



## Gas-Phase Ozonolysis of Furan, Methylfurans, and Dimethylfurans in the Atmosphere

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Electronic Supplementary Information: Figure S1-S11

Figure S1. Structures at M06-2X/6-311++G(2df,2p) level

Figure S2. CASSCF(8,6)/6-311+G(d) calculation on CH<sub>2</sub>=CHCHO

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Figure S5. Interconversions and isomerizations of 2,5-DMF-CI1-*syn* at RHF-CCSD(T)-F12a/cc-pVDZ-F12 level. Energies are relative to separate 2,5-DMF and O<sub>3</sub>

Figure S6. The profiles of fractional yield of product channels in the ozonolysis of 2,5-DMF at 298 K and 760 Torr, obtained from RRKM-ME calculations based on F12/VDZ energies

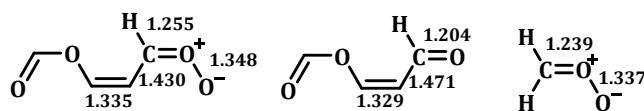
Figure S7. Interconversions and isomerizations of 3-MF-CI1-*syn* and 3-MF-CI3-*syn* at RHF-CCSD(T)-F12a/cc-pVDZ-F12 level. Energies are relative to separate 2,3-DMF and O<sub>3</sub>

Figure S8. Potential energy diagrams for reaction between 2-methylfuran and O<sub>3</sub> at levels of CCSD(T)-F12a/cc-pVDZ-F12 [and CCSD(T)-F12a/cc-pVTZ-F12]

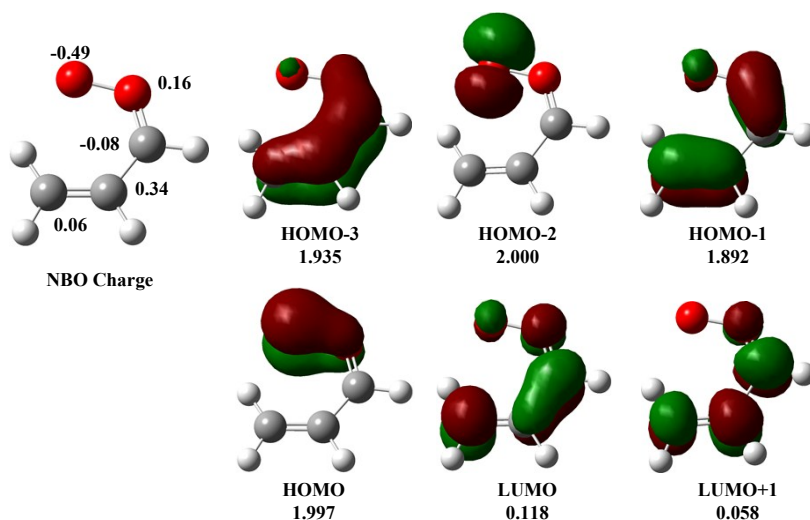
Figure S9. Interconversions and isomerizations of 3-MF-CI1-*syn* and 3-MF-CI3-*syn* at RHF-CCSD(T)-F12a/cc-pVDZ-F12 level. Energies are relative to separate 2,3-DMF and O<sub>3</sub>

Figure S10. Potential energy diagrams for reaction between 2,3-dimethylfuran and O<sub>3</sub> at levels of CCSD(T)-F12a/cc-pVDZ-F12 [and CCSD(T)-F12a/cc-pVTZ-F12]

