GasThermo - web application for computations thermodynamic properties of diatomic ideal gases

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Databases on the thermodynamic properties of substances play an essential role in solving engineering problems, which require thermodynamic modeling. To maintain the relevance of thermodynamic databases, the information in them must be regularly updated and supplemented. This requires the development of modern software that include new ab initio methods that allow for obtaining results for substances that are difficult to study experimentally.
This work aims to solve two main problems by developing a new web application GasThermo. The first is to provide modern software solutions for updating thermodynamic databases and in particular the information system IVTANTHERMO [1]. And the second is to develop tools to estimate the errors introduced by background ions in inductively coupled plasma mass spectrometry (ICP-MS) [2].
GasThermo is a set of web applications, which provide tools for calculation thermodynamic functions of diatomic ideal gases based on traditional molecular constants or potential energy curves of interatomic interactions (which can be obtained using ab initio quantum chemical computations). Also GasThermo has models aimed at assessing the impact of background ions on ICP-MS by thermodynamic modeling. The data for thermodynamic modeling will be taken from the application itself and also from IVTANTHERMO.
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[1] Belov G V and et al 2018 *J. Phys. Conf. Ser.* **946** 012120
[2] Pupyshev A A and et al 2025 *Journal of Analytical Chemistry* **80** 864 – 876