Electronic structure with dipole moment and rovibrational calculations of the MgLi and MgNa Molecules

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Electronic structure with dipole moment and rovibrational calculations of the MgLi and MgNa Molecules

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Abstract

We investigate an orderly study of the adiabatic potential energy curves for 29 and 30 low-lying $2s+1\Lambda^{+/-}$ electronic states of the molecules MgLi and MgNa respectively. The calculation has been done by using the Complete Active Space Self Consistent Field (CASSCF) followed by Multi-Reference Configuration Interaction with Davidson correction (MRCI+Q). For the investigated electronic states, the static and transition dipole moment curves are calculated along with the Einstein coefficients, the emission oscillator strength, the spontaneous radiative life time, the line strength, the classical radiative decay rate of the single-electron oscillator, the spectroscopic constants T_e , ω_e , $\omega_e x_e$, B_e , R_e , and the equilibrium dissociation energy D_e . By means of the canonical functions approach, the ro-vibrational constants E_v , B_v , D_v and the abscissas of the turning points $R_{\min}$ and $R_{\max}$, have been calculated for the considered electronic states up to the vibrational level $v = 79$. The Franck-Condon factors have been calculated and plotted for the transition between the low-lying electronic states of the two considered molecules. A good agreement is revealed between our calculated values and those available in literature. Fifty new electronic states are investigated in the present work for the first time.

1. Introduction

The research field of cold and ultracold molecules revealed that they caused a revolution in the physical chemistry and many body physics. The vibrational and rotational motions of the molecules offer degrees of freedom which motivate the theoretical and experimental studies for these molecules. They provide the opportunity for studying chemical reactions [1, 2], quantum computations [3], high precession measurement of the variation of the fine structure constant α [4], the proton to electron mass ratio $\mu=m_p/m_e$ [5-8], electron dipole moment [9, 10], high resolution molecular spectroscopy [11] and permanent electric dipole moments (PDMs) that lead to long-range dipole-dipole interactions [12]. The interatomic reactions determine many phenomena observed in Bose-Einstein Condensation material [13].

The importance of our theoretical study of the diatomic molecules MgLi and MgNa is twofold. First, magnesium atom has been considered as helping agents for cooling the decelerated molecules such as NH or NH₃ to the ultracold regime [14-16]. Second, Li is the lightest atom that can be cooled in the ground state because the Alkaline Earth Metals (AEM)-Li molecules are the attractive systems in the ultracold domain and their vibrational and rotational transitions frequencies are the largest among the ultracold molecules. Accordingly, the properties of such molecules are needed for the determination of the low-energy scattering properties and for modeling the corresponding experiments at ultracold temperature. These species have additional advantages as it is possible to keep the molecules in the single quantum state for a long period [17]. Therefore, the alkaline earth metal-lithium is proposed to be laser-cooling molecules where the magnesium lithium has received a particular interest.

Due to the lack of potential energy curves for the higher electronic states of MgLi and MgNa diatomic molecules in the literature, we investigated excessively the lowest 29 and 30 doublet and quartet electronic states of these molecules by using MRDSCI calculations where 50 electronic states have been studied here for the first time. Based on our previous theoretical calculations and the canonical functions approach [18-20], the eigenvalue E_v , the rotational constant B_v , and the abscissas of the turning points $R_{\min}$ and $R_{\max}$ have been calculated for several vibrational levels of selected electronic states. In addition to the spectroscopic constants T_e , ω_e , $\omega_e x_e$, B_e , and R_e , the Einstein coefficients and the Franck-Condon-Factor (FCF) are calculated as well.

2. Results and discussion

2.1 *ab Initio* calculation

The aim of the present work is the study of the low-lying doublet and quartet electronic states of the molecules MgLi and MgNa using the complete active space self-consistent field (CASSCF) followed by a multireference configuration interaction (MRDSCI with Davidson correction) procedure. Hence, the required calculations are performed by the computational chemistry program MOLPRO [21] using the graphical user interface GABEDIT [22]. The basis set cc-PVnZ is considered as the current state of the art of the correlated or post-Hartree-Fock calculations for Alkali and alkaline earth metal. Therefore, the basis sets used for the three atoms Mg, Na, Li are the correlation-consistent polarized valence triple zeta cc-pVTZ for the atomic orbitals s , p , d . The added f functions for the two atoms Li and Mg are cc-pVTZ.

Based on the aforesaid calculations, we were able to plot the diverse set of the curves for the adiabatic potential energy and the static and transition dipole moments in terms of the internuclear distance R . Fig. (1-4) and Figs. (FS1-FS4) (Figures in the supplementary file) represent respectively the potential energy (PECs) and static dipole moment (DMCs) curves of the low lying 14 doublet and 16 quartet electronic states of MgNa molecule. While Figs. (5-8) and Figs. (FS5-FS8) (Figures in the supplementary file) represent respectively the PECs and DMCs curves for the low-lying 14 doublet and 15 quartet electronic states for MgLi molecule.

The electric dipole moment lies at the heart of a widely used experimental method for probing the vibrational dynamics of a system [23, 24]. It is obtained because of the non-uniform distribution of charges between the two atoms of a heteropolar molecule. All applications of molecules confined in optical lattices rely on the long-range dipole-dipole interactions therefore the magnitude of the permanent electric dipole moment is a figure of merit for experiments with lattice-confined molecules [25, 26]. As it is shown in Figs. (FS1-FS8) of DMCs, the sign of the dipole moment curves can vary positively and negatively. This is due to the direction of the internuclear axis as it is originated from the nucleus Mg atom to the nuclei Li and Na atoms. The positive values signify that the excess of electron density is closer to the alkaline earth Mg atom more than the alkali Li and Na atoms whereas the negative is the opposite. For a neutral compound, and as general trend, the DMCs must tend smoothly to zero at large value of the internuclear distance R . Some electronic states, of the two considered molecules, are not obeying this rule because of the singularities in the electronic Hamiltonian operator which is giving the appearance of cusps in the exact wave function and undulation in the PECs. Which also can be explained by the breakdown of the Born-Oppenheimer (B.O) approximation where the responsible term for the so-called 'non-adiabatic effects' cannot be neglected.