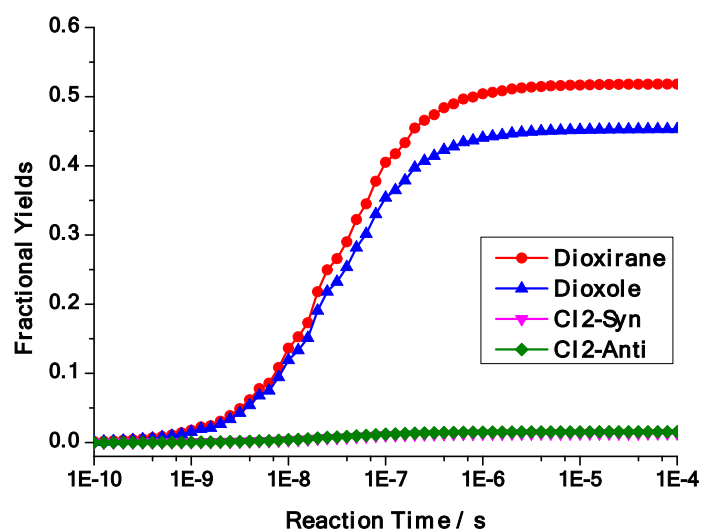
Figure S11. Interconversions and isomerizations of 2,3-DMF-CI1-*syn* and 2,3-DMF-CI3-*syn* at RHF-CCSD(T)-F12a/cc-pVDZ-F12 level. Energies are relative to separate 2,3-DMF and O<sub>3</sub>



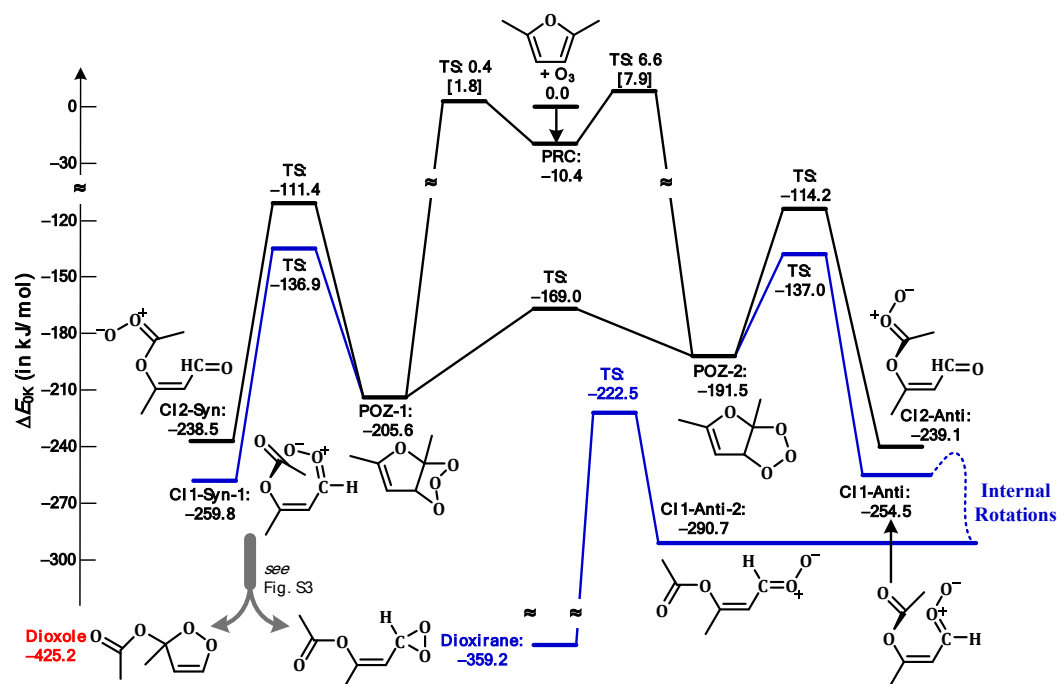
**Figure S1.** Structures at M06-2X/6-311++G(2df,2p) level (bond lengths in Ångström).



