

## An *ab initio* study of the ground and low-lying excited states of $\text{LiBe}^+$

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**Abstract.** By using multi-reference configuration interaction method and large all-electron basis sets aug-cc-pwCV5Z, we have calculated the dense potential energy curves (PECs) of  $1^1\Sigma^+$ ,  $1^3\Sigma^+$ ,  $1^1\Pi$ , and  $1^3\Pi$  states of  $\text{LiBe}^+$  molecule. Based on the obtained PECs, the analytical potential energy functions (APEF) have been constructed with a Morse long-range potential function and nonlinear least squares method. The rotational and vibrational energy levels of the four states are determined by solving Schrödinger equation of nuclear movement with the APEFs. The spectroscopic parameters are deduced with the obtained rotational and vibrational energy levels.

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**Key words:** analytical potential energy function, excited state, spectroscopic parameters.

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## 1 Introduction

Ultra-cold molecules have been brought in a great deal of interests in the past twenty years [1, 2], and now still arouse many researchers' interesting. Recently, some researchers have started to pay attention to the diatoms comprise of alkali and alkaline-earth metal elements. In 1993, using several theoretical methods and basis sets, Boldyrev *et al.* [1] studied the electronic structures of lithium containing diatomic molecules and ions. The equilibrium internuclear distance  $R_e$  and the harmonic vibrational frequency  $\omega_e$  were obtained by using correlated second-order Moller-Plesset (MP2) with 6-311+G\* For the dissociation energy  $D_e$ , they used two methods, PMP4 and quadratic configuration interaction with single and double (triplet) (QCISD (T)) excitation, with the basis sets 6-311+G (2df). They found the QCISD (T) can give better results than PMP4 when compared with

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the experimental values. Marino *et al.* [2] reported the potential energy curves (PEC) for the ground state and fourteen excited states of LiBe and LiBe<sup>+</sup>. Several spectroscopic parameters were also presented in their work. Safonov *et al.* [3] also performed a study on LiBe and LiBe<sup>+</sup> by using self-consistent field method. The PECs and some spectroscopic parameters of 1<sup>1</sup>Σ<sup>+</sup>, 1<sup>3</sup>Σ<sup>+</sup>, and 2<sup>1</sup>Σ<sup>+</sup> states of LiBe<sup>+</sup> are also obtained. Using MRCI+Q and multi-reference averaged quadratic coupled-cluster (MRAQCC) methods including Davidson correction, Sun *et al.* [4] calculated the PECs for the X<sup>1</sup>Σ<sup>+</sup>, a<sup>3</sup>Σ<sup>+</sup>, A<sup>1</sup>Σ<sup>+</sup>, c<sup>3</sup>Σ<sup>+</sup>, C<sup>1</sup>Σ<sup>+</sup>, B<sup>1</sup>Π, and b<sup>3</sup>Π states. Their results showed that X<sup>1</sup>Σ<sup>+</sup>, a<sup>3</sup>Σ<sup>+</sup>, B<sup>1</sup>Π, and b<sup>3</sup>Π are weakly bound, while A<sup>1</sup>Σ<sup>+</sup>, c<sup>3</sup>Σ<sup>+</sup>, and C<sup>1</sup>Σ<sup>+</sup> states are repulsive. The calculated spectroscopic parameters for the bound states with two methods show a little difference.

Beyond all question, these investigations should not be ignored and have made a significant effort for the later theoretical work. However, obvious differences occur in the reported spectroscopic parameters from the different author, especially for the  $D_e$  in the ground state. Besides, the analytical potential energy functions (APEF) of the PECs, which are very important for constructing an analytical function for the system containing more atoms or dynamical calculations such as photoassociation or photoassociation dissociation investigation, have not constructed. Therefore, the present paper focus on performing high accurate *ab initio* calculations for the PECs of LiBe<sup>+</sup> and constructing the APEF for both the ground and the low-lying states.

