International Journal of Chemistry, Mathematics and Physics (IJCMP)
[Vol-9, Issue-2, Apr-Jun, 2025]
https://dx.doi.org/10.22161/ijcmp.9.2.2
ISSN: 2456-866X

Theoretical investigation of low-lying electronic states of the Be$^+$He molecular ion: Potential energy curves, spectroscopic constants and vibrational levels

Michel Douglas Epée Epée[1], Ghislain P. Tchakouadeu[2] and Polain R. Tchoupo kamdem[2]

[1]Department of Physics, Faculty of Science, University of Douala, P. O. Box: 24157, Douala, Cameroon
[2]Postgraduate Training Unit for Mathematics, Applied Computer Science and Pure Physics, University of Douala, Douala, Cameroon
Corresponding author: epeemichel23@yahoo.fr

Received: 07 May 2025; Received in revised form: 30 May 2025; Accepted: 07 Jun 2025; Available online: 11 Jun 2025

***Abstract*— *Potential energy curves, inter-nuclear equilibrium separations and harmonic frequencies of the low-lying electronic states of Be^+He correlating to the six lowest dissociative channels have been calculated using the cc-pV5Z basis sets and the complete active space self-consistent field (CASSCF) followed by the multi-reference interaction (MRCI) wave function including Davidson correction. Potential curves obtained are all fitted to analytical potential energy functions (APEFs) using the Murrell-Sorbie potential function. The spectroscopic parameters, such as D_e, $\omega_e x_e$, α_e , B_e are determined using the obtained APEFs, and compared with theoretical data available. The vibrational level $G(v)$, inertial rotation constant B_v are predicted for each vibrational states of this electronic states by solving the ro-vibrational Schrödinger equation of nuclear motion using Numerov's method.*

***Keywords*— Potential energy curve, spectroscopic parameters, vibrational level.**

I. INTRODUCTION

Study of the structure and spectrum of molecular species containing beryllium have been the subject of studies over the years for the important role they play in several areas of research. Beryllium is valuable a material for atomic energy, rocket, missile, aviation and metallurgical industry. It is presently chosen as plasma-facing wall material for fusion devices such as International Thermonuclear Experimental Reactor (ITER) and the Joint European Torus (JET) [1-3]. Experimental characterization of Beryllium compounds which are known to cause serious lung diseases [4], is difficult as well as dangerous [5], given the extremely toxic nature of Be dust. The Be$^+$He molecular ion has thus received little attention from theoretical investigations may be because of the absence of experimental information. Of these investigations, only a few theories are involved in its ground state spectroscopic properties. Frenking et al. [6] have reported the result of equilibrium geometries, dissociation energies, vibrational frequencies and total energies at the MP4 (SDTQ)/6-311G(2df,2pd)//MP2/6-31G(d,p) level of theory for the ground state $X\ ^2\Sigma^+$ and the first excited state $^2\Pi$. Spectroscopic constant for Be$^+$He have been determined by Leung and Breckenridge[4] at the QCISD(T) level using the 6-311++G**(3df,3dp) basis set for Be atom and the Dunning augmented correlation consistent polarized basis set aug-cc-pVQZ for He, both for the ground and the first excited states. As part of a study investigating Be$^+$He$_n$ clusters, Be$^+$He has been studied by Bu et al.[7-8] at the MP2/6-311+G(3df,3pd) level. Gardner et al.[9] have reported spectroscopic constants of the ground state of Be$^+$He at the RCCSD(T)daVQZ level of theory. More recently, in a new study, using a one-electron pseudo-potential approach, potential energy and spectroscopic constants of the ground and excited states of Be$^+$He have been investigated by Dhiflaoui et al. [10]. Most of these theories mainly concentrated on the spectroscopic parameters ($D_e, R_e,\ \omega_e,\ \omega_e x_e,\ \alpha_e\ , B_e$) and the values reported still show a wide variation. To the best of our knowledge, no information is available in the literature about vibrational level (v) , inertial rotation constant B_v, though these data have important applications in the vibrational transitions calculations.

