Supplemental Material-I

Impact of Conformational Structures on Low-Temperature Oxidation Chemistry for Cyclohexyl Radical: A Theoretical and Kinetic Modeling Study on First Oxygen Addition

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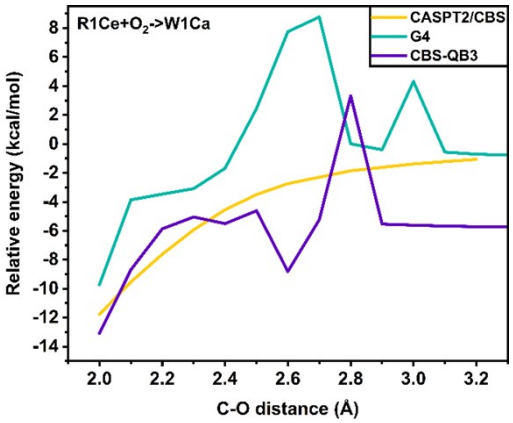

Fig. S1. Interaction potential for O_2 adding onto cyclohexyl in chair form along minimum energy pathway by using CBS-QB3, G4 and CASPT2/CBS methods.

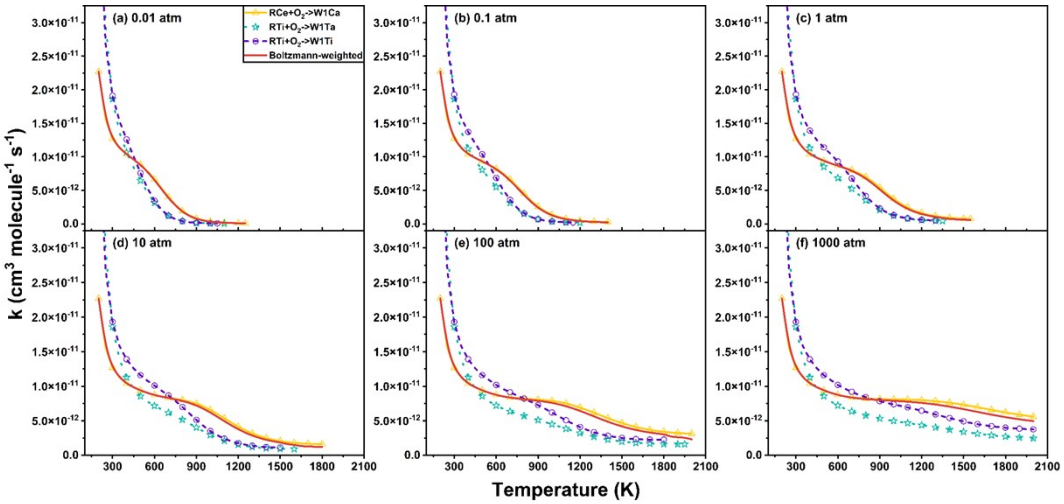

Fig. S2. Boltzmann-weighted rate coefficients for three entrance channels, i.e. RCe + O_2 to W1Ca, at 0.01-1000 atm.

