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## Dissociation Energies of Diatomic Molecules \*

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Molecular dissociation energies of 10 electronic states of alkali molecules of KH,  $^7\text{LiD}$ ,  $^7\text{LiH}$ ,  $^6\text{LiH}$ , NaK, NaLi and NaRb are studied using the highest three accurate vibrational energies of each electronic state, and an improved parameter-free analytical formula which is obtained starting from the LeRoy–Bernstein vibrational energy expression near the dissociation limit. The results show that as long as the highest three vibrational energies are accurate, the current analytical formula will give accurate theoretical dissociation energies  $D_e^{\text{theory}}$ , which are in excellent agreement with the experimental dissociation energies  $D_e^{\text{expt}}$ .

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Accurate molecular dissociation energies  $D_e$  of stable diatomic electronic states play an important role in the studies of molecular structures, reactive scatterings, and astrophysics.<sup>[1–4]</sup> Experimentally, recent extensive efforts have been focused on dissociation energies of a series of electronic states of diatomic alkali molecules<sup>[5–12]</sup> using high resolution experimental apparatus such as the Doppler-free polarization spectroscopy, the polarization labelling spectroscopy, the optical–optical double resonance excitation spectroscopy, and the high-resolution pulse-amplified laser. Theoretically, many studies on  $D_e$  have used ab initio methods which have different features and use many basis functions with variational parameters.<sup>[2–4]</sup> However ab initio studies may have difficulty obtaining accurate values of dissociation energies for many molecular systems due to theoretical limitations such as the breakdown of Born–Oppenheimer approximation in the molecular dissociation region. The values of molecular dissociation energies have also been determined by using Birge–Sponer (B-S) extrapolation approach<sup>[13]</sup> for diatomic systems whose potentials behave like Morse potential functions. On the other hand, the B-S method may produce considerable errors for many potentials having long-range potential tails,<sup>[14]</sup> and it may not work for many diatomic states whose high-lying vibrational energies near dissociation limit are not known.

In this Letter, we propose a parameter-free analytical formula for molecular dissociation energy  $D_e$  based on LeRoy and Bernstein’s energy expression.<sup>[15,16]</sup> For a stable diatomic molecular system having potential energy  $V(R)$ , LeRoy and Bernstein obtained a relation between the vibrational energy  $E_\nu$  and the vibrational quantum number  $\nu$  using the first-order WKB (Wentzel–Kramers–Brillouin) quantum condition<sup>[15]</sup>

$$\nu = \frac{(2\mu)^{1/2}}{\pi\hbar} \int_{R_1(\nu)}^{R_2(\nu)} [E_\nu - V(R)]^{1/2} dR - \frac{1}{2}, \quad (1)$$

where  $\mu$  is the reduced mass, and both  $R_1(\nu)$  and  $R_2(\nu)$  are the classical turning points of energy  $E_\nu$ . Differentiating Eq. (1) with respect to  $E_\nu$  yields

$$\frac{d\nu}{dE_\nu} = (\pi\hbar)^{-1} \left(\frac{1}{2}\mu\right)^{1/2} \cdot \int_{R_1(\nu)}^{R_2(\nu)} [E_\nu - V(R)]^{-1/2} dR. \quad (2)$$

If the vibrational potential  $V(R)$  is replaced near the molecular dissociation limit by a good approximate function which is accurately close to the outer turning point  $R_2(\nu)$  of  $V(R)$ , the integral of Eq. (2) will be nearly unchanged. An asymptotic form for such a good function is chosen as<sup>[15]</sup>

$$V(R) = D_e - \frac{C_n}{R^n}, \quad (3)$$

where  $D_e$  is the dissociation energy of a molecular system, and the potential coefficient  $C_n$  can be given by<sup>[15]</sup>

$$E_\nu = D_e - \frac{C_n}{[R_2(\nu)]^n}. \quad (4)$$

Starting from Eq. (2) one may obtain an alternative expression for molecular dissociation energy  $D_e$ <sup>[15]</sup>