The purpose of the present study is to contribute to a thorough understanding of electronic structure, spectroscopic parameters and molecular constants of Be$^+$He. In order to achieve these purpose, accurate potential energy curves of the low-lying electronic states $X\ ^2\Sigma^+, A\ ^2\Pi, B\ ^2\Sigma^+, C\ ^2\Sigma^+,\ D\ ^2\Sigma^+, E\ ^2\Pi, F\ ^2\Pi,\quad G\ ^2\Delta,$ $H\ ^2\Sigma^+, I\ ^2\Sigma^+,$ of Be$^+$He correlating to the six lowest dissociative channel are first carried out, using the correlation-consistent basis sets cc-pV5Z and the complete active self –consistent field (CASSCF) followed by the multi-reference configuration interaction (MRCI) wave function including Davidson correction. The potential energy curves are fitted to the analytic Murrell-Sorbie function, which is used to determine the spectroscopic parameters. .

II. COMPUTATIONAL DETAILS

Due to the lack of experimental data and the little theoretical information about the diatomic molecular ion Be$^+$He, the first step in the planning of our calculation was the identification of possible electronic states correlating to six lowest dissociation channels using Wigner-Witmer rules[11]. This information is summarized in Table 1, which also includes the energy separation for each channel. We performed ab initio calculations with ORCA[12-14] software package using the correlation-consistent polarized valence quintuple zeta (cc-pV5Z) basis sets for Be(24s8p4d3f2g1h contracted to 6s5p4d3f2g1h) and Helium (8s4p3d2f1g contracted to 5s4p3d2f1g). Calculation of potential energy curves, inter-nuclear equilibrium separations and harmonic frequencies were performed in three steps. In the first step, a Restricted Hartree-Fock (RHF) calculation was performed in order to produce a set of 146 molecular orbitals. This orbitals were then used as initial guess for the Complete Active Space Self-Consistent Field (CASSCF) calculations; the final step was a Multi-Reference Configuration Interaction (MRCI) for which the CASSCF molecular orbitals was used. All our calculations are carried out in the C_{2v} point group. The 146 molecular orbitals resulted from RHF were divide in three groups: one internal orbital, 6 active orbitals of CASSCF accessible to three valence electrons and the 139 external orbitals remained unoccupied in CASSCF were accessible to valence electrons in MRCI calculations. In order to obtain more accurate PECs, the energies were calculated in the range of inter-nuclear separation from 0.5 Å to 15Å in the step of 0.05Å. Over these inter-nuclear distance range, the obtained potential energy curves are smooth and completely convergent.

The potential curves obtained are then fitted to analytical potential energy functions (APEFs) using the Murrell-Sorbie potential function [15]. The general expression of the Murrell potential function is [16]

Table 1: Low-Lying electronic states of Be$^+$He arising from the six lowest dissociation limits

Dissociation channel	**Molecular states**	**Energy Separation**
Be$^+$(2s, ^{2}S) + He (^{1}S)	$X\ ^2\Sigma^+$	0.000000
Be$^+$(2p, ^{2}P) + He (^{1}S)	$A\ ^2\Pi, B\ ^2\Sigma^+$	3.959067
Be$^+$(3s, ^{2}S) + He (^{1}S)	$C\ ^2\Sigma^+$	10.939363
Be$^+$(3p, ^{2}P) + He (^{1}S)	$D\ ^2\Sigma^+\quad E\ ^2\Pi,$	11.964019
Be$^+$(3d, ^{2}D) + He (^{1}S)	$F\ ^2\Pi,\ G\ ^2\Delta, H\ ^2\Sigma^+$	12.157258
Be$^+$(4s, ^{2}S) + He (^{1}S)	$I\ ^2\Sigma^+$	14.315766

$$V(\rho) = -D_e(1 + \textstyle\sum_{i=1}^{n} a_i\, \rho^i \exp(-a_1\rho)) \qquad (1)$$

where $\rho = R - R_e$, R is the inter-nuclear distance of diatomic molecule, R_e is it equilibrium inter-nuclear distance and is regarded as a fixed parameter in the fitting process. The parameters D_e and $a_i\ (i = 1{,}2{,}3 \ldots..n)$ are determined by fitting. The quadratic, cubic, and quartic force constants $f_n\ (f_n = \frac{d^nV}{dR^n},\ n = 2, 3$ and $4)$ could be derived from function at the equilibrium position as followed