In Figs. (9-10) we present the transition dipole moment curves in terms of the internuclear distance. These curves are crucial in the molecular spectroscopy for astrophysical, environmental sciences and for the research of chemical reactions for biology where the detailed microscopic properties of the molecular objects are needed [27, 28]. Due to spin forbidden transitions between two atomic orbitals at asymptotic limits most of the TDMCs vanish at large value of the internuclear distance R . In these figures one can notice changes and jumps in some TDMCs at different internuclear distances which can be explained by the radiationless electronic transitions where the electronic motion suddenly switches from one electronic state to another. These transitions occur when the electronic wavefunctions of these states are mixed or most probable when two potential energy curves cross or come very close to one another.

For the two considered molecules, some PECs undergo avoided crossings where the DMCs can support the validity of the positions of these points by their crossings between the respective states in the DMCs (Figs. (1-8) and Figs (FS1-FS8)). One can notice that the positions of the avoided crossing of the PECs agree very well with the positions of crossings of dipole moment curves of these states. Moreover, the calculations of the energy difference ΔE_{AC} and the position of the internuclear distance between two avoided crossing states R_{AC} for the different states are given in Table 1 in addition to the positions of the crossings between the permitted states R_C . The abrupt crossing between the two different DMCs in the same symmetry and with the same quantum number Λ can be explained by the reverse of the polarity of the two atoms where the electronic character is interchanged in this region.

Fig. (FS9) compares the electronic transition energies with respect to the ground state T_e of the different excited electronic states for the two molecules MgNa and MgLi. From this figure, one can notice that the 2 molecules have the same ground state $X^2\Sigma^+$ with a similar order of the first 7 excited electronic states. The change in the order of the electronic states is due to the absence of some electronic states from the energy level diagram. This absence is due to the presence of crossing or avoided crossing at the positions of the internuclear distance R_e or due to the presence of undulations in the PECs for higher excited electronic states of the two considered molecules.

Due to the significance of the Frank-Condon factor in the prediction of the probability of transition between electronic and vibrational levels, Figs. (FS10-FS11) display the spontaneous radiative transitions $f_{v'v}$ between $0 \leq v' \leq 9$ for the upper state and $0 \leq v \leq 9$ for the lower states (Tables TS1-TS2). the diagonal Franck-Condon array $f_{00}=0.750$ for the $X^2\Sigma^+-(1)^2\Sigma^+$ transition of the MgLi molecule shows that this molecule is a suitable candidate for the laser cooling experiment between these electronic states. Unfortunately, the intervening of the electronic state

(1)²Π to which the upper state could radiate threaten the closed-loop cooling cycle of the transition. Moreover, the other transitions of Tables (TS1-TS2) for the two considered molecules have the lowest probabilities of transitions.

Tables (2-3) list the different values of transition dipole moments, cross sections, f values (oscillator strengths) and Einstein coefficients for the different allowed electronic transitions between the following five states (X)²Σ⁺, (2)²Σ⁺, (3)²Σ⁺, (1)²Π and (2)²Π. These molecular parameters are significant in the determination of the strength of atomic and molecular optical transitions [29].

To simplify and clarify the discussion of the data for the two diatomic molecules MgLi and MgNa, we separated the analysis of the results for the remaining tables for each molecule:

2.2 MgNa molecule

In literature, one can find several theoretical calculations of the spectroscopic constants for the X²Σ⁺ and (1)⁴Σ⁺ electronic states of the molecule MgNa. Our calculations of the spectroscopic constants in Table 4 are based on the correlation-consistent polarized valence triple zeta basis set cc-PVTZ with three valence electrons were included in the active space. To confirm the reliability of our work, we computed the spectroscopic constants for the X²Σ⁺ and (1)⁴Σ⁺ electronic states by increasing the number of valence electrons to 7 in the active space. The comparison of our calculated values of ω_e and R_e with those obtain theoretically in literature [30-33], for the X²Σ⁺ and (1)⁴Σ⁺ electronic states, shows a very good agreement either calculated by using 3 or 7 valence electrons. Similar results are obtained by comparing our calculated values of D_e with those given in Refs. [30-33] and less agreement by comparing with those given in Refs. [31-32]. The agreement deteriorates by comparing the values of the static dipole moment μ given in Ref. [31] with our calculated values for the ground state (either using 3 valence electrons or 7 valence electrons) and becomes good agreement by comparing with those calculated in Ref. [33]. While a disagreement is obtained by comparing this constant given in Ref. [33] with our investigated value for the (1)⁴Σ⁺ electronic state. The inclusion of the 7 valence electrons in our calculation could not show an improvement in the results by comparing with the theoretical values given in the literature. The investigation of experimental data on the molecule MgNa may will confirm the validity and the accuracy of our results.

2.3 MgLi molecule

By fitting the calculated energy values of different investigated electronic states into a polynomial in terms of the internuclear distance at equilibrium R_e , the spectroscopic constants R_e , ω_e , B_e and

T_e have been calculated for MgLi molecule. The comparison of these values with those given in literature either theoretically or experimentally [30-40] are given in Table 5. However, the absence of the values of some constants, for the investigated potential energy curves, is due to the crossing or avoided crossing near the minima of these curves.