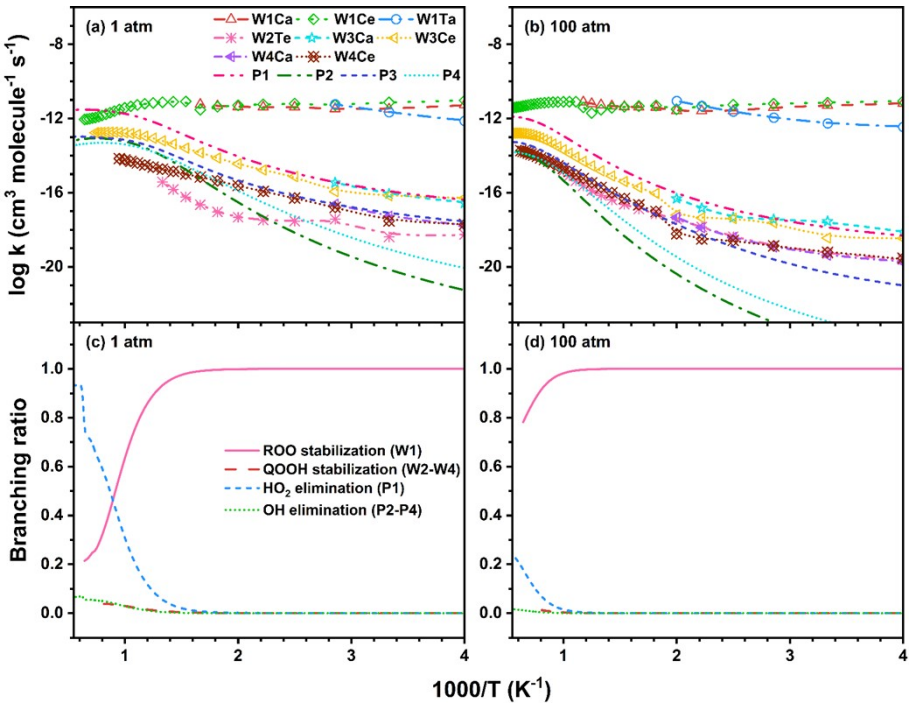

Fig. S3. Temperature-dependent rate constants (a and b) and branching ratios (c and d) for main consumption channels in cyclohexyl + O_2 system at 0.1 and 10 atm with Ar as the bath gas.

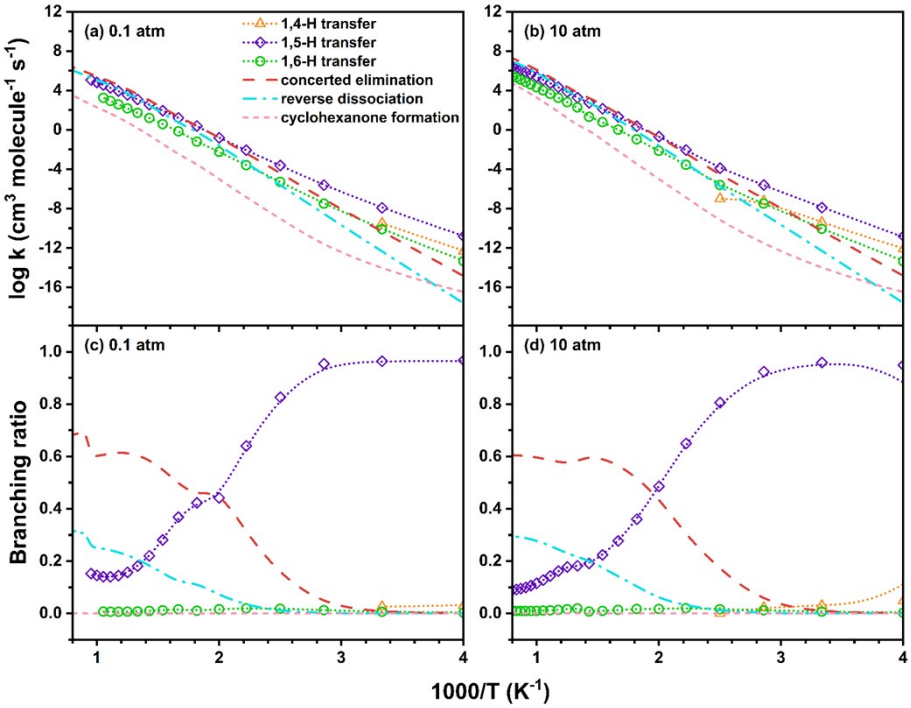

Fig. S4. Boltzmann-weighted rate constants for product channels in W1 at (a) 0.1 and (b) 10 atm with Ar as bath gas and branching ratio for six channels at (c) 0.1 and (d) 10 atm.