$$f_2 = D_e(a_1^2 - 2a_2) \qquad (2)$$

$$f_3 = -6D_e(a_3 - a_1a_2 + \tfrac{1}{3}a_1^3) \qquad (3)$$

$$f_4 = D_e(3a_1^4 - 12a_1^2a_2 + 24a_1a_3) \qquad (4)$$

The expression relating the spectroscopic constants with the force constants f_2, f_3 and f_4 for diatomic molecules may be found as

$$B_e = \frac{h}{8\pi c\mu R_e^2} \qquad (5)$$

$$\omega_e = \sqrt{\frac{f_2}{4\pi^2 mc^2}} \qquad (6)$$

$$\alpha_e = -\frac{6B_e^2}{\omega_e}\left(\frac{f_3R_e}{3f_2} + 1\right) \qquad (7)$$

$$\omega_e x_e = \frac{B_e}{8}\left[-\frac{f_4R_e^2}{f_2} + 15\left(1 + \frac{\omega_e\alpha_e}{6B_e^2}\right)^2\right] \qquad (8)$$

Based on the relationship equations among spectroscopic parameters and force constants (6)-(8), the spectroscopic data of diatomic molecule can be calculated. Using the potential energy curves obtained at the MRCI/ cc-pV5Z level of theory, the radial Schrödinger equation of nuclear motion is numerically solved using the Numerov method [17] to get the vibrational states when $J = 0$. The complete vibrational levels $\mathrm{G(v)}$, inertial rotation constant $\mathrm{B_v}$ are calculated.

III. RESULTS AND DISCUSSION

In the present work, a total of 10 electronic states of the Be$^+$He species dissociating into Be$^+$ (2s, 2p, 3s, 3p, 3d, 4s) + He have been investigate, namely six $^2\Sigma^+$, three $^2\Pi$ and one $^2\Delta$. The potential energy curve are graphically displayed in Fig.1 for $^2\Sigma^+$and Fig. 2 for $^2\Pi$ and $^2\Delta$. The spectroscopic constants (D_e, R_e, ω_e, $\omega_e x_e$, α_e , B_e) of the ten electronic states obtained in this work are presented in Table 2 along with the theoretical results available. To the best of our knowledge, there is no experimental work on Be$^+$He system. As shown in Table 2, our equilibrium distance R_e obtained for the ground state $X\ ^2\Sigma^+$ is 2.9064 Å, that compares favorably with the 2.924 Å results of Gardner et al. [9]. In the case of the spectroscopic constants (ω_e, $\omega_e x_e$, α_e , B_e), our results (78.8658 cm^{-1} , 10.2876 cm^{-1}, 0.0976 cm^{-1}, 0,7252 cm^{-1}) are reasonably in good agreement with those obtained by Gardner et al. (76.3 cm^{-1}, 11.7cm^{-1}, 0.142 cm^{-1}, 0.723 cm^{-1}). Concerning the dissociation energy De, we obtained 122.6205 cm^{-1} that compares well with 124 cm^{-1} of Leung et al. [6]. The disagreement ranges with the other theoretical results for the ground state are between 0.017 and 0.226 Å for R_e, 12.621 and 86.380 cm^{-1} for D_e, 2.566 and 14.866 cm^{-1} for ω_e, 1.412 and 4.878 cm^{-1} for $\omega_e x_e$, 0.002 and 0.47 for B_e.

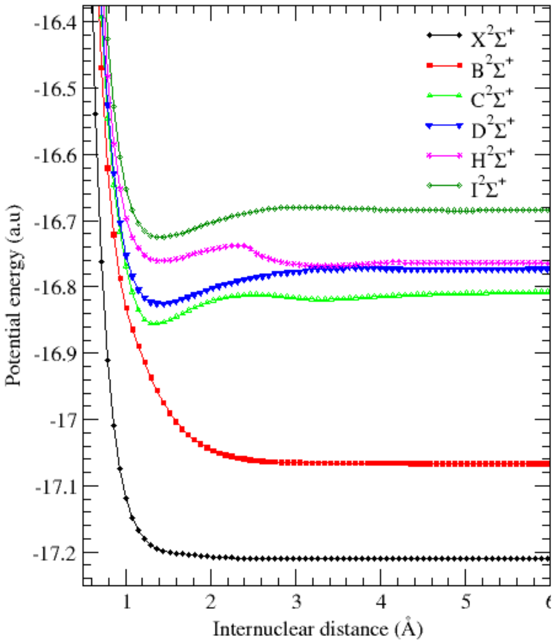

Figure 1: *Potential energy curves for the ground and excited $^2\Sigma$ states of Be$^+$He*

