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MOLECULAR CONSTANTS OF THE $2^1\Pi$ STATE OF NaLi MOLECULE

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Abstract. *We report our determination of the molecular constants for the $2^1\Pi$ state of NaLi from a set of 732 spectral lines. Using the linear least-squares fitting method, an optimum set of molecular constants, which corresponds to dimensionless root mean of squares of deviation $\sigma = 0.62$ within 0.1 cm^{-1} experimental uncertainty, have been derived.*

I. INTRODUCTION

The alkali-metal diatomic molecules with their main absorption bands in the UV-VIS region are very appropriated for modern laser spectroscopy techniques. Experimental investigations for these molecules have further promoted since the emergence of molecular Bose-Einstein condensates (see [1] and references therein). As several experimental techniques related to cold molecules involve optical excitation either in the formation and/or detection stages, a precise spectroscopic characterization of excited molecular states is necessary.

Among alkali-metal diatomic molecules NaLi is particularly interested because it is the lightest hetero-nuclear type and has permanent dipole moment, thus can be manipulated with external electric fields. Several experimental investigations for the $^1\Sigma^+$ and $^1\Pi$ symmetric types were performed to study up to the $9^1\Sigma^+$ and $7^1\Pi$ excited states [2-7]. Among those, the $2^1\Pi$ state was still known only at vibrational resolution [4].

In this paper we determine the molecular constants for the $2^1\Pi$ state of NaLi based our recent experimental data [8].

II. MOLECULAR CONSTANTS OF THE $2^1\Pi$ STATE

The experimental data used in this work consist of 732 spectral lines in the $2^1\Pi \leftarrow 1^1\Sigma^+$ band. The data were obtained by the polarization labeling spectroscopy technique [8] within to 0.1 cm^{-1} experimental uncertainty. Distribution of the data field corresponding

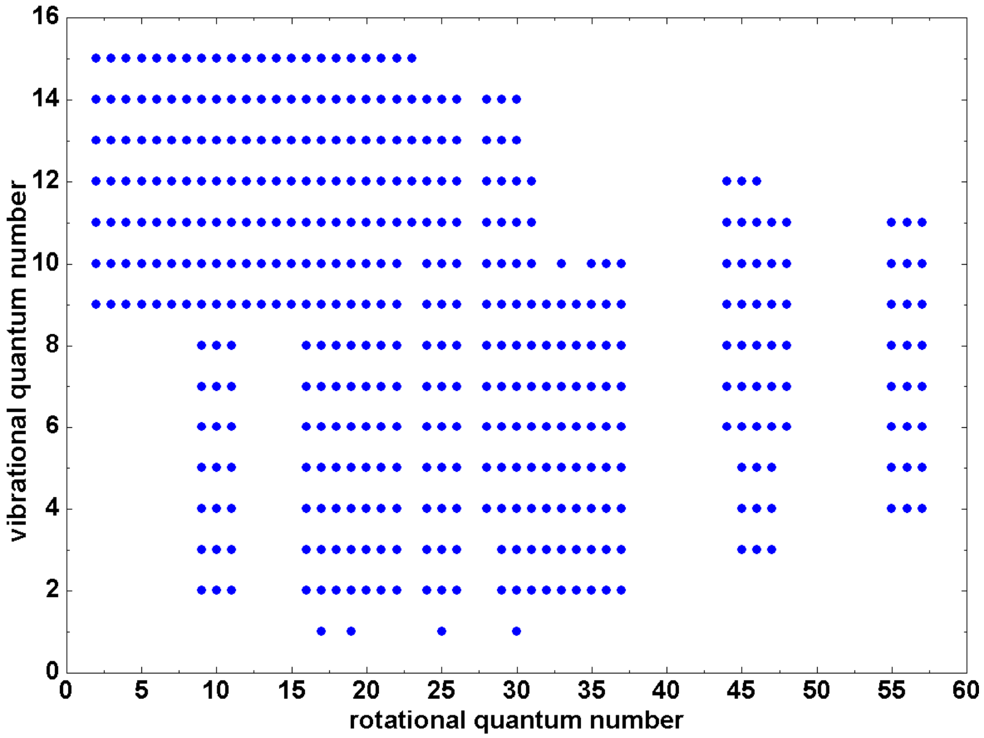

Fig. 1. Distribution of data field with the corresponding vibrational and rotational quantum numbers in the $2^1\Pi$ state.

to rotational and vibrational quantum numbers in the $2^1\Pi$ state is presented in detail in Fig. 1.