$$D_e = E_\nu - \left(\frac{n+2}{2n}\right) \frac{[E'_\nu]^2}{E''_\nu}, \quad (5)$$

where the derivative of the high-lying vibrational energies may be obtained using the following approximation<sup>[16]</sup> when a molecular system is near its dissociation limit

$$E'_\nu = \frac{dE_\nu}{d\nu} \approx \frac{1}{2} [E_{\nu+1} - E_{\nu-1}] + \dots \dots \quad (6)$$

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It is not easy for one to apply Eq. (4) or Eq. (5) to diatomic electronic systems since these equations are the functions of the long-range potential quantities  $n$  and  $C_n$ . In their example studies,<sup>[15,16]</sup> Eq. (5) and a numerical fitting procedure were applied to calculate molecular dissociation energy using a set of experimental vibrational energies  $E_\nu$  and a group of initial trial values of  $C_2$ ,  $n$  and  $D_e$ . However, it is difficult for one to obtain good initial trial values of  $C_2$ ,  $n$  and  $D_e$  for most diatomic molecular systems, and usually the final result of dissociation energy  $D_e$  from these initial values has errors. In order to have a parameter-free formula for molecular dissociation energy, one may take the first-order derivative and the second-order derivative of  $E_\nu$  in Eq. (4) with respect to  $\nu$ , and obtain

$$E'_\nu = nC_n \cdot [R_2(\nu)]^{-(n+1)} \cdot R_2(\nu)', \quad (7)$$

$$E''_\nu = nC_n \cdot \left( -(n+1)[R_2(\nu)]^{-(n+2)} \cdot [R_2(\nu)']^2 + [R_2(\nu)]^{-(n+1)} \cdot R_2(\nu)'' \right), \quad (8)$$

$$\frac{E'_\nu}{E''_\nu} = \frac{R_2(\nu) \cdot R_2(\nu)'}{R_2(\nu) \cdot R_2(\nu)'' - (n+1)[R_2(\nu)']^2}. \quad (9)$$

Substituting Eqs. (6) and (9) into Eq. (5), one obtains an alternative

$$D_e = E_\nu + \frac{1}{2} \left( \frac{n+2}{2n} \right) [E_{\nu+1} - E_{\nu-1}] \cdot A_n(\nu), \quad (10)$$

where

$$A_n(\nu) = \frac{R_2(\nu) \cdot R_2(\nu)'}{(n+1)[R_2(\nu)']^2 - R_2(\nu) \cdot R_2(\nu)''}. \quad (11)$$

Therefore, when very near the molecular dissociation limit one may take  $\nu+1 = \nu_{\max}$ , and Eq. (10) becomes

$$D_e = E_{\nu_{\max}-1} + \frac{1}{2} \left( \frac{n+2}{2n} \right) \cdot [E_{\nu_{\max}} - E_{\nu_{\max}-2}] \cdot A_n(\nu_{\max}-1). \quad (12)$$

Similarly, for  $\nu = \nu_{\max}$ , Eq. (10) can be rewritten as

$$D_e = E_{\nu_{\max}} + \frac{1}{2} \left( \frac{n+2}{2n} \right) \cdot [E_{\nu_{\max}+1} - E_{\nu_{\max}-1}] \cdot A_n(\nu_{\max}). \quad (13)$$

