

Theoretical study on spectroscopy and molecular constants of the ground and low-lying excited states of GeO molecule

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Abstract. The potential energy curves (PECs) of $X^1\Sigma^+$, $a^3\Sigma^+$, $a^3\Pi$, $A^1\Pi$ states for GeO molecule are calculated by the multireference configuration interaction method (MRCI) and MRCI with the Davidson's corrections (MRCI+Q) with aug-cc-pVTZ basis set. All these states involved dissociate into the same dissociation channel $\text{Ge}(^3\text{P})+\text{O}(^3\text{P})$. For the four states, the spectroscopic parameters (R_e , D_e , ω_e , B_e , $\omega_e\chi_e$ and T_e) have been obtained, which shows that our results are in very good agreement with the experimental value and other theoretical data at MRCI+Q level. The dipole moments of these states are also obtained. In addition, based on the accurate results of spectroscopic constants at MRCI+Q level, the first 30 vibrational states are determined for the four low-lying electronic states when $J=0$. The vibrational levels $G(v)$ and inertial rotation constants B_v at MRCI+Q level are calculated when $J=0$, the results of $X^1\Sigma^+$ and $A^1\Pi$ states are in concordance with the available other theoretical values and experimental work. The dissociation limits, dissociation energies, electronic configurations at equilibrium internuclear distance for $a^3\Sigma^+$, $a^3\Pi$ states also are predicted for the first time.

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Key words: GeO molecule, spectroscopic constants, vibrational levels, molecular constants

1 Introduction

Germanium monoxide (GeO) as one of the important oxides of group IVa elements, has been studied very extensively. A variety of experiments have been reported including chemiluminescence studies of low-lying electronic states [1, 2], microwave spectroscopy

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[3, 4], photoelectron spectroscopy [5], emission spectroscopy and gas phase infrared spectroscopy [6]. The geometry and energy structures for the molecule attracted much more research interests.

In recent years, there have been numerous theoretical studies of GeO. Raymonda *et al.* [7] calculated the electric dipole moments of GeO in the lower vibrational states. The chemiluminescent reaction $\text{Ge}(^3\text{P})+\text{N}_2\text{O} \rightarrow \text{GeO}+\text{N}_2$ have been studied, since such reaction has been shown to warrant investigation as potential chemical laser systems [8, 9]. Mummigatti *et al.* [10] applied the RKR (Rydberg–Klein–Rees–Vanderslice) method to calculate potential energy curves (PECs) for $A^1\Pi$ and $X^1\Sigma^+$ states and Franck-Condon factors for $A^1\Pi \rightarrow X^1\Sigma^+$ band system of GeO molecule in 1977. Later, in 1993, molecular structures and vibrational IR spectra of GeX (X = O, S, Se) were studied by *ab initio* Hartree-Fock and Post-Hartree-Fock methods [11], respectively. Then Barandiarán and Seijo [12] presented the results of a systematic comparison between the values of the bond lengths and vibrational frequencies of group IV monoxides (XO, X = Ge, Sn, Pb), calculated with the spin-free quasi-relativistic *ab initio* core model potential method (AIMP) and the all-electron Dirac-Hartree-Fock method. In 1995, absolute oscillator strengths and related radiative properties of the $A^1\Pi - X^1\Sigma^+$ transition of the GeO molecule have been determined from accurate multireference configuration interaction (MRCI) calculations [13]. An accurate analytical potential energy function is determined for the ground $X^1\Sigma^+$ state of GeO molecule by Lee *et al.* [14] in 1999. Later, analytical potential energy functions and theoretical spectroscopic constants for MX/MX⁻ (M = Ge, Sn, Pb; X = O, S, Se, Te, Po) and LuA (A = H, F) systems were presented by Jalbout *et al.* [15] with the LSDA/SDD, BLYP/SDD and B3LYP/SDD methods. Shi *et al.* [16] calculated the spectroscopic constants and molecular constants for $X^1\Sigma^+$, $A^1\Pi$, $C\Sigma^-$ and $b^3\Pi$ states with the aid of module VIBROT presented in the MOLCAS 7.4 program package.

