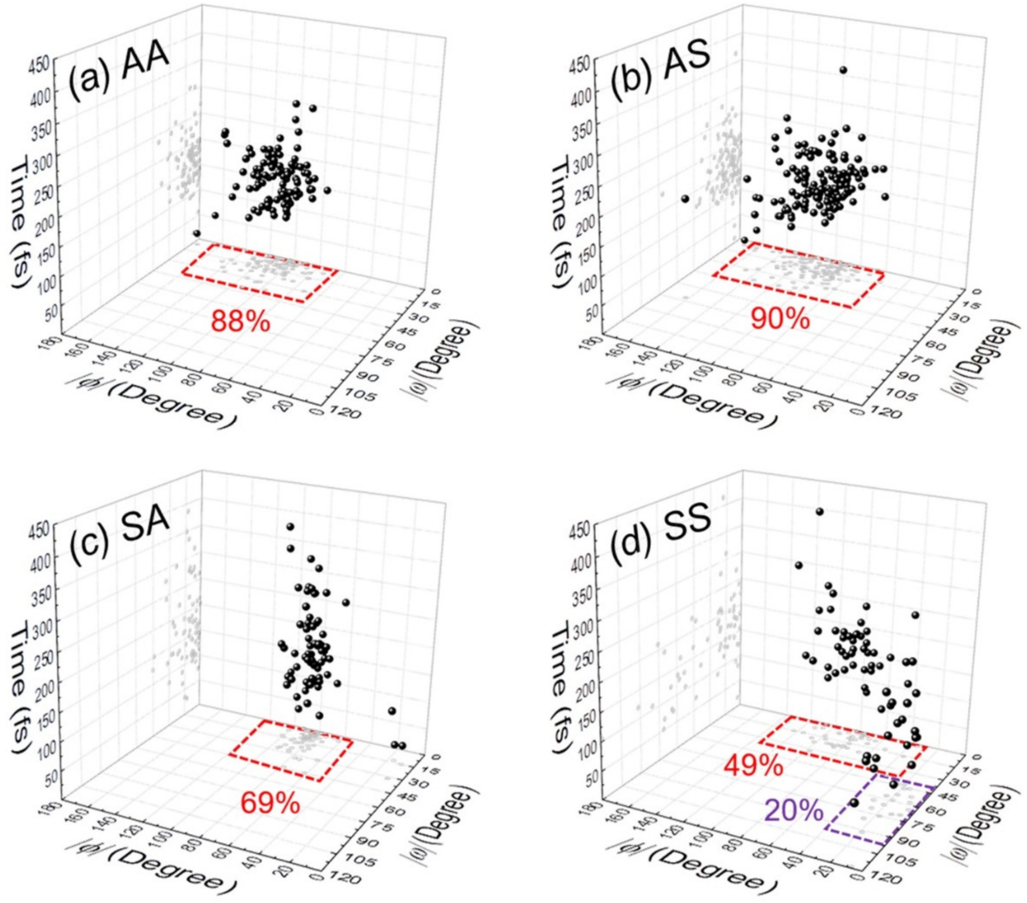

Figure S10. (a)-(d) Geometry distribution of the first hopping points in trajectories starting from the S_1 state of the AA, AS, SA and SS respectively. In this figure, the black balls show the hop of $S_1 \rightarrow S_0$. The projection of the hopping points of $S_1 \rightarrow S_0$ on the ω-ϕ and Time-ω is light gray. The hopping points of SS are obviously divided into two parts. One part is concentrated at the O-O bond length of 1.5Å and the ϕ dihedral angle of 90°, which is close to the S_1/S_0 ConInt. The other part is concentrated on the initial structure of AA, AS, SA and SS, which hop in the FC region. The purple box is the proportion of hopping points in the FC region, and the ratio of points that hop in FC region of SS configuration is 20%, which has the highest proportion of the four configurations.

