4.074 Hydrogen Shift Reactions in four Methyl-Buten-Ol (MBO) Peroxy Radicals and its impact on the Atmosphere.

Early Career Scientist

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Abstract:

Methyl-buten-ol (MBO) molecules are emitted from many different natural sources. The most important biogenic emitted MBO is the 2-methyl-3-buten-2-ol (MBO232), with an estimated global emission around 1.6-2.2 Tg yr^{-1}. The oxidation of MBO232 produces secondary organic aerosols (SOA), when the NO concentration is low.
We investigate the possible hydrogen shift (H-shift) reactions in the peroxy radicals derived from four different MBOs; 2-Methyl-3-buten-2-ol (MBO232), 2-Methyl-3-buten-1-ol (MBO231), 3-Methyl-3-buten-2-ol (MBO332) and 3-Methyl-3-buten-1-ol (MBO331), with quantum mechanical calculations. The rate constants of the forward 1,5 H-shift reactions in all four MBO peroxy radicals are greater than the rate constant of the forward 1,4 or 1,6 H-shift reactions. The rate constants for the 1,5 H-shift reaction from a CH group or OH group are approximately 1 s^{-1} and 10^{-3} s^{-1}, respectively. The atmospheric impact of OH oxidation of MBO232 is investigated. The major atmospheric reactions of the MBO232 peroxy radical are the reactions with NO and HO_2, with reaction yield of 84 % and 12 %, respectively. The H-shift reactions of MBO232 peroxy radical play a minor role with a total yield of about 4 %.