## 2 Theoretical details

### 2.1 Computational details

The multi-reference configuration interaction (MRCI) [5, 6] method shows a good performance in dealing with the electron correlation. Combined with suitable basis sets and active space, MRCI can give the accurate PEC for molecule. The MRCI calculations are based on the optimized orbitals with the complete-active-space-self-consistent field (CASSCF) method. In the present work, the all-electron basis sets aug-cc-pwCV5Z [7] are used, which implies that (9s,4p,1d) [3s,2p,1d] for both Li and Be atoms. Orbitals and occupation schemes are referring to the irreducible representation (A<sub>1</sub>/B<sub>1</sub>/B<sub>2</sub>/A<sub>2</sub>) of C<sub>2v</sub> group. All calculations are performed in the C<sub>2v</sub> subgroup of the C<sub>∞v</sub> point group because of the limit of the program. No core orbitals is used to include the correlation effect of the inner 1s electrons. That is to say, the orbitals of 2p of Li and Be are included in the active space for the excited states, which mean the active space consisted of 2 closed-shell orbitals (2,0,0,0) and 8 active orbitals (4,2,2,0). Hence there are 2 active electrons in 8 orbitals in the correlation energy calculations. The PECs spanning a range from 1.50 to 21.45 Å with a step of 0.05 Å are used for both the ground and the low-lying excited states. All calculations are carried out with MOLPRO package [8].

## 2.2 Expression of APEF

The Morse long-range (MLR) potential function suggested by Le Roy [9, 10] is adopted to fit the PECs of  $\text{LiBe}^+$  because it can accurately reproduce the PECs in both the long and short separate distances. The general MLR function form is

$$V_{MLR}(R) = D_e \left\{ 1 - \frac{u_{LR}(R)}{u_{LR}(R_e)} \exp[-\phi_{MLR}(R)Y_p(R)] \right\}, \quad (1)$$

Where the  $R$  and  $R_e$  are the interatomic distance and the equilibrium bond length, respectively. The corrected long-range (attractive) interaction energy is defined as

$$u_{LR}(R) = \sum_{i=1}^{last} D_{mi}(R) \frac{C_{mi}}{R^{mi}}, \quad (2)$$

and

$$Y_p(R) = (R^p - R_e^p) / (R^p + R_e^p), \quad (3)$$

where  $D_{mi}(R)$  is the damping function, which has been fairly widely used in recent years and especially proposed by Douketis *et al.* [11] The generalized damping function is

$$D_m^{DS(s)}(R) = \left\{ 1 - \exp \left[ -\frac{b^{ds}(s)\rho R}{m} - \frac{c^{ds}(s)(\rho R)^2}{m^{1/2}} \right] \right\}^{m+s}. \quad (4)$$

The parameters  $b(s)$  and  $c(s)$  are system-independent constants determined by optimizing the agreement with the *ab initio* ( $m = 6, 8, 10$ ) damping function behavior that was determined by Kreek and Meath [12]. Here, we used the standard, as recommended by Douketis *et al.* [11] In addition, the system-dependent range parameter  $\rho$  for interacting atoms  $A$  and  $B$  is presented as

$$\rho \equiv \rho_{AB} = \frac{2\rho_A\rho_E}{\rho_A + \rho_E}, \quad (5)$$

in which

$$\rho_A = \left( \frac{I_\rho^A}{I_\rho^H} \right)^{2/3}, \quad (6)$$

and

$$\rho_B = \left( \frac{I_\rho^B}{I_\rho^H} \right)^{2/3}. \quad (7)$$

Here,  $\rho$  is defined in terms of the ratio of the ionization potential of the atom in question ( $I_\rho^A$ ) to that of the H atom ( $I_\rho^H$ ). Finally, the function  $u_{LR}(R)$  defines the long-range behavior of the potential energy function

$$V(R) \approx D_e - u_{LR}(R) = D_e - \sum_{i=1}^{last} D_{mi}(R) \frac{C_{mi}}{R^{mi}}, \quad (8)$$

where  $m_i$  (6, 8, and 10) are the dispersion coefficients. The exponent coefficient function is

$$\phi_{MLR}(R) = [1 - Y_p(R)] \sum_{i=1}^{17} \phi_i Y_p(R)^i + Y_p(R) \phi_{\infty}, \quad (9)$$

and

$$\phi_{\infty} = \text{In} \left\{ \frac{2D_e}{u_{LR}(R)} \right\}. \quad (10)$$

