Quantum chemical study of the interatomic interaction of ArN^+

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Argon is often used as a buffer gas for the inductively coupled plasma mass spectrometry (ICP-MS). However, given the high density of argon in the ICP-MS experiments it can interact with the other plasma components forming argides. Even a small fraction of argide can significantly affect the mass spectra obtained due to its signal overlapping with the ones coming from the studied substances [1]. Positively charged argon nitride (ArN^+) is one of the most common argide in ICP-MS experiments. To quantify the prevalence of this argide in plasma, thermodynamic data are needed. The calculation of the thermodynamic functions of diatomic molecules is based typically on the use of molecular constants. However, this method can be improved via using the interatomic potentials obtained from the quantum chemistry methods [2,3]. Here we report the results of the quantum chemistry calculations of ArN^+ interatomic potential for the low-lying triplet and singlet electronic states. The MRCI (multireference configuration interaction) method has been employed. The spin–orbit and spin–spin interactions have been accounting for. The potential energy curves have been compared with other computational results reported in the literature. Using these interatomic potentials, the Shrödinger equation has been solved numerically to get the rovibronic partition function. Finally, the thermodynamic properties have been obtained for the ArN^+ species in the gas phase.

[1] Witte T M and Houk R S 2012 *Spectrochim. Acta, Part B* **69** 25–31

[2] Maltsev M A, Morozov I V and Osina E L 2020 *High Temp.* **58** 184–189

[3] Maltsev M A, Morozov I V and Osina E L 2021 *J. Phys.: Conf. Ser.* **1787** 012009