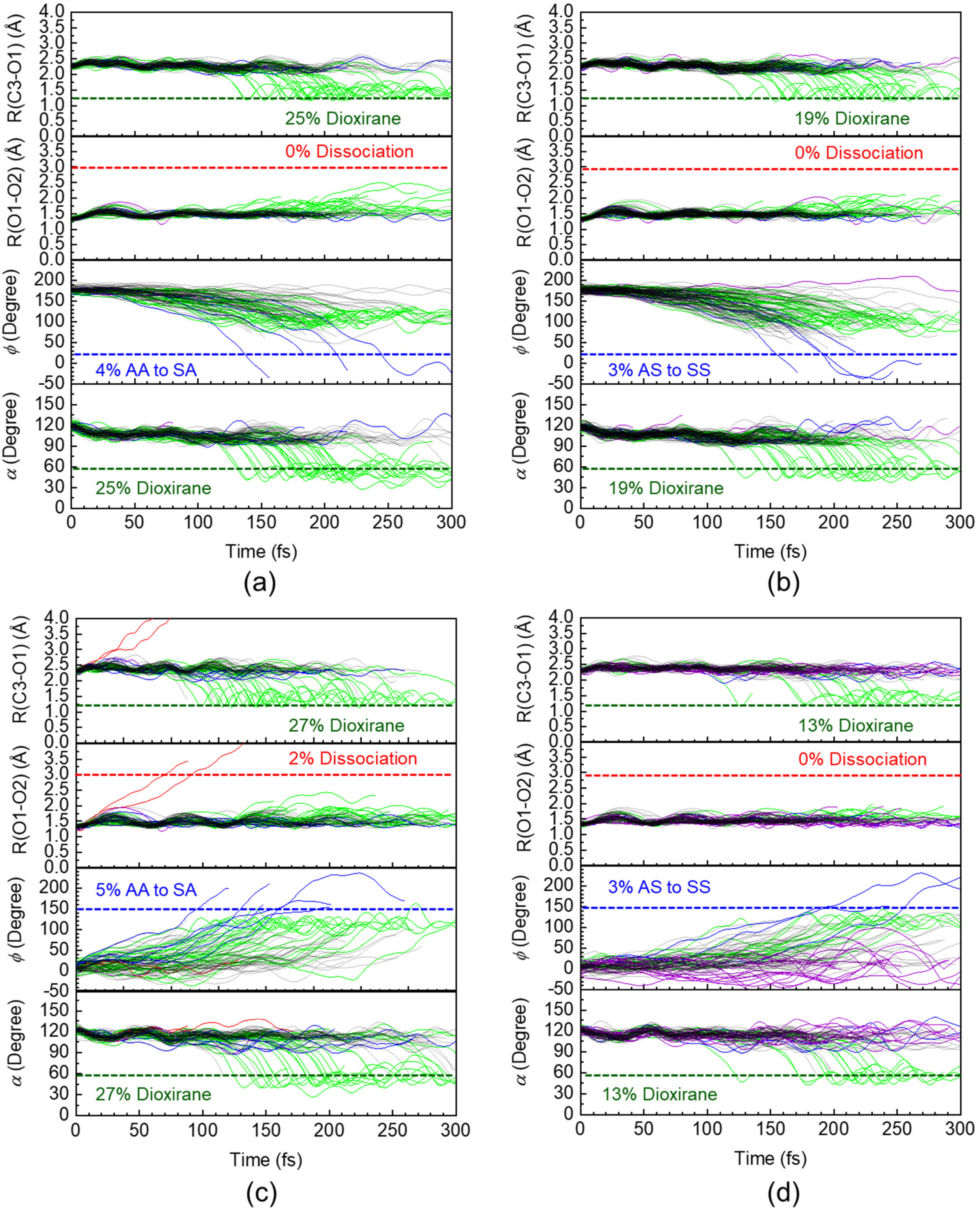

Figure S11. (a)-(d) The evolution of C1-O3 and O2-O3 distance, ϕ dihedral, α angle of trajectories for AA, AS, SA and SS configurations start from the S_1 state, respectively. The trajectories of dissociation (red) show that the O2-O1 bond length is longer than 3 Å. The ring-closure in dioxirane (green) shows that the C3-O1 bond length is shorter than 1.4 Å and α is less than 60˚. The *anti/syn* (CO) isomerization (blue) shows the ϕ change to 180˚ or 0˚. The trajectories of hopping in FC region show in purple and the rest trajectories are in black. The graph also shows the yield of isomerization.

