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Molecular characteristics of water-soluble organics in atmospheric aqueous phase by Fourier transform ion cyclotron resonance mass spectrometry

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Atmospheric aqueous phase is an essential source and sink of organics and provides a medium for the reactions of dissolved gases and aerosols, which can substantially modify the characteristics of the organics. However, little is known regarding its molecular-level compositions. Herein, the molecular characteristics of water-soluble organic matter (WSOM) in fog samples, at Mt. Tianjing in southern China, were analyzed by Fourier transform ion cyclotron resonance mass spectrometry coupled with electrospray ionization (ESI) in negative mode. Thousands of formulas were identified in cloud water, in which CHON formulas were dominant in WSOM and exhibited the highest level of aromaticity, suggesting their enhanced aqueous phase formation. Other organics are mainly originate from biomass burning and oxidation of biogenic volatile organic compounds. The cloud water contains more abundant CHON (calculated by relative abundance fraction) at night, which are primarily contributed by $-N_2O_5$. The most important $-N_2O_5$ compounds, dinitrophenols and their derivatives exist abundantly in cloud water, especially at night, suggesting the contribution of radical nitration on N- containing organics. While more abundant CHO is observed during the daytime, likely due to the photochemical oxidation and photolysis of N- or S-containing formulas. Coupled with an Aethalometer, we also found that the aqueous-phase process can facilitate the formation of brown carbon (BrC), which may change the lifetime of the clouds and ultimately affect precipitation.