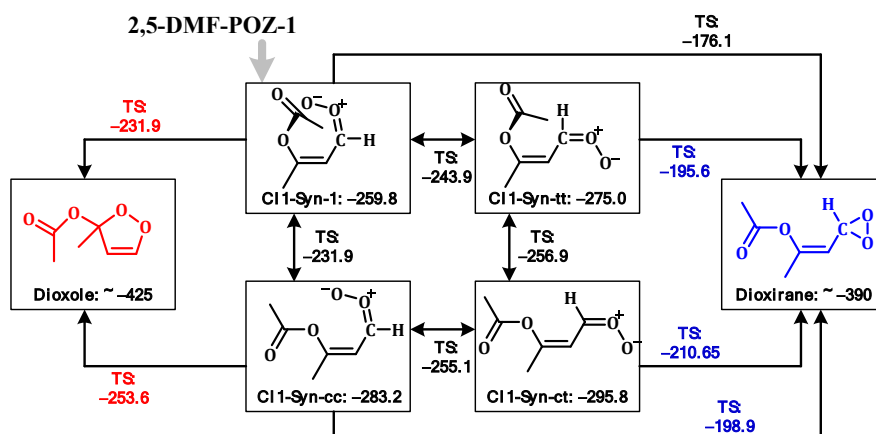
**Figure S2.** CASSCF(8,6)/6-311+G(d) calculation on  $\text{CH}_2=\text{CHCHOO}$ : the NBO charges, the active orbitals and their orbital occupancies.



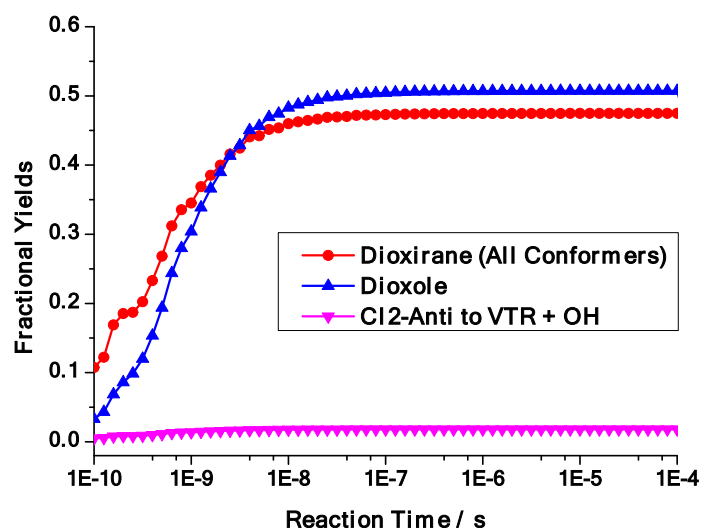
**Figure S3.** The profiles of fractional yield of product channels in the ozonolysis of furan at 298 K and 760 Torr, obtained from RRKM-ME calculations based on F12/VTZ energies.