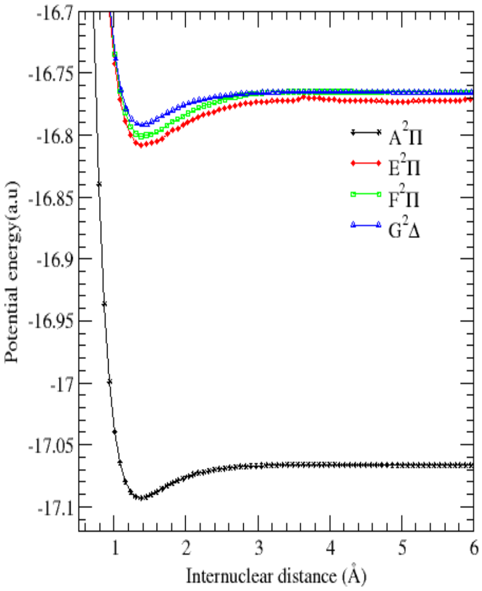

Fig.2: Potential energy curves for the excited $^2\Pi$ states of Be$^+$He

Next in energy, the state $A\ ^2\Pi$ ($T_e = 25\,697\ cm^{-1}$) with $R_e = 1.3763$Å, and ($D_e = 6244.5361 cm^{-1}, \omega_e = 939.0774 cm^{-1}$) is also reasonably in good agreement with the QCISD(T) results of Leung et al.($R_e = 1.38$Å, $D_e = 5845\ cm^{-1}$ $\omega_e = 916 cm^{-1}$). By comparing the available theoretical data of Frenking et al. [5], Leung et al. [6], Bu et al. [7,8], Gardner et al. [9], for the the ground state $X\ ^2\Sigma^+$ and the first excited state $A\ ^2\Pi$ with the recent theoretical study of Dhiflaoui et al. [10] using the pseudo potential, we can find that Although his equilibrium distance R_e(3.1274 Å) for the ground state is in better agreement with the MP2/MP4 calculation of Frenking et al. (3.13 Å) [5], their rest of spectroscopic constants (De, ω_e, $\omega_e x_e$, α_e , B_e) are large or small than the results of the present investigation and the other theoretical data available. For the other electronic states $B\ ^2\Sigma^+, C\ ^2\Sigma^+$, $D\ ^2\Sigma^+, E\ ^2\Pi$, $F\ ^2\Pi$, $G\ ^2\Delta$, $H\ ^2\Sigma^+, I\ ^2\Sigma^+$comparisons with the only theoretical results of Dhiflaoui et al. [10] ($B\ ^2\Sigma^+, 3\ ^2\Sigma^+, 4\ ^2\Sigma^+$, $5\ ^2\Sigma^+ 6\ ^2\Sigma^+$, $2\ ^2\Pi, 3\ ^2\Pi, 1\ ^2\Delta$) respectively show that their equilibrium distances are slightly larger when compared with the present ones. A more noticeable discrepancy in Dhiflaoui et al. lies on the harmonic frequencies ω_e which are underestimated by about 78.89 % for $B\ ^{2}\Sigma^{+}$, 68.50% for , $C\ ^{2}\Sigma^{+}$, 59.08% for $D\ ^{2}\Sigma^{+}$, 50.45 for $E\ ^{2}\Pi$, 58.20 for $F\ ^{2}\Pi$, 45.05 for $G\ ^{2}\Delta$, 45.93 for $H\ ^{2}\Sigma^{+}$, 51.68 for $I\ ^{2}\Sigma^{+}$. Their values of anharmonic frequencies $\omega_e x_e$ are substantially lower than the ones presented in this work. The adiabatic excitation energies T_e of Dhiflaoui et al. [10] are slightly lower than this work. The dissociation energies of the present work and the ones of Dhiflaoui et al. [10] show a wide variation. Dipole moments for the ground state $X\ ^{2}\Sigma^{+}$ calculated at the MRCI level of theory are plotted in Fig. 3. As it is seen in the figure , the slope of the dipole moment is positive. Based on the potential energy curve of $X\ ^{2}\Sigma^{+}, A\ ^{2}\Pi, B\ ^{2}\Sigma^{+}, C\ ^{2}\Sigma^{+}$, $D\ ^{2}\Sigma^{+}, E\ ^{2}\Pi$, $F\ ^{2}\Pi$, $G\ ^{2}\Delta$, $H\ ^{2}\Sigma^{+}, I\ ^{2}\Sigma^{+}$, electronic states, we have obtained the maximum vibrational levels to be : 4 for $X\ ^{2}\Sigma^{+}$, 8 for $B\ ^{2}\Sigma^{+}$, 17 for $C\ ^{2}\Sigma^{+}$, 21 for $D\ ^{2}\Sigma^{+}$, 16 for $H\ ^{2}\Sigma^{+}$, 13 for $I\ ^{2}\Sigma^{+}$, 14 for $A\ ^{2}\Pi$, 23 for $E\ ^{2}\Pi$, 19 for $F\ ^{2}\Pi$ and 16 for $G\ ^{2}\Delta$. We summarize these results in Table 3 and the inertial rotation constants in Table 4. In Fig. 4 we have shown the variation of vibrational levels spacing $G(v+1) - G(v)$ between the adjacent vibrational states for the ten electronic states as a function of vibrational quantum number.

