

Solvation of divalent ions in organic solvents

Orekhov M A^{1,2,3}

¹ National Research University Higher School of Economics, Myasnitskaya 20, Moscow 101000, Russia

² Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

³ Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141701, Russia

mo2411@mail.ru

Molecular dynamics simulation of divalent ion solvation in organic solvents is carried out. Various liquids are considered as solvents. It is shown that solvent molecules are bound to ions via oxygen atoms. As a consequence ion coordination number is weakly dependent on the solvent. A theoretical model of the ion solvation in organic solvent is developed and tested. It is in a good agreement with results of the molecular dynamics.

This work is an output of a research project implemented as part of the Basic Research Program at the National Research University Higher School of Economics (HSE University).