

Quantum-chemical modeling of the hydroxide ion gas-phase adsorption on IB metal clusters Me_n ($n = 2-8$)

© Alexander A. Doroshenko,⁺ Igor V. Nechaev, and Alexander V. Vvedensky*

Department of Physical Chemistry. Voronezh State University. Universitetskaya sq., 1.
Voronezh, 394006. Russia. Phone: +7 (473) 220-85-46. E-mail: doroshenko@chem.vsu.ru

*Supervising author; ⁺Corresponding author

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Abstract

The gas-phase adsorption of hydroxide ion on small IB-metals clusters simulation has been carried out within the framework of the density functional theory. The enthalpies and Gibbs energy of metal-cluster interaction was calculated. Similarities in geometry and charge states of the adsorbed OH-radical and OH-anion were revealed. The analysis of the vibrational spectra of adsorption complexes was carried out. It was established that the hydroxide ion is chemisorbed on small IB-metals clusters on top or in bridge position. It was shown that the OH bond frequency of adsorbed OH-ion is increased relative to the corresponding values in the isolated state, while the intensity of the oscillations is considerably reduced.