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

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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.

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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: \(R_e = 5.657\ \text{Å}, \quad D_e = 182\ \text{cm}^{-1}\) [4]; \(R_e = 5.161\ \text{Å}, \quad D_e = 542\ \text{cm}^{-1}\) [5] and \(R_e = 5.144\ \text{Å}, \quad D_e = 621\ \text{cm}^{-1}\) [3] (where \(R_e\) is equilibrium internuclear distance, \(D_e\) is dissociation energy). In this connection it is important to compare the calculated characteristics of other alkali-metal–ytterbium diatomic molecules: LiYb, NaYb, KYb, and RbYb.

The dissociation energies calculated at the different levels of theory for the alkali-metal–ytterbium diatomics are: 1151 cm\(^{-1}\) (Tohme et al. [6], MRCI), 1403 cm\(^{-1}\) (Shao et al. [5], MRCI), 1422 and 1490 cm\(^{-1}\) (Gopakumar et al. [7], CASPT2), 1577 cm\(^{-1}\) (Zhang et al. [8], CCSD(T)), 1641 cm\(^{-1}\) (Brue and Hutson [3], CCSD(T)), 2289 cm\(^{-1}\) (Kotochigova et al. [9], CCSD(T)) for the LiYb molecule; 248–1291 cm\(^{-1}\) (Tohme and Korek [10], MRCI), 912 cm\(^{-1}\) (Shao et al. [5], MRCI), 1012 cm\(^{-1}\) (Brue and Hutson [3], CCSD(T)) for the NaYb molecule; 696 cm\(^{-1}\) (Shao et al. [5], MRCI), 737 cm\(^{-1}\) (Brue and Hutson [3], CCSD(T)), 858 and 971 cm\(^{-1}\) (Tohme and Korek [11], MRCI) for the KYb molecule; and 193 cm\(^{-1}\) (Meyer and Bohn [4], MRCI), 531 cm\(^{-1}\) (Shundalau and Minko [12], XMCQDPT2), 565 cm\(^{-1}\) (Shao et al. [5], MRCI), 591–868 cm\(^{-1}\)
Lately MRPT calculations at the CASSCF/XMCQDPT2 (Extended Multi-Configuration Quasi-Degenerate 2nd Order Perturbation Theory) [16] level of theory were performed for the KRB [17] and RbYb [12] molecules. In study [17] we obtained the spectroscopic parameters of the ground state for the KRB molecule with a high accuracy. As a result of calculations in [12] the energies obtained for the first two asymptotic limits exactly respond to the experimental data for rubidium and ytterbium atoms. An explanation of sufficient results of the calculations is also discussed in [12]. Thus we use the same technique expecting to achieve the best results for CsYb molecule.

The aim of this work is to carry out ab initio calculations of PECs of the low-lying electronic states taking into account the spin-orbit coupling (SOC), to determine molecular spectroscopic constants, vibrational energies, Franck–Condon factors (FCS) for the vibronic transitions of diatomic polar CsYb molecule at the high level of theory. Particular attention is paid to the ground \( X^2\Sigma^+ \) state and low-lying excited \( 1\Sigma^+ \), \( 2\Sigma^+ \), and \( 2\Sigma^+ \) states.

2. Computations

The electronic configuration and the ground state term for the cesium atom are \([\text{Xe}]^6s^2\) and \( ^2\Sigma^+ \), respectively. The first three excited configurations, atomic terms and corresponding to them energies are: \( 5p^66s^1 \rightarrow 5p^53d^2 \) (11 178.268 cm\(^{-1}\)), \( ^2P_{3/2} \) (11 732.308 cm\(^{-1}\)), \( 5p^53d^2 \rightarrow 2d_{5/2} \) (14 499.358 cm\(^{-1}\)), \( 5p^53d^2 \rightarrow 7d_{5/2} \) (14 596.842 cm\(^{-1}\)), and \( 5p^57s \rightarrow 5s^1 \) (18 535.529 cm\(^{-1}\)) [18]. The SOC splittings of the \( ^2P \) and \( ^2D \) terms are 554.040 and 98.484 cm\(^{-1}\), respectively.

