

Figure 1. Elementary reactions of the 1-propynyl radical studied under single-collision conditions. [1] – 1-propynylallene is also formed at a ratio of dimethyldiacetylene versus 1‑propynylallene of 9 : 0.1. [2] – 1,3-heptadien-5-yne, 5-methylene-1,3-cyclohexadiene, 3-methylene-1-hexen-4-yne are also formed as minor products.

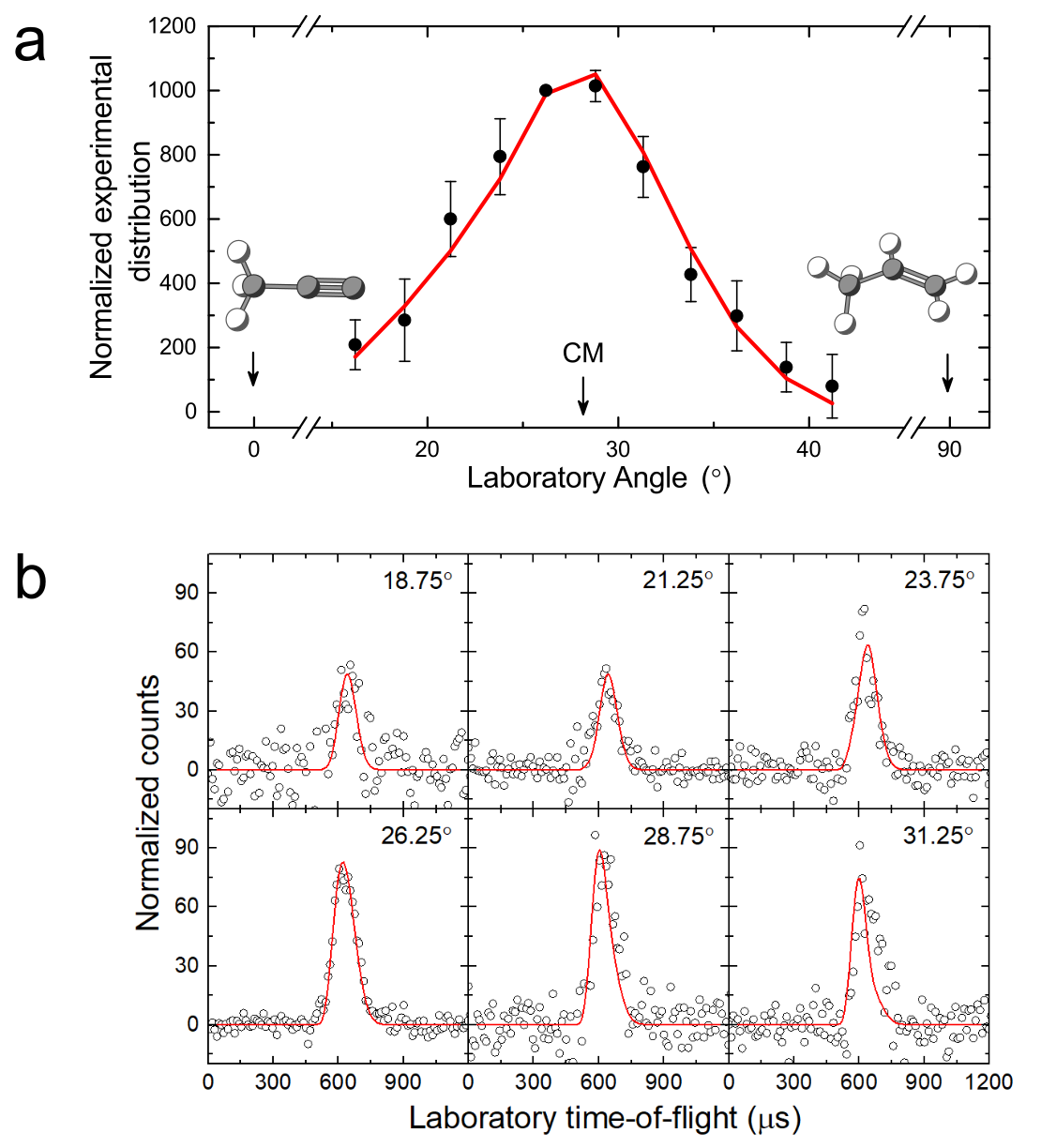


Figure 2. (a) Time-of-flight spectra and (b) laboratory angular distribution recorded at *m/z* 79 (C6H7+) for products formed in the reaction of the 1-propynyl radical with propylene. The circles represent the experimental data and the solid lines the best fit.

