Web application for computation of rovibronic spectrum from potential energy curves

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Equilibrium thermodynamic modeling serves as an instrumental method for examining the composition of a low-temperature plasma. For execution of this methodology, a comprehensive understanding of the thermodynamic functions of all molecular structures and ions constituting the system under scrutiny is requisite. A pivotal step in the calculation of these thermodynamic functions involves the determination of the rovibronic spectrum of the molecules. Calculations of the rovibronic spectrum for argides were carried out in the works [1–4]. They demonstrated that for a more accurate calculation, it is necessary to take into account quasi-bound energy levels and determine the spectrum for complex potentials of interatomic interaction. To execute this computations, it is essential to deploy a software application equipped with an intuitive user interface. This study unveils a novel algorithm designed to accomplish the entire process of determining the rovibronic spectrum of diatomic molecule, commencing with the entry of data in a user-friendly format, concurrently confirming the arrived values, and concluding with the display and portrayal of results. The cultivated web application, constructed through Django and Vue.js frameworks, is envisaged to be incorporated into the existing GasThermo software suite.

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