Except the experimental data in Refs. [27, 30] most of the published works on the molecule MgLi are obtained theoretically either by using different techniques of calculation or different basis sets where can find the influence of these different techniques and basis sets on the results. The comparison of our calculated value of T_e , for all the investigated electronic states given in literature, with our calculated values shows a good agreement with the relative difference $0.10\%((1)^4\Pi)[34^{b5}] < \Delta T_e / T_e < 7.36\%((1)^2\Pi)[34^{b1}]$ (Table TS4). One can notice also the good agreement with relative difference $0.27\% < \Delta\omega_e / \omega_e < 4.55\%$ by comparing our calculated values of ω_e , for the ground state, with those obtained theoretically in the Refs. [30, 33^{f1-f2} , $34^{b1-b5, b11-b13, b17}$, 36]. This agreement becomes less by comparing our calculated data with those given in the Refs. [$34^{b6-b8, b10}$, 33^{f3}] with the relative difference $9.26\% < \Delta\omega_e / \omega_e < 12.71\%$ and deteriorates by comparing with the values given in Ref. [35] with $\Delta\omega_e / \omega_e = 33.7\%$. While the comparison of our calculated values of ω_e with those given in Ref. [34^{b1-b5}] shows a very good agreement for the electronic states $(1)^2\Pi$, $(2)^2\Sigma^+$, $(1)^4\Pi$ and less agreement with the electronic states $(2)^2\Pi$, $(3)^2\Sigma^+$. For this constant the comparison of our value for ground state with that obtained experimentally [40] shows a good agreement with the relative difference 3.95%. The comparison of the present calculated values of the rotational constant B_e with those obtained either theoretically or experimentally in literature shows a very good agreement for all the investigated electronic states except the results obtained in Refs. [$34^{b2, b11-12}$, 36]. For the internuclear distance at equilibrium R_e always there is an agreement between our calculated values with those given in literature except the data of Ref. [37] for the electronic states $(2)^2\Pi$, $(2)^2\Sigma^+$ and Ref. [40] for the electronic states $(2)^2\Pi$, $(3)^2\Sigma^+$. The predicted values of dipole moment μ_e are of great importance for some experiments of ultracold polar MgLi molecules and can provide access to many laser cooling applications. The static dipole moment at equilibrium is given in literature only for the ground and $(1)^4\Sigma^+$ states. For the ground state, the values of μ_e given in Ref. [$33^{f1-f2, f5}$] are in good agreement with our calculated value, the agreement becomes less with Ref. [33^{f3}] and deteriorate with Ref. [33^{f4}] while there is a disagreement for the value of $(1)^4\Sigma^+$ electronic state. From this comparison, no one can predict the advantage of one technique or basis on the other. The excellent agreement of a constant for one state, obtained by one technique and a given basis, may become less or deteriorate for other

constant or state. A highly precision experimental work, for large number of electronic states, is needed to confirm the accuracy of the investigated data

By using the canonical function approach [18-21], the eigenvalue E_v , the rotational constant B_v , the centrifugal distortion constant D_v , and the abscissas of the turning points $R_{\min}$ and $R_{\max}$ of the molecules MgNa and MgLi have been calculated for the ground (Table 6) and 17 excited electronic states (Tables (TS3-TS5)). This approach can give the values of the eigenvalue of energy even near the dissociation. Therefore, one can notice the variation of the vibrational quantum number from $v=2$ ($(2)^4\Sigma^+$ of MgLi molecule) until $v=44$ ($(2)^4\Pi$ of MgLi molecule) (Tables TS3) according to the deepness of the corresponding potential energy curves.

The comparison of our results for the ground state of the molecule MgLi with 4 vibrational levels available in literature shows a good agreement with the relative difference $0.883\% \leq \Delta E_v/E_v \leq 4.140\%$ [36] and $5.548\% \leq \Delta B_v/B_v \leq 10.395\%$ [36]. There is no comparison with data in literature for the other investigated vibrational levels of MgLi and all the investigated rovibrational values of the MgNa molecule since they are calculated here for the first time. However, these data can be validated by referring to the term value of energy E_v and the rotational constant B_v of anharmonic oscillator:

$$E_v = \omega_e \left(v + \frac{1}{2} \right) - \omega_e x_e \left(v + \frac{1}{2} \right)^2 \dots \quad (1)$$

$$B_v = B_e - \alpha_e (v + 1/2) \dots \quad (2)$$

By using these relations for the MgNa molecule for the ground state with $v=0$, $E_v=42.0 \text{ cm}^{-1}$ and $B_v=11.3 \text{ cm}^{-1}$ (data from Table 4), while $E_v=42.6 \text{ cm}^{-1}$ and $B_v=11.12 \text{ cm}^{-1}$ are obtained by using the canonical function approach given in Table 6. One can notice the very good agreement of E_v and B_v calculated by two different ways.

3. Conclusion

We used the CASSCF/MRCI method to investigate 59 low-lying doublet and quartet excited electronic states of the MgLi, and MgNa molecules. Fifty new electronic states are studied here for the first time. The potential energy, the permanent dipole moment and the transition dipole moment curves along with the spectroscopic constants T_e , ω_e , $\omega_e x_e$, B_e , R_e and D_e allowed us to calculate the Einstein coefficients A_{21} and B_{21}^ω with several important parameters such as the emission oscillator strength f_{21} , the spontaneous radiative lifetime τ_{spont} , the classical radiative decay rate of the single-electron oscillator γ_{cl} , the absorption cross section σ_0 and the line

strength S_{21} . The results of the considered transitions are reported for the first time. The relative short lifetime ($\tau = 59.1$ ns) of the $(2)^2\Sigma^+$ upper state for the $X^2\Sigma^+-(2)^2\Sigma^+$ transition of the MgLi molecule and the large oscillator strength ($|f_{21}| = 0.3228$) of this transition increase the spontaneous scattering forces, which are benefit for rapid laser cooling. Moreover, the intermediate state $(1)^2\Pi$ cannot terminate the cycling transition between $X^2\Sigma^+$ and $(2)^2\Sigma^+$ electronic states, since it is strongly suppressed. Consequently, the $X^2\Sigma^+-(2)^2\Sigma^+$ can be considered the optimal electronic transition for laser cooling of the MgLi species. Based on the off-diagonal Franck-Condon factors for the considered lowest electronic transitions, the MgLi and MgNa molecules cannot be considered a laser-cooled candidate. By using the canonical functions approach, the eigenvalues E_v , the rotational constant B_v , the centrifugal distortion constant D_v and the abscissas of the turning points $R_{\min}$ and $R_{\max}$ have been calculated for different electronic states of the molecules MgLi and MgNa up to the vibrational level $v = 79$. The present investigation of the electronic structure of the two molecules MgNa and MgLi may stimulate more experimental works on the excited electronic states of these molecules.

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Figures Captions:

Fig.1: Potential energy curves of the $^2\Sigma^+$ and $^2\Delta$ electronic states of the molecule MgNa.

Fig.2: Potential energy curves of the $^4\Sigma^+$ and $^4\Delta$ electronic states of the molecule MgNa.

Fig.3: Potential energy curves of the $^2\Pi$ electronic states of the molecule MgNa.

Fig.4: Potential energy curves of the $^4\Pi$ electronic states of the molecule MgNa.

Fig.5: Potential energy curves of the $^2\Sigma^+$ and $^2\Delta$ electronic states of the molecule MgLi.

Fig.6: Potential energy curves of the $^2\Pi$ electronic states of the molecule MgLi.

