Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Formation of C_3H_2, C_5H_2, C_7H_2, and C_9H_2 from Reactions of CH, C_3H, C_5H, and C_7H Radicals with C_2H_2

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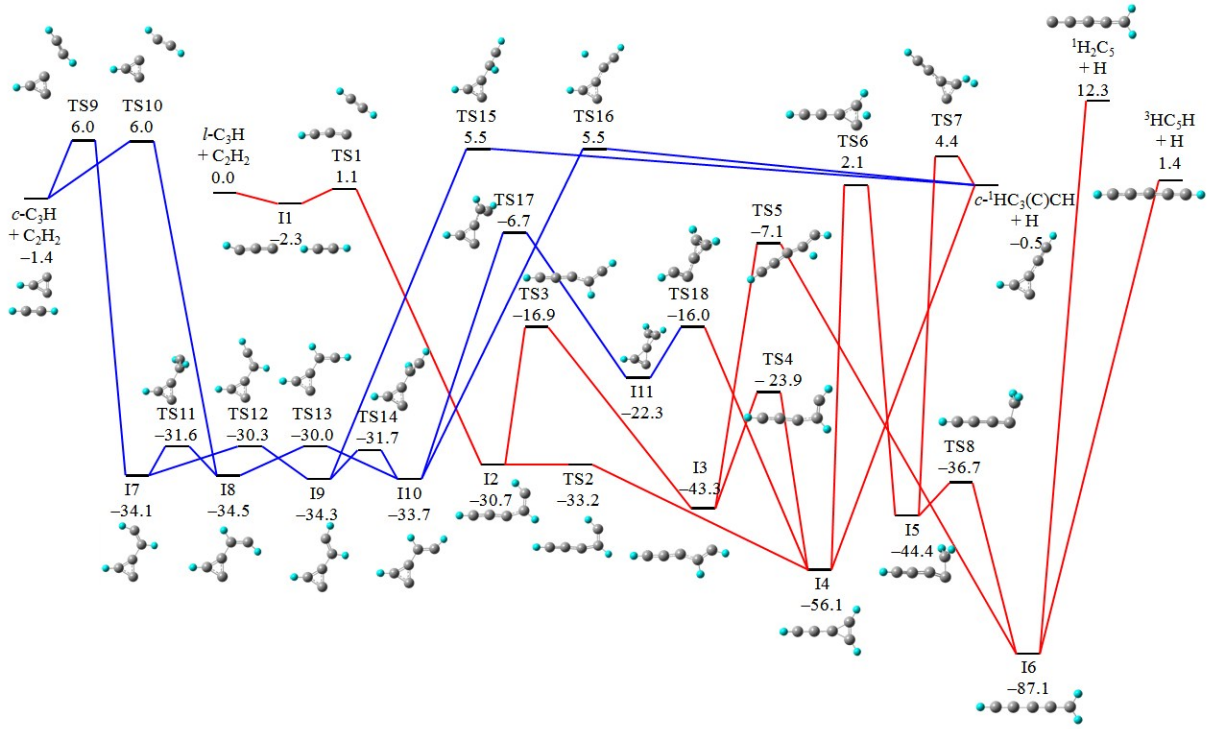

Figure S1. Potential-energy surface of the reaction $C_3H + C_2H_2 \rightarrow C_5H_2 + H$. The red (blue) line is for the linear (cyclic) C_3H reaction. The molecular structures are presented along with the corresponding potential-energy levels. The relative potential energies are given in kcal mol^{-1}. An intermediate is labeled with I# and a transition structure is labeled with TS#. TS2 lies above I2 at the B3LYP/aug-cc-pVDZ level but TS2 becomes below I2 at the level of CCSD(T)/aug-cc-pVTZ + ZPE, indicating that TS2 is negligible at the latter level of theory.

