Thermodynamic function calculation for ideal gases using the "GasThermo" web application

Maltsev M.A.[1,2,@], **Kravchenko A.V.**[1,2] **and Shcherba A.A.**[1,2]

[1] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, 141701, Russia
[2] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow, 125412, Russia

[@] maksim.malcev@phystech.edu

Inductively coupled plasma mass spectrometry (ICP-MS) is a highly sensitive analytical technique that plays a pivotal role in detecting and quantifying trace elements and isotopes in complex samples. Its precision and versatility make it indispensable across various fields, including environmental monitoring, clinical diagnostics, and materials science.

A critical challenge in ICP-MS analysis is the interference caused by background ions, which can hinder the accurate detection of target analytes and reduce the overall sensitivity of the method. Addressing this issue is essential for ensuring reliable results, particularly when analyzing samples with complex matrices.

This work introduces a set of web applications, collectively referred to as "GasThermo", designed to calculate the thermodynamic functions of diatomic gases using quantum chemical methods. These applications provide valuable insights into the molecular interactions of atoms, aiding in the evaluation of plasma environments.

As part of this study, argon nitrides (species commonly formed in inductively coupled plasma during the analysis of organic substances) were investigated. "GasThermo" contributes to a broader suite of tools aimed at assessing the impact of background ions on ICP-MS performance, offering researchers enhanced capabilities for tackling this significant analytical challenge.

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