Gas-phase Formation of 1-Methylcyclopropene and 3-Methylcyclopropene via the Reaction of the Methyldyne Radical (CH; X^2Π) with Propylene (CH₃CHCH₂; X¹A’)

Chao He,¹ Aaron M. Thomas,¹ Galiya R. Galimova,²,³ Alexander M. Mebel,²,³,* Ralf I. Kaiser¹,*

¹ Department of Chemistry, University of Hawai‘i at Manoa, Honolulu, Hawaii 96822, United States
² Department of Chemistry and Biochemistry, Florida International University, Miami, Florida 33199, United States
³ Samara National Research University, Samara 443086, Russia

Supporting Information

Potential energy surface (PES) figures for isotopic reactions of CD + CH₃CHCH₂, CH + CD₃CHCH₂, and CD + CD₃CHCH₂.

* Corresponding Authors:
  Prof. Ralf I. Kaiser: ralfk@hawaii.edu
  Prof. Alexander M. Mebel: mebela@fiu.edu
Figure S1. Portion of the C₄H₆D potential energy surface (PES) following CD radical addition to the carbon-carbon double bond of propylene. Energies are given for the fully hydrogenated reactant; energies of the (partially) deuterated species differ by a few kJ mol⁻¹ at most.
Figure S2. Portion of the C₄H₄D PES corresponding to CD radical insertion into the terminal C-H bond of propylene. Energies are given for the fully hydrogenated reactant; energies of the (partially) deuterated species differ by a few kJ mol⁻¹ at most.
Figure S3. Portion of the C₄H₆D PES corresponding to CD radical insertion into the middle C–H bond of propylene. Energies are given for the fully hydrogenated reactant; energies of the (partially) deuterated species differ by a few kJ mol⁻¹ at most.
Figure S4. Portion of the C₄D₆H PES following CH radical addition to the carbon-carbon double bond of propylene-d₆. Energies are given for the fully hydrogenated reactant; energies of the (partially) deuterated species differ by a few kJ mol⁻¹ at most.
Figure S5. Portion of the C₄D₈H PES corresponding to CH radical insertion into the terminal C-D bond of propylene-d₆. Energies are given for the fully hydrogenated reactant; energies of the (partially) deuterated species differ by a few kJ mol⁻¹ at most.
Figure S6. Portion of the C₄D₆H PES corresponding to CH radical insertion into the middle C−D bond of propylene-d₆. Energies are given for the fully hydrogenated reactant; energies of the (partially) deuterated species differ by a few kJ mol⁻¹ at most.
Figure S7. Portion of the C₄D₄H₃ PES following CD radical addition to the carbon-carbon double bond of propylene-3,3,3-d₃. Energies are given for the fully hydrogenated reactant; energies of the (partially) deuterated species differ by a few kJ mol⁻¹ at most.
Figure S8. Portion of the C₄D₄H₃ PES corresponding to CD radical insertion into the terminal C-H/C-D bond of propylene-3,3,3-d₃. Energies are given for the fully hydrogenated reactant; energies of the (partially) deuterated species differ by a few kJ mol⁻¹ at most.
Figure S9. Portion of the C$_4$D$_4$H$_3$ PES corresponding to CD radical insertion into the middle C–H bond of propylene-3,3,3-d$_3$. Energies are given for the fully hydrogenated reactant; energies of the (partially) deuterated species differ by a few kJ mol$^{-1}$ at most.