Modelling the physical states of aqueous solution containing mixed organic/inorganic electrolytes and dicarboxylic acids

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Abstrak

We suggest a chemical model for the composition and atmospheric processing of mixed organic-inorganic aerosol. The PITZER model
was modified and parameterized to better
describe atmospheric relevant conditions and mixture compositions. Using the wide range of data for the following systems containing malonic acid (H2Malo): H+? Na+? HMalo-? Cl-?H2Malo ? H2O and H2Malo ? H2SO4? H2O. With these modifications the activities of inorganic
salt solutions and acids are well represented up to high ionic strength. The first model is a result of mixtures containing NaCl, water and either malonic acid, succinic, oxalic, glutaric or adipic
at room temperature. The parameterization of direct inorganic/organic
interactions strongly improves the agreement between experimental
and modelled activity coefficients for the
diacids/ water/ salt solutions. The system compositions are given in terms of ions in the cases where acid dissociation was considered. Tropospheric aerosols contain a mixture of inorganic
salts, acids, water and organic compounds. An
interaction between neutral or charged components in such a mixture leads to discrepancies from ideal thermodynamic behavior.
Using component activities instead of molar concentrations one can co
unt for this non idea behavior.