

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 (H_2Malo): H^+ ? Na^+ ? HMalo^- ? Cl^- ? H_2Malo ? H_2O and H_2Malo ? H_2SO_4 ? H_2O . 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 count for this non ideal behavior.