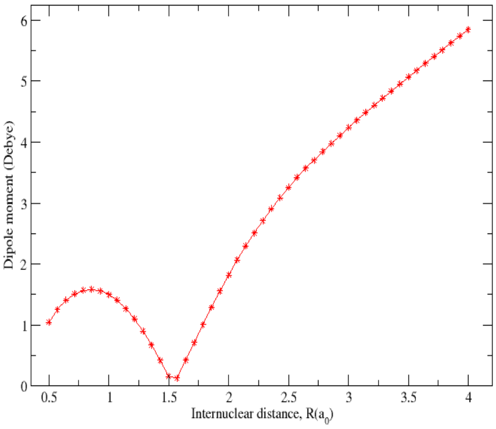

Fig.3: Permanent dipole moment curve for the ground state of Be$^+$He

Unfortunately, no theoretical results, no experiments can be found in the literature about $G(v)$ and B_v of both ground and excited states of Be$^+$He. We cannot make any direct comparison. According to the good agreement between our spectroscopic parameters and the available theoretical results, we have reasons to believe that the results presented in Tables 3 and 4 are reliable and accurate.

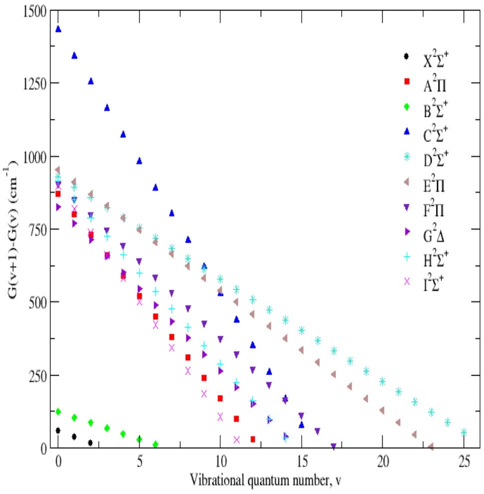

Fig.4: Vibrational energy levels spacing for ground and excited electronic states

IV. CONCLUSION

This work investigates the potential energy curves, spectroscopic parameters and vibrational levels of $X\ ^{2}\Sigma^{+}, A\ ^{2}\Pi, B\ ^{2}\Sigma^{+}, C\ ^{2}\Sigma^{+}$, $D\ ^{2}\Sigma^{+}, E\ ^{2}\Pi$, $F\ ^{2}\Pi$, $G\ ^{2}\Delta$, $H\ ^{2}\Sigma^{+}, I\ ^{2}\Sigma^{+}$ electronic states. By using Murrell-Sorbie function the spectroscopic constants are calculated and a good agreement between our calculation and those of the theoretical study available is observed. A total of 151 vibrational states have been predicted for the first time. For each vibrational state, the vibrational level and inertial rotation constants are determined when J = 0. The overall view of the electronic states, their spectroscopic constants, as well vibrational levels provided should be an important guide to the experimentalist in the search and identification of this species.

