Quantum chemical computations of argon carbides in the gas phase

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The demand for accurate data regarding the energy structure of argon carbides is primarily driven by the applications of Inductively Coupled Plasma Mass Spectrometry (ICP-MS) and thermodynamic modeling involving argon-containing ions to resolve the equilibrium state of complex mixtures. Furthermore, such data are essential for subsequent studies aimed at determining the thermodynamic and transport properties of argon-carbon plasmas [1]. These results may also be relevant for specific problems utilizing the low reactivity of argon to model fluid flow through carbon-based structures [2].
This study presents quantum-chemical calculations for the ArC^+ molecule, along with a comparison of the calculated potential energy curves (PECs) with experimental data reported in [3]. The simulations were performed using the ORCA software package [4] employing the multireference configuration interaction (MRCI) method. Results were obtained for several basis sets, followed by extrapolation to the complete basis set (CBS) limit.
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