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Hygroscopicity of organic compounds as a function of organic functionality, water solubility, molecular weight and organic oxidation level

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Hygroscopic properties of 23 organic compounds with different physico-chemical properties including carboxylic acids, amino acids, sugars and sugar alcohols were measured using a Hygroscopicity Tandem Differential Mobility Analyzer (HTDMA). We converted our experimental GF data of organics at 90% RH to κ to facilitate the comparison and we find that organic compounds with different molecular functionality present quite different hygroscopicity. Compounds with extra functional groups usually show higher hygroscopicity compared to their parental molecular compounds. Moreover, some compounds share the same molecular structure or functionality but vary differently in hygroscopicity. In general, the hygroscopicity of organics increase with functional groups in the following order: (-CH3/-NH2) < (-OH) < (-COOH/C=C/C=O). For highly soluble organics, the hygroscopicity decreases with molecular weight; while for slightly soluble organics which are not fully dissolved in aerosol droplets, their hygroscopicity can be divided into two categories. One is non-hygroscopic compounds, which may not fully deliquesce in the aerosol droplets. The other is moderate hygroscopic compounds, of which the hygroscopicity is mainly limited by their water solubility. Moreover, the hygroscopicity of organic compounds generally increased linearly with O:C ratios, although some of them have the same O:C ratio of but with different hygroscopicity. The experimental determined hygroscopicity are also compared with model predictions using the Extended Aerosol Inorganics Model (E-AIM) and the UManSysProp at 10-90% RH. Both models poorly represent the hygroscopic behavior of some organics, which may due to that the phase transition and intermolecular interactions are not considered in the simulations.