Geophysical Research Abstracts, Vol. 9, 00813, 2007
SRef-ID: 1607-7962/gra/EGU2007-A-00813

Atmospheric chemistry of acetylacetone

Sh. Zhou(1,2), I. Barnes(2), T. Zhu(1), and Th. Benter(2)

(1) College of Environmental Sciences, Peking University, Beijing, China (2) Physikalische Chemie/FBC, Bergische Universitaet Wuppertal, Wuppertal, Germany
(barnes@uni-wuppertal.de / phone: +49-202-4392510)

The atmospheric chemistry of acetylacetone (AcAc, 2,4-pentadione) has been investigated by studying its reaction with OH, O_3 and Cl atom in a 405 liter Duran glass chamber at the University of Wuppertal, Germany.

A relative kinetic method has been applied to determine the rate constants for the reaction of AcAc with OH radical, ozone and Cl atom. The kinetic study on OH reaction with AcAc was also performed in 1080 l quartz chamber at University of Wuppertal. The obtained rate coefficient for OH radical reaction determined in both chambers were in good agreement and were considerably higher than the value reported earlier in the literature. The possible reason for this large discrepancy is given. Relative to ethene the rate constant for O_3 reaction with AcAc was determined. AcAc was found to react with molecular Cl_2 and very rapid with Cl atoms. The slow dark reaction of AcAc with Cl atom precluded an accurate measurement of the rate coefficient for Cl with AcAc. Using n-butane as reference an upper limit for the rate coefficient in air has been estimated.

Products from the OH radical, Cl atoms were investigated in 405 liter Duran glass chamber. In the reaction of OH with AcAc two products, i.e. methyl glyoxal and acetic acid were positively identified and quantified. Infrared analysis seems to indicate the formation of vicinal triketone 2,3,4-pentatrione and its hydrated analogue pentan-2,3-dione-4-diol are main products. The dark reaction of AcAc with molecular chlorine produces 3-chloroacetylacetone, HCl in considerable yield and 2,3,4-pentatrione. In AcAc/Cl_2/N_2 system acetyl chloride and HCl are major products, CO and 3-chloroacetylacetone are minor products and the remaining IR bands could be attributed to the formation of 2,3,4-pentatrione. In AcAc/Cl_2/air HCl, CO and 3-chloroacetylacetone are observed but these are much weaker than those observed in

N_2 and 2,3,4- pentatrione seems to be major product.

A simplified mechanisms for OH radical and Cl atom reactions with AcAc were postulated.