POTENTIAL ENERGY SURFACES OF THE GROUND AND EXCITED STATES OF ^{11}BH MOLECULE IN THE MULTIREFERENCE COUPLED CLUSTER THEORY

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S u m m a r y

The multireference state-specific coupled cluster theory is used for the calculation of the potential energy surfaces (PES) of ^{11}BH molecule in the ground and excited states. The PESs are approximated by a number of analytical functions generalizing the Morse potential. The solution of a radial Schrödinger equation and the values of spectroscopic constants depending on the accuracy of the PES approximation are analyzed.