Gas-phase Formation of 1-Methylcyclopropene and 3-Methylcyclopropene via the Reaction of the Methylidyne Radical (CH; $X^2\Pi$) with Propylene (CH_3CHCH_2; X^1A')

Chao He,[a] Aaron M. Thomas,[a] Galiya R. Galimova,[b,c] Alexander M. Mebel,[b,c,*] Ralf I. Kaiser[a,*]

[a] *Department of Chemistry, University of Hawai'i at Manoa, Honolulu, Hawaii 96822, United States*

[b] *Department of Chemistry and Biochemistry, Florida International University, Miami, Florida 33199, United States*

[c] *Samara National Research University, Samara 443086, Russia*

Supporting Information

Potential energy surface (PES) figures for isotopic reactions of CD + CH_3CHCH_2, CH + CD_3CHCH_2, and CD + CD_3CHCH_2.

* Corresponding Authors:
Prof. Ralf I. Kaiser: ralfk@hawaii.edu
Prof. Alexander M. Mebel: mebela@fiu.edu

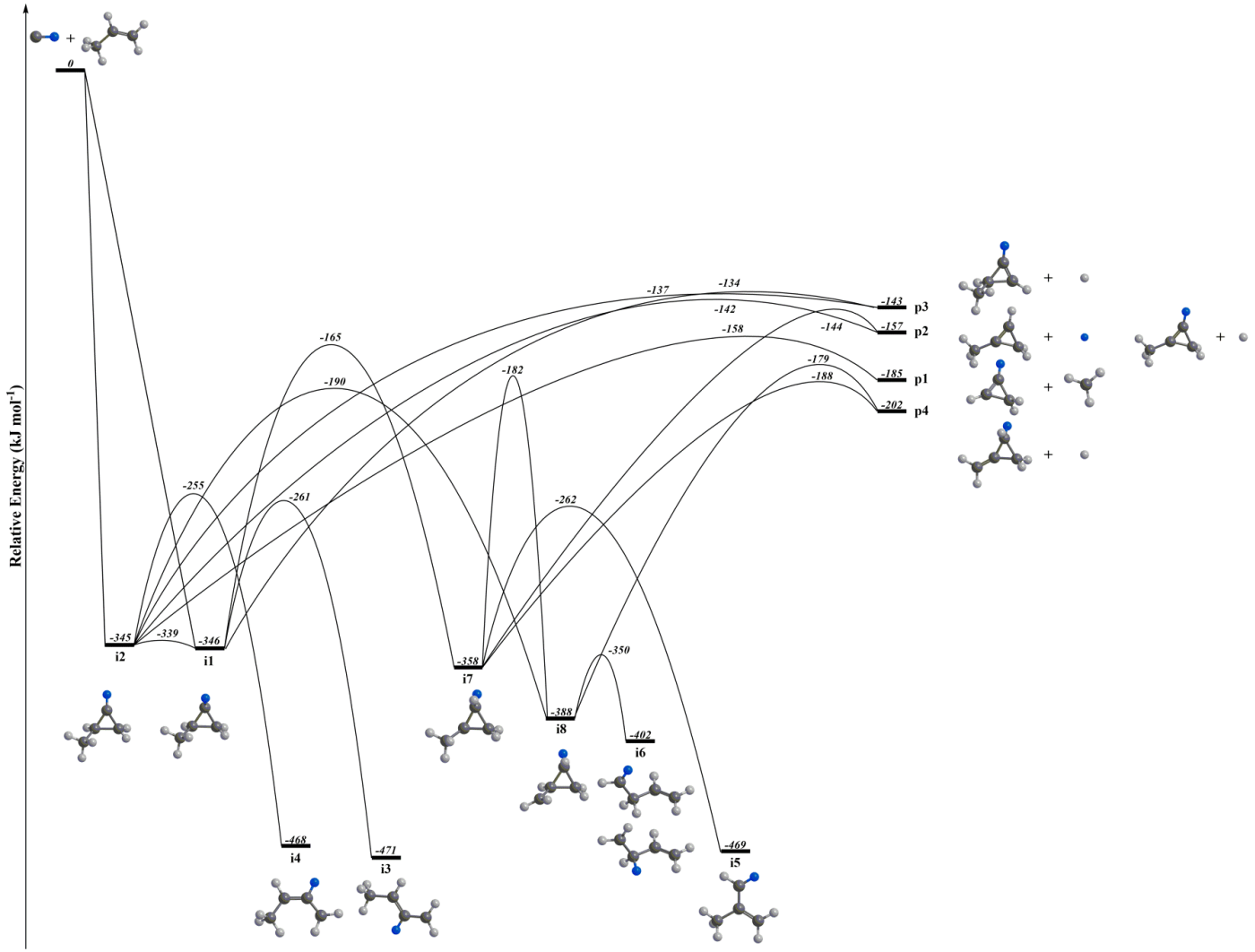

Figure S1. Portion of the C_4H_6D potential energy surface (PES) following CD radical addition to the carbon-carbon double bond of propylene. Energies are given for the fully hydrogenated reactant; energies of the (partially) deuterated species differ by a few kJ mol^{-1} at most.