However, to our knowledge, the dissociation limits, electronic configurations at equilibrium internuclear distance for $X^1\Sigma^+$, $a^3\Sigma^+$, $a^3\Pi$, $A^1\Pi$ states and the PECs, vibrational levels for $a^3\Sigma^+$, $a^3\Pi$ states have not been reported. The main goal of this paper is to investigate the PECs for $X^1\Sigma^+$, $a^3\Sigma^+$, $a^3\Pi$, $A^1\Pi$ states of GeO. According to the accurately results, we also predict the well depths, electronic configurations at the equilibrium internuclear distance, spectroscopic constants, vibrational levels of these states.

2 Computational details

The calculations of electronic structure and PECs are performed with the MOLPRO 2010.1 program package [17]. The spectroscopic constants and molecular constants are investigated by solving the nuclear Schrödinger equations with Le Roy's LEVEL8.0 program [18]. The molecular orbitals of the ground state for GeO molecule are first calculated through the spin-restricted Hartree-Fock (RHF) method. Then, the state-averaged complete active space self-consistent-field (CASSCF) calculations are performed by using the preceding RHF orbitals as a starting point. Moreover, by utilizing the CASSCF wave

functions as a zero-order function, the energies of these states are gotten through the MRCI method and MRCI+Q method, which is a MRCI method with the Davidson's corrections [19]. The GeO molecule belongs to the $C_{\infty v}$ point group. So it can be replaced by C_{2v} symmetry on the yz plane and the z axis was chosen as the molecular axis in MOLPRO program. There are four irreducible representations (A_1 , B_1 , B_2 and A_2) in C_{2v} point group. Corresponding relationship is $\Sigma^+ = A_1$, $\Sigma^- = A_2$, $\Pi = B_1 + B_2$, and $\Delta = A_1 + A_2$ [20]. Thirteen molecular orbits (6, 3, 3, 1) are put into the active space, which correspond to the $2s^2 2p^6 3s^2$ shell of O atom and $3d^{10} 4s^2 4p^6$ of Ge atom, and the $1s^2$ electrons of O atom and $1s^2 2s^2 2p^6 3s^3 3p^6$ electrons of Ge atom are frozen core orbits. So we used these molecular orbits (13, 5, 5, 1) to calculate the PECs of GeO.

In the present calculations for the O and Ge atoms, the basis set aug-cc-pVTZ (O: (10s, 5p, 2d, 1f) / [4s, 3p, 2d, 1f], Ge: (20s, 13p, 9d, 1f) / [6s, 5p, 2d, 1f]) are employed. In present work, all PECs calculations are performed with an interval of 0.1 Å over the distance from 1.2 Å to 10.0 Å. The value declines to 0.002 Å nearby the equilibrium distance. Then, according to the adiabatic PECs calculated by using MRCI and MRCI+Q method, the spectroscopic constants including the equilibrium internuclear distance (R_e), the harmonic frequency and anharmonic vibrational constants (ω_e and $\omega_e \chi_e$), the rotational constants (B_e), dissociation energy (D_e) and the adiabatic relative electronic energy referred to the ground state (T_e) of $X^1\Sigma^+$, $a^3\Sigma^+$, $a^3\Pi$, $A^1\Pi$ states are evaluated.

3 Results and discussion

3.1 The PECs

The adiabatic PECs of the $X^1\Sigma^+$, $a^3\Sigma^+$, $a^3\Pi$, $A^1\Pi$ states for GeO molecule are obtained by using the MRCI+Q method with aug-cc-pVTZ basis set, which are plotted in Fig. 1. We can clearly see that there is the same dissociation channel Ge (3P) + O (3P) for $X^1\Sigma^+$, $A^1\Pi$, $a^3\Sigma^+$, $a^3\Pi$ states of GeO molecule. On the basis of the adiabatic PECs, the spectroscopic constants of $X^1\Sigma^+$, $a^3\Sigma^+$, $a^3\Pi$, $A^1\Pi$ states are calculated in Table 1. In addition, the experimental and other calculated data are collected in Table 1.

