

Pseudopotential calculations on the ground state of the alkaline-earth monohydride ions

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The ground state potential energy curves of alkaline-earth monohydride ions have been investigated. A pseudopotential formalism including a corepolarization potential has been used. For the valence correlation energy a local spin density functional with corrections for self interaction has been employed. Dissociation energies, bond lengths and vibrational frequencies are reported, and so are the vertical and adiabatic ionization potentials of the alkali and alkaline-earth monohydrides, which were obtained using the same theoretical model. A discussion and a comparison with other values, both theoretical and experimental, are also included. © 1987 Taylor & Francis Group, LLC.