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Possible schemes of photoassociation processes in the KLi molecule with newly calculated potential energy curves

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Abstract: We present four promising schemes for photoassociative formation of KLi molecule in its ground electronic state. Analysis is based on newly calculated adiabatic potentials supported by transition dipole moments and Franck-Condon factors.

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1. Introduction

Heteronuclear alkali metal dimers have started to attract more attention from both experimentalists and theoreticians. Spectroscopic investigations of these dimers may provide valuable insights into several basic phenomena, such as perturbations in excited states, potential curve crossings and avoided crossings, photodissociation and photoassociation. They also may serve as prototypes for studies of the properties of ultracold two-fermionic species or bosonic heteronuclear molecules. On the one hand, the heteronuclear alkali metal pairs present a challenge for experimental handling, due to two different melting points and the presence in abundance of two species of homonuclear molecules (Li_2, K_2). Nevertheless, the progress of spectroscopic methods allows for very accurate measurements, providing data on the ground and excited states. On the other hand, heteronuclear alkali metal dimers are very attractive objects to test theoretical methods, because of simple electronic structure and the possibility of treating them as effective two-electron systems with well separated atomic cores. Pseudopotential methods with long-tail core polarization model potentials are very well suited to treat such systems.

KLi was an object of a few early spectroscopic experiments, e.g. Walter and Barrat [1], Weizel and Kulp [2]. We also note the more recent works of Dagdigian and Wharton [3] on molecular beam electric resonance spectra, Zmbov [4] et al. who demonstrate the application of the mass spectrometry method, and Engelke et al. [5] on high-resolution laser excitation spectra. Quite recently, a notable series of experiments on the KLi system were performed by the Warsaw group with different coworkers [6–18]. Primarily using Doppler-free polarization labeling spectroscopy, they reinvestigated earlier spectra of band systems with ground and low-lying excited states. They also investigated for the first time transitions to more highly excited states like $4^1\Sigma^+$, asymptotically correlating to K(5s) and Li(2s) [17].

Recently, in the emerging field of ultracold atomic and molecular gases, Wille et al. [19] performed experiments on strongly interacting two-fermionic species consisting of ^{40}K and ^{6}Li atoms; in turn, Voight et al. [20] presented the production of ultracold KLi molecules. The photoassociative formation of ultracold heteronuclear alkali dimers, including KLi, was the subject of recent paper by Stwalley et al. [21]. In very recent work done by Ridinger et al. [22], the formation of KLi was investigated by a single-photon photoassociation in a magneto-optical trap.

In 1984, Müller and Meyer [23] presented a theoretical description of the ground state properties of several alkali metal dimers, including KLi. They performed extensive all-electron SCF calculations along with two-electron CI calculations. To describe intershell correlation effects, they used effective core potentials with one adjustable parameter. In 1999 Rousseau et al. [24] calculated 58 electronic states. They performed CI calculations with non-empirical one-electron pseudopotentials and appropriate polarization potentials by means of the CIPSI program package [25, 26]. A theoretical paper of Ingamells and Sadlej [27] on electronic and vibrational contributions to the electric properties of KLi is also worthy of mention. Very recently, an extensive theoretical *ab initio* study, including the electronic structure and transition dipole moments of the KLi molecule, has been performed by Dardouri et al. [28].

The calculations we present here use the SCF CI method with a rich basis set of Gaussian functions centered on atoms. The use of pseudopotentials describing the interaction of valence electrons with atomic cores and effective core polarization potentials allows for the reduction of a 22-electron system to the much simpler two-effective-electron problem. Calculations of adiabatic potential energy curves and electronic transition dipole moment functions are performed by means of the MOLPRO program package[1]. All spectroscopic parameters and Franck-Condon factors are calculated using the Level 8.0 program [29].

A brief overview of our computational method is given in the next section. In Section 3, we discuss the obtained potential curves, comparing them with available experimental data and other theoretical results. We also present four ways of achieving the effective photoassociative formation of cold and ultracold KLi molecules.

2. Computational method

In this section, we provide an insight into some technical details of the computational method implemented in MOLPRO. More detailed theoretical formulas are given in our other contributing papers [30–33].