The calculations shows that the ground state of GeO is $X^1\Sigma^+$ state with electronic configuration (core) $7\sigma^2 8\sigma^2 9\sigma^2 10\sigma^2 11\sigma^2 3\pi_x^2 4\pi_x^2 3\pi_y^2 4\pi_y^2 1\delta^2$. The ground state of GeO molecule has been studied extensively in the past. Our results (R_e , ω_e , $\omega_e \chi_e$, B_e and D_e) both MRCI and MRCI+Q method for this state are in very good agreement with the results of Huber and Herzberg [21], which means that the present calculation is reasonable, but general speaking, the spectroscopic constants at MRCI+Q level are more closer the data of Huber and Herzberg. For example, the R_e equals 1.6370 Å at MRCI+Q level, which differs from Huber and Herzberg's value by only 0.0114 Å. We also observe excellent agreement for D_e . Our D_e is equal to 6.9365 eV, the value of Huber and Herzberg is 6.841 eV, the difference is about 0.0955 eV, while the theoretical value by Jalbout *et al.* [15] and Shi *et al.* [16] is 6.8440 and 7.0053 eV, respectively. The same excellent agreement is observed

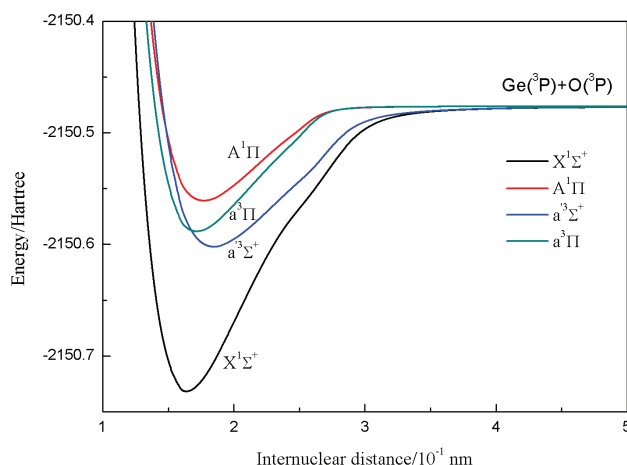


Figure 1: The PECs and the dissociation channel at MRCI+Q method for GeO molecule.

Table 1: Spectroscopic parameter of $X^1\Sigma^+$, $a^3\Sigma^+$, $a^3\Pi$, $A^1\Pi$ states for GeO molecule: comparison with experiments and other theories value.

states	method	R_e (Å)	ω_e (cm^{-1})	$\omega_e\chi_e$ (cm^{-1})	B_e (cm^{-1})	D_e (ev)	T_e (cm^{-1})	μ (Debye)
$X^1\Sigma^+$	MRCI	1.6360	990.33	4.0989	0.4800	6.9605	0	2.9781
	MRCI+Q	1.6370	984.47	4.0618	0.4792	6.9365	0	2.9816
	Expt. [5]	1.6246	989	-	-	6.83	0	
	Expt. [6]	-	986.5	-	0.4857	-	0	
	Ref. [15]	1.68	982.21	3.4337	0.4571	6.8440	0	
	Ref. [16]	1.6364	989.04	4.5820	0.4787	7.0053	0	
	Ref. [21]	1.6246	985.5	4.29	0.4857	6.8410	0	
	Expt. [9]	-	985.7	4.32	-	-	0	
	Ref. [11]	1.64	-	-	-	-	0	2.806
Expt. [27]	1.627	-	-	-	-	0	3.2824	
$a^3\Sigma^+$	MRCI	1.8595	632.47	3.0848	0.3717	3.4001	28650.88	2.2618
	MRCI+Q	1.85	636.22	3.2468	0.3754	3.4274	28423.7	2.2135
	Ref. [21]	1.815	633.3	2.7	0.389	-	27733	
$a^3\Pi$	MRCI	1.7095	756.69	4.7499	0.4396	2.9518	31156.6	2.7556
	MRCI+Q	1.7145	748.67	4.6726	0.4371	3.0347	31491.5	2.7462
	Ref. [21]	1.711	734.9	5.3	0.438	-	32132	
$A^1\Pi$	MRCI	1.7757	653.03	3.8006	0.4075	2.1273	37803.3	1.8639
	MRCI+Q	1.7697	652.63	3.8215	0.4102	2.2781	37588.48	1.8365
	Ref. [22]	1.7590	648.8	4.02	0.4143	2.2996	37762.5	
	Ref. [16]	1.7764	644.20	4.1966	0.4078	2.2728	38276.3	
	Ref. [21]	1.761	650.4	4.21	0.4133	-	37766.9	

