New web application for approximation of thermodynamic functions of diatomic gases

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Temperature-dependent thermodynamic functions are essential for thermodynamic modeling, providing the foundation for realistic descriptions of physicochemical processes. Such data must be structured to represent the behavior of reactants across any temperature range. Traditionally, the Glushko handbook and IVTANTHERMO-online information system [1] utilizes polynomial representations for thermodynamic functions:

$$\Phi^\circ(T) = \phi_1 + \phi_2 \ln X + \phi_3 X^{-2} + \phi_4 X^{-1} + \phi_5 X + \phi_6 X^2 + \phi_7 X^3,$$

$$C_p^\circ(T) = \phi_2 + 2\phi_3/X^2 + 2\phi_5 X + 6\phi_6 X^2 + 12\phi_7 X^3$$

This study introduces a modern web application designed to approximate fundamental thermodynamic functions using specified polynomial forms. The approximation algorithm is based on dividing the entire temperature range into a variable number of intervals, as described in [2]. This approach ensures higher accuracy and adaptability for a wide range of temperature-dependent datasets.
The developed application also features a dedicated API (Application Programming Interface), enabling users to remotely approximate dependencies of thermodynamic functions for ideal gases.
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[1] Belov G V and et al 2018 *J. Phys.: Conf. Ser.* **946** 012120
[2] Belov G, Aristova N, Morozov I and Sineva M 2017 *J. Math. Chem.* **55** 1683–1697