Fig.7: Potential energy curves of the $^4\Sigma^+$ and $^4\Delta$ electronic states of the molecule MgLi.

Fig.8: Potential energy curves of the $^4\Pi$ electronic states of the molecule MgLi.

Fig.9: Transition dipole moment curves between $^2\Sigma^+-^2\Sigma^+$ and $^2\Sigma^+-^2\Pi$ electronic states of the molecule MgNa.

Fig.10: Transition dipole moment curves between $^2\Sigma^+-^2\Sigma^+$ and $^2\Sigma^+-^2\Pi$ electronic states of the molecule MgLi.

Fig. FS1: Permanent Dipole moment curves of the $^2\Sigma^+$ and $^2\Delta$ electronic states of the molecule MgNa.

Fig. FS2: Permanent Dipole moment curves of the $^4\Sigma^+$ and $^4\Delta$ electronic states of the molecule MgNa.

Fig. FS3: Permanent Dipole moment curves of the $^2\Pi$ electronic states of the molecule MgNa.

Fig. FS4: Permanent Dipole moment curves of the $^4\Pi$ electronic states of the molecule MgNa.

Fig. FS5: Permanent Dipole moment curves of the $^2\Sigma^+$ and $^2\Delta$ electronic states of the molecule MgLi.

Fig. FS6: Permanent Dipole moment curves of the $^2\Pi$ electronic states of the molecule MgLi.

Fig. FS7: Permanent Dipole moment curves of the $^4\Sigma^+$ and $^4\Delta$ electronic states of the molecule MgLi.

Fig. FS8: Permanent Dipole moment curves of the $^4\Pi$ electronic states of the molecule MgLi.

Fig. FS9: Permanent Relative position of the lowest-lying states for the MgLi and MgNa molecules.

Fig. FS10: The FCFs of the $^2\Sigma^+ - ^2\Sigma^+$ and $^2\Sigma^+ - ^2\Pi$ and transitions of the MgNa molecule.

Fig. FS11: The FCFs of the $^2\Sigma^+ - ^2\Sigma^+$ and $^2\Sigma^+ - ^2\Pi$ and transitions of the MgLi molecule.

For Review Only

Fig1.

Fig2.

Fig3.

Fig4.

Fig.5

Fig. 6

Fig.7

Fig.8

Fig.9

Fig.10

Table 1: Position of the crossings R_c and avoided crossing R_{ac} with the energy difference ΔE of the molecules MgLi, and MgNa

	Crossing		Avoided crossing		$\Delta E \times 10^3$ (Hartree)
	State1/ State2	$R_c(\text{\AA})$	State1/ State2	$R_{ac}(\text{\AA})$	
MgLi	$(3)^2\Sigma^+/(1)^2\Delta$	1.92			
	$(4)^2\Sigma^+/(1)^2\Delta$	2.14			
	$(5)^2\Sigma^+/(1)^2\Delta$	2.62	$(3)^2\Pi/(4)^2\Pi$	2.2	4690.01
	$(6)^2\Sigma^+/(1)^2\Delta$	3.4	$(5)^4\Sigma^+/(6)^4\Sigma^+$	5.0 4.4 3.96 2.64	462.10 1365.42 657.88 217.24
	$(8)^2\Sigma^+/(1)^2\Sigma^-$	2.58	$(4)^4\Pi/(5)^4\Pi$	3.92 5.98	2264.01 362.73
	$(7)^2\Sigma^+/(1)^2\Sigma^-$	4.02			
	$(1)^4\Sigma^-/(1)^4\Sigma^+$	2.78			
	$(1)^4\Delta/(2)^4\Sigma^+$	3.92			
	$(2)^4\Sigma^-/(3)^4\Sigma^+$	2.34			
	$(2)^4\Delta/(4)^4\Sigma^+$	2.36			
	$(2)^4\Delta/(3)^4\Sigma^+$	2.06			
	$(2)^4\Delta/(5)^4\Sigma^+$	2.78			
	$(2)^4\Sigma^-/(4)^4\Sigma^+$	5.78			
	$(6)^4\Sigma^+/(2)^4\Delta$	3.3			
MgNa					
	$(1)^2\Delta/(4)^2\Sigma^+$	1.90	$(3)^2\Sigma^+/(4)^2\Sigma^+$	1.74 3.28	0.861 10.59
	$(1)^2\Delta/(5)^2\Sigma^+$	2.52	$(4)^2\Sigma^+/(5)^2\Sigma^+$	2.4	2.30
	$(1)^2\Delta/(1)^2\Sigma^-$	5.68	$(1)^2\Pi/(2)^2\Pi$	4.5	21.70
	$(1)^2\Sigma^-/(2)^2\Delta$	2.3 2.58	$(2)^2\Pi/(3)^2\Pi$	3.22 4.48	35.37 28.95
	$(1)^4\Sigma^+/(1)^4\Sigma^-$	3.02	$(3)^2\Pi/(4)^2\Pi$	1.92	21.82
	$(2)^4\Sigma^-/(3)^4\Sigma^+$	2.38	$(4)^2\Pi/(5)^2\Pi$	3.64	11.11
	$(2)^4\Sigma^-/(4)^4\Sigma^+$	7.58	$(4)^4\Sigma^+/(5)^4\Sigma^+$	3.42 5.3 8.5	23.27 36.12 38.89
	$(3)^4\Sigma^-/(5)^4\Sigma^+$	2.48	$(1)^4\Pi/(2)^4\Pi$	4.68	51.97
	$(3)^4\Sigma^-/(2)^4\Delta$	4.34 6.62	$(2)^4\Pi/(3)^4\Pi$	4.04	17.52
			$(3)^4\Pi/(4)^4\Pi$	3 4.3	36.93 44.75
			$(4)^4\Pi/(5)^4\Pi$	3 3.84	1.58 1.57
			$(5)^4\Pi/(6)^4\Pi$	2.16 4.68	5.25 6.85

Table 2: Calculation of the spontaneous and induced emissions Einstein coefficients A_{21} and B_{21} , the spontaneous radiative lifetime τ , the absorption cross section σ_0 , the classical radiative decay rate γ_{cl} and the emission oscillator strength f_{21} .