for spectroscopic constants ω_e , $\omega_e\chi_e$ and B_e , which is 984.47, 4.0618, 0.4792 cm^{-1} , respectively. The value of Huber and Herzberg are 985.5, 4.29, 0.4857 cm^{-1} , while Jalbout *et al.* [15] and Shi *et al.* [16] have found, respectively, 982.21, 3.4337, 0.4571 cm^{-1} and 989.04, 4.5820, 0.4787 cm^{-1} .

Good agreement is also observed for $a^3\Sigma^+$, $a^3\Pi$, $A^1\Pi$ states. For $a^3\Sigma^+$ state, the electronic configuration is (core) $7\sigma^2 8\sigma^2 9\sigma^2 10\sigma^2 11\sigma^2 3\pi_x^2 4\pi_x^2 3\pi_y^2 4\pi_y 5\pi_y 1\delta^2$. The $a^3\Sigma^+$ state has been reported by Huber and Herzberg [21], and the spectroscopic constants (R_e , ω_e , $\omega_e\chi_e$, B_e and T_e) are 1.815 Å, 633.3, 2.7, 0.389, 27733 cm^{-1} , which were in concordance with our spectroscopic data at MRCI+Q level, 1.85 Å, 636.22, 3.2468, 0.3754 and 28423.7 cm^{-1} , respectively. For $a^3\Pi$ state, the electronic configuration is (core) $7\sigma^2 8\sigma^2 9\sigma^2 10\sigma^2 11\sigma 3\pi_x^2 4\pi_x^2 5\pi_x 3\pi_y^2 4\pi_y^2 1\delta^2$. The $a^3\Pi$ state has been studied by Huber and Herzberg [21]. They have found the following spectroscopic data: 1.711 Å, 734.9, 5.3, 0.438 and 32132 cm^{-1} for R_e , ω_e , $\omega_e\chi_e$, B_e and T_e , respectively, which are in very good agreement with our results, 1.7145 Å, 748.67, 4.6726, 0.4371 and 31491.5 cm^{-1} . The electronic configuration of $A^1\Pi$ state is (core) $7\sigma^2 8\sigma^2 9\sigma^2 10\sigma^2 11\sigma 3\pi_x^2 4\pi_x^2 5\pi_x 3\pi_y^2 4\pi_y^2 1\delta^2$. The same good agreement is observed for $A^1\Pi$ state with the theoretical work of Shi *et al.* [16], Lagerqvist *et al.* [22] and the results of Huber and Herzberg [21]. They have found the R_e , ω_e , $\omega_e\chi_e$, B_e and T_e , corresponding with 1.7764 Å, 644.20, 4.1966, 0.4078, 38276.3 cm^{-1} ; 1.759 Å, 648.8, 4.02, 0.4143, 37762.5 cm^{-1} and 1.761 Å, 650.4, 4.21, 0.4133, 37766.9 cm^{-1} , respectively. Our calculated values at MRCI+Q level are 1.7697 Å, 652.63, 3.8215, 0.4102, 37588.48 cm^{-1} . Our D_e is 2.2781 eV, while Shi *et al.* [16] and Lagerqvist *et al.* [22] obtained 2.2996 eV and 2.2728 eV, respectively.

In addition, the dipole moments μ at R_e of GeO molecule ($X^1\Sigma^+$, $a^3\Sigma^+$, $a^3\Pi$, $A^1\Pi$) are calculated, which are listed in Table 1. For the ground state, our value at MRCI+Q level is 2.9816 Debye, the value of Leszczynski *et al.* [26] is 2.806 Debye, it is very obvious that our result is more closer the experimental data of Lovas *et al.* [27]. The μ values at MRCI+Q level for $a^3\Sigma^+$, $a^3\Pi$, $A^1\Pi$ states are 2.2135, 2.7462 and 1.8365 Debye, respectively. To the best of our knowledge, there are no experimental results or other theoretical results can be found in the literature.

