Energy and size distribution of $(H_2O)_n$ and $H^+(H_2O)_n$ clusters

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Hydrated ions and water clusters play an essential role in the physics and chemistry of the atmosphere [1]. In this work, the structures and thermodynamic characteristics of $(H_2O)_n$ and $H^+(H_2O)_n$ clusters were studied theoretically. The clusters of size $n \leq 30$ were investigated using the GFN2-XTB method [2].

The results of numerical calculations were used to parameterize the analytical dependence of the cluster energies on their sizes. The data obtained using quantum chemical modeling for $(H_2O)_n$ and $H^+(H_2O)_n$ are well approximated by the analytical functions, which indicates a qualitative agreement between the analytical and numerical models. Comparison of the model parameters with the reference data also indicates a reasonable accuracy of the analytical approximation. Comparison of the calculated size distribution of $H^+(H_2O)_n$ clusters with the experimental data from [3] also supports the proposed model.

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