Quantum-chemical computation and thermodynamic functions of argon fluorides in the gas phase

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Argon fluorides are among the argon-containing ions observed in inductively coupled plasma mass spectrometry (ICP-MS) with argon plasma sources. To estimate the errors introduced by these ions into mass spectrometric measurements, it is necessary to know their thermodynamic properties. In previous studies, thermodynamic functions were calculated for several argides [1–4].

This work presents the potential energy curves of interatomic interactions for ArF and ArF^+ molecules, computed using various basis sets. The computations were performed with the ORCA software package [5] using the multireference configuration interaction (MRCI) method. Based on these results, the corresponding thermodynamic functions were calculated using the developed web application "GasThermo".

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