The μ as a function of R at MRCI+Q level are displayed in Fig. 2. From Fig. 2, we can see that the μ of these four states approach zero at large distances, it can be say that the dissociation channels of these states are Ge+O, which is corresponding to Ge(3P)+O(3P). The Dipole moment functions have reached a maximum value of 4.2807, 2.9623, 3.9634 and 3.8404 Debye at about 2.3, 2.4, 2.3 and 2.3 Å for $X^1\Sigma^+$, $A^1\Pi$, $a^3\Sigma^+$, $a^3\Pi$ states, respectively.

3.2 Vibrational manifolds

According to the PECs of these electronic states obtained here, the vibrational level $G(v)$ and inertial rotation constant B_v are determined with the aid of solving the Schrödinger equation of the nuclear motion with LEVEL8.0 package [18]. Considering the length limitations of the present paper, we only collect the $G(v)$ and B_v for the first 30 vibrational

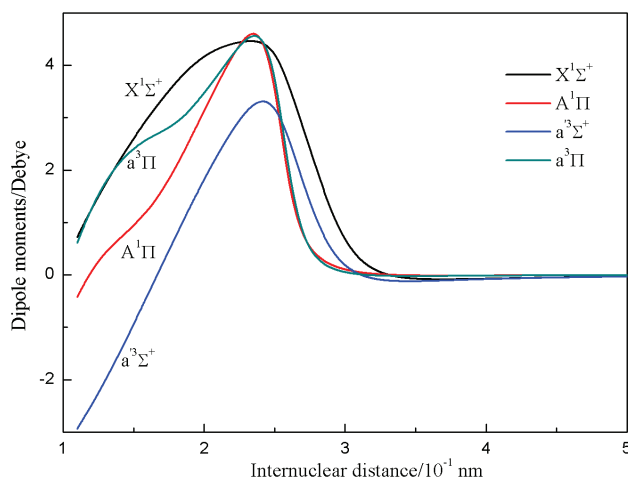


Figure 2: The dipole moments at MRCI+Q method for GeO molecule.

states of the $X^1\Sigma^+$, $a^3\Sigma^+$, $a^3\Pi$, $A^1\Pi$ states at MRCI+Q level, and which is listed in Tables 2-4, respectively. For the vibrational levels, only the results of GeO ($X^1\Sigma^+$) and GeO ($A^1\Pi$) states were reported by Shi *et al.* [16] in 2010 and Nair *et al.* [25] in 1965. To avoid congestion, we do not tabulate all data in these tables, only the data of Shi *et al.* is listed in Tables 2 and 4 for comparison. It is obvious that our data is in very good agreement with the work of Shi *et al.*, though no experimental data can be presented for comparison. For the GeO ($X^1\Sigma^+$) and GeO ($A^1\Pi$) states, the greatest differences between them are only 20.89 cm^{-1} (which corresponds to $v = 7$) and 248.63 cm^{-1} (which corresponds to $v = 28$), and it is only equal to 0.29% and 1.62%, respectively. The vibrational levels of $a^3\Sigma^+$ and $a^3\Pi$ states are tabulated in Tables 3.

For inertial rotation constant B_v , to our knowledge, only the experimental results about GeO ($X^1\Sigma^+$) and GeO ($A^1\Pi$) states can be found in the literature [3, 22-24]. From Table 2 and 4, excellent agreement can be found between our results and the experimental data, and it is in very good agreement with the theoretical work of Shi *et al.* [16] For inertial rotation constant of $a^3\Sigma^+$ and $a^3\Pi$ states, to our knowledge, no B_v data can be found in the literature for all these states, either experimentally or theoretically. Thus, we cannot make any direct comparison between them. As above mentioned, excellent agreement of the spectroscopic data exists between the present theoretical results and experimental values, in addition, our $G(v)$ and B_v of $X^1\Sigma^+$ and $A^1\Pi$ states are in very good agreement with theoretical results and experimental ones. According to this, it is believed that the present calculations in Tables 3 about GeO ($a^3\Sigma^+$) and GeO ($a^3\Pi$) are both reliable and accurate. They should be good predictions for future experimental research.

