



HKUST

Division of Environment

MPhil Thesis Presentation

Oligomeric products and formation mechanisms from acid-catalyzed reactions of methyl vinyl ketone on acidic sulfate particles

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Abstract

Methyl vinyl ketone (MVK) is a key first-generation product from atmospheric isoprene photo-oxidation, especially under high-NO_x conditions. In this work, acid-catalyzed reactions of gas-phase MVK with ammonium sulfate (AS), ammonium bisulfate (ABS), and sulfuric acid (SA) particles were investigated in a flow reaction system at relative humidity (RH) of 40% and 80%. Ultra-performance liquid chromatography with electrospray ionization time-of-flight mass spectrometry (UPLC/ESI-TOFMS) and gas chromatography-mass spectrometry (GC-MS) were utilized to identify particle-phase products for developing the reaction mechanisms. High-order oligomers were detected when ABS and SA particles were used, while no oligomeric products were found when AS particles were used. Particle-phase oligomeric products were formed via i) acid-catalyzed aldol reaction with or without dehydration and/or ii) acid-catalyzed hydration followed by oligomerization. Reactions on SA particles yield more abundant and higher-order oligomers up to hexamers than on ABS particles. Moreover, aldol reaction occurred only on SA particles, but hydration followed by oligomerization occurred in both ABS and SA particles. The high RH condition with the same type of acidic particles was found to favor hydration and facilitate the subsequent oligomerization, while the low RH condition with the same type of acidic particles was found to favor aldol reaction with dehydration (aldol condensation). Overall, the findings suggest acidic particles can facilitate the formation of high-order oligomers in the particle phase, with particle acidity and RH as key factors.

Date: 8 January 2013 (Tuesday)

Time: 3:00pm

Venue: Room 4475 (Lift 25-26), HKUST

~ All are welcome ~