Since  $E_{\nu_{\max}}$  is the maximum vibrational energy of a stable diatomic electronic state, therefore  $E_{\nu_{\max}+1}$  is a non-existing 'vibrational energy' being very close to  $E_{\nu_{\max}}$ , and in fact  $E_{\nu_{\max}+1} < E_{\nu_{\max}}$ . In Eq. (13),  $[E_{\nu_{\max}+1} - E_{\nu_{\max}-1}]$  is not physical and may be a negative value, which may cause  $D_e < E_{\nu_{\max}}$ . As a result of  $D_e \geq E_{\nu_{\max}}$  and as a rational approximation, one may replace  $E_{\nu_{\max}+1}$  by  $E_{\nu_{\max}}$  in Eq. (13), and obtain

$$D_e = E_{\nu_{\max}} + \frac{1}{2} \left( \frac{n+2}{2n} \right) \cdot [E_{\nu_{\max}} - E_{\nu_{\max}-1}] \cdot A_n(\nu_{\max}). \quad (14)$$

Under the first-order WKB quantum condition, the difference between  $A_n(\nu_{\max})$  and  $A_n(\nu_{\max}-1)$  is very small in the dissociation limit, thus one may take  $A_n(\nu_{\max}-1) \approx A_n(\nu_{\max}) = A$  for a diatomic molecular system. Subtracting Eq. (12) from Eq. (14), and solving for parameter  $A$ , one obtains

$$A = 2 \left( \frac{2n}{n+2} \right) \cdot \left\{ \frac{\Delta E_{\nu_{\max}, \nu_{\max}-1}}{\Delta E_{\nu_{\max}, \nu_{\max}-2} - \Delta E_{\nu_{\max}, \nu_{\max}-1}} \right\}. \quad (15)$$

Substituting Eq. (15) into Eq. (14) yields

$$D_e \cong E_{\nu_{\max}} + \frac{\Delta E_{\nu_{\max}, \nu_{\max}-1}^2}{\Delta E_{\nu_{\max}, \nu_{\max}-2} - \Delta E_{\nu_{\max}, \nu_{\max}-1}} = E_{\nu_{\max}} + F(\nu_{\max}, \nu_{\max}-2), \quad (16)$$

where

$$\begin{aligned} \Delta E_{\nu_{\max}, \nu_{\max}-1} &= E_{\nu_{\max}} - E_{\nu_{\max}-1}, \\ \Delta E_{\nu_{\max}, \nu_{\max}-2} &= E_{\nu_{\max}} - E_{\nu_{\max}-2}. \end{aligned}$$

Equation (16) is an analytical formula for molecular dissociation energy, and does not depend on any molecular potential quantities such as  $C_n$  and  $n$ . It indicates that one can obtain the molecular dissociation energy  $D_e$  of a stable diatomic molecular electronic state by using its highest three vibrational energies  $E_{\nu_{\max}}$ ,  $E_{\nu_{\max}-1}$  and  $E_{\nu_{\max}-2}$ . Since the right-hand side of Eq. (6) is always smaller than the left-hand side by a very small quantity,  $D_e$  generated using Eq. (16) will be slightly smaller than the correct experimental dissociation energy  $D_e^{\text{expt}}$ , namely

$$D_e \lesssim D_e^{\text{expt}}. \quad (17)$$

If Eq. (17) is violated, the highest three vibrational energies used to calculate  $D_e$  will have errors, and so does the vibrational spectrum  $E_\nu$ .

The key condition to obtain correct diatomic molecular dissociation energy  $D_e$  using Eq. (16) is that one must use accurate high-lying vibrational energies near molecular dissociation limit. However, modern experimental methods and quantum methods usually give a vibrational energy subset  $[E_\nu]$  which may not be very close to the dissociation limit of a given diatomic system. In our previous study,<sup>[17]</sup> an algebraic method (AM) is suggested to generate a full set of vibrational energy spectrum  $\{E_\nu\}$  using a known experimental vibrational energy subset  $[E_\nu]$ . Together with the AM method, Eq. (16) is applied to study molecular dissociation energies for 10 electronic states of alkali molecules of KH, <sup>7</sup>LiD, <sup>7</sup>LiH, <sup>6</sup>LiH, NaK, NaLi and NaRb respectively. Table 1 gives the maximum vibrational quantum number, the highest three vibrational energies calculated either using the AM or the literature vibrational spectroscopic constants respectively, the approximate molecular dissociation energy  $D_e^{\text{app}} = E_{\nu_{\max}} + \Delta E_{\nu_{\max}, \nu_{\max}-1}$ , the molecular dissociation energy  $D_e^{\text{calc}}$  obtained using the new

