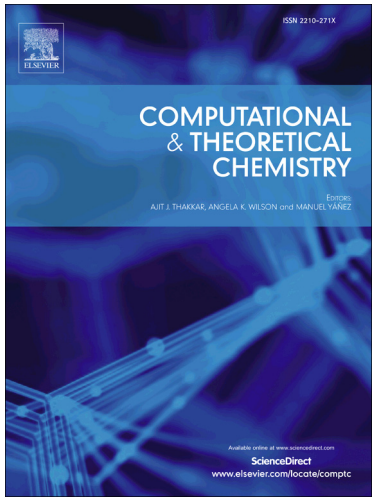

Multi-reference perturbation theory study on the CsYb molecule including the spin-orbit coupling

Darya N. Meniailava, Maksim B. Shundalau

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Multi-reference perturbation theory study on the CsYb molecule including the spin-orbit coupling

Darya N. Meniailava [a], Maksim B. Shundalau [a,b] *

[a] *Physics Department, Belarusian State University, 4 Nezaležnaści Ave., 220030, Minsk, Belarus*
[b] *A.N. Sevchenko Institute of Applied Physical Problems at Belarusian State University, 7 Kurčataŭ Str., 220108 Minsk, Belarus*
** Corresponding author, e-mail: shundalov@bsu.by*

Abstract. We present CASSCF/XMCQDPT2 level of theory calculations of the ground and sixteen low-lying excited electronic states of the CsYb molecule taking into account the spin-orbit coupling. Spectroscopic constants (electronic term energies, equilibrium internuclear distances, dissociation energies, harmonic vibrational frequencies), transition dipole moments, Franck–Condon factors and vibrational energies of the CsYb molecule have been obtained. The energies of the ground and first exited states at the asymptotic limits definitely satisfy the experimental data for cesium and ytterbium atoms. All the data obtained allow to predict and realize two-photon schemes for producing ultracold CsYb molecules and carry out spectral experiments with them.

Keywords. Multi-reference perturbation theory calculations; CsYb molecule; Potential energy curves; Spin-orbit coupling; Vibrational states; Franck–Condon factors

1. Introduction

Nowadays in the field of cold and ultracold molecules theoretical and practical studying of a new class of heteronuclear diatomic molecules, which include an atom of alkali metals and one of transition metals, is of great interest. In a diatomic molecule consisting of an alkali metal atom and, for example, of an atom of the lanthanide series with even atomic number one of the electrons is found out to be unpaired. This means that such a molecule besides a permanent electric dipole moment also has a permanent magnetic dipole moment. Thus, it is possible to effectively manipulate of the molecular quantum matter by external magnetic field. Moreover these molecules offer the possibilities for high precision measurements of fundamental constants, for quantum many-body physics and quantum information, for testing fundamental models etc. [1,2]. The CsYb molecule is proposed to be an attractive candidate for the possibilities mentioned. For efficient production of ultracold CsYb molecules by two-photon schemes the knowledge of exact potential energy curves (PECs), vibrational energies, molecular spectroscopic and dynamic parameters are crucial.

Up to our knowledge, no experimental data are evaluable for a system of electronic states of the CsYb molecule, and there are only three *ab initio* calculations for the ground $X^2\Sigma^+$ state in CCSD(T) (Coupled Cluster) [3] and CASSCF/MRCI (Complete Active Space Self-Consistent Field / Multi-Reference Configuration Interaction) approximation [4,5] respectively, and for the first excited states (namely spin-free $1^2\Pi$ and $2^2\Sigma^+$ states), performed by Meyer and Bohn [4] at the CASSCF/MRCI level of theory. The results of these calculations for the ground state are quite different: R_e = 5.657 Å, D_e = 182 cm^{-1} [4]; R_e = 5.161 Å, D_e = 542 cm^{-1} [5] and R_e = 5.144