MgLi					
Transition (1-2)	$ \mu_{21} $ (a.u.)	$\mu_{21} \times 10^{30}$ (C.m)	$\omega_{21} \times 10^{-15}$ (rad.s ⁻¹)	A_{21} (s ⁻¹)	$\tau_{spont(2-1)}$ (ns)
X ² Σ ⁺ - (2) ² Σ ⁺	2.741	23.24	1.953	16915552.6	59.1
X ² Σ ⁺ - (3) ² Σ ⁺	0.028	0.24	3.529	10661.0	93799.8
X ² Σ ⁺ - (1) ² Π	2.021	17.14	1.175	2003890.5	499.03
X ² Σ ⁺ - (2) ² Π	0.053	0.448	3.394	32957.9	30341.7
MgNa					
Transition (1-2)	$ \mu_{21} $ (a.u.)	$\mu_{21} \times 10^{30}$ (C.m)	$\omega_{21} \times 10^{-15}$ (rad.s ⁻¹)	A_{21} (s ⁻¹)	$\tau_{spont(2-1)}$ (ns)
X ² Σ ⁺ - (1) ² Π	0.572	4.85	1.462	309580.8	3230.2
(1) ² Π - (2) ² Σ ⁺	0.75	6.36	0.739	68811.8	14532.4
X ² Σ ⁺ - (2) ² Σ ⁺	3.015	25.56	2.202	29358342.0	34.1
(2) ² Σ ⁺ - (2) ² Π	0.75	6.36	1.200	294123.5	3399.9
(1) ² Π - (2) ² Π	2.036	17.26	1.940	9150312.8	109.3
X ² Σ ⁺ - (2) ² Π	1.656	14.04	3.402	32665136.3	30.6
(2) ² Π - (3) ² Σ ⁺	0.342	2.90	0.204	298.3	3352121.7
(2) ² Σ ⁺ - (3) ² Σ ⁺	0.375	3.18	1.404	117645.0	8500.1
(1) ² Π - (3) ² Σ ⁺	0.095	0.81	2.143	26874.3	37210.3
X ² Σ ⁺ - (3) ² Σ ⁺	2.014	17.07	3.606	57515662.9	17.4

Table 2: Continue

MgLi						
Transition (1-2)	$B_{21}^{\omega} \times 10^{-18}$ ($\text{m}^3 \cdot \text{J}^{-1} \cdot \text{s}^{-2}$)	$\sigma_0 \times 10^9$ ($\text{m}^2 \cdot \text{s}^{-1}$)	λ_{21} (nm)	$\gamma_{cl} \times 10^{-6}$ (s^{-1})	$ f_{21} \times 10^4$	$S_{21} \times 10^{59}$ ($\text{C}^2 \cdot \text{m}^2$)
$X^2\Sigma^+ - (2)^2\Sigma^+$	5742.17	3941.22	965.39	23.84	2.3655	108.00
$X^2\Sigma^+ - (3)^2\Sigma^+$	0.61	0.76	534.08	77.88	0.4563	0.01
$X^2\Sigma^+ - (1)^2\Pi$	3123.34	2579.60	1604.55	8.63	774.1366	117.48
$X^2\Sigma^+ - (2)^2\Pi$	2.13	5.08	555.44	72.00	1.5257	0.08
MgNa						
Transition (1-2)	$B_{21}^{\omega} \times 10^{-20}$ ($\text{m}^3 \cdot \text{J}^{-1} \cdot \text{s}^{-2}$)	$\sigma_0 \times 10^7$ ($\text{m}^2 \cdot \text{s}^{-1}$)	λ_{21} (nm)	$\gamma_{cl} \times 10^{-6}$ (s^{-1})	$ f_{21} $	$S_{21} \times 10^{58}$ ($\text{C}^2 \cdot \text{m}^2$)
$X^2\Sigma^+ - (1)^2\Pi$	2.50	2.57	1288.91	13.37	0.0077	0.94
$(1)^2\Pi - (2)^2\Sigma^+$	4.30	0.56	2549.01	3.42	0.0067	0.81
$X^2\Sigma^+ - (2)^2\Sigma^+$	69.48	53.78	856.05	30.32	0.3228	13.07
$(2)^2\Sigma^+ - (2)^2\Pi$	4.30	3.63	1570.66	9.01	0.0109	1.62
$(1)^2\Pi - (2)^2\Pi$	31.69	21.60	971.83	23.52	0.1297	11.92
$X^2\Sigma^+ - (2)^2\Pi$	20.96	50.14	554.07	72.37	0.1505	7.88
$(2)^2\Pi - (3)^2\Sigma^+$	0.89	0.0320	9261.37	0.26	0.0004	0.17
$(2)^2\Sigma^+ - (3)^2\Sigma^+$	1.07	0.5304	1342.91	12.32	0.0032	0.20
$(1)^2\Pi - (3)^2\Sigma^+$	0.0689	0.0260	879.54	28.72	0.0003	0.01
$X^2\Sigma^+ - (3)^2\Sigma^+$	31.01	39.30	522.79	81.28	0.2359	5.83

Table 3: the spontaneous radiative lifetime τ_{spont} for MgNa Molecule

State	$\tau_{\text{spont}}(\text{MgNa})$ (ns)
$(2)^2\Sigma^+$	34.0
$(2)^2\Pi$	23.7
$(3)^2\Sigma^+$	17.3

Table 4: Spectroscopic constants of the low-lying doublet and quartet electronic state the molecule MgNa