The electronic configuration and the ground state term for the ytterbium atom are \([\text{Xe}]^4f^{13}6s^2 \) and \( ^5S_0 \), respectively. The first excited configuration, appropriate triplet and singlet terms, and energies of the states for the Yb atom are: \( 4f^{13}5d6s^2 \rightarrow 4p^53d^3 \) (17 288.499 cm\(^{-1}\)), \( 4P_1 \) (17 992.007 cm\(^{-1}\)), \( 4P_2 \) (19 710.388 cm\(^{-1}\)), and \( 4P_3 \) (25 068.222 cm\(^{-1}\)) [18]. The SOC splittings of the triplet \( ^2P \) term are 703.508 and 1718.381 cm\(^{-1}\).

The next excited term (7/2, 3/2) \( 2S_{1/2} \rightarrow 4f^{13}5d6s^2 \) originates from the \( 4f^{13}5d6s^2 \) excited configuration with energies of the states lying in the range of 23 288–28 184 cm\(^{-1}\) [18]. The triplet \( ^2D_{1/2,2} \) term arising from the \( 4f^{13}5d6s^2 \) configuration with the energies ranging 24 489–25 271 cm\(^{-1}\) [18] and the \( ^2P \) term (see above) are located between the components of the (7/2, 3/2) \( 2S_{1/2,3/2} \) term. Therefore calculations of the molecular electronic states corresponding to given or higher excited configurations of the Yb atom require including f-electrons into the active space. The states just mentioned are not considered here.

We carry out the PECs calculations for spin-free (doublet and quartet) and spin-mixed states corresponding to the five lowest dissociation limits: \( Cs(6s) + Yb(6s^2) \) (limit I), \( Cs(6p) + Yb(6s^2) \) (limit II), \( Cs(5d) + Yb(6s^2) \) (limit III), \( Cs(7s) + Yb(6s^2) \) (limit IV), \( Cs(6s) + Yb(6s6p) \) (limit V). It is worth mentioning that \( ^2S_{1/2} \) term of the Cs atom occurs between the \( ^3P \) and \( ^3P \) components of the \( ^3P \) term of the Yb atom. The molecular electronic terms relating to the Cs \( (5d) + Yb(6s^2) \) and Cs \( (7s) + Yb(6s^2) \) dissociation limits are supposed to be highly perturbed by the terms relating to the Cs \( (6s) + Yb(6s6p) \) dissociation limit. As we do not take into account during the calculations the terms corresponding to the Cs \( (6s) + Yb \) \( (4f^{13}5d6s^2) \) limit, situated much more above just mentioned terms, the terms corresponding to the Cs \( (5d) + Yb(6s^2) \) dissociation limit lift up and the term corresponding to the Cs \( (7s) + Yb(6s^2) \) dissociation limit is pushed out. Consequently, if excitations of the f-electrons of the Yb atom are not taken into account in the active space, PECs of these terms [6,10,11,14] will be of the artifact character.

The asymptotic limit I comprises the ground \( X^2\Sigma^+ \) state, the asymptotic limit II comprises the doublet \( 2\Sigma^+ \) and \( 1\Sigma^+ \) states, the asymptotic limit III comprises the doublet \( 3\Sigma^+ \), \( 2\Pi \), and \( 1\Delta \) states, the asymptotic limit IV comprises only one doublet \( 4\Sigma^+ \) state, and the asymptotic limit V comprises the doublet \( 5\Sigma^+ \), \( 3\Pi \), \( 0\Pi \), and \( 1\Sigma^+ \) states. As one takes into account spin-orbit effects the \( X^2\Sigma^+ \), \( 2\Sigma^+ \), \( 3\Sigma^+ \), \( 4\Sigma^+ \), \( 5\Sigma^+ \) states transform into the \( X^2\Sigma^+, 2\Sigma^+, 3\Sigma^+, 4\Sigma^+, 5\Sigma^+ \) states, respectively; the \( 1\Pi \), \( 2\Pi \), and \( 3\Pi \) states split into the \( 1\Sigma^+, 2\Sigma^+, 3\Sigma^+ \) states, \( 1\Sigma^+, 2\Sigma^+, 3\Sigma^+ \) states, respectively; the \( 1\Sigma^+ \) state splits into the \( 1\Sigma^+ \) and \( 2\Sigma^+ \) states; the \( 1\Sigma^+ \) state splits into the \( 1\Sigma^+ \) and \( 2\Sigma^+ \) states.