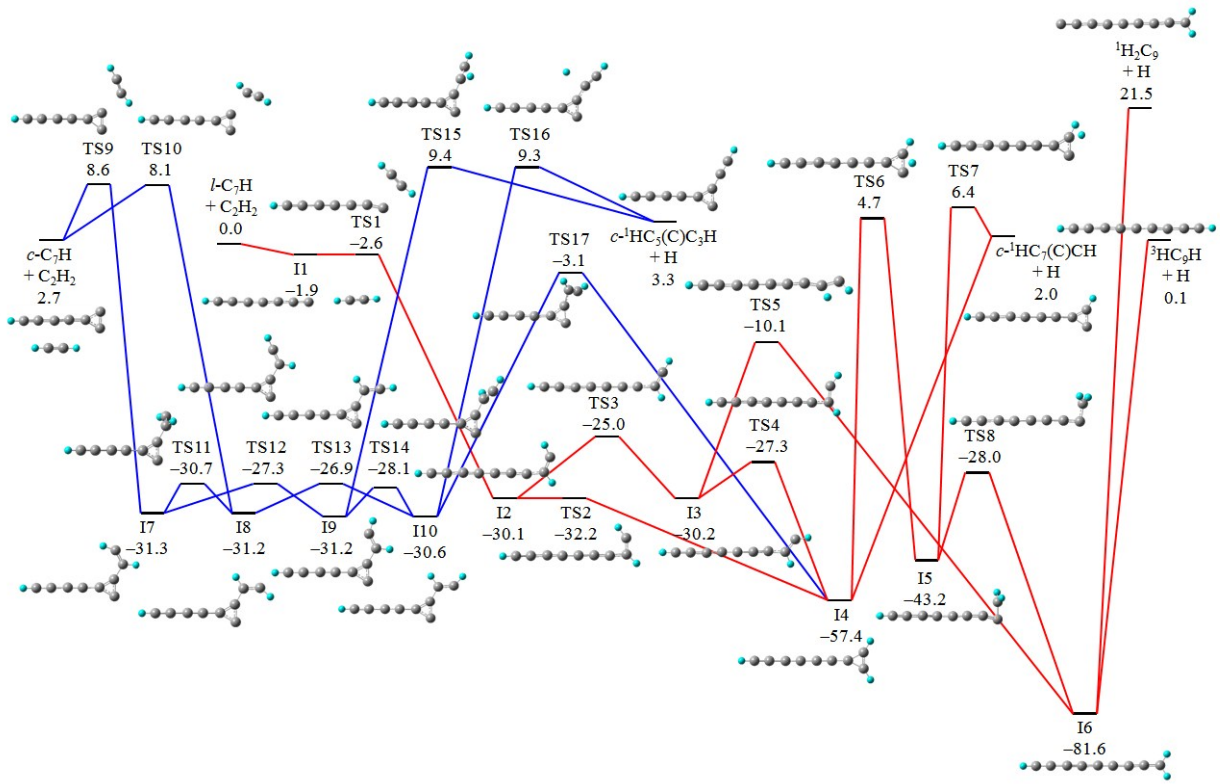

Figure S2. Potential-energy surface of the reaction $C_7H + C_2H_2 \rightarrow C_9H_2 + H$. The red (blue) line is for the linear (cyclic) C_7H reaction. The molecular structures are presented along with the corresponding potential-energy levels. The relative potential energies are given in kcal mol^{-1}. An intermediate is labeled with I# and a transition structure is labeled with TS#. TS1 (TS2) lies above I1 (I2) at the B3LYP/aug-cc-pVDZ level but TS1 (TS2) becomes below I1 (I2) at the level of CCSD(T)/aug-cc-pVTZ + ZPE, indicating that TS1 (TS2) is negligible at the latter level of theory. Compared with the $C_3H + C_2H_2$ (or $C_5H + C_2H_2$) reaction, I11 and TS18 cannot be optimized in the $C_7H + C_2H_2$ reaction. The calculation of intrinsic reaction coordinate (IRC) also confirms the absences of I11 and TS18 in the $C_7H + C_2H_2$ reaction.