To minimize the possibility of long-range irregular potential function behavior, the power  $p$  in the definition of  $Y_p(R)$  is chosen to be a small positive integer. Meanwhile, if the potential is to achieve the long-range behavior of Eq. (1), then  $p > (m_{last} - m_1)$ . In the entire function,  $\phi_{MLR}(R)$  contains only a series of  $\phi_i$  coefficients obtained by fitting. In addition, to estimate quantitatively the quality of the fitting process, the root mean square error (RMS) is also given by

$$\text{RMS} = \frac{1}{N} \sqrt{\sum_{i=1}^N (V_{APEF} - V_{ab \text{ initio}})^2}, \quad (11)$$

where  $V_{APEF}$  and  $V_{ab \text{ initio}}$  are the energies given by the fitted and *ab initio* calculations, respectively, and  $N$  is the number of points.

### 2.3 Calculations of ro-vibrational energy levels and spectroscopic parameters

Based on the obtained APEFs, the ro-vibrational energy levels of each state are obtained by solving the Schrödinger equation of nuclear movement using LEVEL8.0 [13] program package, and then the spectroscopic parameters are fitted with the Dunham series expansion [14]. According to the Dunham expression, the ro-vibrational energy  $T(v, N)$  of a given level is represented by

$$T(v, N) = \sum_{m,n} Y_{m,n} (v + 1/2)^m [N(N+1)]^n, \quad (12)$$

where  $Y_{m,n}$  are the Dunham coefficients. They are determined with the calculated energy levels using a least squares fitting procedure. The spectroscopic parameters are related to the coefficients as follows:

$$\begin{aligned} Y_{10} &\approx \omega_e, & Y_{20} &\approx -\omega_e X_e, & Y_{30} &\approx \omega_e Y_e \\ Y_{40} &\approx \omega_e Z_e, & Y_{01} &\approx B_e, & Y_{11} &\approx -\alpha_e \\ Y_{21} &\approx \gamma_e, & Y_{02} &\approx D_{rot}, & Y_{12} &\approx -\beta_e. \end{aligned} \quad (13)$$

Thus, the spectroscopic parameters can be obtained. The  $R_e$  and dissociation energy  $D_e$  are obtained with the fitted APEFs.

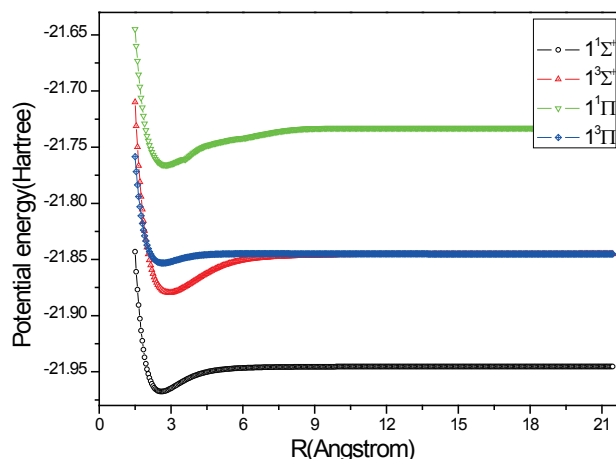


Figure 1: PECs for the  $1^1\Sigma^+$ ,  $1^3\Sigma^+$ ,  $1^1\Pi$ , and  $1^3\Pi$  states of  $\text{LiBe}^+$ .

### 3 Results and discussion

#### 3.1 PECs and APEFs

The *ab initio* PECs for the  $1^1\Sigma^+$ ,  $1^3\Sigma^+$ ,  $1^1\Pi$ , and  $1^3\Pi$  states of  $\text{LiBe}^+$  are depicted in Fig. 1. From the figure, it is obvious to see that the  $1^1\Sigma^+$  state is the lowest one, which means that it is the ground state. Although the higher  $1^1\Pi$  state demonstrates unsmooth to some extent, we can still obtain the APEF with an acceptable error. It may be improved with a larger active space.