It is typical for heavy diatomic molecules containing an alkali metal to use \((n \pi\sigma)\) notation, as spin-mixed states arise from interaction between the states with the different spin. But it is worth using \((2n \pi \sigma)\) notation to lay stress on the relationship between the spin-mixed and the spin-free states. Both notations \((2n \pi \sigma)\) and \((n \pi\sigma)\) are given in Table 1.

We used Stuttgart fully relativistic large core effective core potential (ECP) for ytterbium [19] and Stuttgart fully relativistic small core ECP for cesium [20] atoms during the calculations. The corresponding Gaussian basis sets are \((7s7p6d) \) (ECP60MDF) for ytterbium atom [19] and \((12s11p5d3f2g) \rightarrow [8s8p5d3f2g] \) (ECP46MDF) for cesium atom [20].

The CASSCF calculations were done for active space including 3 electrons in 12 orbitals. The SA-procedure was realized for 11 doublet and quartet states. Both notations \((2n \pi \sigma)\) and \((n \pi\sigma)\) were used. The eight lowest double occupied orbitals were involved in the perturbation calculations, the ISA shift [21] of 0.190 [22] being used. The dimensions of the effective Hamiltonian were \( 11 \times 11 \) and \( 5 \times 5 \) for doublet and quartet states, respectively.

For the spin-orbit coupling (SOC) calculations we used the one-electron Pauli–Breit operator. The effective nuclear charges \( Z_{eff} \), which always turn out to be of high value due to errors caused by nodeless ECPs wave functions (for details see [23–25]), for Yb and Cs were 7137.0 and 7965.0 respectively.

We obtained potential curves for CsYb using the Firefly quantum chemical package [26]. For determining the electronic energy terms \( T_e \) and the equilibrium internuclear distances \( R_e \) we used the fourth degree polynomial approximation of the \( ab \) \( in \) \( itio \) PECs near minima.

The calculations of transition dipole moments (TDMs) are performed at the CASSCF/XMCQDPT2 + SOC level of theory using GAMESS suit of codes [27].
The calculations of the vibrational states energies and the Franck-Condon factors are performed using the LEVEL program package [28]. The perturbations of the vibrational states, which belong to different electronic terms with the equal $\Omega$ values (for example, $1^1\Pi_{1/2}$ and $2^2\Sigma_{1/2}$) and overlap in some region of energies, were not calculated.

### 3. Results and discussion

#### 3.1. Electronic states

The calculated PECs are performed in Fig. 1 and are also given in the Supplementary Material. The calculated molecular spectroscopic constants (the electronic term energy $T_n$, the equilibrium internuclear distance $R_n$, the binding energy $D_n$, and the harmonic vibrational frequency $\omega_n$) are presented in Table 1. Table 1 also shows the results of the ab initio calculations [3–5].

As there is no experimental values of spectroscopic parameters for ground and excited states to determine the accuracy of the calculations in Table 1 we compare the calculated energies of molecular states at the dissociation limits (at the internuclear distance of 17.0 Å) with the sum of the experimental energies [18] of separated atoms. The energies obtained for the $1^1\Pi_{1/2}$, $1^1\Pi_{3/2}$, and $2^2\Sigma_{1/2}$ states corresponding to the limit II are 11728.9 Å and 11728.7 Å respectively, 11728.9 Å and 11728.7 Å respectively, and 11728.9 Å and 11728.7 Å respectively. These data are in agreement with the experimental ones (see Table 1).