Table 2: Spectroscopic constants of the ground and excited $^2\Sigma^+$, $^2\Pi$ *and* $^2\Delta$ *electronic states of* Be^+He.

State		$R_e(Å)$	$E_e(cm^{-1})$	$D_e(cm^{-1})$	$T_e(cm^{-1})$	$\omega_e(cm^{-1})$	$\omega_e x_e(cm^{-1})$	$B_e(cm^{-1})$	$\alpha_e(cm^{-1})$
$X\ ^2\Sigma^+$	This work	2.9064	-17.210093	122.6205	0	78.8658	10.2876	0.7252	0.0916
	RCCSD(T)[a]	2.924		133.1		76,3	11.7	0.723	0.142
	QCISD(T)[b]	2.96		124		73			
	MP2/MP4[c]	3.132	-17, 1740	110		68			
	MP2 (full)[d]	3.095	-17.184355			64			
	Pseudo[e]	3.1274		209	0	66.49	5.41	0.2552	
$B\ ^2\Sigma^+$	This work	3.4401	-17.066317	434.0330	31556	143.9209	9.3959	0.514119	0.0226
	Pseudo[e]	4.2969		44	32966	30. 37	4.54	0.132432	
$C\ ^2\Sigma^+$	This work	1.3408	-16.855776	10638.6530	77764	1524.0239	45.1759	3.384404	0.1079
	Pseudo[e]	1.6087		3821	83865	480	10.18	0.962891	
$D\ ^2\Sigma^+$	This work	1.4286	-16.825369	11919.6013	84437	965.3998	17.5571	2.981179	0.0964
	Pseudo[e]	1.7622		3228	93224	395.04	11.33	0.804161	
$H\ ^2\Sigma^+$	This work	1.3936	-16.705982	-700.4094	98653	976.0478	31.2873	3.132759	0.1025
	Pseudo[e]	1.6669		-9819	107504	527.72	10.56	0.895581	
$I\ ^2\Sigma^+$	This work	1.4075		8755.1941	106713	977.0192	39.5455	33.384525	0.2216
	Pseudo[e]	1.6034		3826	111157	472.04	11.03	0.971556	
$A\ ^2\Pi$	This work	1.3763	-17.093010	6244.5361	25697	939.0774	35.0012	3.212106	0.1411
	QCISD(T)[b]	1.38		5845		916			
	MP2/MP4[c]	1.415	-17.0522	5460					
	Pseudo[e]	1.5875		5264	27746	504.25	12.35	0.991742	
$E\ ^2\Pi$	This work	13836	-16.809105	8354.6749	88007	993.6234	20.5778	3.168627	0.1478
	Pseudo	1.5822		4959	91494	492.33	12.33	0.999341	
$F\ ^2\Pi$	This work	1.4375	-16.8002203	7995.6276	89957	856.6448	26.4011	2.985815	0.11170
	Pseudo[e]	1.6775		2113	95572	358.10	16.51	0.885723	
$G\ ^2\Delta$	This work	1.4068	-16.792773	6440.8781	91591	882.8881	28.0979	3.118421	0.1298
	Pseudo[e]	1.5928		5090	92595	485.11	11.84	0.985233	

[a] RCCSD (T) Calculation of Gardner et al. [9]

[b] QCISD(T) Calculation of A. W. H. Leung and W. H. Breckenridge [6]

[c] MP2/MP4 Calculation of Frenking et al. [5]

[d] MP2(full)/6-311+G(d,2p) calculation of Bu et al. [7-8]

[e] One-electron pseudo-potential approach of Dhiflaoui et al. [10]

Table 3: Vibrational levels $G(v)$ for the lowest $^2\Sigma^+$, $^2\Pi$, $^2\Delta$ electronic states of Be^+He