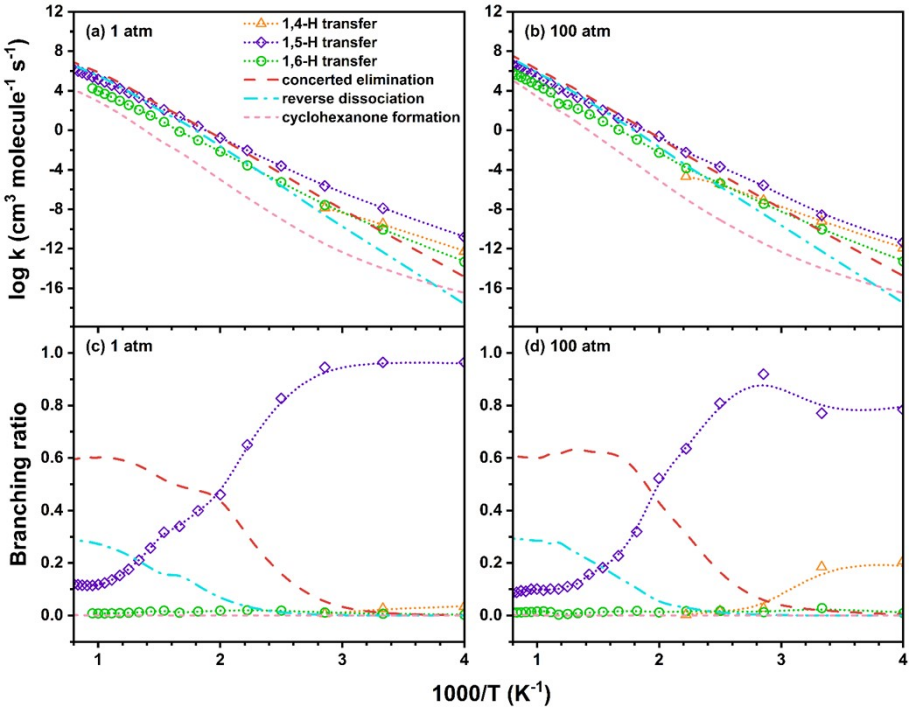

Fig. S5. Boltzmann-weighted rate constants for product channels in W1 at (a) 1 and (b) 100 atm with Ar as bath gas and branching ratio for six channels at (c) 1 and (d) 100 atm.

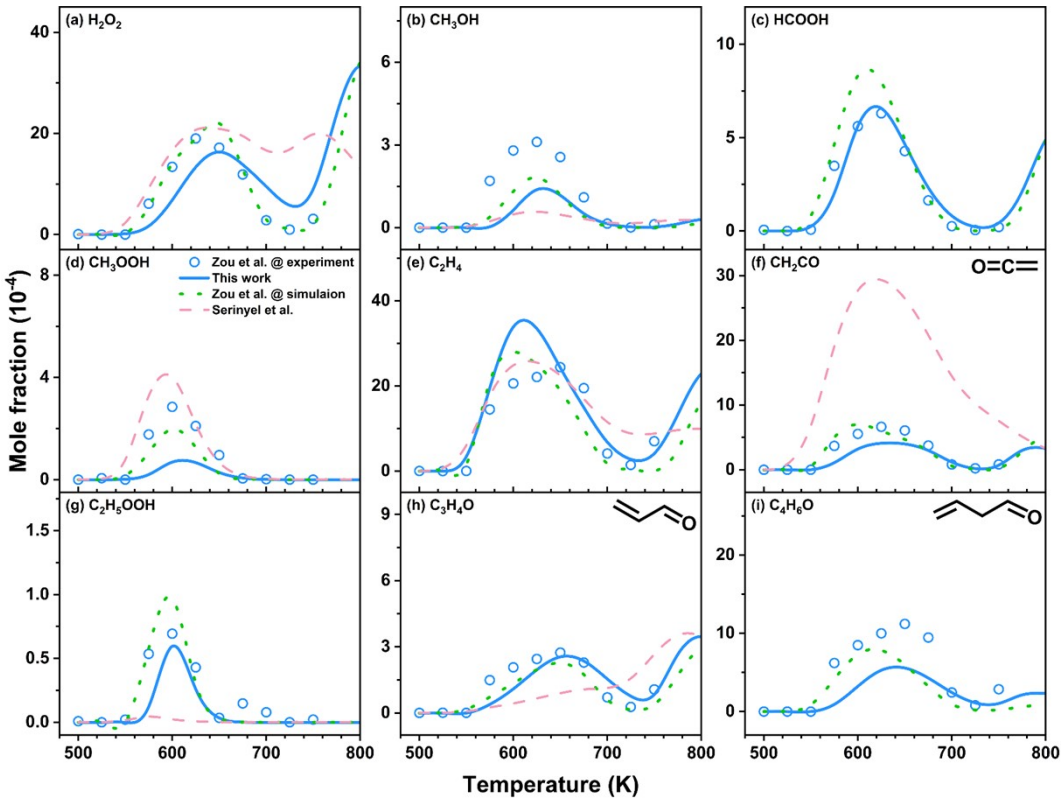

Fig. S6. Mole fraction profiles of C_0-C_6 products in low temperature oxidation of cyclohexane at 1.04 bar, $\phi = 0.25$, and $\tau = 4$s. Open symbols are JSR SVUV-PIMS data by Zou et al.[11], lines are simulation results using new model (solid) and former kinetic models by Zou et al. (dotted)[11] and Serinyel et al. (dashed)[13].