States Λ^{2S+1}	T_e (cm^{-1})	ω_e (cm^{-1})	$\omega_e x_e$ (cm^{-1})	$B_e \times 10$ (cm^{-1})	R_e ($\text{\AA}$)	D_e (cm^{-1})	$ \mu_e $ (Debye)
$X^2\Sigma^+$	0.00 ^a 0.00 ^{a_1}	86.5 ^a 87.6 ^{a_1} 85 ^b 82.6 ^{d_1} 90 ^c	4.99 ^a 4.79 ^{a_1}	1.13 ^a 1.14 ^{a_1} 1.29 ^{d_1}	3.558 ^a 3.541 ^{a_1} 3.564 ^b 3.59 ^c 3.519 ^{d_1} 3.529 ^{d_2} 3.47 ^e	887 ^a 913 ^{a_1} 887 ^b ≤ 800 ^c 825 ^{d_1} 808 ^{d_2} 946 ^e	0.93 ^a 0.88 ^{a_1} 0.72 ^{d_1} 0.72 ^{d_2} 0.86 ^e
(1) $^2\Pi$	7764.55 ^a	211.7 ^a	1.10 ^a	1.671 ^a	2.922 ^a	9029 ^a	4.93 ^a
(2) $^2\Sigma^+$	11690.72 ^a	153.3 ^a	1.30 ^a	1.265 ^a	3.359 ^a	5078 ^a	1.51 ^a
(2) $^2\Pi$	18062.46 ^a	101.3 ^a	1.51 ^a	1.092 ^a	3.614 ^a	3879 ^a	0.43 ^a
(3) $^2\Sigma^+$	19143.06 ^a	95.8 ^a	0.76 ^a	0.871 ^a	4.047 ^a	2791 ^a	1.87 ^a
(1) $^4\Pi$	19501.16 ^a	129.1 ^a	2.21 ^a	1.230 ^a	3.406 ^a	2451 ^a	4.13 ^a
(1) $^4\Sigma^+$	21814.69 ^a 21823.60 ^{a_1}	21.8 ^a 23.5 ^{a_1} 21 ^c	3.23 ^a	0.473 ^a 0.472 ^{a_1}	5.504 ^a 5.496 ^{a_1} 5.71 ^c	125 ^a 127 ^{a_1} 131 ^c	1.41 ^a 1.39 ^{a_1} 0.99 ^c
(3) $^2\Pi$	24987.04 ^a	202.4 ^a	0.98 ^a	0.574 ^a	4.983 ^a	6664 ^a	9.15 ^a
(1) $^4\Sigma^-$	26517.27 ^a	204.3 ^a	0.72 ^a	1.727 ^a	2.874 ^a	11344 ^a	5.06 ^a
(4) $^2\Pi$	29059.57 ^a	154.7 ^a	1.59 ^a	1.177 ^a	3.481 ^a		1.38 ^a
(5) $^2\Sigma^+$	29178.33 ^a	135.7 ^a	0.23 ^a	1.332 ^a	3.274 ^a	3253 ^a	6.33 ^a
(2) $^4\Pi$	31259.19 ^a	113.8 ^a	0.55 ^a	0.979 ^a	3.818 ^a	6512 ^a	1.49 ^a
(5) $^2\Pi$	31576.34 ^a	136.4 ^a	1.45 ^a	1.112 ^a	3.575 ^a		1.33 ^a
(1) $^2\Delta$	32416.52 ^a	195.9 ^a	2.11 ^a	1.668 ^a	2.925 ^a	5461 ^a	3.08 ^a
(3) $^4\Pi$	35181.67 ^a	103.6 ^a	1.85 ^a	0.925 ^a	3.927 ^a	2667 ^a	0.84 ^a
(2) $^4\Sigma^+$	37663.39 ^a	39.4 ^a	0.73 ^a	0.585 ^a	4.938 ^a	196 ^a	5.01 ^a
(1) $^2\Sigma^-$	37764.47 ^a	53.3 ^a	0.18 ^a	0.572 ^a	4.993 ^a	87 ^a	0.33 ^a
(2) $^2\Delta$	39636.82 ^a	102.8 ^a	3.10 ^a	1.208 ^a	3.440 ^a	1832 ^a	1.85 ^a
(2) $^4\Sigma^-$	41909.51 ^a	61.9 ^a	0.12 ^a	0.603 ^a	4.865 ^a	7168 ^a	9.40 ^a
(4) $^4\Pi$ (2 nd min)	44169.38 ^a	53.4 ^a	0.01 ^a	0.383 ^a	6.105 ^a	4201 ^a	14.60 ^a
(2) $^2\Sigma^-$	44508.16 ^a	189.2 ^a	3.08 ^a	1.460 ^a	3.123 ^a		6.10 ^a
(4) $^4\Sigma^+$ (1 st min) (2 nd min)	45433.84 ^a 45131.03 ^a	104.2 ^a 60.6 ^a	2.85 ^a 0.00 ^a	1.080 ^a 0.334 ^a	3.635 ^a 6.540 ^a	2541 ^a 2844 ^a	0.323 ^a 15.48 ^a
(5) $^4\Pi$ (2 nd min)	46577.13 ^a	81.78 ^a	0.05 ^a	0.452 ^a	5.619 ^a	6212 ^a	16.37 ^a
(5) $^4\Sigma^+$	48154.50 ^a	140.5 ^a	1.64 ^a	0.958 ^a	3.858 ^a	3477 ^a	8.17 ^a
(2) $^4\Delta$	51545.93 ^a	176.8 ^a	2.94 ^a	1.433 ^a	3.143 ^a	2071 ^a	0.57 ^a
(3) $^4\Sigma^-$	52691.50 ^a	95.9 ^a	3.73 ^a	1.234 ^a	3.400 ^a	930 ^a	1.97 ^a

a :Present work using MRCI method (3ves-core 6,2,2,0;)

a₁:Present work using MRCI method (7ves-core 6,1,1,0;)

b: Ref[30]

c: Ref[32]

d₁: Ref[31] using UCCSD(T)/aug-cc-pCV5Zd₂: Ref[31] using RCCSD(T)/aug-cc-pCV5Z

e : Ref[33]

Table 5. Calculated spectroscopic constants for the bound electronic Λ -states of the Molecule MgLi

