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Atmospheric Reactions of a Series of Hexenols with OH Radical and Ozone

Yanbo Gai (1,2), Xiaoxiao Lin (1,2), Qiao Ma (1,2), Chengqiang Yang (1,2), Weixiong Zhao (1,2), Weijun Zhang (1,2,3)

(1) Key Laboratory of Atmospheric Composition and Optical Radiation, Anhui Institute of Optics and Fine Mechanics, Chinese Academy of Sciences, Hefei 230031, Anhui, China (wjzhang@aiofm.ac.cn), (2) Laboratory of Atmospheric Physico-Chemistry, Anhui Institute of Optics and Fine Mechanics, Chinese Academy of Sciences, Hefei, 230031, Anhui, China, (3) School of Environmental Science and Optoelectronic Technology, University of Science and Technology of China, Hefei, 230026, Anhui, China

C6 hexenols are one of the most significant groups of biogenic volatile organic compounds (BVOCs). Because of their antibacterial properties, C6 hexenols can be emitted by a wide number of plants in response to changes in the ambient environment. The oxidation of these compounds in the atmosphere is involved in the formation of tropospheric ozone and secondary organic aerosols (SOA), thus causing significant effects on atmospheric chemistry and the climate. The lack of corresponding kinetic parameters and product information of their oxidation reactions will result in incomplete atmospheric chemical mechanisms and models.

In this paper, we will overview our recent research progress on the study of the atmospheric reactions of a series of C6 hexenols with OH radicals and ozone. A series of studies were conducted using both experimental and theoretical methods. Corresponding rate constants were obtained, and reaction mechanisms were also analyzed. It could be concluded that both the nature of the substituent and its position play a fundamental role in the reactivity of the C6 hexenols toward OH radicals and O_3. An activating effect of the –OH group in OH radical reactions was found, thus making the H-abstraction channel non-negligible in reactions of these unsaturated alcohols with OH radicals. The removal of these C6 hexenols by ozone also showed great importance and could be competitive with the major recognized sinks by OH radicals. These studies are of great significance for understanding the mechanism of atmospheric chemical reactions of hexenols and improving the atmospheric chemistry model. Experimental detail and corresponding results will be presented.

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