INTERACTION OF DIMETHYLIMIDAZOLIUM CHLORIDE WITH WATER MOLECULE AT $T=400~{\rm K}$

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Summary

The work presents data on the structure and the energy characteristics in the case of the interaction of a water molecule with dimethylimidazolium chloride $(\dim m^+/CL^-)$ at the temperature T = 400 K calculated using the molecular dynamics method. We established the existence of hydrogen bonds between a water molecule and molecules of dimethylimidazolium $(\dim m^+)$ and chlorine (CL^-) and determined the orientation position of the water molecule with respect to those of chlorine and dimethylimidazolium.