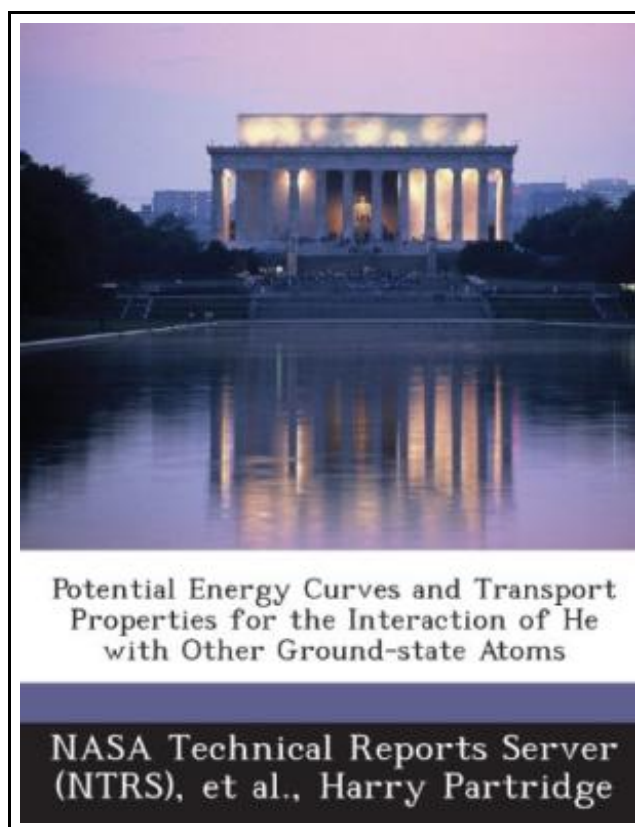


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POTENTIAL ENERGY CURVES AND TRANSPORT PROPERTIES FOR THE INTERACTION OF HE WITH OTHER GROUND-STATE ATOMS



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Bibliogov, United States, 2013. Paperback. Book Condition: New. 246 x 189 mm. Language: English . Brand New Book ***** Print on Demand *****.The interactions of a He atom with a heavier atom are examined for 26 different elements, which are consecutive members selected from three rows (Li - Ne, Na - Ar, and K, Ca, Ga - Kr) and column 12 (Zn, Cd) of the periodic table. Interaction energies are determined using high-quality ab initio calculations for the states of the molecule that would be formed from each pair of atoms in their ground states. Potential energies are tabulated for a broad range of interatomic separation distances. The results show, for example, that the energy of an alkali interaction at small separations is nearly the same as that of a rare-gas interaction with the same electron configuration for the closed shells. Furthermore, the repulsive-range parameter for this region is very short compared to its length for the repulsion dominated by the alkali-valence electron at large separations (beyond about 3-4 a_0). The potential energies in the region of the van der Waals minimum agree well with the most accurate results available. The ab initio energies are applied to calculate scattering cross sections and obtain the collision integrals that are needed to determine transport properties to second order. The theoretical values of Li-He total scattering cross sections and the rare-gas atom-He transport properties agree well (to within about 1%) with the corresponding measured data. Effective potential energies are constructed from the ab initio energies; the results have been shown to reproduce known transport data and can be readily applied to predict unknown transport properties for like-atom interactions.



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