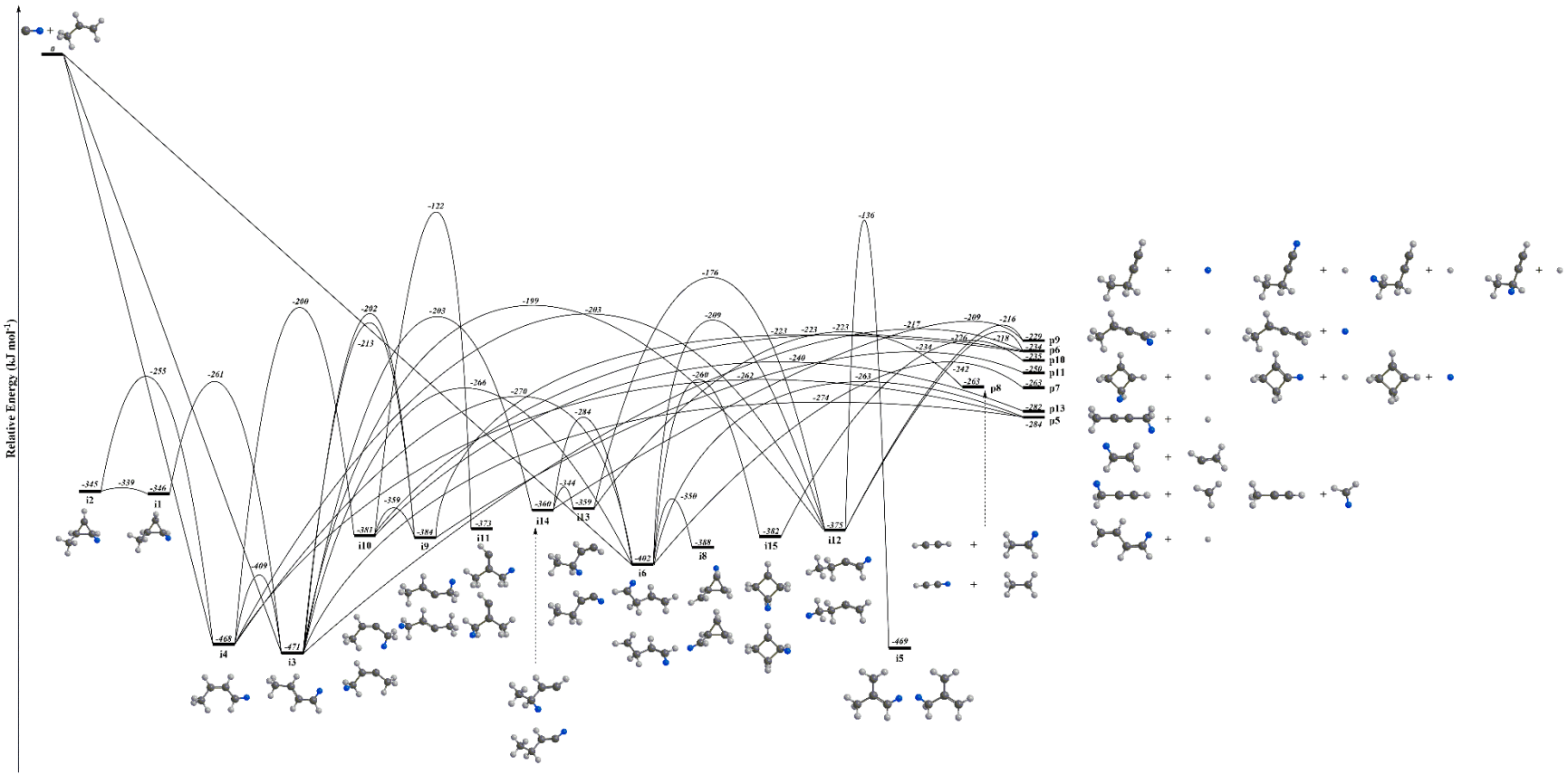

Figure S2. Portion of the C_4H_6D PES corresponding to CD radical insertion into the terminal C-H bond of propylene. Energies are given for the fully hydrogenated reactant; energies of the (partially) deuterated species differ by a few kJ mol^{-1} at most.