Table 2: Vibrational levels and inertial rotation constant of GeO($X^1\Sigma^+$) when $J = 0$.

V	$G(v)/\text{cm}^{-1}$		B_v/cm^{-1}				
	This work	Shi [16]	This work	Shi [16]	Expt. [23]	Expt. [24]	Expt. [3]
0	491.60	493.23	0.477708	0.477247	-	-	-
1	1469.26	1473.23	0.474672	0.474305	0.48107	0.4822	0.481083
2	2438.85	2444.64	0.471763	0.471364	0.47796	0.4780	0.478007
3	3398.52	3407.46	0.468984	0.468428	0.47503	0.4754	0.474932
4	4348.77	4361.71	0.466161	0.465494	-	-	-
5	5290.69	5307.39	0.463255	0.462561	-	-	-
6	6225.02	6244.51	0.460278	0.459626	-	-	-
7	7152.19	7173.08	0.457262	0.456696	-	-	-
8	8072.31	8093.10	0.454299	0.453764	-	-	-
9	8984.92	9004.59	0.451473	0.450831	-	-	-
10	9889.46	9907.55	0.448741	0.447898	-	-	-
11	10785.33	10802.00	0.445941	0.444964	-	-	-
12	11671.71	11687.93	0.442968	0.442033	-	-	-
13	12548.49	12565.35	0.439991	0.439101	-	-	-
14	13417.01	13434.29	0.437186	0.436170	-	-	-
15	14277.81	14294.73	0.434412	0.433239	-	-	-
16	15130.47	15146.70	0.431692	0.430309	-	-	-
17	15975.27	15990.19	0.428893	0.427377	-	-	-
18	16811.07	16825.23	0.425782	0.424444	-	-	-
19	17637.58	17651.81	0.422763	0.421509	-	-	-
20	18456.04	18469.94	0.419834	0.418572	-	-	-
21	19266.52	19279.64	0.416917	0.415633	-	-	-
22	20069.07	20080.90	0.413964	0.412692	-	-	-
23	20863.73	20873.74	0.411011	0.409747	-	-	-
24	21650.29	21658.17	0.407817	0.406802	-	-	-
25	22427.46	22434.20	0.404620	0.403854	-	-	-
26	23196.16	23201.82	0.401600	0.400905	-	-	-
27	23956.31	23961.06	0.398609	0.397956	-	-	-
28	24708.04	24711.92	0.395629	0.395008	-	-	-
29	25451.09	25454.40	0.392635	0.392062	-	-	-

4 Conclusion

The PECs for the $X^1\Sigma^+$, $a^3\Sigma^+$, $a^3\Pi$, $A^1\Pi$ states of GeO molecule have been calculated using MRCI and MRCI+Q method with aug-cc-pVTZ basis set. It is found that there is the same dissociation channel $\text{Ge}(^3\text{P})+\text{O}(^3\text{P})$ for these states. The electronic configuration of $X^1\Sigma^+$, $a^3\Sigma^+$, $a^3\Pi$,

Table 3: Vibrational levels and inertial rotation constant of GeO($a^3\Sigma^+$ and $a^3\Pi$) when $J = 0$.