We consider the interaction between two different alkali metal atoms and solve the Schrödinger equation using the Born-Oppenheimer approximation. In the present approach, only the valence electrons are treated explicitly, so effectively we consider only two-electron system. The atomic cores are represented by l-dependent pseudopotentials and model polarization potentials. The total Hamiltonian of the considered system can be written as

$$\hat{H} = \hat{T} + \hat{V}, \qquad (1)$$

where $\hat{T}$ is the kinetic energy operator of the valence electrons and $\hat{V}$ is the interaction operator. The latter is put into the form

$$\hat{V} = \sum_{\lambda} (\hat{V}^{\lambda} + \hat{V}^{\lambda}_{pol}) + \sum_{j>i=1}^{N} \frac{1}{r_{ij}} + \hat{V}_{cc}, \qquad (2)$$

where the index λ goes over two atomic cores of atoms A and B. Here, A denotes potassium, while B denotes lithium. $\hat{V}^{\lambda}$ describes the Coulomb and exchange interactions and the Pauli repulsion between the valence electrons and core λ. $\hat{V}^{\lambda}$ is defined as

$$\hat{V}^{\lambda} = \sum_{i=1}^{N} \left(-\frac{Q_{\lambda}}{r_{\lambda i}} + \sum_{l,k} B^{\lambda}_{l,k} \exp(-\beta^{\lambda}_{l,k} r^{2}_{\lambda i}) \hat{P}^{\lambda}_{l} \right), \qquad (3)$$

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[1] *MOLPRO, version 2006.1, a package of ab initio programs, H.-J. Werner, P.J. Knowles, R. Lindh, F.R. Manby, M. Schütz, P. Celani, T. Korona, A. Mitrushenkov, G. Rauhut, T.B. Adler, R.D. Amos, A. Bernhardsson, A. Berning, D.L. Cooper, M.J.O. Deegan, A.J. Dobbyn, F. Eckert, E. Goll, C. Hampel, G. Hetzer, T. Hrenar, G. Knizia, C. Köppl, Y. Liu, A.W. Lloyd, R.A. Mata, A.J. May, S.J. McNicholas, W. Meyer, M.E. Mura, A. Nicklaß, P. Palmieri, K. Pflüger, R. Pitzer, M. Reiher, U. Schumann, H. Stoll, A.J. Stone, R. Tarroni, T. Thorsteinsson, M. Wang, A. Wolf, see http://www.molpro.net.*

where Q_λ is the net charge of core λ, $\hat{P}_l^\lambda$ is the projection operator onto the Hilbert subspace of angular symmetry l with respect to core λ and N is the number of the valence electrons. The parameters $B_{l,k}^\lambda$ and $\beta_{l,k}^\lambda$ define the semi-local energy-consistent pseudopotentials. The second interaction term in Eq. (2) is the polarization term, which describes core-valence correlation. In the case of atom A, it is taken as

$$\hat{V}_{pol}^{A} = -\frac{1}{2}\alpha_A \mathbf{F}_A^2, \tag{4}$$

where $\alpha_A = 5.354\ a_0^3$ [34] is the dipole polarizability of the A^+ core and $\mathbf{F}_A$ is the electric field generated at its site by the valence electrons and the other core. In the case of the atom B, $\alpha_B = 0.1915\, a_0^3$ [34]. The electric field can be written as

$$\mathbf{F}_A = \sum_{i=1}^{N} \frac{\mathbf{r}_{Ai}}{r_{Ai}^3}[1 - \exp(-\delta_A r_{Ai}^2)] - \frac{Q_B \mathbf{R}}{R^3}[1 - \exp(-\delta_A R^2)], \tag{5}$$

where the cutoff parameter is $\delta_A = 0.29651\ a_0^{-2}$ for K and $\delta_B = 0.831\ a_0^{-2}$ for Li [34]. The third term in Eq. (2) represents the Coulomb repulsion between the valence electrons, whereas the last term describes the core-core interaction. Since the alkali atomic cores are well separated, we choose a simple point-charge Coulomb interaction in the latter case.

All calculations of adiabatic potentials and electronic transition dipole moments reported in this paper are performed by means of the MOLPRO program package. The core electrons of K atoms are represented by pseudopotential ECP18SDF [34]. We use the basis sets for potassium which come with ECP18SDF [34] for s and p functions and ECP10MDF pseudopotential [35] for d, f, g functions. Additionally, these basis sets are augmented by seventeen s functions (76.345701[2], 26.791999, 18.608373, 4.535573, 1.618743, 1.014043, 0.577728, 0.465037, 0.213265, 0.097803, 0.065676, 0.009433, 0.007466, 0.005909, 0.004326, 0.001984, 0.000849), six p functions (17.126069, 4.012627, 0.940156, 0.004358, 0.001929, 0.000854), ten d functions (25.549602, 10.052166, 3.954897, 1.680236, 0.713847, 0.240858, 0.010789, 0.003932, 0.001433, 0.000522) and six f functions (4.611628, 1.680236, 0.029604, 0.010785, 0.003929, 0.001431). In turn for Li, the core electrons are represented by pseudopotential ECP2SDF [34]. This basis set is augmented by nine s functions (1979.970927, 392.169555, 77.676373, 15.385230, 5.269282, 0.119550, 0.010159, 0.003894, 0.001493) and eleven p functions (470.456384, 96.625417, 19.845562, 4.076012, 0.567670, 0.141468, 0.035314, 0.015774, 0.007058, 0.002598, 0.000956). Additionally, for d, f and g functions we use the cc-pv5z basis set[3] augmented by ten d functions (7.115763, 3.751948, 1.978300, 1.043103, 0.600714, 0.321311, 0.152909, 0.026579, 0.011581, 0.005046) and eight f functions (2.242072, 1.409302, 0.885847, 0.556818, 0.138286, 0.055000, 0.027500, 0.01375).

We check the quality of our basis sets performing the CI calculations for the ground and several excited states of isolated potassium and lithium atoms. The calculated adiabatic potentials correlate to the K(4s) + Li(2s), K(4p) + Li(2s) and K(4s) + Li(2p) atomic asymptotes. The comparison with experimental [36] and theoretical [24, 28] asymptotic energies for different states is shown in Table 1. Rousseau et al. [24] additionally fitted the l-dependent cutoff parameters in effective core-polarization potentials to reproduce experimental atomic energies. The potential energy curves for KLi are calculated using the complete-active-space self-consistent-field (CASSCF) method to generate the orbitals for the subsequent CI calculations. The corresponding active space in the $C_{\infty v}$ point group involves the molecular counterparts of the 4s, 4p valence orbitals of the K atom and 2s, 2p valence orbitals of the Li atom. Since the spin-orbit coupling in KLi is relatively weak, our calculations do not take it into account.

3. Results and discussion

Our calculated potential energy curves are presented in Figure 1. Here, we notice characteristic avoided crossing between the potential curves of the $1^1\Pi$ and $2^1\Pi$ states. We also confirm the existence of the strong resonant coupling between the $1^1\Pi$ and $3^1\Sigma^+$ states (e.g. [21]) due to two crossings between potential curves at around 7 and 10 a_0. Table 2 lists our results for molecular constants alongside other theoretical and experimental values. Our potential depths (D_e) are systematically larger than those given by other authors. At the same time, in the case of $3^1\Sigma^+$ and $1^1\Pi$, our depths are much closer to the experimental values of Pashov et al. [8] than any other listed theoretical results. For the other molecular constants,

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[2] *The numbers listed in parenthesis are the exponential coefficients of the Gaussian Type Orbitals (GTO).*

[3] *D. Feller, unpublished*

Table 1. Comparison of asymptotic energies with experimental data (denoted as "exp.") and other theoretical results. Energies are shown in cm^{-1} units.

	Present work	Moore [36] exp.	Rousseau et al. [24]	Dardouri et al. [28]
K(4p) + Li(2s)	13023.63	13023.65	13023.64	13030.00
K(4s) + Li(2p)	14903.84	14903.87	14903.89	14903.66

such as R_e, ω_e and T_e, we find good agreement with the theoretical results of Rousseau et al. [24]. This is noteworthy given that their results were obtained through the use of a different computer program. Figures 2 and 3 show our results for the transition dipole moments, which evidently depend on the internuclear distance. These functions, as well as the chosen sets of Franck-Condon factors given in Figures 4-6, are useful for setting photoassociation (PA) schemes (see Fig. 7) leading to the formation of the KLi molecule in its ground electronic state. The one-color PA produces an excited molecule from the potassium and lithium atoms. This is followed by very fast decay by spontaneous emission, which conveys this molecule to the ground state with a certain distribution of the vibrational and rotational energy levels.

Experimentally (e.g. [22]), the laser precooled K and Li atoms are loaded into a magneto-optical trap (MOT). Next, the free-bound transitions are induced by a continuous-wave laser at a frequency which is red detuned from the chosen resonance atomic line. Subsequent spontaneous emission may produce the bound ground-state molecule. There are two indirect experimental approaches which may be used in order to estimate the number of produced ground state molecules. The first relies on the counting of atoms remaining in the MOT by probing them with laser light and recording the induced fluorescence. The second method relies on using a laser to ionize some of the excited molecules and then counting the ions. The molecules in their ground state can achieve high vibrational levels. At the same time, since the colliding atoms in the MOT are ultracooled, the rotational levels are kept low, typically up to $J = 4$.

In the first PA scheme, a double crossing between $3^1\Sigma^+$ and $1^1\Pi$ states indicates some possibility of resonant coupling which can be used, as noticed by Stwalley et al. [21], in setting a PA scheme (Fig. 7). Still, since the density of states is relatively small as compared with much heavier heteronuclear alkali dimers, one cannot expect that this coupling will be as strong as in the KRb molecule, for instance. Nevertheless, it is worthwhile to analyze this case using our detailed theoretical results. We identify the vibrational level $v' = 26$ of the $1^1\Pi$ state which may be resonantly coupled with the level $v' = 15$ of the $3^1\Sigma^+$ state. Since the level $v' = 15$ of the $3^1\Sigma^+$ state is of short range with the classical outer turning point at $R = 11$ a_0, it can not be reached by PA. Therefore even the relatively small resonant coupling with the $v' = 26$ of the $1^1\Pi$ state may populate $v' = 15$ of the $3^1\Sigma^+$ state. Since the wavefunction of the $v' = 15$ level of $3^1\Sigma^+$ begins at around $R = 6$ a_0, it may provide good PA probability for red detuning of 52 cm^{-1} from the potassium resonance energy. In turn, with the appropriate Franck-Condon factor reaching a value around 0.15 (Fig. 4), we may assume that there is a substantial overlap with the vibrational wavefunction for $v'' = 0$ of the electronic ground state $1^1\Sigma^+$. The transition dipole moment between $3^1\Sigma^+$ and $1^1\Sigma^+$ at the internuclear distance of 6.09 a_0 is around 0.35 $a.u.$ (Fig. 3).

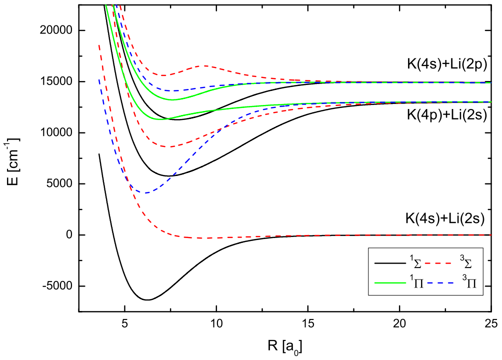

Figure 1. Calculated molecular potential energy curves of the ground and excited states.

The second PA scheme (Fig. 7) was studied, both experimentally and theoretically, by Ridinger et al. [22]. According to them, this scheme relies on the direct access to the high vibrational level of the $1^1\Pi$ state. Due to the spatial coincidence between the classical inner turning point of the upper level and the inner turning point of the level $v'' = 3$ of the ground electronic state, the substantial overlap between appropriate vibrational wavefunctions is expected. Our results indicate that with relatively small red detuning of 26 cm^{-1} the vibrational level $v' = 28$ of $1^1\Pi$ can be reached. The Franck-Condon factor between the wavefunction of the latter vibrational state and the one of $v'' = 3$ of the ground state has the value of 0.01 (Fig. 5), three times bigger than it is for $v'' = 2$. In this case the transition dipole moment equals 3.09 a.u. (Fig. 2), which helps in achieving good efficiency.

Table 2. Molecular constants R_e, D_e, ω_e, T_e for the ground and excited states of the KLi molecule. The experimental results are denoted in the table as "exp.".

State	Dissociation	Author	$R_e[a_0]$	D_e [cm^{-1}]	ω_e [cm^{-1}]	T_e [cm^{-1}]
$1^1\Sigma^+$	K(4s) + Li(2s)	Present work	6.28	6379	211.48	0
		Müller [23] exp.	6.29	6138	210.9	0
		Bednarska [6] exp.	6.27	–	212.03	0
		Bednarska [7] exp.	6.28	–	212.04	0
		Martin [9] exp.	6.28	6216	212.02	0
		Tiemann [16] exp.	6.27	6217	–	0
		Rousseau [24]	6.20	6220	211.59	0
		Dardouri [28]	6.22	6197	210.75	0
$2^1\Sigma^+$	K(4p) + Li(2s)	Present work	7.40	7262	137.38	12140
		Grochola [18] exp.	7.46	7105	137.08	12097
		Rousseau [24]	7.40	7186	135.50	12056
		Dardouri [28]	7.43	7167	133.74	12798
$3^1\Sigma^+$	K(4s) + Li(2p)	Present work	7.86	3637	115.03	17645
		Pashov [8] exp.	7.92	3619	115.41	17501
		Grochola [10] exp.	7.92	3619	115.41	17501
		Rousseau [24]	7.86	3477	114.27	17647
		Dardouri [28]	7.91	3554	115.20	17767
$1^1\Pi$	K(4p) + Li(2s)	Present work	6.94	1723	138.59	17677
		Bednarska [6] exp.	7.04	–	–	17534
		Pashov [8] exp.	7.02	1686	135.84	17573
		Rousseau [24]	7.10	1517	131.00	17725
		Dardouri [28]	7.19	1454	122.97	17672
$2^1\Pi$	K(4s) + Li(2p)	Present work	7.61	1685	128.73	19598
		Grochola [11] exp.	7.64	1664	128.98	19456
		Rousseau [24]	7.60	1684	128.73	19598
		Dardouri [28]	7.69	1300	120.92	20410
$1^3\Sigma^+$	K(4s) + Li(2s)	Present work	9.31	299.76	44.02	6079
		Salami [12] exp.	9.43	287.00	–	–
		Tiemann [16] exp.	9.43	287	–	5930
		Rousseau [24]	9.40	273.00	43.97	5947
		Dardouri [28]	9.42	276.33	37.98	5760
$2^3\Sigma^+$	K(4p) + Li(2s)	Present work	7.35	4405	142.88	14997
		Rousseau [24]	7.40	4309	141.89	14931
		Dardouri [28]	7.43	4099	135.65	15996
$3^3\Sigma^+$	K(4s) + Li(2p)	Present work	7.20	937.22	–	21984
		Dardouri [28]	7.13	917.60	–	22616
$1^3\Pi$	K(4p) + Li(2s)	Present work	6.08	8923	208.55	10479
		Rousseau [24]	6.10	8767	208.39	10475
		Dardouri [28]	6.09	8504	204.57	10534
$2^3\Pi$	K(4s) + Li(2p)	Present work	7.62	812.42	103.62	20470
		Rousseau [24]	7.60	736	108.90	20388
		Dardouri [28]	7.58	612.49	123.60	21090

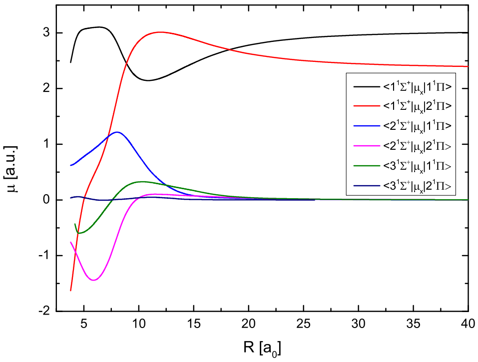

Figure 2. Transition dipole moment functions between states of symmetries $^1\Sigma^+$ and $^1\Pi$.

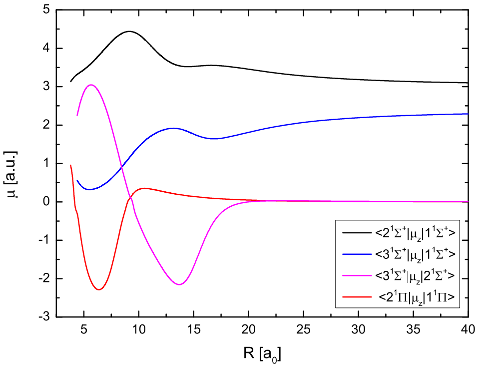

Figure 3. Transition dipole moment functions between states of the same symmetry.

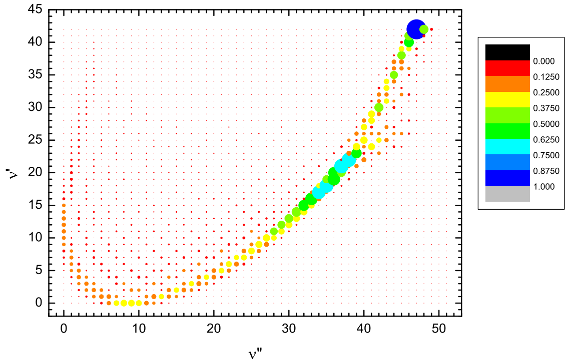

Figure 4. Franck-Condon factors for transitions between all v'' vibrational levels of the $1^1\Sigma^+$ ground state with all v' vibrational levels of the $3^1\Sigma^+$ excited state.

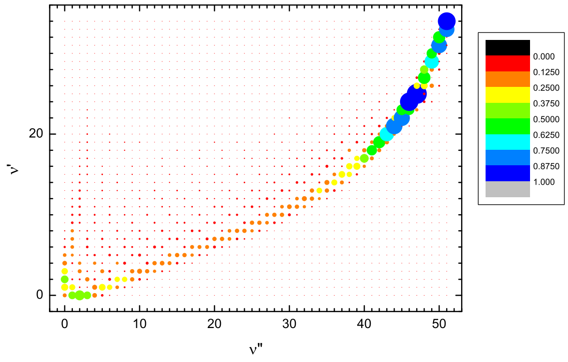

Figure 5. Franck-Condon factors for transitions between all v'' vibrational levels of the $1^1\Sigma^+$ ground state with all v' vibrational levels of the $1^1\Pi$ excited state.

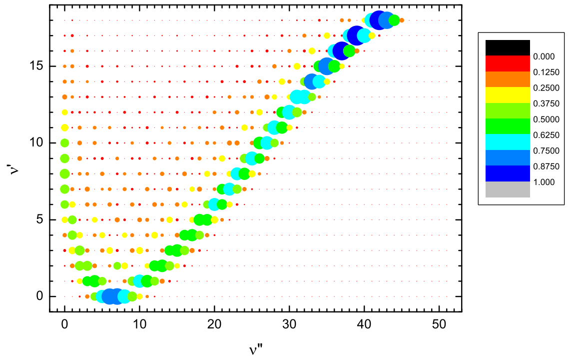

Figure 6. Franck-Condon factors for transitions between all v'' vibrational levels of the $1^1\Sigma^+$ ground state with all v' vibrational levels of the $2^1\Pi$ excited state.

In Fig. 7, the PA transition for the third and fourth PA schemes is shown at a smaller internuclear distance than the one for the first and second schemes. The reason for this lies in the existence of the low and broad potential barrier of the $3^1\Sigma^+$ state; this causes its outer turning points to lie at shorter distances than in the case of the $1^1\Pi$ state.

The third PA scheme (Fig. 7) again takes the promising probability of spontaneous emission from the $3^1\Sigma^+$ state to low vibrational level $v'' = 3$ of the ground electronic state $1^1\Sigma^+$. In order to populate one of the high vibrational states, such as $v' = 38$, 39 or 40 of $3^1\Sigma^+$, the PA light has to be red detuned from the lithium resonance energy by values 98, 51 and 10 cm^{-1}, respectively. The upper-state vibrational wavefunctions have the best overlap with the $v'' = 3$ level of the ground state $1^1\Sigma^+$. The appropriate

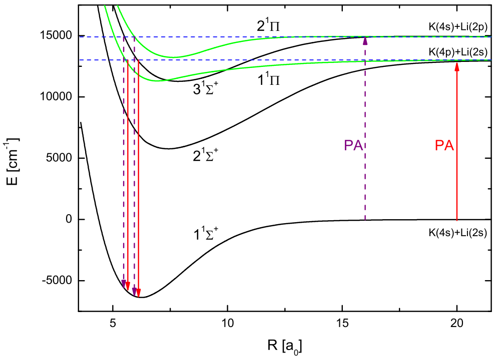

Figure 7. Calculated molecular potential energy curves of singlet states. The vertical arrows indicate photoassociation and radiative decay while the horizontal broken blue lines correspond to the K(4p)+Li(2s) and K(4s)+Li(2p) atomic asymptotes. From the right, the radiative-decay arrows are connected with the first, fourth, second and third PA schemes as described in Section 3. The red arrows are associated with the first and second PA scheme, the purple broken ones with the third and fourth PA schemes.

Franck-Condon factors are around 0.02 (Fig. 4) and classical inner turning points are around 5.52 a_0 (Fig. 7). The value of the transition dipole moment at an internuclear distance around 5.5 a_0 is quite large and is equal to 0.32 $a.u.$ (Fig. 3).

The fourth presented PA scheme (also Fig. 7) is in fact a variant of the previous scheme. We assume the existence of resonant couplings between the vibrational states $v' = 38$, 39 and 40 of $3^1\Sigma^+$ and the vibrational states $v' = 15, 16$ and 17 of $2^1\Pi$. The energy differences between these levels are very small. For instance, the energy difference between $v' = 39$ of $3^1\Sigma^+$ and $v' = 16$ of $2^1\Pi$ does not exceed 2 cm^{-1}. These resonant couplings make it possible to access the vibrational level $v'' = 0$ of $1^1\Sigma^+$ from $v' = 15, 16$ and 17 of the $2^1\Pi$ state. In this PA scheme the Franck-Condon factors are relatively large reaching the value of 0.13 (Fig. 6). The classical inner turning points for three vibrational levels $v' = 15$, 16 and 17 of the $2^1\Pi$ state are 5.99, 5.96 and 5.95 a_0, respectively (Fig. 7). In turn, the value of the transition dipole moment for these internuclear distances is around 0.47 $a.u.$ (Fig. 2). As mentioned above in relation to the previous scheme, in order to populate the vibrational levels $v' = 38, 39$ and 40 of $3^1\Sigma^+$ laser light with red detuning from 10 to 98 cm^{-1} should be used. In our estimation of detuning we do not take into account the thermal energy of ultracold colliding atoms, since they are very slow.

4. Conclusions

We have performed nonrelativistic *ab initio* calculations of adiabatic potential energy curves of KLi. The studied molecular states correlate for large internuclear distance to three atomic asymptotes: K(4s) + Li (2s), K(4p) + Li(2s) and K(4s) + Li(2p). We have drawn comparisons between the molecular constants derived from our curves and those from other theoretical and experimental studies, finding some good agreement overall. We have also presented transition dipole moments and chosen sets of Franck-Condon factors. These results have been used in the description of four photoassociation schemes. Two of these schemes have been previously discussed by other authors, though we have added some useful theoretical details concerning vibrational levels and the values of expected red detunings. The two other schemes use the laser light at an energy very near the resonance energy (2s-2p) in the lithium atom. One of these schemes is direct, involving only the $3^1\Sigma^+$ state and enabling the population of the vibrational level $v'' = 3$ of the $1^1\Sigma^+$ ground state. The other relies on the resonant couplings between the vibrational levels of the $3^1\Sigma^+$ and $2^1\Pi$ states and allows the population of the vibrational level $v'' = 0$ of the $1^1\Sigma^+$ state. We also expect that some high resolution spectra of the bound-free absorption may be experimentally recorded once the detunings suggested in this paper are taken into account. The small region around the given detuning value has to be systematically scanned; this particularly applies to PA schemes connected with the resonant transition (2s-2p) in the lithium atom. All of our detailed numerical results are available at `http://aqualung.mif.pg.gda.pl/kli/photoassociation`.

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