The solvent effect on the hydrogen bond of a neutral complex (^{-}OH, H_3O^{+}) molecular dynamics of the simulations water

F.Benyettou[1*], S.Hiadsi[2], A.Bendraoua[2].

[1,2]Chemistry Department, University of Mohamed Boudiaf, USTO -BP 1505 El Mnaouer -ORAN –Algeria
[1]Applied Hydrology Laboratory-department science technology -University Ain Temouchent, Bellabes Sidi Road, PO Box 284 Ain Temouchent (46000) Algeria.
*Email leau_lautoprotolyse@yahoo.fr

In recent years, molecular dynamics simulations on water-based deep eutectic solvents (DES) have increased. Most of these studies highlight the fact that to faithfully reproduce the dynamic properties of the latter using an atomic force field (TIP3P, Mulliken and SPC / E) at a fixed charge, it is necessary to resort to updating. scale of the load. In this work, we propose an alternative to the scaling of the charges on the complex (^{-}OH, H_3O^{+}) and show that the only refinement of the LENNARD-JONES parameters of oxygen and hydrogen of the hydroxyl function in TIP3P and SPC / E, allows an accurate description of the static, dynamic and structural property parameters of two commonly used DES. Various physicochemical properties calculated for mixtures with our modified version of TIP3P and SPC / E are in good agreement with the experimental data. Finally, the calculated radial distribution functions correspond to those reported in the literature.

Keywords: Water ; the hydrogen bond ; TIP3P ; SPC / E ; molecular dynamics.