V	$a^3\Sigma^+$		$a^3\Pi$	
	$G(v)/\text{cm}^{-1}$	B_v/cm^{-1}	$G(v)/\text{cm}^{-1}$	B_v/cm^{-1}
0	318.10	0.374017	373.63	0.435172
1	948.84	0.371156	1113.20	0.431280
2	1570.33	0.368100	1842.99	0.427402
3	2185.57	0.365466	2563.52	0.423547
4	2796.24	0.362588	3275.26	0.419733
5	3398.93	0.359668	3978.07	0.415891
6	3995.74	0.356978	4670.82	0.411963
7	4587.39	0.354278	5352.95	0.408178
8	5172.39	0.351364	6026.10	0.404662
9	5750.91	0.348597	6690.88	0.401033
10	6323.20	0.345915	7346.34	0.397333
11	6890.38	0.343204	7992.58	0.393609
12	7450.93	0.340405	8630.18	0.390083
13	8005.29	0.337595	9260.26	0.386492
14	8553.30	0.334886	9881.99	0.382850
15	9095.78	0.332240	10495.83	0.379169
16	9632.19	0.329425	11101.37	0.375558
17	10162.30	0.326632	11699.49	0.372081
18	10685.71	0.323746	12289.99	0.368600
19	11202.33	0.320882	12872.72	0.365197
20	11712.57	0.318088	13447.90	0.361798
21	12216.81	0.315578	14015.19	0.358472
22	12716.64	0.313218	14575.02	0.355151
23	13211.67	0.310584	15127.51	0.351954
24	13700.23	0.307830	15673.40	0.348938
25	14183.57	0.305675	16213.71	0.346009
26	14665.76	0.304640	16748.30	0.343084
27	15150.52	0.304176	17277.27	0.340171
28	15638.79	0.303649	17801.06	0.337493
29	16129.17	0.302861	18320.15	0.334915

$A^1\Pi$ states also are obtained. The spectroscopic parameters (D_e , R_e , ω_e , B_e and T_e) of these states have been derived by solving the nuclear Schrödinger equations with Le Roy's LEVEL program, which is in very good agreement with the experimental work and other theoretical values at MRCI+Q level. And the dipole moments for the $X^1\Sigma^+$, $a^3\Sigma^+$, $a^3\Pi$, $A^1\Pi$ states of GeO molecule are also obtained. Based on the accurate results, the first 30 vibrational states are determined for the four low-lying electronic states when $J = 0$. The $G(v)$ and B_v at MRCI+Q level are calculated when $J = 0$, the results of $X^1\Sigma^+$ and $A^1\Pi$

Table 4: Vibrational levels and inertial rotation constant of GeO($A^1\Pi$) when $J = 0$.

V	$G(v)/\text{cm}^{-1}$		B_v/cm^{-1}			
	This work	Shi [16]	This work	Shi [16]	Expt. [22]	Expt. [23]
0	325.80	321.05	0.408369	0.404424	0.41236	0.41247
1	971.38	956.91	0.404700	0.400803	0.40868	-
2	1609.68	1584.53	0.401104	0.397216	0.40485	0.40482
3	2240.41	2204.0	0.397427	0.393652	0.40087	-
4	2861.95	2815.45	0.393616	0.390111	0.39732	-
5	3474.99	3418.97	0.390071	0.386594	0.39367	-
6	4081.79	4014.65	0.386611	0.383097	0.38947	-
7	4680.85	4602.60	0.3828790	0.379617	-	-
8	5271.57	5182.93	0.379255	0.376148	-	-
9	5854.95	5755.73	0.375815	0.372691	-	-
10	6431.74	6321.11	0.372361	0.369241	-	-
11	7000.48	6879.17	0.368765	0.365792	-	-
12	7561.44	7430.02	0.365262	0.362348	-	-
13	8114.56	7973.74	0.361885	0.358911	-	-
14	8660.94	8510.46	0.358508	0.355479	-	-
15	9199.57	9040.27	0.355034	0.352050	-	-
16	9730.71	9563.26	0.351575	0.348629	-	-
17	10254.26	10079.55	0.348122	0.345227	-	-
18	10770.72	10589.24	0.344802	0.341869	-	-
19	11280.21	11092.43	0.341408	0.338573	-	-
20	11783.16	11589.21	0.338233	0.335324	-	-
21	12280.20	12079.70	0.335112	0.332104	-	-
22	12771.64	12564.00	0.332052	0.328954	-	-
23	13257.76	13042.20	0.328995	0.325922	-	-
24	13737.67	13514.41	0.325674	0.322859	-	-
25	14210.70	13980.73	0.322276	0.319577	-	-
26	14677.45	14441.27	0.319345	0.316618	-	-
27	15139.26	14896.12	0.316440	0.315373	-	-
28	15594.02	15345.39	0.312348	0.316036	-	-
29	16035.31	15789.19	0.306390	0.316700	-	-

states are in concordance with the available other theoretical values and experimental work. They should be good predictions and references for future experimental research.