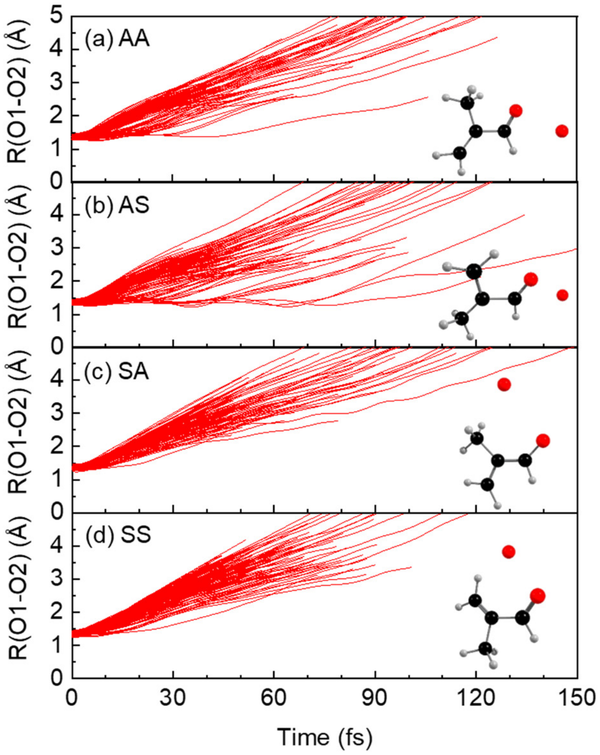

Figure S12. Geometrical evolution of trajectories in four configurations (a) AA, (b) AS, (c) SA and (d) SS, starting from the S_2 state. Trajectories in red represent O-O dissociation isomerization.