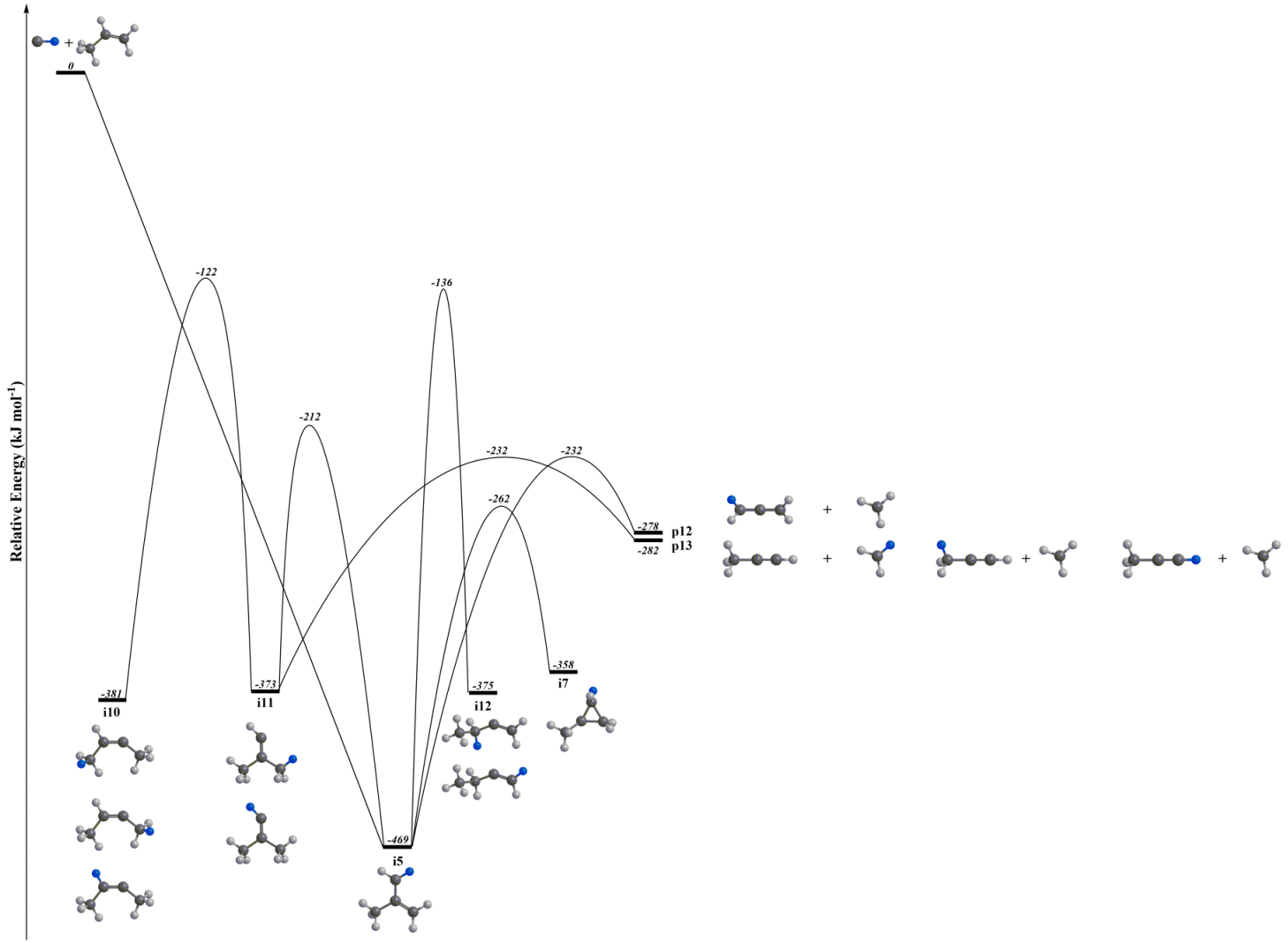

Figure S3. Portion of the C_4H_6D PES corresponding to CD radical insertion into the middle C−H bond of propylene. Energies are given for the fully hydrogenated reactant; energies of the (partially) deuterated species differ by a few kJ mol^{-1} at most.

