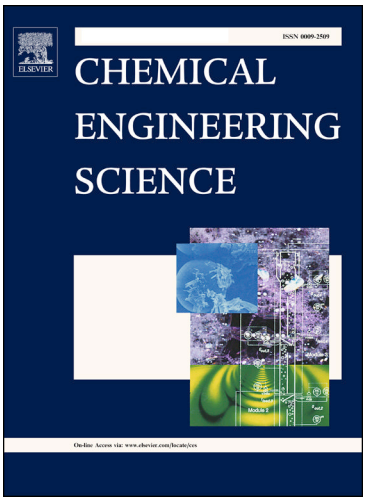

Short Communication

Entropy of gaseous phosphorus dimer

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Entropy of gaseous phosphorus dimer

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Abstract. Based on the improved Rosen-Morse oscillator for describing the internal vibration of a molecule, we establish an explicit representation of molar entropy for gaseous substances. Using the dissociation energy, equilibrium internuclear distance and harmonic vibrational frequency, we calculate the molar entropy values of the gaseous phosphorus dimer. Our calculated results show an excellent agreement compared to the experimental data in a wide variety of temperatures ranging from 298 up to 6000K.

Keywords: Entropy; Mathematical modeling; Gaseous phosphorus dimer

1. Introduction

Entropy is an important thermodynamic quantity, which involves in many fields, including dissolution [1], thermal conductivity [2], phase transition [3-5], fluid transport [6-8], and adsorption [9-11]. Investigation of the adsorption entropy has attracted much interest because it provides information about the order and disorder of the adsorbate on the adsorbent surface. A multitude of approaches have been proposed for the calculation of molar entropy of the thermodynamic system under consideration [12-18]. A universal mathematical expression of molar entropy for gaseous substances is useful for giving simple explanations of chemical phenomena involving entropy change. Based on the improved Tietz oscillator [19] for representing the internal vibration of a molecule, we [18] established a mathematical expression of molar entropy for gaseous substances in terms of four molecular constants, and successfully predicted the molar entropy values for some gaseous substances, including the carbon monoxide, hydrogen chloride, hydrogen fluoride, deuterium fluoride, nitrogen monoxide, and gaseous boron monobromide. Hydrochloric acid (HCl) and the mixture of HCl and hydrofluoric acid (HF) are often used to acidize