Our calculated equilibrium internuclear distance ($R_0 = 5.763$ Å) for the $X^2\Sigma_{1/2}^+$ state is higher than $R_0 = 5.673$ Å for the $X^2\Sigma_{1/2}^+$ state calculated by 253 cm$^{-1}$ in comparison with NIST energies [18]. Nevertheless, the total SOC splitting of this limit equals to 2 421.9 cm$^{-1}$, which almost coincides with experimental one (2 421.9 cm$^{-1}$).

Table 1 shows the calculated and experimental values (for 1$^1\Pi_{1/2}$, 1$^1\Pi_{3/2}$, and 2$^2\Sigma_{1/2}$) of the 6s state of Cs atom and signals the van der Waals' character of the molecule. In contrast to the ground state PEC, the first excited states (1$^1\Pi_{1/2}$, 1$^1\Pi_{3/2}$, and 2$^2\Sigma_{1/2}$) have deeper wells due to stronger polarizability of the 6p state of cesium atom.

During the calculations the $2^2\Sigma_{1/2}$ states that should belong to limit III disappeared, the remaining ones being shifted and SOC splitting of this limit being overestimated by 1633.8 cm$^{-1}$. This may be caused by the not including f-electrons of Yb atom in active space through the calculations.

The term, related to limit IV, must appear according to experimental data between fine-structure components of limit V. However, within the calculations such a situation did not arise. "Intruded" term $5^2\Sigma_{1/2}$ caused a perturbation and as a result dropped down by 2739.8 cm$^{-1}$ and affected terms belonging to limit III.

The PECs obtained for limit V are shifted down approximately by 253 cm$^{-1}$ in comparison with NIST energies [18]. Nevertheless, the total SOC splitting of this limit equals to 2 422.5 cm$^{-1}$, which almost coincides with experimental one (2 421.9 cm$^{-1}$).

Table 1: Molecular spectroscopic constants of $^{133}$Cs$^{173}$Yb molecule.

| Term | $\Omega_1$,$\Omega_2$ | $T_n$, cm$^{-1}$ | $R_n$, Å | $\omega_n$, cm$^{-1}$ | $D_n$, cm$^{-1}$ | Asymptotic limit, cm$^{-1}$ |
|------|---------------------|-----------------|---------|---------------------|----------------|--------------------------|
| $X^2\Sigma_{1/2}$ | $(1)\frac{1}{2}$ | 158.7 | 5.763 | 12.1 | 158.7 | 0.0 |
| | $(2)\frac{1}{2}$ | 182$^a$ | 5.66$^b$ | 9.9$^b$ | 182$^a$ | 542$^b$ |
| | $(3)\frac{1}{2}$ | 621$^c$ | 5.144$^d$ | 19.56$^d$ | 621$^c$ | 542$^b$ |
| | $(4)\frac{1}{2}$ | 7425.2 | 4.100 | 58.6 | 4307.1 | 11728.9 |
| | $(5)\frac{1}{2}$ | 2710$^e$ | 5.09$^f$ | 35.0 | 1283.3 | 17842.9 |
| | $(6)\frac{1}{2}$ | 9908.2 | 4.932 | 41.2 | 1196.5 | 14409.3 |
| | $(7)\frac{1}{2}$ | 15074.5 | 5.621 | 19.5 | 1256.7 | 14596.8 |
| | $(8)\frac{1}{2}$ | 13502.0 | 4.777 | 55.0 | 693.1 | 19456.7 |
| | $(9)\frac{1}{2}$ | 7425.2 | 4.932 | 41.2 | 1196.5 | 14409.3 |
| | $(10)\frac{1}{2}$ | 15074.5 | 5.621 | 19.5 | 1256.7 | 14596.8 |
| | $(11)\frac{1}{2}$ | 18763.6 | 5.582 | 14.6 | 721.0 | 17288.5 |
| | $(12)\frac{1}{2}$ | 18763.6 | 5.582 | 14.6 | 721.0 | 17288.5 |

* $a$ NIST [18].
* $b$ Meyer and Bohn [4], spin-free states.
* $c$ Brue and Hutson [3].
* $d$ Shao et al. [5].
3.2. Vibrational states

