Atmospheric oxidation of N-PAC and nitro substituted N-PAC in water droplets

A pulse radiolysis technique was used to study the formation of OH-adducts of quinoline (Q) and 5-nitroquinoline (5NQ) and the subsequent reactions of the OH-adducts with O-2 in both acidic and alkaline aqueous solution. The rate constants in alkaline solution were: 
\[ k(Q+OH) = (9.0+/-1.0)\times10^9 \text{ dm}^3\text{mol}^{-1}\text{s}^{-1}, \]
\[ k(5NQ+OH) = (5.4+/-0.5)\times10^9 \text{ dm}^3\text{mol}^{-1}\text{s}^{-1}, \] 
\[ k(Q-OH+O_2) = (9.9+/-0.9)\times10^8 \text{ dm}^3\text{mol}^{-1}\text{s}^{-1}, \]
\[ k(5NQ-OH+O_2) = (1.1+/-0.1)\times10^6 \text{ dm}^3\text{mol}^{-1}\text{s}^{-1}. \]
The rate constants in acidic solution were: 
\[ k(Q+OH) = (4.0+/-0.5)\times10^9 \text{ dm}^3\text{mol}^{-1}\text{s}^{-1}, \]
\[ k(5NQ+OH) = (1.4+/-0.1)\times10^9 \text{ dm}^3\text{mol}^{-1}\text{s}^{-1}, \]
\[ k(Q-OH+O_2) = (9.9+/-0.9)\times10^8 \text{ dm}^3\text{mol}^{-1}\text{s}^{-1}, \]
\[ k(5NQ-OH+O_2) = (8.7+/-0.6)\times10^5 \text{ dm}^3\text{mol}^{-1}\text{s}^{-1}. \] Absorption spectra of the OH-adducts were also measured. The results suggest that the lifetime of quinoline and 5-nitroquinoline with respect to reaction with OH in water droplets in the atmosphere is less than 1 hour. It is estimated that the degradation of Q is accelerated in the presence of aqueous droplets with comparable contributions from aqueous and gas phase chemistry at neutral pH. Under acidic conditions the aqueous phase degradation is predicted to dominate. For 5NQ the aqueous phase degradation is predicted to dominate regardless of pH.

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