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A new analytical potential energy surface for (H2+)He cluster

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We present a new potential energy surface (PES) for the interaction between the Hydrogen molecule ion and the Helium atom in its electronic ground state. The PES of (H2+)He cluster is represented by two contributions: a polarization energy term due to the electric field generated by the molecular cation in the position of the polarizable He atom and dispersion-repulsion forces characterized by an "atom-bond" potential between the bond of H2+ and the He atom. All parameters of this new PES have been chosen and fitted from post Hartree-Fock calculations at CCSD(T) level and performed with the NWCHEM Quantum Chemistry Software. By assuming pair-wise interactions and considering the Azis-Slaman potential for the interaction between Helium atoms, we define a PES for H2+(He)N clusters and study their energetic and structural properties employing classical and quantum
simulations.

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