For calculations of vibrational energies and frequencies reduced mass of the molecule is important. The Yb atom has seven stable isotopes: $^{168}\text{Yb}$ (0.13%), $^{170}\text{Yb}$ (3.04%), $^{171}\text{Yb}$ (14.28%), $^{172}\text{Yb}$ (21.83%), $^{173}\text{Yb}$ (16.13%), $^{174}\text{Yb}$ (31.83%) and $^{176}\text{Yb}$ (12.76%). For Cs atom there is only one ($^{133}\text{Cs}$) stable isotope. We calculate the vibrational energies for $^{133}\text{Cs}^{174}\text{Yb}$ molecule, as the most abundant isotopomer, and some other isotopomers for all spin-mixed PECs up to the dissociation limit of the corresponding state, and then we obtained the harmonic vibrational frequencies for these electronic states (see Table 1).

For the ground $^1\Sigma^+_{1/2}$ state and excited $^1\Sigma^+_{3/2}$, $^1\Delta^+_{3/2}$, $^1\Pi^+_{1/2}$ states we obtained 37, 145, 137 and 120 vibrational levels, respectively. Fig. 3, as an example, shows vibrational energies $E_v$ and vibrational intervals $D_v(v_0 + 1/2)$ for the ground $^1\Sigma^+_{1/2}$ state and "shelf-like" $^3\Sigma^+_{1/2}$ state. Kinks on such dependencies (see Fig. 3c, d) usually indicate the existence of some peculiarities on the potential curves: several minima, flat areas, etc. Since the highly excited vibrational states located near the dissociation limit of the ground $^1\Sigma^+_{1/2}$ state are of primary concern to optical production of the ultracold molecules, we used approximation function $C_0 + C_3/r^3 - C_6/r^6$ to reproduce more proper values of bound states of the ground electronic state near the threshold starting from 11 Å. The coefficients $C_3$ and $C_6$ are 6496.53 cm$^{-1}$Å$^3$ and 1.60325 x 10$^{-7}$ cm$^{-1}$Å$^6$, respectively. With this outer part of the ground state PEC we already obtained 45 bound vibrational states, and well depth became 160.8 cm$^{-1}$. The insert in Fig. 3a shows differences in sequences of vibrational energies calculated without and with asymptotic function. For other excited states $(^2\Pi^+_{1/2}, ^2\Pi^+_{3/2}, ^2\Sigma^+_{1/2}, ^4\Sigma^+_{1/2}, ^4\Pi^+_{1/2}, ^4\Pi^+_{3/2}, ^4\Pi^+_{5/2}, ^4\Sigma^+_{1/2}, ^4\Sigma^+_{3/2}, ^4\Sigma^+_{5/2})$ we obtained 55, 57, 134, 85, 110, 111, 89, 131, 147, 44, 59, 78, and 115 bound vibrational states, respectively.

Fig. 1. The low-lying terms of the CsYb molecule calculated at the CASSCF(3,12)/XMCQDPT2 + SOC level of theory.

Fig. 2. Calculated transition dipole moments for the transitions from the ground (1) $^1\Sigma^+_{1/2}$ state to the states (2) $^1\Pi^+_{1/2}$, (3) $^1\Pi^+_{3/2}$, (4) $^3\Pi^+_{1/2}$, (5) $^3\Pi^+_{3/2}$, (6) $^3\Sigma^+_{1/2}$, (7) $^5\Sigma^+_{1/2}$, (8) $^3\Pi^+_{1/2}$, (9) $^3\Pi^+_{3/2}$, (10) $^1\Delta^+_{3/2}$, (11) $^3\Delta^+_{3/2}$, (12) $^1\Pi^+_{3/2}$, (13) $^3\Pi^+_{1/2}$, (14) $^3\Pi^+_{3/2}$, (15) $^3\Pi^+_{5/2}$, and (16) $^3\Pi^+_{5/2}$.
3.3. Franck–Condon factors

On the basis of calculated PECs we obtain the Franck–Condon factors (FCFs) between the pointful states of the $^{133}\text{Cs}^{174}\text{Yb}$ molecule. Using the $\Delta \Omega = 0, \pm 1$ selection rules we have calculated FCFs for vibronic transitions between the spin-mixed electronic states. We concern the transitions between the fixed vibrational level $v_0$ of the upper electronic state and a sequence of vibrational levels $v'_0$ of the lower electronic state applying the selection rules $\Delta J = 0$ or $\Delta J = \pm 1$.

