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Intramolecular CH_3-Migration-Controlled Cation Reactions in the VUV Photochemistry of 2-Methyl-3-Buten-2-ol Investigated by Synchrotron Photoionization Mass Spectrometry and Theoretical Calculations

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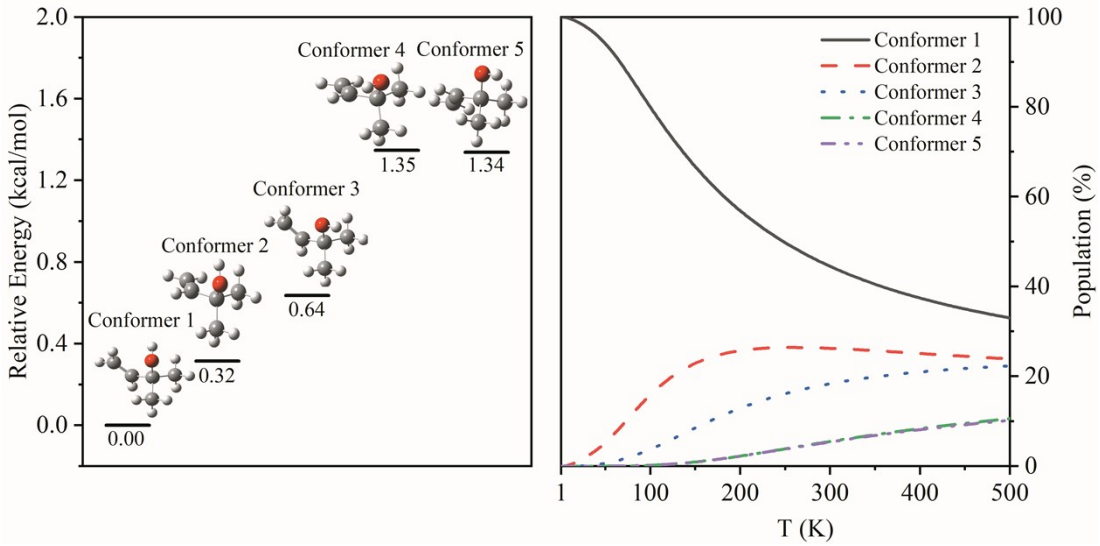

Figure S1. (a) Energies of five conformers of MBO232 calculated at the CCSD(T)/CBS//M06-2X/def2-TZVP level at 0K (zero-point energy corrected). The energies are relative energies to the lowest energy conformer (Conformer 1). (b) Boltzmann distribution probability of five conformers of MBO232 at 1–500K.

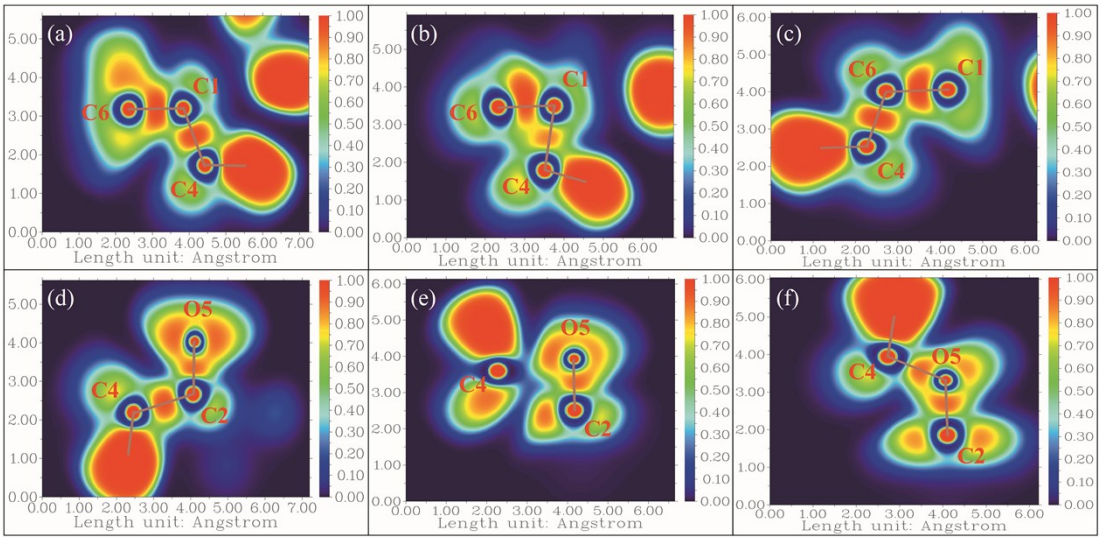

Figure S2. Color-filled maps of the electron localization function (ELF) in the molecular plane defined by the plane of the C4−C6=C1 for (a) INT1, (b) TS2 and (c) INT2, and the plane defined by the plane of the C4−O5−C2 for (d) cationic MBO232, (e) TS12 and (f) INT12. The ELF values [0–1] are mapped on a blue–green–red color scale indicated on the right of each representation. Blue and red colors indicate no electron and high electron localization, respectively.