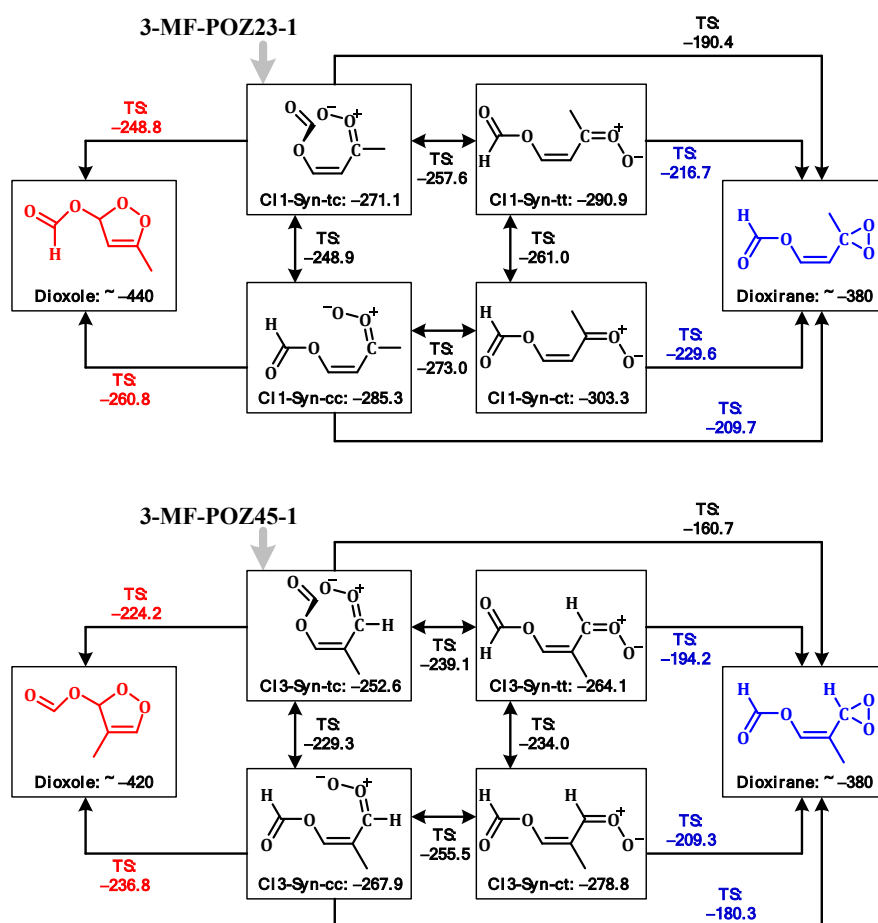
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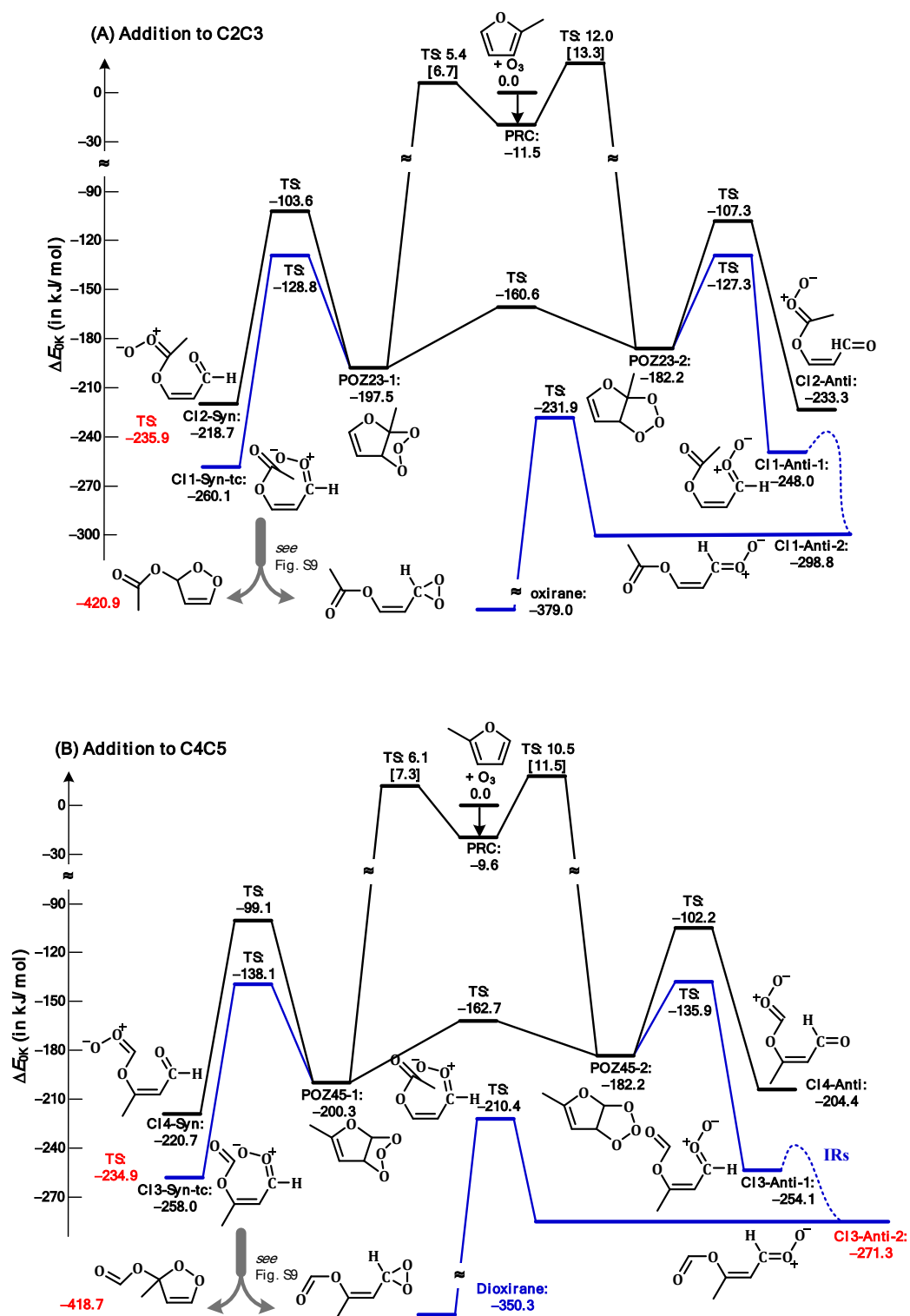
**Figure S5.** Interconversions and isomerizations of 2,5-DMF-CI1-*syn* at RHF-CCSD(T)-F12a/cc-pVDZ-F12 level. Energies are relative to separate 2,5-DMF and  $O_3$ .