As is known to all, the PECs in numerical form is not convenient for further applications, especially for dynamical calculation or construction of analytical potential energy surfaces containing many atoms. Therefore, we fitted the PECs into APEFs with the MLR function and non-linear squares fitting method. All parameters including  $\phi_1$  to  $\phi_{17}$ ,  $D_e$ ,  $R_{ef}$ ,  $R_e$ , the long-range coefficients  $C_6$ ,  $C_8$ ,  $C_{10}$ , and RMS are provided in Table 1. The smallest RMS is  $0.427 \text{ cm}^{-1}$  for the  $1^1\Sigma^+$  state shows the suitability of the MLR function for these states and the high quality of the fitting process. Because of the unsmooth PEC of the  $1^1\Pi$  state, it has the largest RMS of  $11.600 \text{ cm}^{-1}$ , however, which is acceptable because it is still far less than the chemical accuracy  $349.755 \text{ cm}^{-1}$ .

#### 3.2 Ro-vibrational energy levels and spectroscopic parameters

In order to calculate the vibrational and rotational energy levels for  $\text{LiBe}^+$ , we use LEVEL8.0 [13] program package to solve the Schrödinger equation of the nuclear motion based on the obtained APEFs. We have found 31, 49, 53, and 12 levels for the  $1^1\Sigma^+$ ,  $1^3\Sigma^+$ ,  $1^1\Pi$ , and  $1^3\Pi$  states, respectively. For the sake of brevity, we only list the first 12 levels in the Table 2. They can be used as a helpful reference for further investigation because there is no theoretical or experimental data for these states in the literature.

Table 1: The parameters of MLR for LiBe<sup>+</sup>. ( $D_e$  and RMS are in cm<sup>-1</sup>, and  $R_e$  in Å.)

	1 <sup>1</sup> Σ <sup>+</sup>	1 <sup>3</sup> Σ <sup>+</sup>	1 <sup>1</sup> Π	1 <sup>3</sup> Π
$\phi_1$	-2.114964383761	-2.101630782656	-3.273987893657	-3.289110244343
$\phi_2$	-4.56015005360010 <sup>-1</sup>	-5.880960498423	4.296882414934×10 <sup>-1</sup>	5.774979399070
$\phi_3$	-8.479874817989×10 <sup>-1</sup>	-1.010893013755×10 <sup>1</sup>	6.781378841748×10 <sup>-2</sup>	1.000226737263×10 <sup>1</sup>
$\phi_4$	-7.052308767331×10 <sup>-1</sup>	-1.245785921524×10 <sup>1</sup>	5.649769650444	1.078073906733×10 <sup>1</sup>
$\phi_5$	-4.670449284978	-2.501588513311×10 <sup>1</sup>	-4.800171313213×10 <sup>1</sup>	1.584471978961
$\phi_6$	-4.311598391878×10 <sup>1</sup>	-6.334568612041×10 <sup>1</sup>	-1.012190695041×10 <sup>2</sup>	1.219681953033×10 <sup>1</sup>
$\phi_7$	-6.798963326036×10 <sup>1</sup>	1.399125448361×10 <sup>-1</sup>	2.653529989442×10 <sup>2</sup>	1.706804027643×10 <sup>2</sup>
$\phi_8$	1.942297391442×10 <sup>2</sup>	2.609553787274×10 <sup>2</sup>	1.648954205712×10 <sup>2</sup>	1.431759261419×10 <sup>2</sup>
$\phi_9$	5.537005603724×10 <sup>2</sup>	6.822911767751×10 <sup>1</sup>	-8.060433587352×10 <sup>2</sup>	-9.349212834273×10 <sup>2</sup>
$\phi_{10}$	-2.831273187700×10 <sup>2</sup>	-9.861895440541×10 <sup>2</sup>	9.504936600774×10 <sup>2</sup>	-1.198579965498×10 <sup>3</sup>
$\phi_{11}$	-1.928044560659×10 <sup>3</sup>	-9.831775105220×10 <sup>2</sup>	1.673560238893×10 <sup>3</sup>	2.728385588932×10 <sup>3</sup>
$\phi_{12}$	-8.407552217229×10 <sup>2</sup>	1.158949174812×10 <sup>3</sup>	-4.548332134539×10 <sup>3</sup>	4.691667396637×10 <sup>3</sup>
$\phi_{13}$	2.604063907177×10 <sup>3</sup>	2.083937094551×10 <sup>3</sup>	-3.415136955694×10 <sup>3</sup>	-2.933134355532×10 <sup>3</sup>
$\phi_{14}$	2.585422462587×10 <sup>3</sup>	3.389866159192×10 <sup>1</sup>	6.981119098006×10 <sup>3</sup>	-7.927725519817×10 <sup>3</sup>
$\phi_{15}$	-8.271197969562×10 <sup>2</sup>	-1.561103837762×10 <sup>3</sup>	4.840315158740×10 <sup>3</sup>	-5.224890144534×10 <sup>2</sup>
$\phi_{16}$	-1.959558050074×10 <sup>3</sup>	-1.006124359730×10 <sup>3</sup>	-3.654437025084×10 <sup>3</sup>	5.074112215088×10 <sup>3</sup>
$\phi_{17}$	-6.770827853067×10 <sup>2</sup>	-1.911481397861×10 <sup>2</sup>	-2.715033360966×10 <sup>3</sup>	2.290940264178×10 <sup>3</sup>
$D_e$	4.903607989794×10 <sup>3</sup>	7.527014468295×10 <sup>3</sup>	7.224677680126×10 <sup>3</sup>	1.754200282361×10 <sup>3</sup>
$R_{ef}$	5.447656520127	7.144759770531	4.719602222884	8.488570525563
$R_e$	2.599829038210	2.935215460676	2.784947543327	2.661490398269
$C_6$	1.048646823287×10 <sup>7</sup>	4.089246441117×10 <sup>6</sup>	-2.000140733514×10 <sup>8</sup>	-2.585549529673×10 <sup>9</sup>
$C_8$	3.333820962753×10 <sup>8</sup>	1.593938031969×10 <sup>8</sup>	1.648158213712×10 <sup>10</sup>	4.764999401183×10 <sup>7</sup>
$C_{10}$	3.963128665362×10 <sup>8</sup>	1.704954876670×10 <sup>9</sup>	5.333071974397×10 <sup>10</sup>	1.710070420243×10 <sup>12</sup>
RMS	4.27×10 <sup>-1</sup>	7.43×10 <sup>-1</sup>	1.16×10 <sup>1</sup>	7.20×10 <sup>-1</sup>

Based on the obtained ro-vibrational levels of those states, we have determined the spectroscopic parameters by using Dunham expansion of Eq. (12) and nonlinear least squares fitting method. The calculated spectroscopic parameters with the previously reported values [1-4] are tabulated in Table 3. It should be noticed that the values of  $D_e$  and  $R_e$  are fitted from the PECs with the MLR function.

For the ground state 1<sup>1</sup>Σ<sup>+</sup>, our value of  $R_e$  is 2.600 Å, which is close to 2.629 Å of Boldyrev *et al.* [1], 2.635 Å of Marino *et al.*, [2] and 2.634 Å of Sun *et al.* [4] but smaller than 2.66 Å of Safonov *et al.* [3], respectively. The present dissociation energy  $D_e$  of 4903.6 cm<sup>-1</sup> is different from all the previously reported values. For examples, it is 286.8 cm<sup>-1</sup> larger than that of Boldyrev *et al.* [1], 391.9 cm<sup>-1</sup> larger than that of Marino *et al.* [2], 298.6 cm<sup>-1</sup> larger than that of Sun *et al.* [4], and 97.0 cm<sup>-1</sup> smaller than Safonov *et al.* [3]. It is shown that the calculational method and basis sets play more obvious effect on the  $D_e$  than that of  $R_e$ . The full CI with the Gaussian expansions of Slater-type orbitals (STO-6G) by Marino *et al.* [2] gives smaller  $D_e$  than that of QCISD(t)/6-311+G\* by Boldyrev *et al.* [1]. The present large basis sets aug-cc-pwCV5Z is responsible for the larger  $D_e$ . As

Table 2: The vibrational levels ( $N = 0$ ) for NaBe. (in  $\text{cm}^{-1}$ ).

$v$	$1^1\Sigma^+$	$1^3\Sigma^+$	$1^1\Pi$	$1^3\Pi$
0	160.2783	136.4554	141.8240	121.3875
1	473.2341	405.8650	418.9235	354.4488
2	776.1739	670.8786	677.6471	573.1145
3	1069.1745	931.5224	911.0826	776.2302
4	1352.2139	1187.8030	1126.1489	963.0179
5	1625.1970	1439.7132	1339.6056	1133.1242
6	1887.9806	1687.2373	1558.5264	1286.5425
7	2140.3941	1930.3548	1782.8431	1423.3456
8	2382.2513	2169.0437	2011.2360	1543.265
9	2613.3529	2403.2829	2242.1027	1645.288
10	2833.4842	2633.0523	2473.7126	1727.5563
11	3042.4119	2858.3324	2704.2081	1787.975

for the largest  $D_e$  given by Safonov *et al.*, [3] may be less reliable because the calculation was based on the SCF method. Our  $\omega_e$  is in good agreement with those from all the four reports [1-4]. Our anharmonic frequency  $\omega_e x_e$  is close to that of Boldyrev *et al.* [1], but both smaller than that of Safonov *et al.* [3] and Sun *et al.* [4] For the excited states ( $1^3\Sigma^+$  and  $1^3\Pi$ ), the differences between our results and the reports in the literature [1-4] show a similar tendency. The reader can easily find the details in Table 3. Therefore, we omit the repetitive description. Unfortunately, no experimental data can be found for all the considered states. The present results can be used as a helpful reference for further investigation because they are performed with the high theoretical level of and the large all-electron basis sets, and are in agreement with the available theoretical reports in the literature.

## 4 Conclusions

The *ab initio* PECs of the ground and three low-lying excited states of  $\text{LiBe}^+$  are obtained using the high accurate CASSCF/MRCI method with large all-electron basis sets aug-cc-pwCV5Z. By using the MLR function and the nonlinear least squares method, we deduce the APEFs for each state. The ro-vibrational levels and the spectroscopic parameters of the states are determined by solving the Schrödinger equation of nuclear movement based on the obtained APEFs. It is found that all the theoretical method, the basis sets and the active space impact on the spectroscopic properties. The obtained APEFs for the  $1^3\Sigma^+$  and  $1^3\Pi$  states with very little RMS should be reliable for further investigation, while that of  $1^1\Pi$  state need improve because of the relative larger RMS. These results could be helpful in the dynamical investigation of photoassociation or light dissociation of  $\text{LiBe}^+$  molecule.

Table 3: The spectroscopic parameters (in  $\text{cm}^{-1}$  except  $R_e$  in  $\text{\AA}$ ) for the  $1^1\Sigma^+$ ,  $1^3\Sigma^+$ ,  $1^1\Pi$ , and  $1^3\Pi$  states of  $\text{LiBe}^+$ .

	$1^1\Sigma^+$	$1^3\Sigma^+$	$1^1\Pi$	$1^3\Pi$
$R_e$	2.600	2.935	2.785	2.661
	2.629 <sup>a</sup>	2.953 <sup>b</sup>	2.839 <sup>d</sup>	2.694 <sup>b</sup>
	2.635 <sup>b</sup>	2.97 <sup>c</sup>		2.701 <sup>d</sup>
	2.66 <sup>c</sup>	2.966 <sup>d</sup>		
	2.634 <sup>d</sup>			
$D_e$	4903.6	7527.0	7224.7	1754.2
	4616.8 <sup>a</sup>	7339.6 <sup>b</sup>	3395.6 <sup>d</sup>	1532.5 <sup>b</sup>
	4511.7 <sup>b</sup>	7420.3 <sup>c</sup>		6976.7 <sup>d</sup>
	5000.6 <sup>c</sup>	1669.6 <sup>d</sup>		
	4605.0 <sup>d</sup>			
$\omega_e$	318.4	274.2	281.1	244.6
	320 <sup>a</sup>	274 <sup>b</sup>	256.3 <sup>d</sup>	235 <sup>b</sup>
	311 <sup>b</sup>	274 <sup>c</sup>		236.5 <sup>d</sup>
	320 <sup>c</sup>	270.8 <sup>d</sup>		
	315.3 <sup>d</sup>			
$\omega_e X_e$	4.310	2.290	$1.572 \times 10^1$	5.501
	4.8 <sup>b</sup>	2.2 <sup>b</sup>	4.696 <sup>d</sup>	7.0 <sup>b</sup>
	8.2 <sup>c</sup>	5.4 <sup>c</sup>		6.954 <sup>d</sup>
	4.762 <sup>d</sup>	2.173 <sup>d</sup>		
$\omega_e Y_e$	$-2.409 \times 10^{-2}$	$7.748 \times 10^{-3}$	1.872	$4.845 \times 10^{-1}$
	$-5.241 \times 10^{-2d}$	$-0.074 \times 10^{-2d}$	$-2.703 \times 10^{-2d}$	$-3.025 \times 10^{-2d}$
$\omega_e Z_e$	$-1.855 \times 10^{-3}$	$-2.379 \times 10^{-4}$	$-9.333 \times 10^{-2}$	$4.547 \times 10^{-2}$
	$2.529 \times 10^{-3d}$	$0.211 \times 10^{-3d}$	$-0.468 \times 10^{-3d}$	$-2.020 \times 10^{-3d}$
$B_e$	$6.173 \times 10^{-1}$	$4.949 \times 10^{-1}$	$5.329 \times 10^{-1}$	$5.984 \times 10^{-1}$
	0.616 <sup>b</sup>	0.490 <sup>b</sup>	0.533 <sup>d</sup>	0.590 <sup>b</sup>
	0.601 <sup>c</sup>	0.482 <sup>c</sup>		0.589 <sup>d</sup>
	0.620 <sup>d</sup>	0.489 <sup>d</sup>		
$D_{rot}$	$-4.869 \times 10^{-6}$	$-5.747 \times 10^{-6}$	$-6.846 \times 10^{-6}$	$-1.249 \times 10^{-5}$
	$9.565 \times 10^{-6d}$	$-6.539 \times 10^{-6d}$	$0.923 \times 10^{-6d}$	$14.61 \times 10^{-6d}$
$\alpha_e$	$9.179 \times 10^{-3}$	$6.894 \times 10^{-3}$	$4.875 \times 10^{-3}$	$1.402 \times 10^{-2}$
	0.013 <sup>b</sup>	0.006 <sup>b</sup>	$1.232 \times 10^{-2}$	0.021 <sup>b</sup>
	$1.83 \times 10^{-2c}$	$1.19 \times 10^{-2c}$		$2.048 \times 10^{-2d}$
	$1.261 \times 10^{-2d}$	$0.664 \times 10^{-2d}$		
$\gamma_e$	$-3.234 \times 10^{-4}$	$5.267 \times 10^{-5}$	$-1.549 \times 10^{-4}$	$-1.257 \times 10^{-3}$
	$-2.09310^{-4d}$	$0.051 \times 10^{-4d}$	$-1.631 \times 10^{-4d}$	$-3.415 \times 10^{-4d}$
$\beta_e$	$9.066 \times 10^{-7}$	$3.737 \times 10^{-8}$	$2.258 \times 10^{-7}$	$2.739 \times 10^{-6}$
	$7.017 \times 10^{-8d}$	$6.856 \times 10^{-8d}$	$-15.94 \times 10^{-8d}$	$-50.47 \times 10^{-8d}$

<sup>a</sup> Data from Ref. 1. <sup>b</sup> Data from Ref. 2. <sup>c</sup> Data from Ref. 3. <sup>d</sup> Data from Ref. 4.

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