formula in Eq. (16), the experimental molecular dissociation energy  $D_e^{\text{expt}}$ , and the relative error  $E_{\text{rroR}} = (D_e^{\text{expt}} - D_e^{\text{calc}})/\Delta E_{\nu_{\text{max}}, \nu_{\text{max}}-1}$  of the calculated dis-

sociation energy  $D_e^{\text{calc}}$  for each electronic state. These states are listed in a way such that the  $E_{\text{rroR}}$  of AM study is increasing.

Table 1. Theoretical molecular dissociation energies  $D_e$  and the related data of some diatomic electronic states (all quantities but  $\nu_{\text{max}}$  and  $E_{\text{rroR}}$  are in units of  $\text{cm}^{-1}$ ).

State		$\nu_{\text{max}}$	$E_{\nu_{\text{max}}-2}$	$E_{\nu_{\text{max}}-1}$	$E_{\nu_{\text{max}}}$	$(D_e^{\text{app}})^{\text{a}}$	$D_e^{\text{calc}}$	$(D_e^{\text{expt}})^{\text{b}}$	$E_{\text{rroR}}^{\text{c}}$
KH- $X^1\Sigma^+$	AM	24	14638.63	14761.32	14771.80	14782.28	14772.69 <sup>d</sup>	14772.7	0.001
	Ref. [18]	23	14423.49	14633.73	14749.35	14864.97	14812.93 <sup>e</sup>		-0.348
NaK- $B^1\Pi$	AM	28	1116.421	1124.550	1127.723	1159.453	1128.962 <sup>d</sup>	1129.17 <sup>f</sup>	0.007
	Ref. [19]	30	1150.335	1157.062	1160.069	1163.076	1161.413 <sup>e</sup>		-10.72
$^6\text{LiH}-X^1\Sigma^+$	AM	23	19995.83	20205.52	20268.36	20331.20	20287.20 <sup>d</sup>	20287.7	0.008
	Ref. [20]	21	19232.10	19664.54	19995.83	20327.12	20249.63 <sup>e</sup>		0.115
$^7\text{LiH}-X^1\Sigma^+$	AM	23	19939.73	20169.84	20254.79	20339.74	20286.14 <sup>d</sup>	20287.7	0.018
	Ref. [20]	22	19581.14	19932.13	20169.84	20407.54	20330.83 <sup>e</sup>		-0.181
NaK- $d^3\Pi$	AM	46	1959.306	1963.474	1963.929	1964.384	1963.979 <sup>d</sup>	1964 <sup>g</sup>	0.046
	Ref. [21]	45	1950.541	1957.870	1961.582	1965.294	1963.462 <sup>e</sup>		0.145
NaK- $c^3\Sigma^+$	AM	68	2506.599	2507.653	2507.919	2508.185	2507.987 <sup>d</sup>	2508	0.049
	Ref. [22]	63	2469.432	2471.960	2473.159	2474.358	2473.728 <sup>e</sup>		28.6
NaLi- $X^1\Sigma^+$	AM	44	7040.381	7058.544	7065.081	7071.618	7067.434 <sup>d</sup>	7067.8	0.056
	Ref. [23]	44	7035.512	7051.282	7054.701	7058.120	7055.442 <sup>e</sup>		3.614
$^7\text{LiD}-X^1\Sigma^+$	AM	31	20101.83	20229.45	20273.55	20317.65	20288.79 <sup>d</sup>	20293.5	0.107
	Ref. [20]	27	18954.15	19320.78	19638.84	19956.94	19914.76 <sup>e</sup>		1.191
NaLi- $A^1\Sigma^+$	AM	64	7763.368	7778.769	7786.098	7793.427	7789.586 <sup>d</sup>	7791	0.193
	Ref. [24]	79	8572.035	8579.544	8583.296	8587.048	8585.171 <sup>e</sup>		-211.67
NaRb- $X^1\Sigma^+$	AM	76	5026.868	5030.191	5030.558	5030.925	5030.598 <sup>d</sup>	5030.75 <sup>h</sup>	0.414
	Ref. [25]	82	5241.481	5245.631	5247.636	5249.641	5248.605 <sup>e</sup>		-108.7