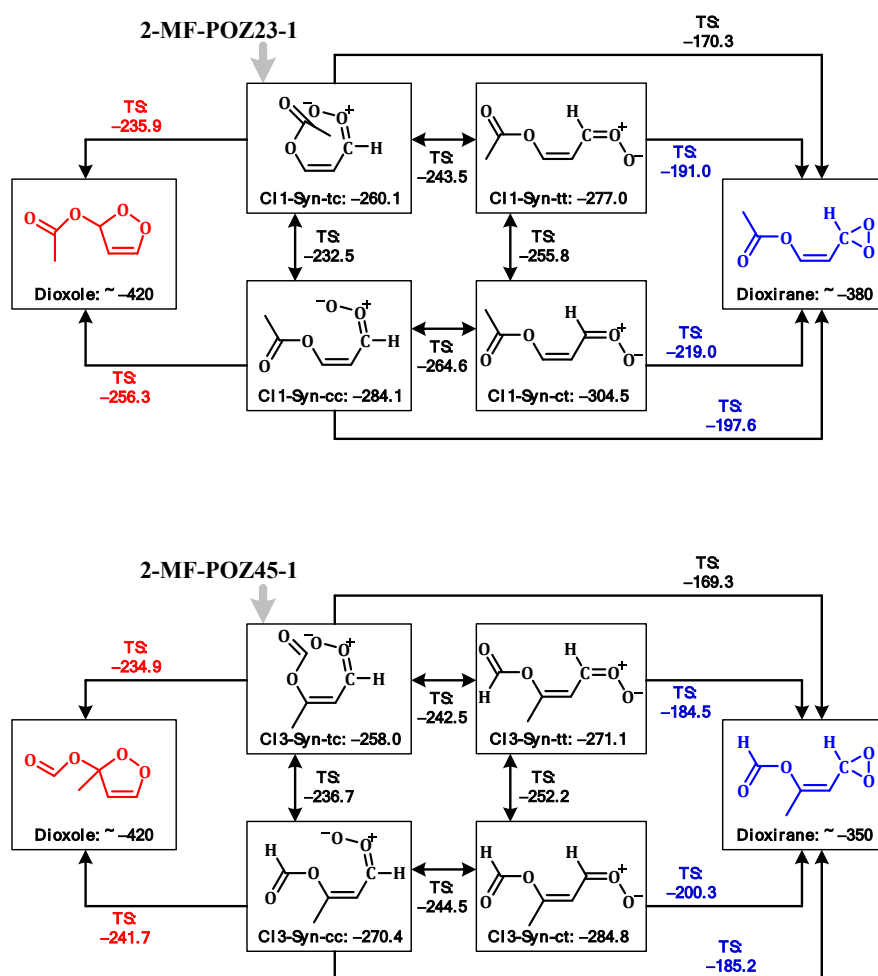
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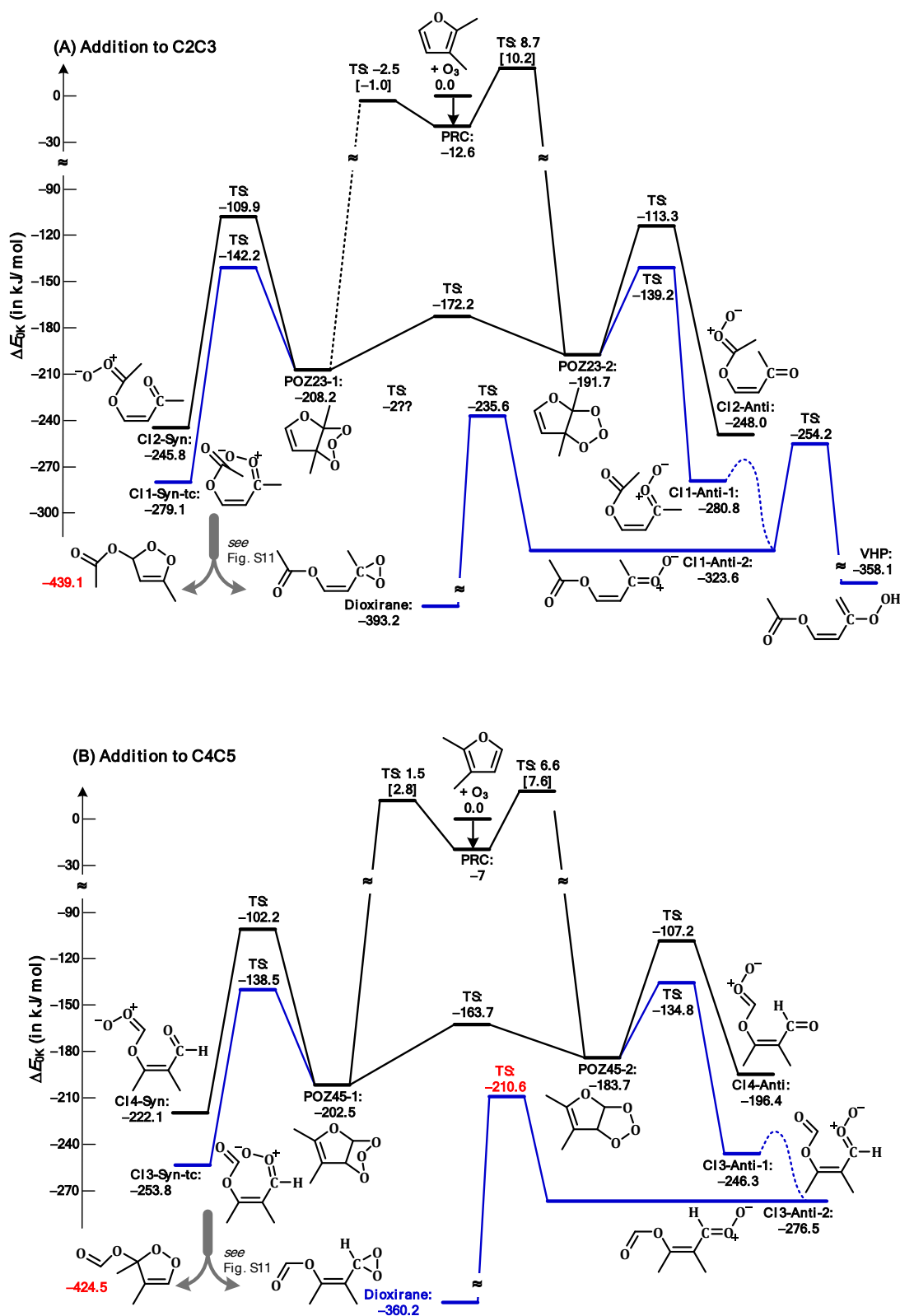
**Figure S7.** Interconversions and isomerizations of 3-MF-CI1-*syn* and 3-MF-CI3-*syn* at RHF-CCSD(T)-F12a/cc-pVDZ-F12 level. Energies are relative to separate 2,3-DMF and O<sub>3</sub>.



