

Supplemental Information

Pericyclic Reactions in Ether Biofuels

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Table S1: Comparisons of different level of calculations for pericyclic reactions in DEE and THF

Table S2: Parameters used in the master equation simulation of the H₂ elimination in DME.

Figure S1: High-pressure limit rate constants calculated for the pericyclic reactions in DMTHF and DMTHP.

Figure S2: Comparisons of high-pressure limit rate constants for similar pericyclic reactions in different cyclic ethers.

Table S1: Comparisons of different levels of calculations for pericyclic reactions in DEE and THF. Units are kcal/mol.

Level	DEE → Ethanol+C ₂ H ₄	DEE → (CH ₃ CH) ₂ O + H ₂
mo6-2x/6-311+G(2d,p)	67.5	81.5
CBS-QB3	68.3	76.9
G4	67.1	77.7
ccsd(t)/VDZ-F12	67.3	77.3
ccsd(t)/VTZ-F12	67.1	77.5

Level	THF → 3-buten-1-ol	THF → C ₄ H ₆ O + H ₂
mo6-2x/6-311+G(2d,p)	82.1	83.8
CBS-QB3	80.4	78.3
G4	79.8	78.6
ccsd(t)/VDZ-F12	80.7	79.2

Table S2: Parameters used in the master equation simulation of the H₂ elimination DME.

Species	$\langle E_{down} \rangle$ (cm ⁻¹)	σ (Å)	ϵ (K)
Kr	100	3.61	190
DME		4.76	252

The collisional energy transfer probability was described by the exponential down model, with $\langle E_{down} \rangle$

$= \langle E_{down} \rangle \times (T/300)^{0.85}$ (cm⁻¹). Pressure dependant rate of DME → CH₃ + CH₃O in Kr was taken from

Sivaramakrishnan et al.

Figure S1: High-pressure limit rate constants calculated for the pericyclic reactions in DMTHF and DMTHP.

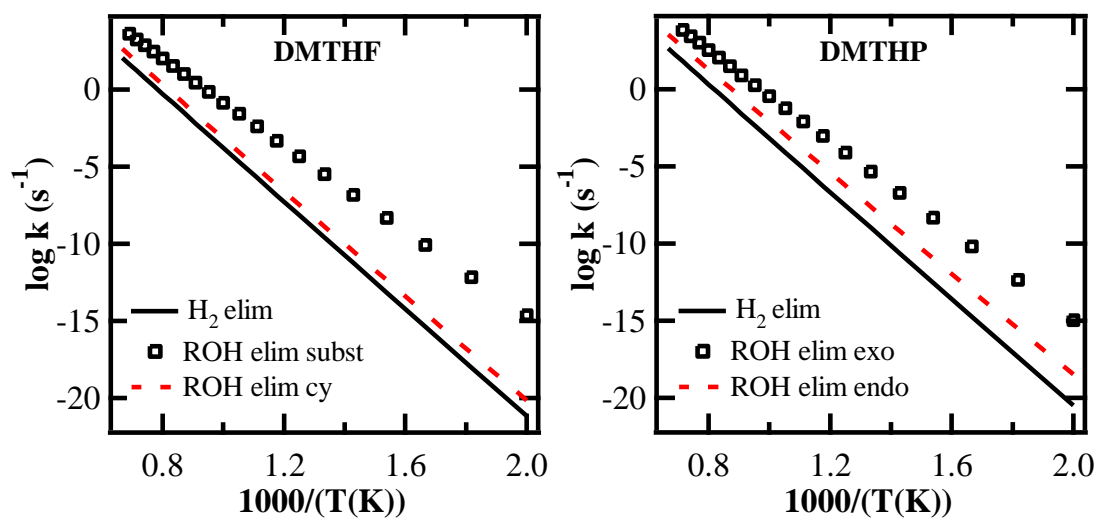


Figure S2: Comparisons of high-pressure limit rate constants for similar pericyclic reactions in different cyclic ethers.

