"GasThermo" code for calculation of thermodynamic functions of diatomic ideal gases

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The determination of thermodynamic functions of diatomic gases holds critical importance within the realm of physical chemistry, playing a key role in comprehending chemical thermodynamics and reactions. An example where such thermodynamic functions are necessary is the calculation of the equilibrium composition of inductively coupled plasma, taking into account diatomic argide ions [1–3]. In order to obtain more accurate thermodynamic functions of diatomic ions and molecules it is necessary to consider quasi-bound energy levels and ascertain the spectrum derived from complicated potentials of interatomic interaction. In order to carry out these computations, it is imperative to utilize a software application that features a user interface of intuitive design.

In this work we present the GasThermo software package that enables the calculation of thermodynamic properties of diatomic molecules, based on the potential of interatomic interactions. The program is capable of approximating potential curves derived either experimentally or via quantum chemistry techniques, and performs the computation of the vibrational-rotational spectrum of molecules while including quasi-bound states. Additional features of the software also allow the computation of thermodynamic functions of diatomic molecules and the determination of the equilibrium compositions of various thermodynamic systems.

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[2] Maltsev M A, Morozov I V and Osina E L 2019 *High Temp.* **57** 335–337
[3] Maltsev M A, Morozov I V and Osina E L 2020 *High Temp.* **58** 184–189