v	$X\ ^2\Sigma^+$	$B\ ^2\Sigma^+$	$C\ ^2\Sigma^+$	$D\ ^2\Sigma^+$	$H\ ^2\Sigma^+$	$I\ ^2\Sigma^+$	$A\ ^2\Pi$	$E\ ^2\Pi$	$F\ ^2\Pi$	$H\ ^2\Delta$
0	36.861	69.112	750.7180	478.311	480.202	478.573	460.788	491.667	471.722	434.416
1	95.152	193.241	2184.3902	1408.596	1393.675	1376.401	1329.864	1444.135	1375.564	1261.101
2	132.877	298.578	3527.7106	2303.768	2244.573	2195.138	2128.936	2355.447	2226.605	2031.591
3	150.007	385.124	4780.6792	3163.825	3032.897	2934.785	2858.007	3225.604	3024.842	2745.884
4		452.878	5943.2960	3988.768	3758.646	3595.340	3517.075	4054.605	3770.278	3403.982
5		501.840	7015.5612	4778.597	4421.820	4176.804	4106.141	4842.451	4462.911	4005.883
6		532.011	7997.4745	5533.311	5022.419	4679.177	4625.205	5589.141	5102.742	4551.589
7		543.389	8889.0361	6252.912	5560.443	5102.459	5074.266	6394.676	5689.771	5041.099
8			9690.2459	6937.398	6035.893	5446.650	5453.325	6959.055	6223.997	5474.413
9			10401.1040	7586.770	6448.768	5711.749	5762.381	7582.279	6705.421	5851.531
10			11021.6103	8201.028	6799.068	5897.758	6001.436	8164.34	7134.043	6171.453
11			11551.7649	8780.171	7086.794	6004.676	6170.488	8705.259	7509.862	6437.180
12			11991.5676	9324.201	7311.944	6032.503	6269.538	9205.016	7832.880	6645.711
13			12341.0186	9833.116	7474.520		6298.585	9663.618	8103.094	6798.045
14			12600.1179	10306.917	7574.521			10081.064	8320.507	6894.184
15			12768.8654	10745.604	7611.948			10457.354	8485.117	6934.127
16			12847.2611	11149.177				10792.489	8596.925	
17				11517.635				11086.469	8655.931	
18				11850.979				11339.292	8662.134	
19				12149.209				11550.961		
20				12412.325				11721.473		

Table 4: Rotational constants B_v for vibrational levels of $^2\Sigma^+$, $^2\Pi$, $^2\Delta$ electronic states

v	$X\ ^2\Sigma^+$	$B\ ^2\Sigma^+$	$C\ ^2\Sigma^+$	$D\ ^2\Sigma^+$	$F\ ^2\Sigma^+$	$I\ ^2\Sigma^+$	$A\ ^2\Pi$	$E\ ^2\Pi$	$G\ ^2\Pi$	$H\ ^2\Delta$
0	0.6795	0.5028	3.3305	2.9330	3.0815	2.9605	3.1415	3.0947	2.9273	3.0535
1	0.5879	0.4801	3.2226	2.8365	2.9791	2.8389	3.0001	2.9469	2.8103	2.9237
2	0.4963	0.4576	3.1147	2.7401	2.8766	2.5172	2.8591	2.7990	2.6933	2.7939
3	0.4047	0.4350	3.0068	2.6437	2.7742	2.2956	2.7179	2.6512	2.5763	2.6642
4	0.3131	0.4124	2.8990	2.5472	2.6717	2.0740	2.5767	2.5034	2.4593	2.5344
5		0.3897	2.7911	2.4508	2.5693	1.8524	2.4355	2.3556	2.3423	2.4046
6		0.3671	2.6832	2.3544	2.4668	1.6308	2.2943	2.2077	2.2254	2.2748
7		0.3445	2.5754	2.2579	2.3644	1.4092	2.1531	2.0599	2.1084	2.1450
8			2.4675	2.1615	2.2619	1.1876	2.0119	1.9121	1.9914	2.0153
9			2.3596	2.0651	2.1595	0.9660	1.8707	1.7642	1.8744	1.8855
10			2.2517	1.9686	2.0570	0.7444	1.7295	1.6164	1.7574	1.7557
11			2.1439	1.8722	1.9546	0.5228	1.5883	1.4686	1.6404	1.6259
12			2.0360	1.7758	1.8521	0.3012	1.4771	1.3207	1.5234	1.4951
13			1.9281	1.6793	1.7497		1.3059	1.1729	1.4064	1.3663
14			1.8203	1.5829	1.6472		1.1647	1.0251	1.2894	1.2365
15			1.7124	1.4865	1.5448			0.8772	1.1724	1.1068
16			1.6045	1.3900				0.7294	1.0554	
17				1.2936				0.5816	0.9385	
18				1.1972				0.4337	0.8213	
19				1.1007				0.2859		
20				1.0043				0.1381		

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