The FCFs obtained for transitions between the vibrational levels of the first three exited electronic states and the vibrational levels of the ground electronic state with $\Delta J = 0$ selection rule are presented in Fig. 4. FCFs shown here are calculated for the transitions from the lowest vibrational levels ($v' = 0...4$) of the excited electronic states (Fig. 4a, d, g) (1), for the transitions with the largest FCFs to the ground rovibronic $X^2\Sigma_{1/2}^+$ ($v'' = 0, J = 0$) state (Fig. 4b, e, h) (2), and for the transitions with the largest values of all possible FCFs (Fig. 4c, f, i) (3).

The FCFs distributions for the $X^2\Sigma_{1/2}^- - 1^2\Pi_{1/2}$ and $X^2\Sigma_{1/2}^- - 1^2\Pi_{3/2}$ transitions have the same character (see Fig. 4a–f). The largest values of FCFs for the transitions to the “absolute” ground state $X^2\Sigma_{1/2}^+$ ($v = 0, J = 0$) are about 0.07 with $v' = 70...74$ for $1^2\Pi_{1/2}$ state and $v' = 61...65$ for $1^2\Pi_{3/2}$ state. The rovibronic transitions between weakly-bound vibrational states near the dissociation limits of the excited electronic states ($v = 139...144$ for $1^2\Pi_{1/2}$ state and $v = 130...137$ for $1^2\Pi_{3/2}$ state) and the ground electronic state ($v' = 40...46$) have the largest probabilities.

For the $X^2\Sigma_{1/2}^- - 2^2\Sigma_{1/2}^+$ transitions to the “absolute” ground state $X^2\Sigma_{1/2}^+$ ($v = 0, J = 0$) the largest FCFs occur for the transitions from the $2^2\Sigma_{1/2}^+$ ($v' = 13...21$) vibronic states with FCFs values of about 0.1. According to predicted average TDM value of about 9.5 D in the 3.5–17.0 Å region for the $2^2\Sigma^+ - X^2\Sigma^+ ((3)1/2 - (1)1/2)$ transition (see Fig. 2), the $2^2\Sigma_{1/2}^+$ (or $3(1/2)$) state is concerned to be a suitable candidate for two-photon optical scheme for the producing CsYb molecules in the ground rovibronic state.
4. Conclusions

The system of the low-lying electronic states of the CsYb molecule taking into account the spin-orbit coupling at the high level of theory was calculated for the first time. PECs of the ground and 16 excited states were constructed, for each of them the system of vibrational levels and vibrational frequencies were computed. The value of 158.7 cm\(^{-1}\) (or 160.8 cm\(^{-1}\) with approximation function) obtained for dissociation energy of the ground state indicates van der Waals’ character of the molecule. The transition dipole moments were calculated, Franck–Condon factors for vibronic transitions were determined. Since at the Cs(6p) + Yb(6s 2) dissociation limit our obtained PECs are in a good agreement with the experimental \cite{18} energies and since the calculations for the KRb \cite{17} and RbYb \cite{12} molecules in the same approximation show accurate values, we expect the results of our current calculations for the ground and low-lying excited states of the CsYb molecule to be close to the correct values. The effective schemes (optical cycles, for example) for transferring CsYb molecules to the ground rovibronic state by initial excitation into overlying states can be developed on the basis of the calculated spectral and dynamic characteristics. The results obtained can be used for spectroscopic studies of CsYb molecule, as well as for the synthesis of such molecules. The ytterbium-containing diatomics (such as RbYb and SrYb) now are considered as perspective molecular systems for the experiments under cold and ultracold conditions \cite{13,29}. We assume that the molecule under consideration also can be used for the purposes mentioned.

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Appendix A. Supplementary material

Supplementary data associated with this article can be found, in the online version, at http://dx.doi.org/10.1016/j.comptc.2017.03.046.
