

pH-Dependent Antioxidant Capacities of N-acetylcysteine Aqueous Nanoaerosols Studied by Aerosol VUV Photoelectron Spectroscopy

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Abstract

N-Acetylcysteine (NAC) is a derivative of the natural amino acid *l*-cysteine. With its antioxidant capacity, NAC protects cell from oxidative damages and has been widely used to treat the chronic obstructive pulmonary disease (COPD) and chronic bronchitis. On the other hand, NAC can act as a precursor of reduced glutathione (GSH), which is the most prevalent antioxidant existing in the lung. To get new molecular insights into the antioxidant capacities and therapeutic efficacies of NAC and GSH, we applied the high-resolution aerosol valence photoelectron spectroscopy, using the undulator-based VUV radiation (BL21B2, NSRRC) to characterize the difference between NAC and GSH. The results showed that NAC and GSH aerosols with an average size ~ 100 nm exhibit distinct molecular orbital characters and ionization energies at varying pH, providing relevant information to further discuss the cellular redox state regulation *in-vivo*. This study unravels new molecular insights of the antioxidant abilities of GSH and NAC in the nano-scaled aqueous aerosol form, shedding new light in formulating aerosol medicines with optimized therapeutic efficacies for treating lung diseases that are induced or associated with excessive metabolic/pathogenic oxidative stress.

Keywords - N-Acetylcysteine (NAC), Reduced glutathione (GSH), Antioxidant capacity, Chronic obstructive pulmonary disease (COPD), Aerosols