States Λ^{2S+1}	T_e (cm^{-1})	ω_e (cm^{-1})	B_e (cm^{-1})	R_e ($\text{\AA}$)	D_e (cm^{-1})	$ \mu_e $ (Debye)
$(X)^2\Sigma^+$	0	182.5 ^a	0.323 ^a	3.11 ^a	1533.8 ^a	1.15 ^a
		174.2 ^{b1}	0.323 ^{b1}	3.1028 ^{b1}	1379.2 ^{b1}	
		174.4 ^{b2}	0.323 ^{b2}	3.1020 ^{b2}	1395.3 ^{b2}	1.22 ^{b2}
		185.9 ^{b3}	0.323 ^{b3}	3.1043 ^{b3}	1588.9 ^{b3}	
		188.4 ^{b4}	0.324 ^{b4}	3.0983 ^{b4}	1629.2 ^{b4}	
		188.8 ^{b5}	0.324 ^{b5}	3.0968 ^{b5}	1645.4 ^{b5}	
		159.3 ^{b6}	0.316 ^{b6}	3.1348 ^{b6}	1080.8 ^{b6}	
		161.9 ^{b7}	0.317 ^{b7}	3.1287 ^{b7}	1121.1 ^{b7}	
		165.6 ^{b8}	0.321 ^{b8}	3.1120 ^{b8}	1153.4 ^{b8}	
		174.4 ^{c1}		3.1010 ^{c1}	1417.0 ^{c1}	
		206.1 ^{c2}		3.1063 ^{c2}	1432.0 ^{c2}	1.12 ^{c2}
		187.0 ^d	0.363 ^d	3.116 ^d	1332.0 ^d	0.86 ^d
		179.9 ^{e1}	0.394 ^{e1}	3.094 ^{e1}	1445.4 ^{e1}	1.02 ^{e1}
		177.8 ^{e2}		3.100 ^{e2}	1414.6 ^{e2}	
		121.0 ^f		3.245 ^f	1452.0 ^f	
		183 ^g		3.110 ^g	1613 ^g	
				3.2 ^h	968.0 ^h	
		180.0 ⁱ		3.196 ⁱ	1371.0 ⁱ	
		190.0 ^j		3.121 ^j	1419.5 ^j	
		181.0 ^k		3.10 ^k	1538.0 ^k	1.18 ^k
$(1)^2\Pi$	6236.8 ^a	354.8 ^a	0.454 ^a	2.62 ^a	10153.4 ^a	2.80 ^a
	6732.4 ^{b1}	361.1 ^{b1}	0.4571 ^{b1}	2.606 ^{b1}	9590.5 ^{b1}	
	6699.9 ^{b2}	363.7 ^{b2}	0.4558 ^{b2}	2.609 ^{b2}	9638.7 ^{b2}	
	6093.2 ^{b3}	353.6 ^{b3}	0.4513 ^{b3}	2.623 ^{b3}	10,372.3 ^{b3}	
	5952.6 ^{b4}	354.7 ^{b4}	0.4537 ^{b4}	2.617 ^{b4}	10,550.9 ^{b4}	
	5929.4 ^{b5}	354.5 ^{b5}	0.4539 ^{b5}	2.616 ^{b5}	10,589.8 ^{b5}	
$(2)^2\Sigma^+$		398.0 ^k		2.588 ^k		
	10366.6 ^a	256.3 ^a	0.346 ^a	3.00 ^a	6004.9 ^a	1.46 ^a
	10,783.5 ^{b1}	256.5 ^{b1}	0.3526 ^{b1}	2.968 ^{b1}	5510.2 ^{b1}	
	10,775.0 ^{b2}	257.3 ^{b2}	0.3526 ^{b2}	2.968 ^{b2}	5498.6 ^{b2}	
	10,307.2 ^{b3}	254.0 ^{b3}	0.3447 ^{b3}	3.002 ^{b3}	6114.9 ^{b3}	
	10,222.8 ^{b4}	255.4 ^{b4}	0.3461 ^{b4}	2.996 ^{b4}	6237.3 ^{b4}	
$(2)^2\Pi$	10,209.7 ^{b5}	255.5 ^{b5}	0.3463 ^{b5}	2.995 ^{b5}	6263.0 ^{b5}	
	18019.6 ^a	219.7 ^a	0.292 ^a	3.27 ^a	4566.3 ^a	1.66 ^a
	18,889.9 ^{b1}	199.2 ^{b1}	0.3155 ^{b1}	3.137 ^{b1}	4387.5 ^{b1}	
	18,860.7 ^{b2}	200.5 ^{b2}	0.3175 ^{b2}	3.128 ^{b2}	4377.2 ^{b2}	
	17,909.7 ^{b3}	176.3 ^{b3}	0.3001 ^{b3}	3.216 ^{b3}	4787.1 ^{b3}	
	17,796.4 ^{b4}	174.2 ^{b4}	0.2996 ^{b4}	3.219 ^{b4}	4921.3 ^{b4}	
$(3)^2\Sigma^+$	17,770.2 ^{b5}	174.8 ^{b5}	0.3009 ^{b5}	3.212 ^{b5}	4990.3 ^{b5}	
				3.882 ^j	3160.4 ^j	
				3.880 ⁱ		
	18738.1 ^a	181.4 ^a	0.227 ^a	3.69 ^a	3832.6 ^a	1.01 ^a
	19,371.2 ^{b1}	169.1 ^{b1}	0.2336 ^{b1}	3.646 ^{b1}	3870.1 ^{b1}	
	19,358.5 ^{b2}	168.6 ^{b2}	0.2337 ^{b2}	3.646 ^{b2}	3836.3 ^{b2}	
$(1)^4\Pi$	18,690.8 ^{b3}	163.4 ^{b3}	0.2307 ^{b3}	3.669 ^{b3}	3961.7 ^{b3}	
	18,670.7 ^{b4}	162.6 ^{b4}	0.2320 ^{b4}	3.659 ^{b4}	4002.2 ^{b4}	
	18,663.9 ^{b5}	161.9 ^{b5}	0.2326 ^{b5}	3.654 ^{b5}	4049.0 ^{b5}	
				4.536 ^j	3840.8 ^j	
				4.534 ⁱ		
	18977.3 ^a	237.3 ^a	0.344 ^a	3.01 ^a	3605.3 ^a	3.62 ^a
$(1)^4\Sigma^+$	19,618.6 ^{b1}	240.2 ^{b1}	0.3482 ^{b1}	2.987 ^{b1}	3667.3 ^{b1}	
	19,587.9 ^{b2}	239.6 ^{b2}	0.3475 ^{b2}	2.990 ^{b2}	3654.1 ^{b2}	
	18,944.3 ^{b3}	236.9 ^{b3}	0.3404 ^{b3}	3.021 ^{b3}	3765.0 ^{b3}	
	18,950.3 ^{b4}	237.3 ^{b4}	0.3413 ^{b4}	3.017 ^{b4}	3780.9 ^{b4}	
	18,958.7 ^{b5}	237.5 ^{b5}	0.3414 ^{b5}	3.016 ^{b5}	3815.9 ^{b5}	
	22363.5 ^a	40.2 ^a	0.1365 ^a	4.45 ^a	214.9 ^a	3.24 ^a
		32 ^k		4.72 ^k	222 ^k	2.52 ^k