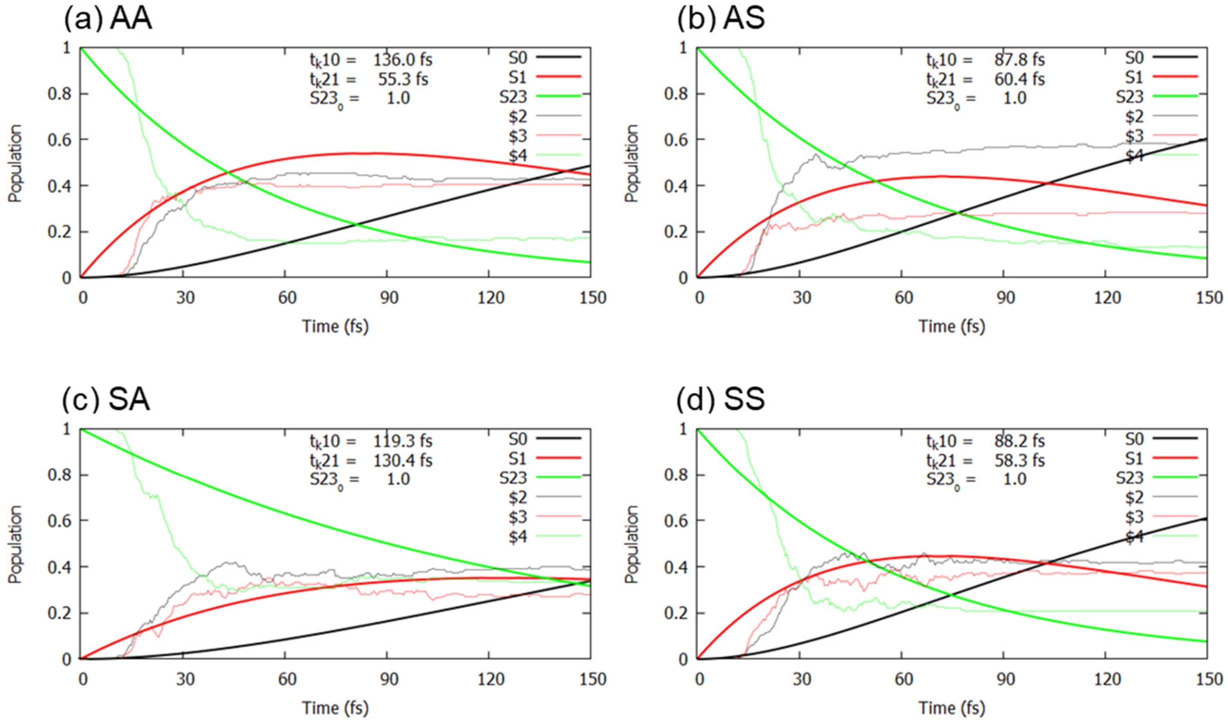

Figure S13. The state population and lifetime of S_2-state trajectories obtained by a kinetic model in SHARC2.1 program.

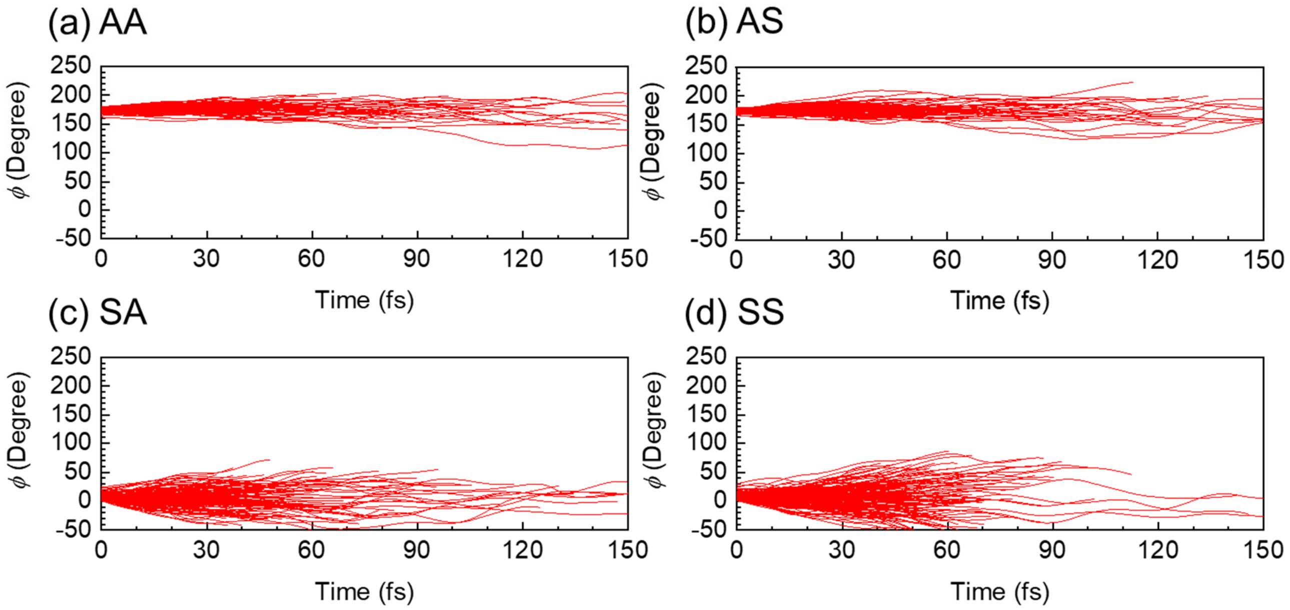

Figure S14. (a), (b), (c) and (d) are the evolutions of ϕ dihedral of trajectories for AA, AS, SA and SS configurations in S_2 state, respectively. And the trajectories of dissociation are in red.

<Coordinates>

SA3-CASSCF/def2-TZVP calculated geometries

S$_0$-AA-MACR-OO

E= -304.72757171

C	0.474776	-0.859600	-0.082764
O	-0.819991	-0.866502	-0.043112
O	-1.411598	-1.694572	0.814967
H	0.980577	-1.527513	0.583813
C	1.126314	0.021493	-0.997548
C	2.484110	0.033020	-1.043678
H	3.012210	0.679837	-1.716257
H	3.072955	-0.603531	-0.410212
C	0.284304	0.909176	-1.880273
H	-0.370645	0.321042	-2.512170
H	-0.341075	1.566541	-1.287907
H	0.915931	1.516574	-2.513463