Once spectral lines had been assigned quantum numbers, their wave number $\bar{v}$ were fitted to the following relation:

$$\bar{v} = T'(v', J') - T"(v", J") + \delta. \tag{1}$$

In the Eq. (1), T' and T'' represent term values of the upper and lower states, respectively; δ describes the Λ-doubling in the $2^1\Pi$ state, given by

$$\delta = q_e[J(J+1) - 1], \tag{2}$$

where, q_e represents lambda-doubling coefficient for e-parity levels which gives rise to P and Q transitions. The spectroscopic term value $T(v, J)$ is represented with the conventional Dunham expansion:

$$T(v, J) = T_e + \sum_k \sum_l Y_{kl}(v + \tfrac{1}{2})^k [J(J+1) - 1]^l, \tag{3}$$

where T_e and and Y_{kl} stand for electronic energy and Dunham coefficient, respectively. The term values for the labelled levels were calculated by using Dunham coefficients obtained from [2] and fixed during the fitting procedure. The final optimum set of Dunham coefficients for the $2^1\Pi$ state corresponding to a dimensionless root mean of squares of deviation $\sigma = 0.62$ has been obtained, and listed in Table 2.

Table 1. Molecular constants of the $2^1\Pi$ state of NaLi

Constants	Value [cm^{-1}]	Error [%]
Y_{00} (T_e)	22296.72539	0.001
Y_{10} (ω_e)	151.3553669	0.061
Y_{20} ($-\omega_e x_e$)	-1.212648477	2.097
Y_{30}	-0.1163013955	2.874
Y_{40}	0.5415371×10^{2}	3.810
Y_{50}	$-0.2242726086\times10^{3}$	2.138
Y_{01} (B_e)	0.2255917721	0.064
Y_{11}	$-0.2459652022\times10^{2}$	2.44
Y_{21}	0.8435599232×10^{4}	9.029
Y_{31}	-0.204878997×10^{4}	1.444
Y_{02}	-0.178619694×10^{5}	2.102
Y_{12}	-0.653086282×10^{7}	16.828
Y_{22}	$-0.1834230918\times10^{7}$	4.254
q_e	$-0.9339851354\times10^{4}$	5.715
D_e	17620	
σ	0.62	

Since the $2^1\Pi$ state associates to Na(3^2P)-Li(2^2S) atomic asymptotes, its dissociation energy can be determined by

$$D_e[2^1\Pi] = \Delta + D_e[1^1\Sigma^+] - T_e[2^1\Pi], \tag{4}$$

where, Δ is energy separation between the Na(3P) and Na(3S) atomic states, $D_e[1^1\Sigma^+]$ is dissociation energy of the ground electronic state $1^1\Sigma^+$. Taking electronic energy $T_e[2^1\Pi]$ from this work; Δ = 16965 cm^{-1} from [9]; and $D_e[1^1\Sigma^+]$ = 7105 cm^{-1} from [2]; the dissociation energy of the $2^1\Pi$ state is estimated to be D_e =1760 cm^{-1}.

From the experimental data and the dissociation energy determined above, the highest vibrational level observed here is only 17 cm^{-1} below the dissociation limit, thus the experimental data cover about 99% depth of the potential well.

Having the molecular constants, we calculated bond length R_e between the Na and Li atoms based on the following conventional relation:

$$R_e = \sqrt{\frac{\hbar}{B_e 4\pi\mu c}}\,, \tag{5}$$

where μ is reduced mass of NaLi, c is the light speed in vacuum. Taking the value of B_e in Table 2, the bond length is determined to be R_e = 3.728438 Å.

III. CONCLUSIONS

Spectroscopic structure of the $2^1\Pi$ state of NaLi has been characterized to rotational resolution for the first time. A set of molecular constants was determined based on the experimental data up to near the dissociation limit. The results give comprehensive spectroscopic characterization of the state and provide a benchmark to check reliability of modern theoretical calculations.

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