



Kinetic investigation of the unsaturated nitriles degradation initiated by OH reaction in atmospheric conditions

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Unsaturated nitriles are usually released from industries and also widely used in the production of plastics, nitrile rubbers, nitrile barrier resins, adiponitrile and acrylamide. Upon its formation this nitrile may decompose and produce poisonous gases like hydrogen cyanide. (1)

Other sources of unsaturated nitriles are minute traces in food packaging and accidental chemical spills. There are believed to be no significant natural sources. (2)

The release of these volatile organic compounds (VOCs) into the atmosphere is likely to contribute to the formation of ozone and other components of photochemical smog found in urban areas through their reactions with OH and NO₃ radicals as well as with O₃ and Cl atoms. In this work, we report rate coefficients for the reactions of OH radicals with (E)-3-pentenenitrile (k_1) and 4-pentenenitrile (k_2).



Relative rate constants were measured by comparing the OH radical reaction rate with the pentenenitriles to that butyl acrylate, 1,3-butadiene and isobutene used as the reference compounds. All the experiments were performed in synthetic air (296 \pm 3 K and 1010 mbar) in 1080 L quartz-glass photoreactor equipped with a White type multiple reflection mirror system operated at a total optical path length of (484.7 \pm 0.8) m coupled to an NEXUS FTIR spectrometer with a MCT detector. (3)

To the best of our knowledge this is the first experimental determination of the rate constants for these reactions. Kinetics data are used to estimate the tropospheric lifetimes for the unsaturated nitriles studied. Lifetimes of few hours were obtained for the OH-initiated degradation of the pentenenitriles indicating that these compounds will be oxidized close their anthropogenic sources indicating their importance in the photochemical smog production.

References

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