(1) ⁴ Σ^-	25025.9 ^a	349.2 ^a	0.489 ^a	2.53 ^a	12411.6 ^a	2.03 ^a
(4) ² Σ^+	25595.8 ^a	268.3 ^a	0.372 ^a	2.90 ^a	8596.9 ^a	4.47 ^a
(5) ² Σ^+	29583.6 ^a	479.6 ^a	0.341 ^a	3.24 ^a	7092.4 ^a	1.45 ^a
(2) ⁴ Π	30760.2 ^a	172.2 ^a	0.252 ^a	3.52 ^a	6619.6 ^a	3.55 ^a
(2) ² Δ	31722.2 ^a	321.5 ^a	0.455 ^a	2.62 ^a	5740.9 ^a	1.41 ^a
(3) ⁴ Π	34581.0 ^a	163.8 ^a	0.244 ^a	3.58 ^a	2852.9 ^a	0.28 ^a
(2) ⁴ Σ^+	37333.8 ^a	59.6 ^a	0.116 ^a	5.19 ^a	103.3 ^a	2.17 ^a
(2) ⁴ Σ^-	43677.7 ^a	108.1 ^a	0.173 ^a	4.25 ^a	9098.2 ^a	9.25 ^a
(4) ⁴ Π						
1 st min	47228.6 ^a	703.4 ^a	0.341 ^a	3.06 ^a	4868.8 ^a	1.71 ^a
2 nd min	45968.8 ^a	84.8 ^a	0.121 ^a	5.16 ^a	6128.6 ^a	8.94 ^a
(4) ⁴ Σ^+						
1 st min	46521.3 ^a	253.3 ^a	0.265 ^a	3.43 ^a	2549.3 ^a	4.51 ^a
2 nd min	45597.0 ^a	176.8 ^a	0.085 ^a	6.22 ^a	3473.5 ^a	16.78 ^a

a :Present work using

MRCI method (3ves-core 6,2,2,0;)

b1-b8: Ref [34] using different basis or method { b1:MRCI/ CVQZ+Q, b2:MRCI/ACVQZ+Q, b3:FCI/AVQZ, b4:MRCI/AVQZ+Q, b5:MRCI/AV5Z+Q, b6:MRCI/AV5Z+CV, b7:MRCI/AV5Z+Q+CV, b8:MRCI/V5Z+Q+CV+3DK }

c1-c2:Ref[38] using different basis or method {c1: RCCSD(T)/aug-cc-pCVQZ , c2: UCCSD(T)/aug-cc-pV5Z-DK }

d: Ref [36]

e1-e2: Ref[31] using different basis or method {e1: UCCSD(T)/aug-cc-pCV5Z, e2: RCCSD(T)aug-cc-pCV5Z }

f:Ref[35]

g:Ref [30]

h:Ref[32]

i:Ref [39]

j:Ref^{EXP}[40]

k:Ref[33]

l:Ref[37]

Table 6: Values of the eigenvalues E_v , the abscissas of the turning points $R_{\min}$ and $R_{\max}$ the constants B_v and D_v for the different vibrational levels of $X^2\Sigma^+$ states of MgLi and MgNa molecules

	States Λ^{2S+1}	v	E_v cm^{-1}	$\Delta E_v/E_v$ %	$B_v \times 10$ cm^{-1}	$\Delta B_v/B_v$ %	$D_v \times 10^7$ cm^{-1}	$R_{\min}$ $\text{\AA}$	$R_{\max}$ $\text{\AA}$
MgLi	$X^2\Sigma^+$	0	90.5 ^a 89.70 ^b	0.88	3.172 ^a 3.54 ^b	10.39	4.047 ^a	2.949 ^a	3.321 ^a
		1	264.2 ^a 259.67 ^b	1.71	3.070 ^a 3.40 ^b	9.70	4.352 ^a	2.849 ^a	3.511 ^a
		2	426.4 ^a 415.58 ^b	2.54	2.959 ^a 3.25 ^b	8.95	4.745 ^a	2.790 ^a	3.671 ^a
		3	576.5 ^a 557.34 ^b	3.32	2.843 ^a 3.01 ^b	5.55	5.204 ^a	2.747 ^a	3.824 ^a
		4	714.4 ^a 684.82 ^b	4.14	2.720 ^a 2.93 ^b	7.17	5.660 ^a	2.714 ^a	3.979 ^a
		5	840.2 ^a		2.589 ^a		6.219 ^a	2.687 ^a	4.140 ^a
		6	953.9 ^a		2.455 ^a		6.809 ^a	2.666 ^a	4.311 ^a
		7	1056.1 ^a		2.319 ^a		7.218 ^a	2.647 ^a	4.495 ^a
		8	1147.7 ^a		2.183 ^a		8.029 ^a	2.632 ^a	4.695 ^a
		9	1228.6 ^a		2.033 ^a		9.054 ^a	2.619 ^a	4.899 ^a
		10	1299.0 ^a		1.880 ^a		10.94 ^a	2.609 ^a	5.149 ^a
		11	1480.7 ^a		1.210 ^a		15.27 ^a	2.583 ^a	6.591 ^a
MgNa	$X^2\Sigma^+$	0	42.6 ^a		11.118 ^a		7.914 ^a	3.395 ^a	3.762 ^a
		1	124.3 ^a		10.805 ^a		8.415 ^a	3.297 ^a	3.949 ^a
		2	201.3 ^a		10.482 ^a		8.976 ^a	3.238 ^a	4.101 ^a
		3	273.6 ^a		10.151 ^a		9.605 ^a	3.195 ^a	4.243 ^a
		4	341.3 ^a		9.810 ^a		10.267 ^a	3.161 ^a	4.383 ^a
		5	404.4 ^a		9.460 ^a		10.980 ^a	3.133 ^a	4.524 ^a
		6	463.0 ^a		9.102 ^a		11.772 ^a	3.110 ^a	4.669 ^a
		7	517.3 ^a		8.737 ^a		12.615 ^a	3.090 ^a	4.819 ^a
		8	567.3 ^a		8.366 ^a		13.441 ^a	3.073 ^a	4.976 ^a
		9	613.1 ^a		7.995 ^a		13.897 ^a	3.059 ^a	5.142 ^a

a:Present work

b:Ref. [36]