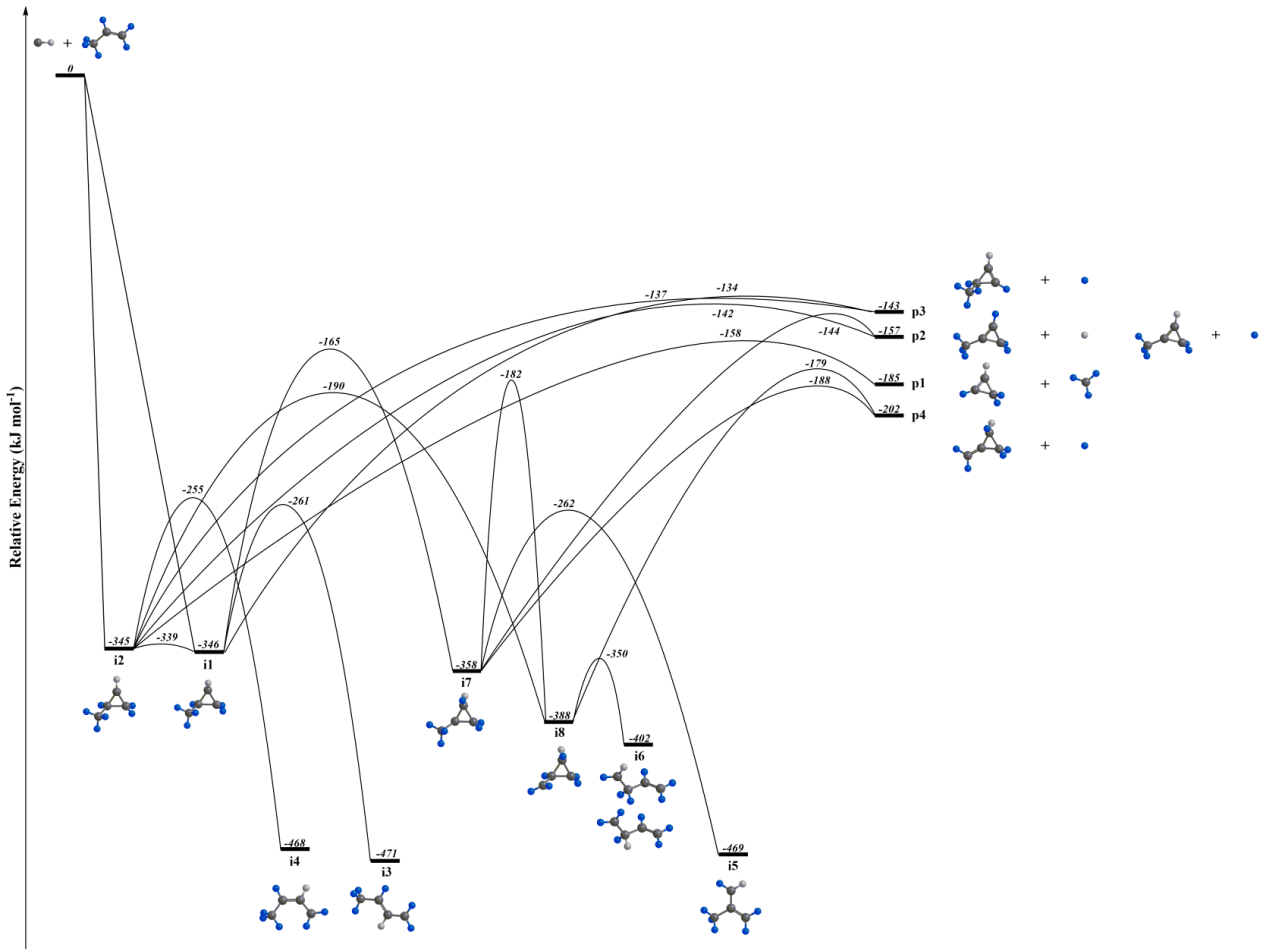

Figure S4. Portion of the C_4D_6H PES following CH radical addition to the carbon-carbon double bond of propylene-d_6. Energies are given for the fully hydrogenated reactant; energies of the (partially) deuterated species differ by a few kJ mol^{-1} at most.