S$_0$-AS-MACR-OO

E= -304.72373235

C	0.461713	-0.898248	-0.076847
O	-0.837397	-0.890793	-0.076796
O	-1.449883	-0.075361	0.776250
H	0.938977	-0.238309	0.618014
C	1.168383	-1.760215	-0.980882
C	0.545826	-2.589007	-1.856953
H	1.115593	-3.216007	-2.514384
H	-0.522790	-2.646301	-1.923184
C	2.673861	-1.680735	-0.889204
H	3.025174	-0.676431	-1.100897
H	3.018854	-1.946585	0.104356
H	3.136418	-2.354492	-1.596824

S$_0$-SA-MACR-OO

E= -304.72117810

C	0.474776	-0.859600	-0.082764
O	-0.819991	-0.866502	-0.043112
O	-1.411598	-1.694572	0.814967
H	0.980577	-1.527513	0.583813
C	1.126314	0.021493	-0.997548
C	2.484110	0.033020	-1.043678
H	3.012210	0.679837	-1.716257
H	3.072955	-0.603531	-0.410212
C	0.284304	0.909176	-1.880273
H	-0.370645	0.321042	-2.512170
H	-0.341075	1.566541	-1.287907
H	0.915931	1.516574	-2.513463

S$_0$-SS-MACR-OO

E= -304.72371450

C	0.431290	-0.916132	-0.001991
O	-0.848232	-0.769552	-0.137556
O	-1.694194	-1.515675	0.567254
H	0.941912	-0.231694	-0.648001
C	1.160885	-1.812713	0.841520
C	0.623069	-2.719527	1.696940
H	1.278477	-3.339368	2.279511
H	-0.426805	-2.848599	1.820315
C	2.663331	-1.671942	0.706389
H	2.985672	-1.869123	-0.310441
H	2.988127	-0.670079	0.966209
H	3.171198	-2.367819	1.359055

S$_1$-AA-MACR-OO

E= -304.72757171

C	0.458193	-0.835199	-0.108344
O	-0.909255	-0.824770	-0.085770
O	-1.341486	-1.794123	0.917424
H	0.946047	-1.507255	0.563068
C	1.111145	0.013771	-0.989219
C	2.497110	0.028198	-1.038833
H	3.018583	0.677444	-1.713001
H	3.086347	-0.607828	-0.406124
C	0.293390	0.914453	-1.885793
H	-0.360816	0.335386	-2.527373
H	-0.330913	1.581644	-1.302684
H	0.939525	1.514244	-2.511954

S$_1$-AS-MACR-OO

E= -304.66430861

C	0.456606	-0.920165	-0.101282
O	-0.909074	-0.943605	-0.133638
O	-1.391669	0.007402	0.863515
H	0.907241	-0.253320	0.600555
C	1.168387	-1.746412	-0.966822
C	0.550418	-2.596360	-1.863726
H	1.130659	-3.218896	-2.515441
H	-0.516860	-2.660360	-1.936448
C	2.678363	-1.672717	-0.880832
H	3.037784	-0.672631	-1.095888
H	3.031442	-1.947628	0.106782
H	3.131431	-2.347793	-1.594127

S_1-SA-MACR-OO

E= -304.66094408

C	0.462844	-0.914259	-0.017388
O	-0.029570	0.362301	0.137627
O	0.217642	0.967649	1.355968
H	0.193607	-1.242614	-0.997358
C	1.177171	-1.697613	0.866765
C	1.555351	-2.978576	0.431503
H	2.109749	-3.634357	1.070999
H	1.301394	-3.335236	-0.547804
C	1.570709	-1.259202	2.261223
H	2.203190	-0.380983	2.240129
H	0.703549	-1.033853	2.868647
H	2.120491	-2.051327	2.750019