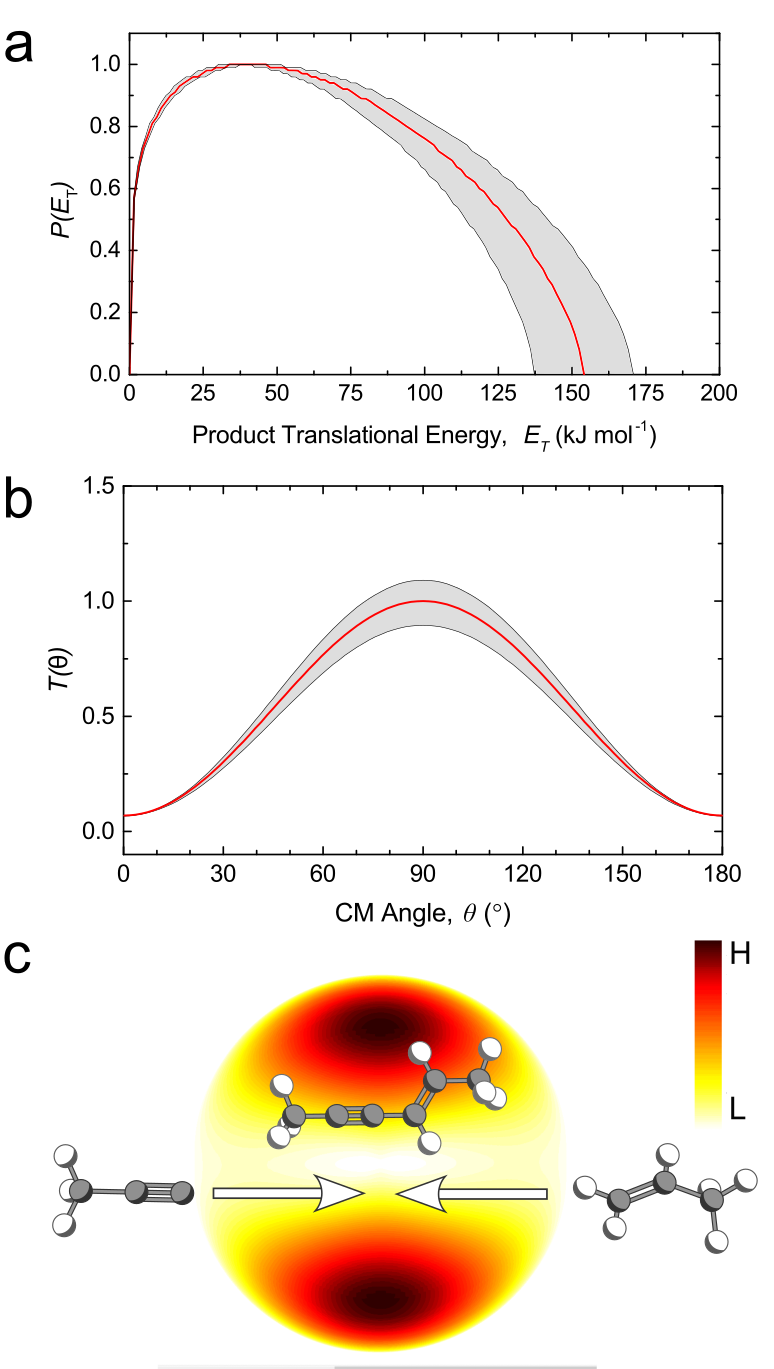


Figure 3. Center-of-mass translational energy (a), angular flux distribution (b), and corresponding flux contour map (c) for the formation of C6H8 plus atomic hydrogen via the reaction of the 1-propynyl radical (CH3CC;X2A1) with propylene (C3H6; X1A′). Grey-filled areas represent regions of acceptable fits.



Figure 4. Potential energy surface for the bimolecular reaction of the 1-propynyl (CH3CC; X2A1) radical with Propylene (CH3CHCH2, X1A′) leading to C6H8 plus H products.

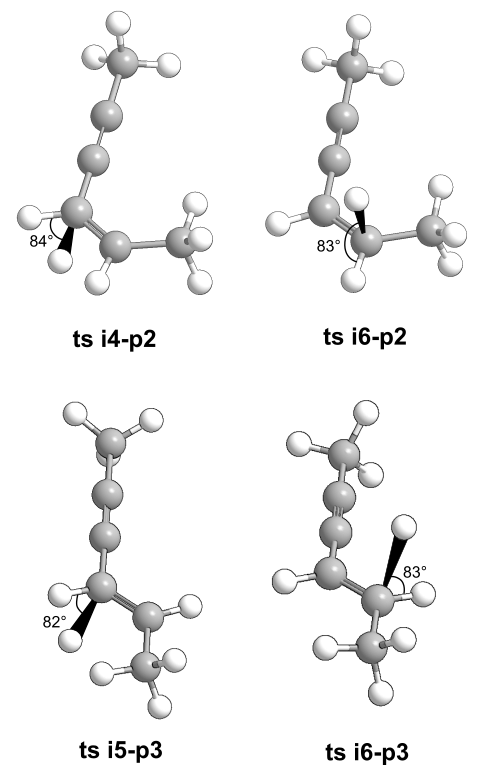


Figure 5. Computed geometries of the the exit transition states from **i4**, **i5**, and **i6** leading to formation of *cis* (**p2**)and *trans* (**p3**) isomers of hex-2-en-4-yne. The angle for each departing hydrogen atom is given with respect to to the rotation plane of the decomposing complex.