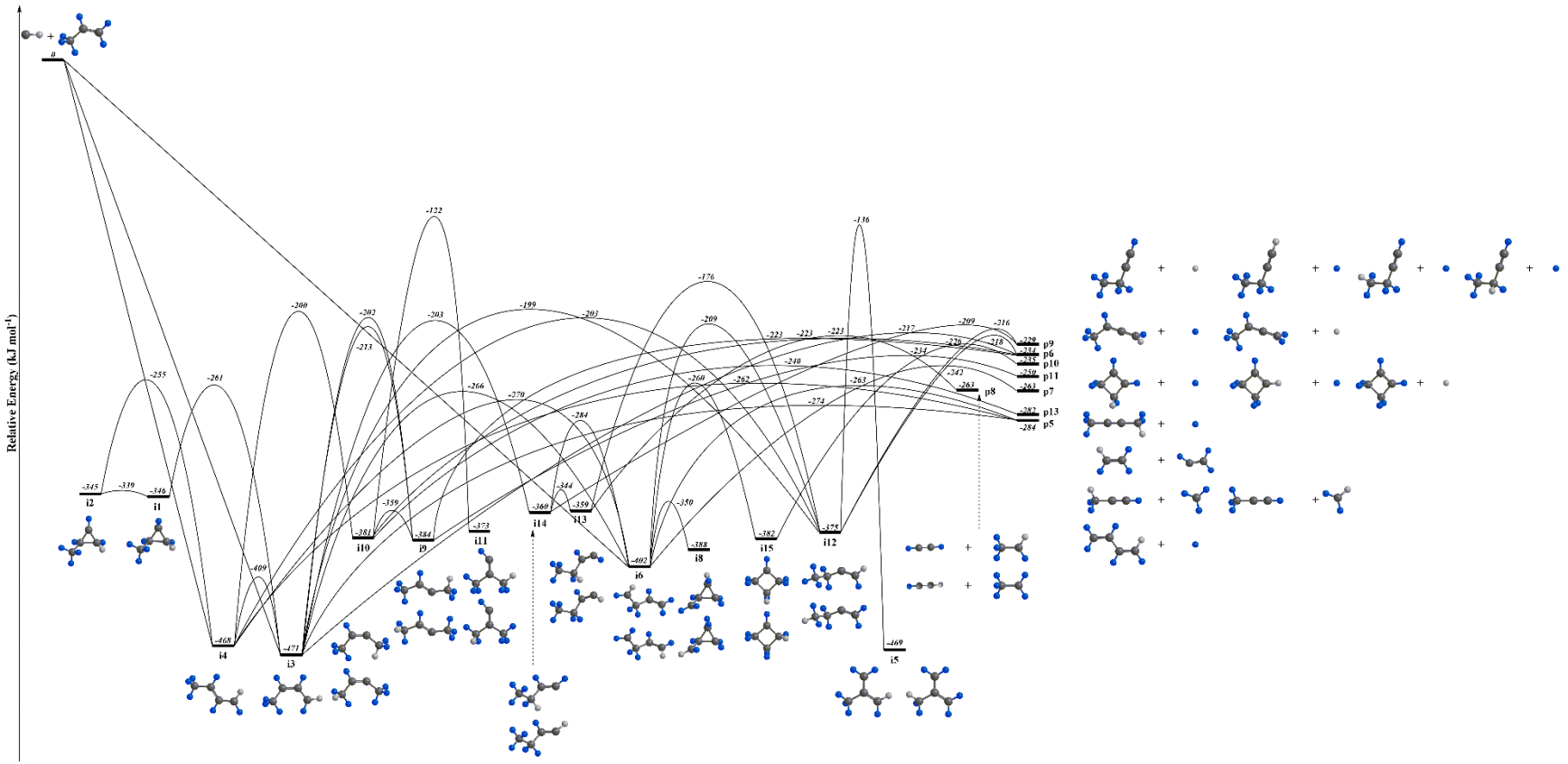

Figure S5. Portion of the C_4D_6H PES corresponding to CH radical insertion into the terminal C-D bond of propylene-d_6. Energies are given for the fully hydrogenated reactant; energies of the (partially) deuterated species differ by a few kJ mol^{-1} at most.