S_1-SS-MACR-OO

E= -304.72757171

C	0.463073	-0.913222	-0.004827
O	-0.892343	-0.734562	-0.170610
O	-1.713839	-1.539028	0.589495
H	0.953705	-0.223401	-0.655754
C	1.154002	-1.787326	0.817562
C	0.623215	-2.725560	1.702551
H	1.286334	-3.338609	2.278932
H	-0.424210	-2.876563	1.846565
C	2.665916	-1.669188	0.703796
H	3.002634	-1.875627	-0.305495
H	3.004977	-0.675430	0.972419
H	3.151265	-2.373708	1.364570

S_0-Heterocyclopentane Dioxole

E= -304.76852597

C	0.463073	-0.913222	-0.004827
O	-0.892343	-0.734562	-0.170610
O	-1.713839	-1.539028	0.589495
H	0.953705	-0.223401	-0.655754
C	1.154002	-1.787326	0.817562
C	0.623215	-2.725560	1.702551
H	1.286334	-3.338609	2.278932
H	-0.424210	-2.876563	1.846565
C	2.665916	-1.669188	0.703796
H	3.002634	-1.875627	-0.305495
H	3.004977	-0.675430	0.972419
H	3.151265	-2.373708	1.364570

S_0-*anti*-Dioxirane

E= -304.72757171

C	0.312617	-1.144413	-0.260080
O	-0.699391	-1.735545	-0.951573
O	-0.909043	-0.973379	0.417969
H	0.989961	-1.828588	0.225436
C	0.955266	0.062331	-0.848475
C	2.272547	0.220169	-0.688182
H	2.790219	1.075454	-1.079912
H	2.865549	-0.503917	-0.159621
C	0.077494	1.042223	-1.578238
H	-0.702821	1.418449	-0.928209
H	0.661451	1.878655	-1.938543
H	-0.406875	0.568770	-2.423511

S_0-*syn*-Dioxirane

E= -304.72757171

C	0.230501	-1.117691	0.277017
O	-1.050529	-0.685573	0.247682
O	0.183635	0.292469	0.350854
H	0.528039	-1.583265	1.206764
C	0.827216	-1.731815	-0.943612
C	0.069629	-2.036509	-1.998434
H	0.495984	-2.485393	-2.876162
H	-0.983876	-1.836047	-2.008733
C	2.310354	-1.977972	-0.870317
H	2.555220	-2.645491	-0.049378
H	2.675540	-2.421735	-1.786344
H	2.849319	-1.050026	-0.705597

$\text{ConInt}_{\text{CO-A}}$

E= -304.68098943

C	0.710911	-0.763807	-0.028451
O	0.553718	0.563929	0.385409
O	1.077154	0.425586	1.695115
H	1.652595	-0.993426	-0.481072
C	-0.318624	-1.749272	0.206754
C	-0.131309	-2.982811	-0.251385
H	-0.870282	-3.753887	-0.130067
H	0.757824	-3.251684	-0.793527
C	-1.584988	-1.324955	0.909924
H	-1.382766	-0.638867	1.720697
H	-2.242255	-0.814932	0.213945
H	-2.109204	-2.185947	1.305310

ConInt$_{\mathrm{CO\text{-}S}}$

E= -304.67953115

C	0.446791	-0.887969	-0.061933
O	-0.943565	-0.917681	-0.195419
O	-1.233917	-0.049380	0.891393
H	0.942075	-0.228326	-0.743684
C	1.174451	-1.827950	0.773828
C	0.591314	-2.747555	1.525032
H	1.176817	-3.442177	2.099599
H	-0.474720	-2.840406	1.585603
C	2.673693	-1.688015	0.675414
H	3.001078	-1.818084	-0.350799
H	2.997428	-0.702990	0.998234
H	3.175738	-2.428126	1.282659

ConInt$_{\mathrm{CC}}$

E= -304.72371410

C	0.175952	-0.909819	-0.225240
O	1.462244	-0.893888	-0.373339
O	2.138290	0.249354	-0.297831
H	-0.184004	-1.913927	-0.318463
C	-0.724459	0.173095	0.026374
C	-0.383261	1.480444	0.161212
H	-1.155225	2.203314	0.347709
H	0.620794	1.828346	0.090869
C	-2.171228	-0.263865	0.133264
H	-2.811810	0.583740	0.331681
H	-2.508092	-0.731183	-0.785925
H	-2.306093	-0.981213	0.935737