عنوان مقاله:

Soret coefficients for binary mixtures of Helium and hydrogen isotopes: The non-adiabatic effects

محل انتشار:

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تعداد صفحات اصل مقاله: 1

نویسندگان:

Samira Kamali - *Department of Chemistry, Faculty of Science, university of Tehran, Tehran, Iran*

Ali Maghari - *Department of Chemistry, Faculty of Science, university of Tehran, Tehran, Iran*

خلاصه مقاله:

In the limit of zero density, the transport coefficients of a gas could be expressed in terms of the collision integrals, which are related to the intermolecular potential energy between two molecules. For different isotopes, the non-adiabatic effects on the potential energy surface could be affected on the collision integrals as well as transport properties of isotopic molecules. The accurate ab initio potential energy between helium/hydrogen and their isotope mixtures developed by bakr [2] and used to calculate the transport cross-sections as well as transport collision integrals. The model potential was fitted as a function of intermolecular separation and the relative orientation of the molecule as [2]In this work, we first utilized a full analytical potential energy function including the non-adiabatic terms to calculate the Soret coefficients of the He-H2 and their isotopic mixtures. The extensive comparisons with experimental data as well as with our calculations in the frame work of the classical kinetic theory demonstrate that the ab initio transport properties can be used as standard values in a wide range of scientific needs. Moreover, the density corrections to the gaseous Soret coefficients are formulated and used to calculate for the isotopic mixtures of hydrogen and helium mixtures. To the best of our knowledge, the formulations for Soret coefficients and thermal diffusion factors are new. The theory was checked with the previous works of Maghari et al. [3,4] studied by the non-equilibrium molecular dynamic simulations

کلمات کلیدی: