

Available online at www.sciencedirect.com



Chemical Physics Letters 402 (2005) 126-132

CHEMICAL PHYSICS LETTERS

www.elsevier.com/locate/cplett

# Preparation of a wave packet through a mixed level in Li<sub>2</sub>; predissociation of one member of the superposition

Xingcan Dai, Elva A. Torres, Eliza-Beth W. Lerch, Dalziel J. Wilson, Stephen R. Leone \*

Department of Chemistry and Department of Physics, University of California, Berkeley, CA 94720, USA

Received 1 November 2004 Available online 22 December 2004

#### Abstract

Through a mixed level, which has characters of both the  $A^1\Sigma_u^+$  and  $b^3\Pi_u$  states of Li<sub>2</sub>, several singlet and triplet Rydberg states are accessed simultaneously using an ultrafast laser. The electronic, vibrational and rotational wave packets of these Rydberg states are detected. Since a single member of the excited superposition,  $2^3\Sigma_g^+$  (v = 12, N = 16), is predissociative, the intensities of the quantum beats that have a component of this state decrease much faster with time ( $\approx 250$  ps) than the other stable states. The polarization dependence of the quantum beats is utilized to assign the spectra.

© 2004 Elsevier B.V. All rights reserved.

## 1. Introduction

Molecular motion has been studied intensely since the introduction of femtosecond laser systems [1,2]. One of the remarkable examples is the study of molecular wave packets using pump-probe techniques. Lithium dimer serves as a benchmark molecule for theoretical and experimental spectroscopic studies because of its simple structure [3,4]; it has also recently become a valuable system for coherent control dynamics research [5–9]. Most molecular dynamics studies of Li2 and other homonuclear alkali diatomic molecules are focused on the singlet states of these molecules because direct transitions from the singlet states to the triplet states are not allowed. However, triplet states contain much more information on the potential molecular dynamics, such as spin-orbit coupling and spin-spin coupling. In high resolution spectroscopy, many experimental methods have been designed to detect the triplet states of molecules; among them, the perturbation facilitated optical-optical double resonance (PFOODR) has proven

\* Corresponding author. Fax: +1 510 643 1376.

E-mail address: srl@berkeley.edu (S.R. Leone).

to be a powerful method to study the high-lying triplet states of diatomic molecules [10–12]. The triplet states can be reached through mixed levels that have characters of both the singlet and triplet states due to the spin–orbit interaction between the singlet and triplet states. Many triplet states of the alkali dimers have been studied and characterized with this method. This Letter extends this method to the study of wave packet dynamics in the time domain.

In this Letter, we use a cw laser to excite a single transition from the ground state of Li<sub>2</sub> to a mixed level of the  $A^{1}\Sigma_{u}^{+}$  state that is perturbed by a level of the  $b^{3}\Pi_{u}$  state and thus has components of both states. Through this mixed level, higher-lying singlet states and triplet states are accessed creating wave packets of these states. The predissociation process of the triplet state,  $2^{3}\Sigma_{g}^{+}$ , is directly observed by the loss of specific quantum beats as a function of time.

# 2. Experimental setup

The experimental setup has been described in detail in previous Letters of this group [5]. In brief, the lithium

<sup>0009-2614/\$ -</sup> see front matter @ 2004 Elsevier B.V. All rights reserved. doi:10.1016/j.cplett.2004.12.014

dimer is prepared by heating lithium to about 1100 K in a stainless steel heat pipe. Fig. 1 shows the excitation steps for the coherent wave packet in Li<sub>2</sub>. A cw laser provides a launch state by exciting a transition from the ground state to an energy level of  $A^1\Sigma_u^+$ , an ultrafast laser pulse then excites the molecule from this level to one or several low-lying Rydberg states, and another time-delayed ultrafast laser pulse is used as the probe beam, exciting the wave packet to the ground state of Li<sub>2</sub><sup>+</sup>. The delay time between the pump and probe pulse is controlled by a precision delay stage. The ion signals are collected by a pair of electrodes located in the heat pipe and are sent to a lock-in amplifier.

The difference between this experiment and our previous ones, as mentioned in Section 1, is that a mixed level of  $A^1\Sigma_u^+$  (or  $b^3\Pi_u$ , in Fig. 1) is selected for a launch level, instead of an unperturbed level. Since this mixed level has characteristics of the singlet states and triplet states, both the singlet and triplet states can be reached using it. Mixed levels have often been used to study the spectra of Li<sub>2</sub>, especially those triplet states that cannot be reached by the usual pump-probe method. Unfortunately, there are only a few mixed levels available for Li2 because of the weak spin-orbit coupling. In this experiment, we choose the mixed level,  $A^{1}\Sigma_{u}^{+}$  (v = 17, J = 15,  $E = 18163.216 \text{ cm}^{-1}$ )- $b^3 \Pi_u$  (v = 22, N = 16, J = 15,  $E = 18163.239 \text{ cm}^{-1}$ ), since the two levels are strongly perturbed by each other, indicating that they are well mixed [11]. From this level, several Rydberg states, including  $2^{3}\Sigma_{g}^{+}$ ,  $2^{3}\Pi_{g}$ , and  $E^{1}\Sigma_{g}^{+}$ , can be accessed with an 807 nm photon generated by the Ti:sapphire ultrafast laser system [11–13]. Under the conditions in this experiment, the Doppler linewidth of  $Li_2$  is about 0.1 cm<sup>-1</sup>, which is larger than the energy difference between two

levels, thus both levels are excited simultaneously in our experiment; however, this does not change the experimental results since both levels have the characters of both states. They are designated a level of  $A^1\Sigma_u^+$  or  $b^3\Pi_u$  because one has a greater component of the  $A^1\Sigma_u^+$  state and the other has a greater component of the  $b^3\Pi_u$  state.

### 3. Results and discussions

#### 3.1. Theoretical model of the wave packet quantum beats

A theoretical model of the pump-probe wave packet experiment has been given in [6]. The results are cited here with some slight modification. The initial state, the wave packet states, and the final ion state are designated as  $|i\rangle$ ,  $|n\rangle$ , and  $|f\rangle$ , respectively. The total photoionization signal as a function of pump-probe delay,  $\tau$ , can be expressed as

$$S(\tau) = \sum_{f} \left( \sum_{n} |a_{ni}|^2 |b_{fn}|^2 + 2 \sum_{n,m,n>m} \Re e[b_{fn}^* b_{fm} a_{ni}^* a_{mi}] \times \cos(\omega_{nm}\tau + \varphi_{nm} + \varphi_{fnm}) \right),$$
(1)

where  $a_{ni} = \varepsilon_{pu}(\omega_{ni})\langle n|\mathbf{\mu}_{pu} \cdot \hat{\mathbf{e}}_{pu}|i\rangle$ ,  $b_{fn} = \varepsilon_{pr}(\omega_{fn}) \times \langle f|\mathbf{\mu}_{pu} \cdot \hat{\mathbf{e}}_{pr}|n\rangle$ ,  $\omega_{nm} = \omega_n - \omega_m$  are the quantum beat frequencies,  $\varepsilon_{pu}(\omega_{ni})$  and  $\varepsilon_{pr}(\omega_{fn})$  are frequency-dependent amplitudes of the pump and probe pulses,  $\mathbf{\mu}_{pu}$  and  $\mathbf{\mu}_{pr}$  are the dipole moment operators of the pump and probe steps, and  $\hat{\mathbf{e}}_{pu}$  and  $\hat{\mathbf{e}}_{pr}$  are the polarizations of the pump and probe pulses,  $\boldsymbol{\mu}_{pu}$  are the relative phases transferred by the pump and probe pulses, respectively.



Fig. 1. The relevant potential curves of Li<sub>2</sub>. The three arrows indicate the three-step excitation in this experiment.

Assuming the molecular state wavefunctions are the products of the electronic, vibrational and rotational wavefunctions, i.e.,  $|n\rangle = |e_n\rangle|v_n\rangle|J_nM_n\rangle$ , the transition probability coefficient for the pump step can be expressed explicitly as

$$a_{ni} = \varepsilon_{\rm pu}(\omega_{ni}) \langle e_n | \mu_{\rm pu}(r) | e_i \rangle \langle v_n | v_i \rangle \langle J_n M_n | \hat{\mathbf{z}} \cdot \hat{\mathbf{e}}_{\rm pu} | J_i M_i \rangle.$$
(2)

Here,  $\hat{z}$  refers to the z-axis of the molecular coordinate system. The other coefficients can be written in similar expressions. The term  $\langle e_n | \mu_{pu}(\mathbf{r}) | e_i \rangle$  is the matrix element of the electronic transition dipole moment;  $\langle v_n | v_i \rangle$  is the vibrational overlap between two states, which is the square root of the Franck-Condon factor of the two states up to a phase factor and provides some insight to the intensity of the different quantum beats we obtain in this experiment. The term  $\langle J_n M_n | \hat{\mathbf{z}} \cdot \hat{\mathbf{e}}_{pu} | J_i M_i \rangle$  is the rotational overlap and gives rise to the polarization dependence of wave packet signals. The intensities of rotational wave packet signals strongly depend upon the polarization of the pump and probe laser pulses [14–16]. As a special case, if  $|\Delta J| = 2$  between two states in a quantum beat, it can be shown that purely rotational beats are completely eliminated when the angle between the pump and probe polarizations is 54.71° ('magic angle'); only non-oscillatory parts remain in the total photoionization signals.

The amplitude of the wave packet signals will decrease with time due to the limited lifetimes of all excited states and the collision-induced dephasing of the superposition states. Since the lifetimes of the different states are not correlated, if one member of the wave packet rapidly predissociates, the amplitudes of quantum beats containing this state will decrease more rapidly with time than the others.

## 3.2. The assignment of quantum beats

Fig. 2a shows the FFT spectra of the wave packet signals obtained in this experiment when the polarization directions of pump and probe pulses are parallel, which is the normal experimental condition. An intense peak at 21.29 cm<sup>-1</sup> and several small peaks at 14.64, 16.41, 37.89 and 79.49 cm<sup>-1</sup> are observed. The differences between Figs. 2a and b, which are caused by the polarization of laser pulses, will be discussed later in this section. By comparing the frequencies of the quantum beats with the spectroscopic data from high resolution spectroscopic measurements, we can assign the beat frequencies to the energy differences between several Rydberg states,  $2^3\Sigma_g^+$ ,  $2^3\Pi_g$ , and  $E^1\Sigma_g^+$ . The results are presented in Table 1 and the energy levels involved are shown in Fig. 3.

All the transitions from the mixed levels to the different electronic states and from the Rydberg states to the ground state of  $Li_2^+$  also are presented in Fig. 3. For the sake of conciseness, only the energy levels of the Rydberg states that can be accessed by the bandwidth  $(\sim 160 \text{ cm}^{-1})$  of the pump and probe pulses and are allowed by the selection rules are shown in Fig. 3. According to the selection rules and the intensities of the rotational lines, transitions from  $b^3 \Pi_u N' = 16$  to  $2^3 \Sigma_g^+$ include only a Q line, i.e.,  $\Delta N = 0$  [11], while transitions from  $b^{3}\Pi_{u} N' = 16$  to  $2^{3}\Pi_{g}$  have a P, a weak Q, and an R line, i.e.,  $\Delta N = 0, \pm 1$  [12], and only a P and an R line are excited during the transitions from the  $A^{1}\Sigma_{n}^{+}$  to the  $E^{1}\Sigma_{g}^{+}$  state. The transition rules from the Rydberg states to the ion state are more complicated. It has been shown that only  $N^+-J = 0$ , -2 are allowed for the  $E^1\Sigma_g^+$  state in the present experiment [6] and the selection rules derived for the two triplet states are  $N^+ - J = 0$ , -2 for the  $2^3 \Pi_{g}$ 



Fig. 2. The FFT spectra when the angle between the pump and probe polarizations is (a)  $0^{\circ}$  or (b) 55°. The assignment of the quantum beats is listed in Table 1.

Table 1The assignment of the observed quantum beats

Peak	Observed position (cm <sup>-1</sup> )	Assignment $(v_m, J_m) \leftrightarrow (v_n, J_n)$	High resolution result (cm <sup>-1</sup> )
Erot	14.64	$E^1\Sigma^+_{\alpha}$ (23, 14) $\leftrightarrow E^1\Sigma^+_{\alpha}$ (23, 16) or	14.68
		$E^{1}\Sigma_{a}^{+}$ (22, 14) $\leftrightarrow E^{1}\Sigma_{a}^{+}$ (22, 16)	14.84
$\Sigma - \Pi(P)$	16.41	$2^{3}\Sigma_{a}^{\ddagger}$ (12, 16) $\leftrightarrow 2^{3}\Pi_{g}^{\ddagger}$ (3, 15)	16.26
П–П	21.29	$2^{3}\Pi_{g}^{s}(3, 15) \leftrightarrow 2^{3}\Pi_{g}(3, 17)$	21.49
$\Sigma - \Pi(\mathbf{R})$	37.89	$2^{3}\Sigma_{g}^{+}$ (12, 16) $\leftrightarrow 2^{3}\Pi_{g}$ (3, 17)	37.75
Evib	79.49	$E^1\Sigma^+_{\sigma}$ (22, 14) $\leftrightarrow E^1\Sigma^+_{\sigma}$ (23, 14) or	79.04
		$E^{1}\Sigma_{\sigma}^{\ddagger}$ (22, 16) $\leftrightarrow E^{1}\Sigma_{\sigma}^{\ddagger}$ (23, 16)	78.88

The numbers in the parentheses are the vibrational and rotational numbers separately.



Fig. 3. The allowed transitions between the states accessed and the energy differences between the energy levels covered by the pump pulses. The numbers in the parentheses are the vibrational and rotational quantum numbers, respectively. 50.82 cm<sup>-1</sup>, which is the energy difference between the level  $2^{3}\Pi_{g}$  (v = 3, N = 15) and E  ${}^{1}\Sigma_{g}^{+}$  (v = 22, N = 14) and serves as a reference energy, is not observed as a quantum beat in this experiment since these two levels do not reach a common final level.

state and  $N^+ - J = -1$  for the  $2^3 \Sigma_g^+$  state [17]. Combining all the transition rules together, the quantum beats that should be present in the spectra are the rotational and vibrational quantum beats of the  $E^1 \Sigma_g^+$  state, the rotational beats of the  $2^3 \Pi_g$  state, and the electronic beats between the  $2^3 \Sigma_g^+$  and  $2^3 \Pi_g$  states. There are no rotational beats of the  $2^3 \Sigma_g^+$  state since only one level is excited.

The vibrational overlap factors between states are calculated with Le Roy's program, LEVEL [18]. The results are presented in Table 2. The calculation results show that the vibrational overlaps between the launch state,  $A^1\Sigma_u^+$  or  $b^3\Pi_u$ , and the Rydberg states are strong for all three Rydberg states, however, only the vibrational overlap between  $2^3\Pi_g$  and  $X^2\Sigma_g^+$  is reasonably large for the probe step. This explains why the intensity of the rotational beat of the  $2^3\Pi_g$  state is extraordinarily large in the spectra.

The intensities of the rotational wave packets depend upon the relative polarization of the pump and probe

 Table 2

 The calculated vibrational overlap factors between the states

	$\mathbf{A}^{1}\boldsymbol{\Sigma}_{\mathrm{u}}^{+} \; (v=17)$	$b^{3}\Pi_{u} (v = 22)$	$X^2 \Sigma_g^+ \ (v = 5)$
$2^{3}\Pi_{g} (v=3)$		$2.82 \times 10^{-1}$	$1.70 \times 10^{-1}$
$2^{3}\Sigma_{\sigma}^{+}$ (v = 12)		$4.51 \times 10^{-1}$	$-1.96 \times 10^{-5}$
$E^{1}\Sigma_{\sigma}^{+}$ (v = 22)	$-1.01 \times 10^{-1}$		$-2.80 \times 10^{-4}$
$E^1 \Sigma_g^{\stackrel{\sim}{+}} (v = 23)$	$1.64 \times 10^{-1}$		$4.17 \times 10^{-4}$

beams, while the intensities of the ro-vibrational or electronic quantum beats, in which two energy levels are from different vibrational levels or different electronic states, do not depend upon the polarization of the pump and probe beams. This property can help us distinguish the purely rotational beats from the other beats. In this experiment, the polarization of the probe is rotated by a half-wave plate. The FFT spectra shown in Fig. 2 are obtained when the polarizations of the pump and probe are either parallel or at the 'magic angle'. The quantum beats at 14.64 and  $21.29 \text{ cm}^{-1}$  are eliminated from the

transient ion signal when the difference in polarization of the pump and probe is set to approximately the magic angle, which indicates that these two beats are rotational and the difference between the rotational quantum numbers of the two components in those quantum beats is two, i.e.,  $|\Delta J| = 2$ . This is in agreement with the previous assignment of those beats as the purely rotational beats of either the  $E^{1}\Sigma_{g}^{+}$  or  $2^{3}\Pi_{g}$  states.

# 3.3. Predissociation of the $2^{3}\Sigma_{g}^{+}$ state

The predissociation of the  $2^{3}\Sigma_{g}^{+}$  state has been observed in high resolution spectra by observation of the  $2p \rightarrow 2s$  atomic fluorescence [11]. In the time domain experiment, we are able to monitor the predissociation process of a single member of the wave packet in real time. Since the intensities of the beats that contain the energy level of the  $2^3\Sigma_g^+$  state are not strong, the wave packet signals of the predissociative beats are noisy. Therefore, the FFT spectra obtained in different time periods are a good way to measure the decrease of the intensities of the predissociative quantum beats. To do this experimentally, we scan the computer-controlled delay stage for the probe pulse for a period of time, which is 133 ps in this experiment, then manually move the compensation mirror in the path of the pump beam with a step size of 66.7 ps to increase the time delay between the pump and the probe beam and scan the probe for the same period of time, 133 ps,

from the new position. The amplitudes of the wave packets in the time domain are proportional to the intensities of the quantum beats in FFT spectra. As shown in Fig. 4, the intensities of two quantum beats that have the components of the  $2^{3}\Sigma_{g}^{+}$  state decrease dramatically compared with the other quantum beats. In Fig. 5, the ratios of the intensities of the quantum beats divided by the intensity of the rotational beat of the  $2^{3}\Pi_{g}$  state are graphed versus time, which clearly shows that the intensities of the two predissociative quantum beats decrease compared with the intensity of the rotational beat of the  $2^{3}\Pi_{g}$  state, while the intensities of the rotational and vibrational quantum beats of the  $E^{1}\Sigma_{g}^{+}$  state remain constant. The average lifetime of the predissociative level can be estimated by fitting the two curves to an exponential decay, which results in 250 ps ( $\pm 30$  ps) in this experiment.

The predissociation of  $2^{3}\Sigma_{g}^{+}$  is caused by the Luncoupling between the  $2^{3}\Sigma_{g}^{+}$  state and the  $1^{3}\Pi_{g}$  state, which is an unbound state and dissociates to 2s + 2p. The L-uncoupling allows for the perturbations between two states with  $\Delta A = \Delta \Omega = \pm 1$  and  $\Delta S = 0$ . The matrix element of the Hamiltonian coupling the two states,  $2^{3}\Sigma_{g}^{+}$  and  $1^{3}\Pi_{g}$ , which can be found in [19], is:

$$\begin{aligned} \mathbf{H}_{v,J;E,J} &= \langle \Psi_{v,J} | - \frac{1}{2\mu R^2} \mathbf{J}^{\pm} \mathbf{L}^{\mp} | \Psi_{E,J} \rangle \\ &\cong - \langle v | \frac{1}{2\mu R^2} | E \rangle \langle^3 \Sigma | \sum_i \mathbf{l}_i^{\mp} |^3 \Pi \rangle [J(J+1)]^{1/2}. \end{aligned} (3)$$



Fig. 4. FFT spectra of the wave packet observed during two different time periods. The top one is the FFT of the wave packet signals when the delay stage scans from 0 to 133 ps, while the bottom one is the FFT when the delay stage scans from 333 to 466 ps. It shows the decrease of the intensities of the predissociative quantum beats, labeled  $\Sigma$ – $\Pi$ .



Fig. 5. The relative intensity of the quantum beats versus time. The *x*-axis is the relative delay time between the pump and the probe beams created by moving the compensation mirror in the path of the pump beam with a step size of 66.7 ps. The intensities of all quantum beats are recorded from the FFT spectra of the wave packet signals by scanning the delay stage in the path of the probe beam for the same period of time, 133 ps, at each step.

Here,  $\langle \Psi_{v,J} |$ ,  $\langle v |$ , and  $\langle {}^{3}\Sigma |$  are the total wavefunction, vibrational wavefunction and electronic wavefunction of the bound state,  $2{}^{3}\Sigma_{g}^{+}$ ; while  $\langle \Psi_{E,J} |$ ,  $\langle E |$ , and  $\langle {}^{3}\Pi |$ are the total wavefunction, vibrational wavefunction and electronic wavefunction of the continuum state,  $1{}^{3}\Pi_{g}$ . The lifetime *T* of the predissociative level, according to Fermi's Golden Rule, has a relationship with the above matrix element of the Hamiltonian, as follows,

$$\frac{1}{T} = \frac{2\pi}{\hbar} \left| H_{\nu,J;E,J} \right|^2. \tag{4}$$

In the treatment of the interaction between  $2^{3}\Sigma_{g}^{+}$  and  $1^{3}\Pi_{g}$ , the second term in the expression of the matrix element,  $\langle {}^{3}\Sigma|\sum_{i} \mathbf{l}_{i}^{+}|^{3}\Pi\rangle \cong \sqrt{l(l+1)} = \sqrt{2}$  since l = 1 for a 2p Rydberg electron. The first term in Eq. (3),  $\langle v|1/2\mu R^{2}|E\rangle$ , can be calculated using the BCONT program [20]. Ab initio potential curves have been used in the calculation since there is no experimental data available for the  $1^{3}\Pi_{g}$  state. The calculated lifetime of  $2^{3}\Sigma_{g}^{+}$  (v = 12, N = 16) is about 950 ps, which is on the same order of magnitude as the experimental measurement,  $\approx 250$  ps.

## 4. Conclusions

The quantum beats of the triplet Rydberg states along with the singlet Rydberg states in Li<sub>2</sub> are observed using a mixed level as a launch state. They are assigned as the rotational quantum beats of the  $2^{3}\Pi_{g}$  state, the electronic quantum beats between  $2^{3}\Pi_{g}$  and  $2^{3}\Sigma_{g}^{+}$ , and rotational and vibrational quantum beats of the  $E^{1}\Sigma_{g}^{+}$  state. The assignment of quantum beats is confirmed by changing the polarization of the probe beam, which allows us to distinguish the purely rotational beats from the other types of quantum beats. Since the  $2^{3}\Sigma_{g}^{+}$  state is predissociated through the  $1^{3}\Pi_{g}$  state, we observed a real time decay of the intensities of only those quantum beats that have the component of the  $2^{3}\Sigma_{g}^{+}$  state. The lifetime of the predissociative energy level,  $2^{3}\Sigma_{g}^{+}$ (v = 12, N = 16), is calculated based on the assumption that the predissociation is caused by the L-uncoupling between  $2^{3}\Sigma_{g}^{+}$  and  $1^{3}\Pi_{g}$ , and the calculation agrees with the experimental observations in approximate magnitude.

#### Acknowledgement

The financial support of this work by the Chemistry Division of the National Science Foundation is gratefully acknowledged.

## References

- [1] A.H. Zewail, J. Phys. Chem. A 104 (2000) 5660.
- [2] M. Dantus, A. Zewail, Chem. Rev. 104 (4) (2004) 1717.
- [3] I. Schmidt-Mink, W. Muller, W. Meyer, Chem. Phys. 92 (1985) 263.
- [4] D.D. Konowalow, J.L. Fish, Chem. Phys. 84 (1984) 463.
- [5] J.M. Papanikolas, R.M. Williams, P.D. Kleiber, J.L. Hart, C. Brink, S.D. Price, S.R. Leone, J. Chem. Phys. 103 (1995) 7269.
- [6] R. Uberna, M. Khalil, R.M. Williams, J.M. Papanikolas, S.R. Leone, J. Chem. Phys. 108 (1998) 9259.

- [7] R. Uberna, Z. Amitay, R.A. Loomis, S.R. Leone, Faraday Discuss. 113 (1999) 385.
- [8] L. Pesce, Z. Amitay, R. Uberna, S.R. Leone, M. Ratner, R. Kosloff, J. Chem. Phys. 114 (2001) 1259.
- [9] Z. Amitay, R. Kosloff, S.R. Leone, Chem. Phys. Lett. 359 (2002) 8.
- [10] L. Li, A.M. Lyyra, Spectrochim. Acta Part A 55 (1999) 2147.
- [11] G. Lazarov, A.M. Lyyra, L. Li, J. Mol. Spectrosc. 205 (2001) 73.
- [12] A. Yiannopoulou, K. Urbanski, S. Antonova, A.M. Lyyra, L. Li, T. An, T.J. Whang, B. Ji, X.T. Wang, W.C. Stwalley, T. Leininger, G.-H. Jeung, J. Chem. Phys. 103 (1995) 5898.
- [13] R.A. Bernheim, L.P. Gold, C.A. Tomczyk, C.R. Vidal, J. Chem. Phys. 87 (1987) 861.
- [14] R.N. Zare, Angular Momentum–Understanding Spatial Aspects in Chemistry and Physics, Wiley, New York, 1988.

- [15] A.J. Cross, D.H. Waldeck, G.R. Fleming, J. Chem. Phys. 78 (1983) 6455.
- [16] P.M. Felker, A.H. Zewail, J. Chem. Phys. 86 (1987) 2460.
- [17] J. Xie, R.N. Zare, J. Chem. Phys. 93 (1990) 3033.
- [18] R.J. Le Roy, LEVEL 7.5: A Computer Program for Solving the Radial Schrödinger Equation for Bound and Quasibound Levels, University of Waterloo Chemical Physics Research Report CP-655, 2002.
- [19] H. Lefebvre-Brion, R.W. Field, Perturbations in the Spectra of Diatomic Molecules, Academic Press, San Diego, 1986.
- [20] R.J. Le Roy, G.T. Kraemer, BCONT 2.1: A Computer Program for Calculating Bound→Continuum Transition Intensities for Diatomic Molecules, University of Waterloo Chemical Physics Research Report CP-650R, 2002.