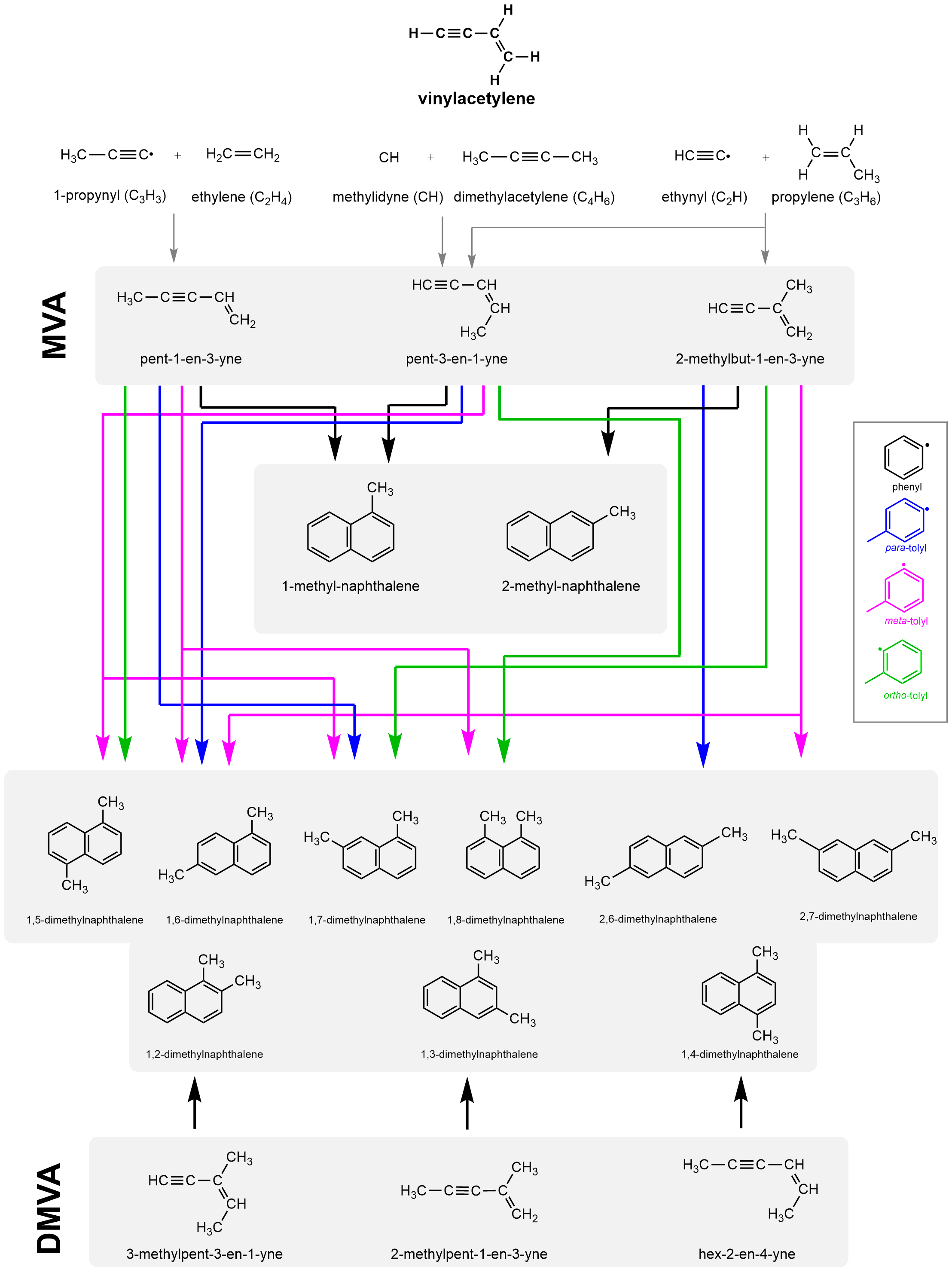


Figure 6. Reaction pathways leading to formation of methyl-substituted naphthalenes.