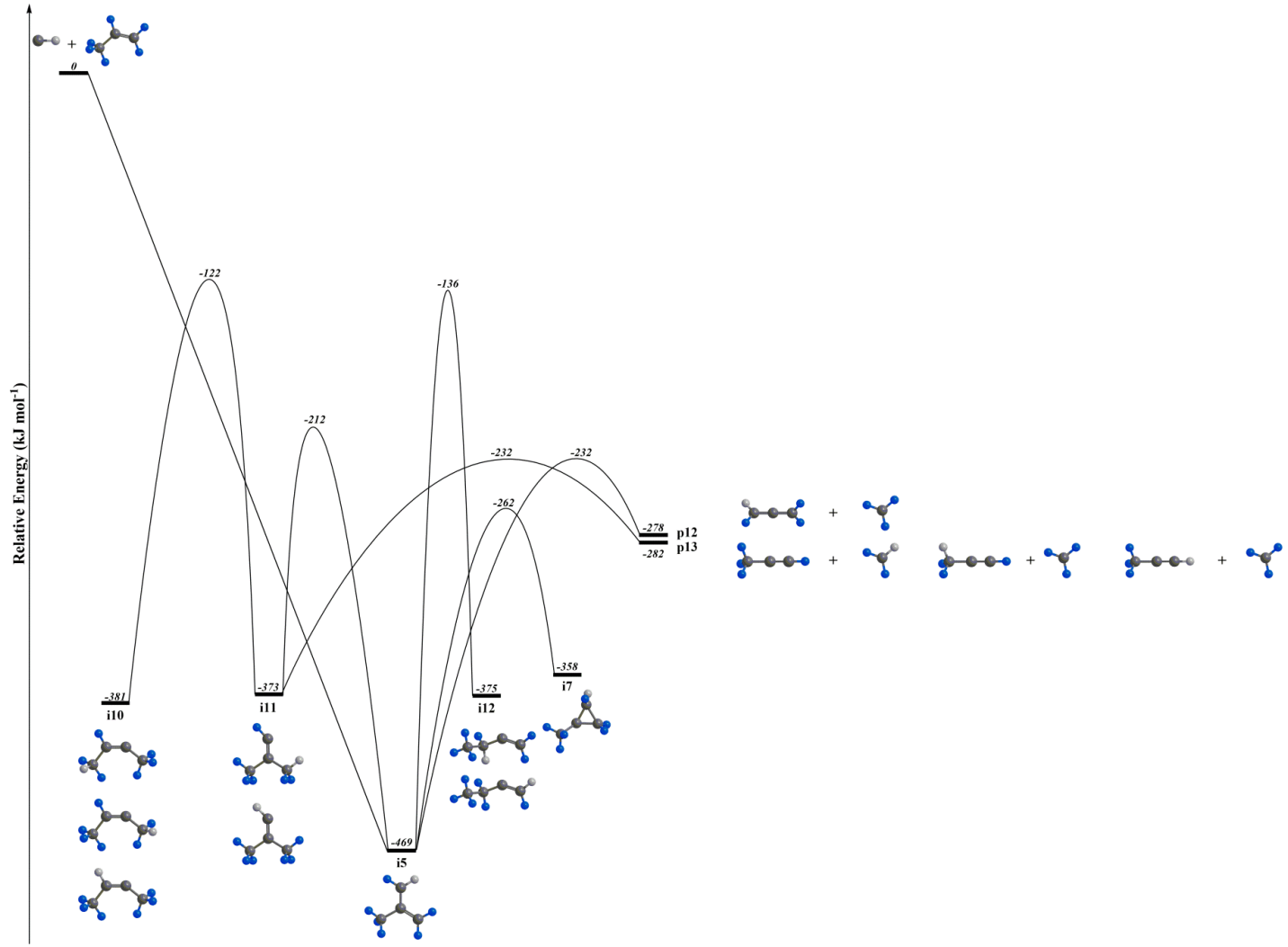

Figure S6. Portion of the C_4D_6H PES corresponding to CH radical insertion into the middle C−D bond of propylene-d_6. Energies are given for the fully hydrogenated reactant; energies of the (partially) deuterated species differ by a few kJ mol^{-1} at most.