<sup>a</sup> $D_e^{\text{app}} = E_{\nu_{\text{max}}} + \Delta E_{\nu_{\text{max}}, \nu_{\text{max}}-1}$ . <sup>b</sup>Experimental value. <sup>c</sup>Relative error  $E_{\text{rroR}} = (D_e^{\text{expt}} - D_e^{\text{calc}})/\Delta E_{\nu_{\text{max}}, \nu_{\text{max}}-1}$ .

<sup>d</sup>Calculated using Eq. (16) and the highest three vibrational energies from algebraic method (AM). <sup>e</sup>Calculated using Eq. (16) and the highest three vibrational energies  $E_{\nu}^{\neq}$  generated using corresponding literature vibrational constants.

<sup>f</sup>Ref. [26]. <sup>g</sup>Ref. [27]. <sup>h</sup>Ref. [28].

It can be seen from Table 1 that the AM dissociation energies  $D_e^{\text{AM}}$  (the  $D_e^{\text{calc}}$  data with superscript d) evaluated using Eq. (16) and the highest three AM vibrational energies are in excellent agreement with the experimental dissociation energies  $D_e^{\text{expt}}$ , and all  $D_e^{\text{calc}}$  satisfy Eq. (17). Table 1 also demonstrates that the AM produces correct maximum vibrational quantum number  $\nu_{\text{max}}$  and the correct maximum vibrational energy  $E_{\nu_{\text{max}}}$  which is very close to the molecular dissociation limit. A typical example is the electronic state  $X^1\Sigma^+$  of NaRb. Kasahara and co-workers<sup>[25]</sup> obtained 31 experimental vibrational energies for this system. Choosing an energy group from Kasahara's energy subset [ $E_{\nu}^{\text{expt}}$ ], the AM approach obtains 77 vibrational energies in full energy spectrum  $\{E_{\nu}\}$ , a correct maximum vibrational energy  $E_{\nu_{\text{max}}=76}^{\text{AM}} (= 5030.558 \text{ cm}^{-1})$  which is very close to  $D_e^{\text{expt}} (= 5030.75 \text{ cm}^{-1})$ , and an accurate dissociation energy  $D_e^{\text{AM}} (= 5030.598 \text{ cm}^{-1})$ .

Table 1 also shows that for the AM studies, the energy difference  $(D_e^{\text{expt}} - D_e^{\text{calc}})$  of an electronic state is within a fraction of its last vibrational spacing  $\Delta E_{\nu_{\text{max}}, \nu_{\text{max}}-1}$  for an accurate theoretical  $D_e^{\text{calc}}$ . In other words, the relative error  $E_{\text{rroR}} = (D_e^{\text{expt}} - D_e^{\text{calc}})/\Delta E_{\nu_{\text{max}}, \nu_{\text{max}}-1}$  of accurate theoretical  $D_e^{\text{calc}}$  is usually smaller than unity. It is clearly seen that all AM  $E_{\text{rroR}}$ 's in Table 1 are smaller than unity.

