Hydrogen bonding in aqueous solutions of sulfuric and methanesulfonic acids: a computer simulation study

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Abstract

One of the current research topics in atmospheric physics is the study of the influence of sulphate aerosols in the atmospheric dynamics; particularly, in the acid rain or in the greenhouse effect. In many cases these aerosols are aqueous clusters of ionized sulfuric or methanesulfonic acids [1]. In the present study, we have performed a series of molecular dynamics simulations of aqueous solutions of sulfuric [2,3] and methanesulfonic [4] acids at different concentrations and temperatures. The dissociation of the acids has been explicitly considered. Calculations have been conducted using reliable force fields, with scaled ionic charges, which allow us to determine density and viscosity values in good agreement with available experimental data. A hydrogen bond analysis, involving only water molecules, has been carried out. To this end, the mean number of hydrogen bonds between water molecules and between ions and water molecules, the percentages of molecular species hydrogen bonded with a given number of water molecules, and the continuous and interrupted lifetimes have been calculated. We have observed that water molecules bonded to the anions are more labile than those bonded to other water molecules or to hydronium ions, the labilities increasing when the temperature rises. Moreover, the characteristic tetrahedral structure of water vanishes when the concentration or the temperatures increases.

REFERENCES

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[3] M. Canales, E. Guardia, J. Mol. Liq. 347 (2022) 118351.
[4] M. Canales, E. Guardia, *to be submited* (2022).

FIGURES

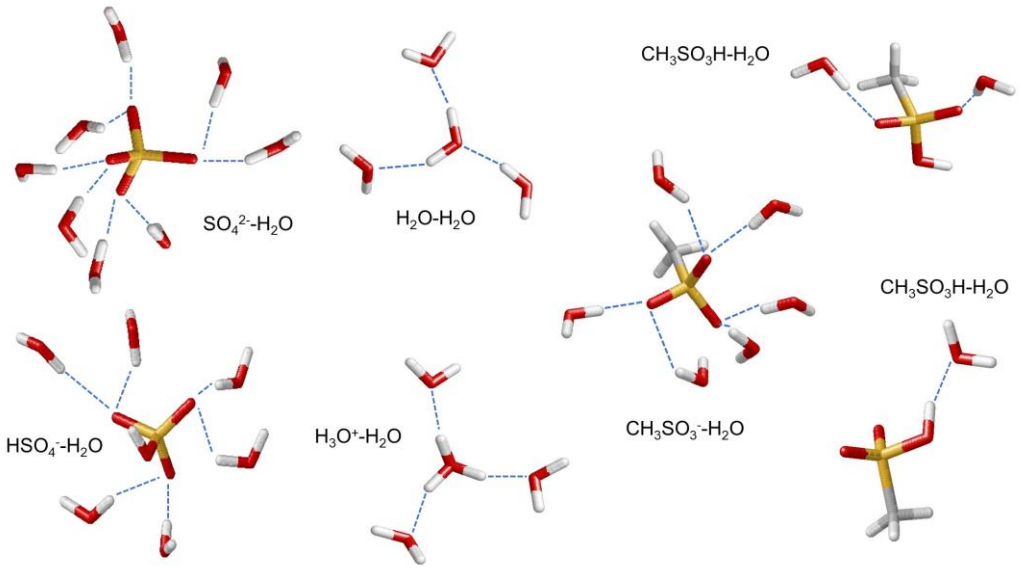

Figure 1: Representative snapshots of ion-water and water-water hydrogen bonds