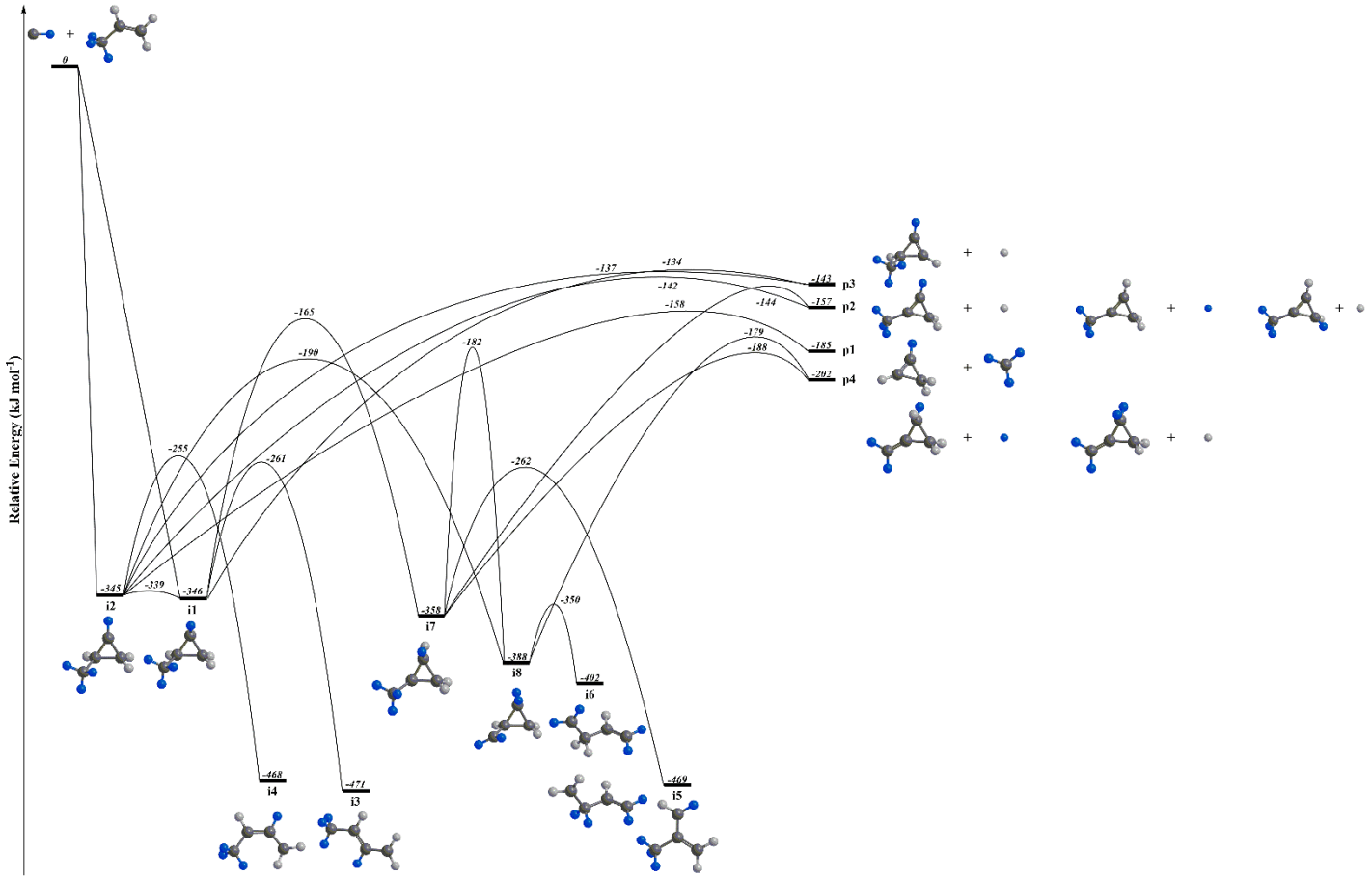

Figure S7. Portion of the $C_4D_4H_3$ PES following CD radical addition to the carbon-carbon double bond of propylene-3,3,3-d_3. Energies are given for the fully hydrogenated reactant; energies of the (partially) deuterated species differ by a few kJ mol^{-1} at most.

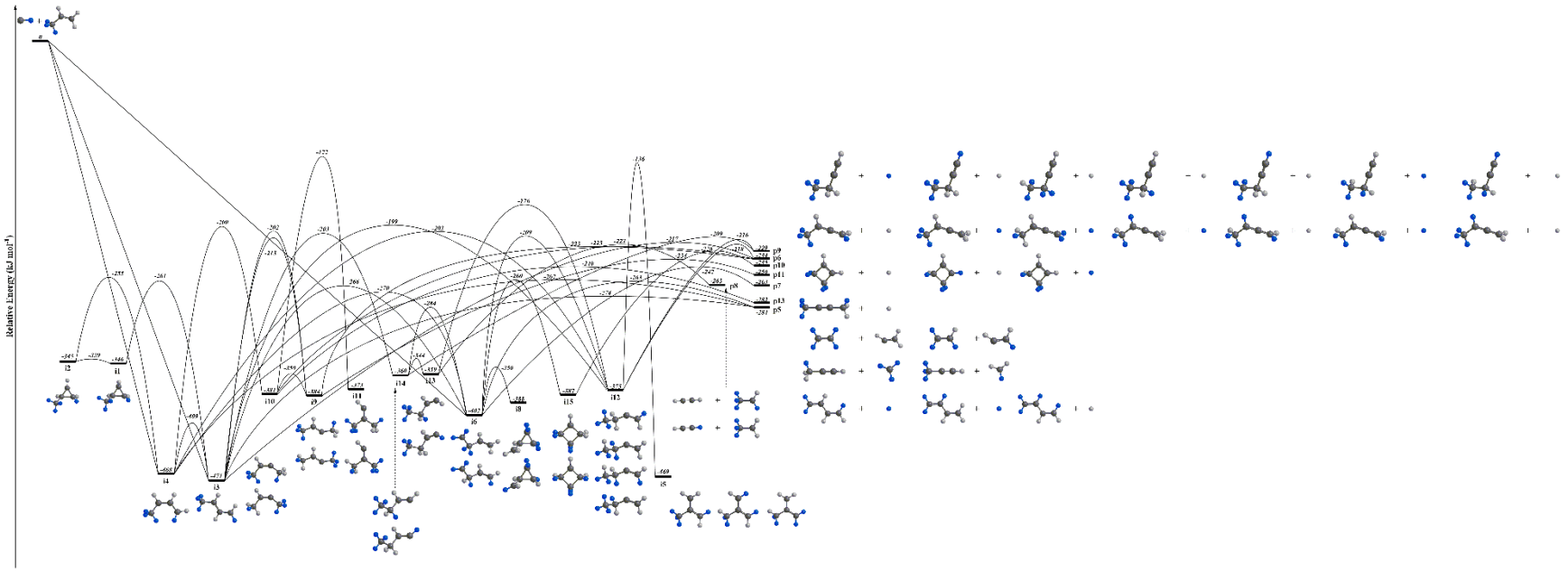

Figure S8. Portion of the $C_4D_4H_3$ PES corresponding to CD radical insertion into the terminal C-H/C-D bond of propylene-3,3,3-d_3. Energies are given for the fully hydrogenated reactant; energies of the (partially) deuterated species differ by a few kJ mol^{-1} at most.