Table 1 gives the dissociation energies  $D_e^{\neq}$  (the  $D_e^{\text{calc}}$  data with superscript e) evaluated using Eq. (16) and the highest three vibrational energies  $E_{\nu}^{\neq}$  generated using literature vibrational spectroscopic constants. Although the dissociation energies  $D_e^{\neq}$  of the  $d^3\Pi$  state of NaK, the  $X^1\Sigma^+$  states of  $^7\text{LiD}$  and  $^6\text{LiH}$  are not as good as their AM counterparts, they have good accuracies (small  $E_{\text{rroR}}$  values). Particularly, the  $D_e^{\neq} (= 1963.462 \text{ cm}^{-1})$  of the  $d^3\Pi$  state of NaK molecule is almost identical to the values of both  $D_e^{\text{expt}} (= 1964 \text{ cm}^{-1})$  and  $D_e^{\text{AM}} (= 1963.979 \text{ cm}^{-1})$ . This fact shows that as long as the accurate experimental/theoretical high-lying vibrational energies near dissociation limit are available, Eq. (16) will give correct molecular dissociation energy. In Table 1, the dissociation energies  $D_e^{\neq}$  of all other electronic states (except the above three) either violate Eq. (17) (for those having negative  $E_{\text{rroR}}$ ) or have greater even much greater  $E_{\text{rroR}}$  than that of corresponding  $D_e^{\text{AM}}$ . If these energies and their corresponding vibrational wavefunctions are used in accurate quantitative studies such as reactive scatterings which may need accurate molecular dissociation energy, accurate high-lying vibrational states and energies, the errors embedded in these data may poison the resulting physical quantities.

The approximate dissociation energies  $D_e^{\text{app}} (=$

$E_{\nu_{\max}} + \Delta E_{\nu_{\max}, \nu_{\max}-1}$ ) listed in Table 1 show that most of these quantities from both the AM and the literature vibrational constants either violate Eq. (17) or have greater  $E_{\text{error}}$  than their corresponding  $D_e^{\text{calc}}$  obtained using Eq. (16). It is this difference that makes the  $D_e^{\text{app}}$  poor or much poor than the  $D_e^{\text{calc}}$ . It should be pointed out that the AM full spectrum  $\{E_\nu^{\text{AM}}\}$  and the AM dissociation energy  $D_e^{\text{AM}}$  from Eq. (16) are the functions of a given (experimental/theoretical) energy subset  $[E_\nu]$ , and the accuracies of  $\{E_\nu^{\text{AM}}\}$  and  $D_e^{\text{AM}}$  depend on the accuracy of the subset  $[E_\nu]$ . Different  $[E_\nu]$  would result in different  $\{E_\nu^{\text{AM}}\}$  and  $D_e^{\text{AM}}$ .

In summary, we have presented a parameter-free analytical formula (16) for dissociation energies of diatomic molecular electronic states. The new formula for  $D_e$  does not depend on any molecular parameters and any molecular potential coefficients, and is only the function of the highest three (experimental/theoretical) vibrational energies near molecular dissociation limit. The accuracy of the theoretical  $D_e$  calculated from Eq. (16) is uniquely determined by the accuracy of these energies. An algebraic method (AM) is proposed recently<sup>[17]</sup> to generate a full set of vibrational spectrum  $\{E_\nu\}$  using a subset of accurate experimental vibrational energies  $[E_\nu]$  which contains nearly all important quantum effects and vibrational information for a given stable diatomic electronic state. Using the highest three accurate AM vibrational energies near dissociation limit and the new analytical formula in Eq. (16), the molecular dissociation energies  $D_e$  of 10 electronic states of alkali molecules of KH,  $^7\text{LiD}$ ,  $^7\text{LiH}$ ,  $^6\text{LiH}$ , NaK, NaLi and NaRb are studied respectively. These AM dissociation energies  $D_e^{\text{AM}}$  have excellent agreement with experimental dissociation energies  $D_e^{\text{expt}}$ . These studies show that the new analytical formula in Eq. (16) together with the accurate high-lying AM vibrational energies supply a simple and useful way to study dissociation energies of diatomic molecules.

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