



Potential Energy Curves and Transport Properties for the Interaction of He with Other Ground-State Atoms (Paperback)

By Harry Partridge

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 doped 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...



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