Interactive comment on “New and extended parameterization of the thermodynamic model AIOMFAC: calculation of activity coefficients for organic-inorganic mixtures containing carboxyl, hydroxyl, carbonyl, ether, ester, alkenyl, alkyl, and aromatic functional groups” by A. Zuend et al.

Anonymous Referee #2

Received and published: 26 July 2011

This paper presents important advances in the thermodynamic model AIOMFAC for estimating activity coefficients in mixed organic-inorganic aerosol systems. The authors should be commended for this huge undertaking. The paper is very well written and the graphs and tables are of excellent quality. I recommend publication in ACP.

General Comments: It is not readily apparent after reading the paper how big the differences are in the activity coefficients of inorganics and organics due to non-ideal behaviour in mixtures. In other words, how much error would one introduce in say the solid-liquid equilibrium of inorganic salts in the presence of some organics by ignoring any changes in the activity coefficients in the mixture compared to their binary values? Can the authors please show 2-3 examples to illustrate the importance of organic-inorganic interactions?

Recent experimental studies (Vaden et al., 2011; Virtanen et al., 2010) indicate that biogenic SOA is in an amorphous solid state and does not readily evaporate upon dilution. These results have challenged the traditional views of the kinetics and thermodynamics of SOA formation (gas-particle partitioning and particle phase state). Can the authors please comment if a comprehensive model such as AIOMFAC can reproduce these behaviors, or is it still quite a ways from addressing these issues.


Minor Comment: Abstract, Line 4: Replace “room temperature” with a number (e.g., 25 C).