

INFLUENCE OF SPIN-ORBIT INTERACTION ON LONG-RANGE POTENTIAL CURVES OF Cs₂, Rb₂ AND Rb-Cs MOLECULES

H. Rakić¹ and R. Beuc²

¹*Infosistem, HR-10000 Zagreb, Croatia*

²*Institute of Physics, HR-10000 Zagreb, Croatia*

E-mail: beuc@ifs.hr

We have studied the long-range interaction potentials of homonuclear and heteronuclear alkali metal dimers Cs₂, Rb₂ and Cs-Rb for molecular states which dissociate into one atom in the ground $n_0S_{1/2}$ state and the other in one of the excited $nS_{1/2}$ or $nP_{1/2,3/2}$ states.

Dominant electrostatic interaction of neutral atoms in the region of large interatomic distances is the dipole-dipole interaction which gives resonance contribution in the case of homonuclear dimers with asymptote $n_0S_{1/2} + nP_{1/2,3/2}$ and van der Waals contribution in all other cases. Various cases were analyzed by Movre and Beuc (1985), Marinescu et al. (1994) and Marinescu and Dalgarno (1995). In all these calculations, atomic radial wave functions dependent on principal and angular quantum numbers (n, l) has been used. Hundred years ago Rasetti (1924) noticed the anomaly in the dipole oscillator strengths in the cesium and rubidium principal series. Fermi (1930) explained the anomaly as a consequence of spin-orbit interaction and suggested an atomic radial wave function dependent on the total angular momentum j .

The aim of our research was to determine the influence of spin-orbit interaction, correctly included in the radial wave function, on the resonance and van der Waals interaction of alkali dimers. In our calculations we use effective valence electron potential described by empirical l - and j - dependent pseudo potential (Hafner and Schwarz, 1978). The energy and wave functions of valence electrons are determined by diagonalization of Hamiltonian on the grid (Vrinceanu and Dalgarno, 2008).

References

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