Thermodynamic properties of diatomic gases from quantum chemistry

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Thermodynamic databases are at the heart of different engineering challenges, such as designing rocket engines and new materials with special properties, chemical engineering, metallurgy, mining, waste processing, etc. Updating these databases can be performed using both new experimental results and contemporary quantum chemistry methods. The computational methods become more essential for the molecules that cannot be studied experimentally due to their short living times and extreme conditions. A particular example of such system is the formation of argon diatomic molecules in plasma at elevated temperatures. Previously, electronic states were studied and thermodynamic functions were calculated for a number of such compounds [1–4]. However, in these studies we relied on quantum chemistry results of other authors. This paper presents our new approach for calculation the thermodynamic functions of positively charged argon nitride (ArN^+) using ab initio quantum chemical calculations. For this molecule, the temperature dependences of the main thermodynamic functions were obtained and the error estimates were given.

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