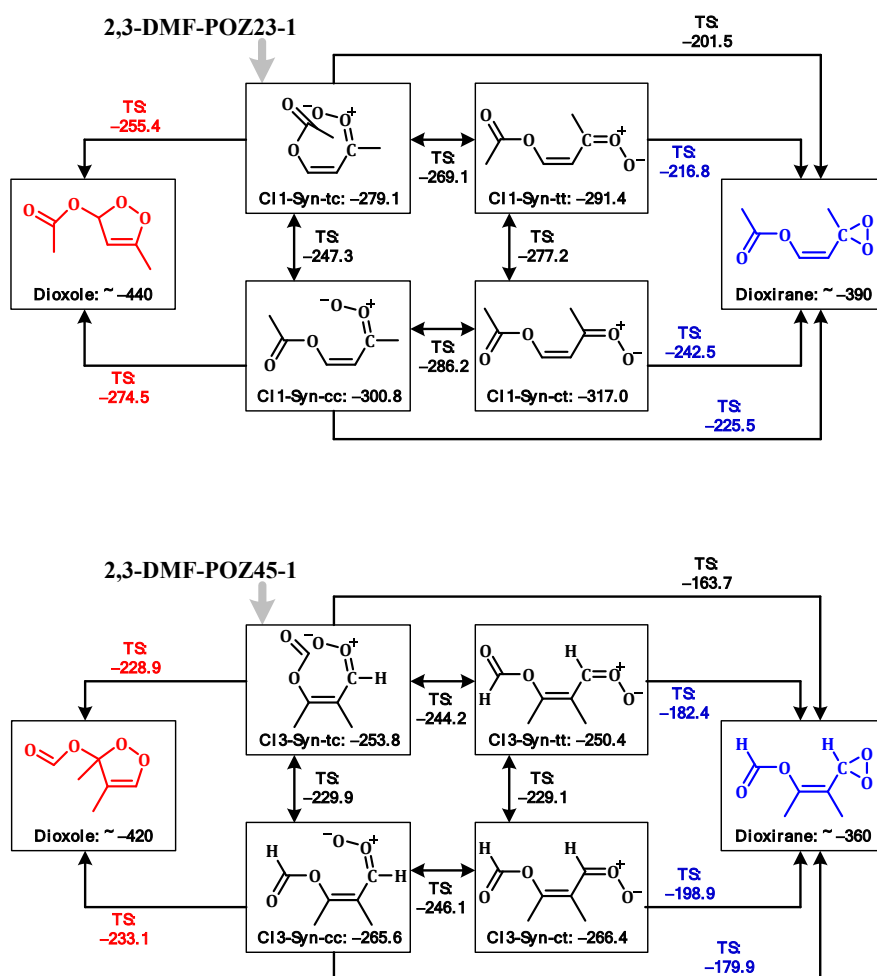
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**Figure S9.** Interconversions and isomerizations of 3-MF-CI1-*syn* and 3-MF-CI3-*syn* at RHF-CCSD(T)-F12a/cc-pVDZ-F12 level. Energies are relative to separate 2,3-DMF and O<sub>3</sub>.



**Figure S10.** Potential energy diagrams for reaction between 2,3-dimethylfuran and  $O_3$  at levels of CCSD(T)-F12a/cc-pVDZ-F12 [and CCSD(T)-F12a/cc-pVTZ-F12]



**Figure S11.** Interconversions and isomerizations of 2,3-DMF-Cl1-*syn* and 2,3-DMF-Cl3-*syn* at RHF-CCSD(T)-F12a/cc-pVDZ-F12 level. Energies are relative to separate 2,3-DMF and O<sub>3</sub>.