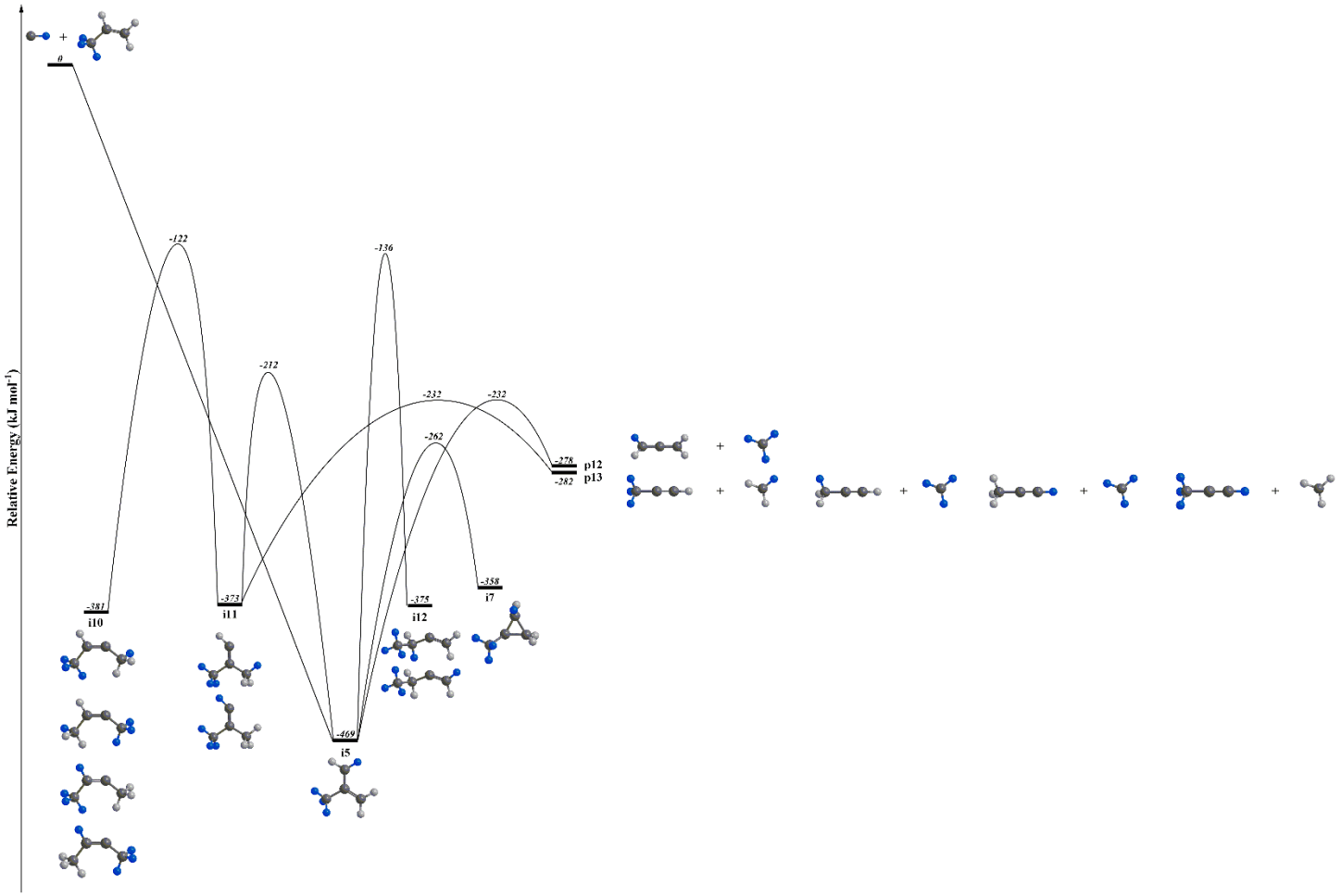

Figure S9. Portion of the $C_4D_4H_3$ PES corresponding to CD radical insertion into the middle C−H bond of propylene-3,3,3-d_3. Energies are given for the fully hydrogenated reactant; energies of the (partially) deuterated species differ by a few kJ mol^{-1} at most.