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References

- [1] G. Hager, L. E. Wilson, and S. G. Hadley, *Chem. Phys. Lett.* 27 (1974) 439.
- [2] G. Hager, R. Harris, and S. G. Hadley, *J. Chem. Phys.* 63 (1975) 2810.
- [3] T. Törring, *Z. Naturforsch. A* 21(1966) 287.
- [4] R. Honerjäger and R. Tischer, *Z. Naturforsch. A* 28 (1973) 1374.
- [5] E. A. Colbourn, J. M. Dyke, A. Fackerell, A. Morris, and I. R. Trickle, *J. Chem. Soc., Faraday Trans. II* 74 (1978) 2278.
- [6] G. A. Thompson, A. G. Maki, and A. Weber, *J. Mol. Spectrosc.* 116 (1986) 136.
- [7] J. W. Raymond, J. S. Muenter, and W. A. Klemperer, *J. Chem. Phys.* 52 (1970) 3458.
- [8] G. Hager, L. E. Wilson, and S. G. Hadley, *Chem. Phys. Letter.* 27 (1974) 439.
- [9] G. A. Capelle and J. M. Brom, *J. Chem. Phys.* 63 (1975) 5168.
- [10] V. M. Mummigatti and B. G. Jyoti, *Acta Physica Academiae Scientiarum Hungaricae* 42 (1977) 99.
- [11] J. Leszczyński and J. S. Kwiatkowski, *J. Phys. Chem.* 97 (1993) 12189.
- [12] Z. Barandiarán and L. Seijo, *J. Chem. Phys.* 101 (1994) 4049.
- [13] F. L. Sefyani, J. Schamps, and D. Duflot, *J. Quant. Spectrosc. Radiat. Transfer.* 54 (1995) 1027.
- [14] E. G. Lee, J. Y. Seto, T. Hirao, P. F. Bernath, and R. J. Le Roy, *J. Mol. Spectrosc.* 194 (1999) 197.
- [15] A. F. Jalbout, X. H. Li, and H. Abou-Rachid, *Int. J. Quantum Chem.* 107 (2007) 522.
- [16] D. H. Shi, H. Liu, J. F. Sun, Z. L. Zhu, and Y. F. Liu, *Journal of Molecular Structure: THEOCHEM* 960 (2010) 40.
- [17] MOLPRO is a package of *ab initio* programs designed by H. J. Werner, and P. J. Knowles. The authors are R. D. Amos, A. Bernhardsson, A. Berning, P. Celani *et al.*
- [18] R. J. Le Roy, Level8.0: A Computer Program for Solving the Radial Schrödinger Equation for Bound and Quasibound Levels' University of Waterloo Chemical Physics Research Report No. CP-663 (2007).
- [19] M. W. Wang, B. W. Wang, and Z. D. Chen, *Science in China Series B: Chemistry* 51 (2008) 521.
- [20] J. Guo, B. Yan and D. L. Zeng, *J. At. Mol. Sci.* 4 (2013) 183.
- [21] G. Herzberg and K. P. Huber, *Molecular Spectra and Molecular Structure of Diatomic Molecules IV* (Van Nostrand Reinhold, New York, 1979).
- [22] A. Lagerqvist and I. Renhorn, *Phys. Scr.* 25 (1982) 241.
- [23] W. Żyrczyński, *J. Mol. Spectrosc.* 89 (1981) 557.
- [24] T. Savithry, D. V. K. Rao, A. A. N. Murthy, and P. T. Rao, *Indian J. Phys. B* 51 (1977) 452.
- [25] K. P. R. Nair, R. B. Singh, and D. K. Rai, *J. Chem. Phys.* 43 (1965) 570.
- [26] J. Leszczyński and J. S. Kwiatkowski, *J. Phys. Chem.* 97 (1993) 12189.
- [27] F. J. Lovas and E. Tiemann, *J. Phys. Chem. Ref. Data* 3 (1974) 609.