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Why is gas phase photolysis of 2-nitrophenol a significant source of OH in the polluted atmosphere?

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The significantly elevated day time nitrous acid (HONO) concentrations compared to those predicted based on the photochemical stationary state between HONO sources and sinks leads to postulate that HONO is produced by photochemical sources. One proposed HONO source is gas phase photolysis of 2-nitrophenol (o-$C_6H_4(NO_2)OH$) over the 300-500 nm region. 2-Nitrophenol is also an important component of brown carbon in the atmosphere. The concentration of 2-nitrophenol is expected to be high in polluted areas where there are increased emissions of aromatic hydrocarbons. To assess the air quality impacts of pollutant emissions, it is important to determine oxidant formation potential of the emitted species. Although photo dissociation dynamics studies of 2-nitrophenol have reported OH formation at photolysis wavelengths of 266 nm, 355 nm, and over the 361-390 nm range, and HONO was observed as a product from 2-nitrophenol photolysis in a smog chamber, the lack of quantitative absorption cross section and product quantum yield information has prevented quantitative assessment of the extent of oxidant formation from 2-nitrophenol photolysis in the atmosphere. The purpose of this study is to determine quantitatively the gas phase absorption cross sections of 2-nitrophenol over the 295-400 nm range, to investigate the HONO and OH formation channels following the 308 and 351 nm photolysis of 2-nitrophenol, and to obtain the OH and the HONO quantum yields. We have estimated the atmospheric oxidant formation rate constants following the gas phase photolysis of 2-nitrophenol using 2-nitrophenol near UV absorption cross sections, and OH and HONO formation quantum yields obtained from this study. Gas phase photolysis rate constant of 2-nitrophenol is about twice that of NO_2 and the sum of OH and HONO formation quantum yields are about unity at 308 nm and 351 nm. OH formation rate constant is fast from the gas phase photolysis of 2-nitrophenol. Recommendations are made to include gas phase 2-nitrophenol photolysis as a significant missing source of OH in the modeling of the chemistry of the polluted atmosphere.

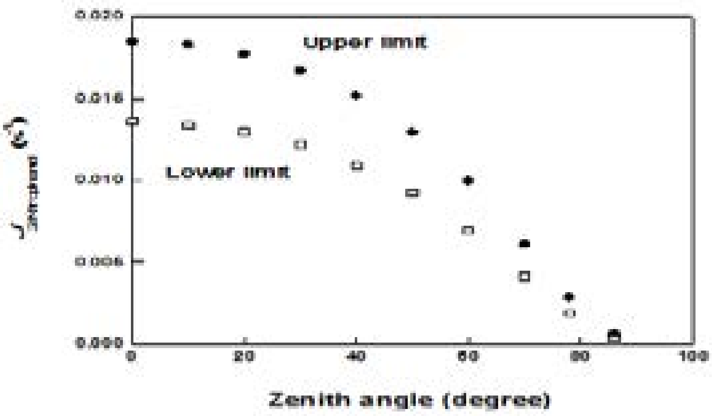

Figure 1: Modeled atmospheric photo dissociation rate constants of 2-nitrophenol as a function of solar zenith angle

Biography

Lei Zhu is a Research Scientist at Wadsworth Center, New York State Department of Health, and a Professor in the Department of Environmental Health Sciences at SUNY-Albany. His research program has been designed to investigate and understand what controls the atmosphere's energy balance and how chemical reactions impact composition, pollutant and oxidant formation in the earth's environment. Her research interests include "Kinetics and photochemistry of homogeneous and heterogeneous atmospheric reactions, atmospheric application of cavity ring-down spectroscopy and its variants, and atmospheric application of time-resolved FT-IR".

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