Surface/bulk partitioning and acid/base speciation of aqueous decanoate: Direct observations and atmospheric implications

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Aqueous sample preparation. The aqueous samples were prepared immediately before each XPS experiment. A binary stem solution was prepared by dissolving DecNa in MilliQ water (18.2 MΩcm resistivity). The solid powder dissolved within a minute to form a clear solution. We are therefore confident that the binary solutions were below the decanoate aqueous solubility limit. The stem solution was subsequently divided into individual samples, and ternary mixed DecNa–inorganic salt solutions were prepared by adding the solid inorganic salt to the appropriate binary samples. The inorganic salts also dissolved readily to form clear ternary solutions, however, upon addition to the more concentrated (25 mM DecNa) binary solutions, it was necessary to shake the sample to ensure rapid dissolution. These ternary samples may therefore be close to the solubility limit of the organic. In determining the yielded molar concentrations, is assumed that the inorganic does not increase solution volume upon dissolution (zero mixing volume, or negative excess mixing volume cancelling the added inorganic volume). The remainder of the stem solution was then kept as the binary solution sample.

Even very small amounts of impurities may dramatically affect the surfactant adsorption properties. Therefore, great care was taken to avoid contamination during preparation of the samples. All glassware was carefully cleaned and handled with clean protective latex gloves and samples were kept under lid as consistently as possible. Futhermore, prior to measuring, each sample was filtered (Whatman Puradisc FP30 syringe filters, 1.2 μm) to remove dust and potential precipitates invisible to the naked eye, and sonicated (VWR ultrasonic cleaner) to remove air bubbles, all of which may disturb the flow in the liquid jet and cause the injection system to fail.