THERMODYNAMIC PROPERTIES OF DIATOMIC ARGON COMPOUNDS

Maltsev M.A.,[*1,2] ***Morozov I.V.,***[1] ***Osina E.L.***[1]

[1] *JIHT RAS, Moscow, Russia,* [2] *MIPT, Dolgoprudny, Russia*

[*] *maksim.malcev@phystech.edu*

The diatomic argon compounds are of importance for different plasma sources that contain argon as a basic gas. One of these applications is the mass spectrometry with inductively coupled plasma (ICP-MS). In such experiments the signals from the argon compounds can disturb measured spectra significantly. Therefore for accurate processing of the ICP-MS results it is necessary to obtain the thermodynamic functions of the compounds of argon with other gases (H, O, etc.) and metal ions. It allows to estimate concentrations of the these compounds in the ICP-MS plasma.

In this work we report on thermodynamic properties of the following substances: ArV^+, $ArCo^+$, ArAr, $ArAr^+$, ArH and ArH^+. As a starting point we use DFT and quantum-chemistry data to find an appropriate model for the interatomic interaction potential. Then the rovibronic spectra is obtained via numerical solution of the Schrödinger equation [1] for each electronic state that contribute to the total internal partition function. The thermodynamic properties are calculated from the partition function within the ideal gas approximation using developed program that described in [2]. This method differs from the typical approach based on the use of molecular constants. Thermodynamic functions are prepared for importing into IVTANTHERMO database [3].

---

1. Le Roy R.J. A Computer program for solving the radial Shroedinger equation for bound and quasibound levels // J. Quant. Spectrosc. Radiat. Transfer. 2016. V. 186. P. 167.
2. Maltsev M.A., Kulikov A.N., Morozov I.V. Thermodynamic properties of vanadium and cobalt argide ions, VAR^+ and $CoAr^+$ // Journal Conference Series. 2016. V. 774. P. 012023
3. Belov G.V., Dyachkov S.A., Levashov P.R. et al. The IVTANTHERMO-Online database for thermodynamic properties of individual substances with web interface // J. Phys. Conf. Ser. 2018. V. 946 P. 012120.