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Investigations on analytic potential energy function, spectroscopic parameters and vibrational manifolds $(J = 0)$ of the $SD^+(X^3\Sigma^-)$ ion*

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This paper investigates the spectroscopic properties of the $SD^+(X^3\Sigma^-)$ ion by employing the coupled-cluster singles-doubles-approximate-triples [CCSD(T)] theory combining with the quintuple correlation-consistent basis set augmented with diffuse functions (aug-cc-pV5Z) of Dunning and co-workers. The accurate adiabatic potential energy function is obtained by the least-squares fitting method with the 100 *ab initio* points, which are calculated at the unrestricted CCSD(T)/aug-cc-pV5Z level of theory over the internuclear separation range from 0.09 to 2.46 nm. Using the potential, it accurately determines the spectroscopic parameters (D_e, $\omega_e\chi_e$, α_e and B_e). The present D_e, R_e, ω_e, $\omega_e\chi_e$, α_e and B_e results are of 3.69119 eV, 0.13644 nm, 1834.949 cm^{-1}, 25.6208 cm^{-1}, 0.1068 cm^{-1} and 4.7778 cm^{-1}, respectively, which are in remarkably good agreement with the experimental findings. A total of 29 vibrational states has been predicted by numerically solving the radial Schrödinger equation of nuclear motion when the rotational quantum number J equals zero. The complete vibrational levels, classical turning points, inertial rotation and centrifugal distortion constants are reported when $J = 0$ for the first time, which are in good accord with the measurements wherever available.

Keywords: spectroscopic parameter, vibrational level, inertial rotation constant, centrifugal distortion constant
PACC: 3520G, 3120D, 3420

1. Introduction

Since Horani *et al*[1] in 1967 made the first observation of the $A^3\Pi$-$X^3\Sigma^-$ transition for the SH^+ and SD^+ ions in the crossed beam experiment, these two ions have attracted considerable interests, both experimentally and theoretically. Because, on the one hand, the SH, SD and their ions are of astrophysical importance. Some of them have been detected in space.[2] On the other hand, these species are expected to play an important role in many industrial processes, such as the fossil fuel combustion and the atmospheric sulfur cycle. Therefore, it is not a surprise that these species have been widely investigated in the past several decades.

In experiment, by using penning ionization, Yencha and Wu[3] and Tsuji *et al*[4] observed the additional bands of this transition, while Edwards *et al*[5,6] measured the hyperfine doubling due to the proton nuclear spin by laser ion beam spectroscopy. In 1984, Rostas *et al*[7] used a special d. c. discharge source to produce the SH^+ and SD^+ ions and gave a very detailed analysis of the $A^3\Pi$-$X^3\Sigma^-$ emission spectra, which has guided several laser spectroscopic studies on the molecular constants of the SH^+ and SD^+ in their $X^3\Sigma^-$ state. In 1987, Zeitz *et al*[8] measured the ground state molecular parameters of SD^+ by employing the Faraday rotation technique[9] and the extracavity co-laser spectrometer. In 1989, Civiš *et al*[10] obtained the spectroscopic parameters of the $SH^+(X^3\Sigma^-)$ and $SD^+(X^3\Sigma^-)$ ions and derived the potential energy curve (PEC). In theory, Khadri *et al*[11] recently reported the reliable theoretical results on spectroscopy for the lowest electronic state of the SH^+ and SD^+ ion. However, the extracted properties from the investigations about these ions mainly focus

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on the spectroscopic constants (D_e, R_e, ω_e, $\omega_e\chi_e$, α_e and B_e). Very few data are available in the literature dealing with their vibrational manifolds (vibrational levels, classical turning points, inertial rotation and centrifugal distortion constants), which are very useful in the rovibrational transition calculations.

This paper reports the accurate adiabatic analytic potential energy function (APEF) and the vibrational manifolds of the $SD^+(X^3\Sigma^-)$ ion. We calculated the equilibrium internuclear separations and the harmonic frequencies by employing the unrestricted coupled-cluster singles-doubles- approximate-triples [UCCSD(T)][12−14] theory with the series of correlation-consistent basis sets, cc-pVnZ and aug-cc-pVnZ (n = 2, 3, 4, 5), of Dunning and co-workers.[15−18] Obtaining the APEF obtained at the UCCSD(T)/aug-cc-pV5Z level of theory, we determine the rest spectroscopic parameters (D_e, $\omega_e\chi_e$, α_e and B_e). The investigations of the $SH^+(X^3\Sigma^-)$ ion will be published elsewhere.

2. Computational details

The harmonic frequencies and the equilibrium structures of the $SD^+(X^3\Sigma^-)$ ion are computed by using the UCCSD(T) theory, which has been proved particularly successful. Especially in recent years, a number of high-quality calculations have been reported for a variety of molecules.[19−22] We also used it to compute several free radicals.[23−25] All the calculations are performed in Gaussian 03 program package[26] at a series of the correlation-consistent basis sets, cc-pVnZ and aug-cc-pVnZ, of Duning and co-workers[15−18] in the valence range. The R_e and ω_e results are all tabulated in Table 1.

Table 1. The equilibrium parameters for the $SD^+(X^3\Sigma^-)$ ion at the UCCSD(T) level of theory and the different correlation-consistent basis sets, cc-pVnZ and aug-cc-pVnZ.

basis sets	D_e/eV	R_e/nm	ω_e/cm^{-1}	basis sets	D_e/eV	R_e/nm	ω_e/cm^{-1}
cc-pVDZ	3.2606	0.13804	1841.592	aug-cc-pVDZ	3.3162	0.13839	1814.786
cc-pVTZ	3.5474	0.13683	1828.571	aug-cc-pVTZ	3.5729	0.13691	1825.871
cc-pVQZ	3.6488	0.13663	1830.883	aug-cc-pVQZ	3.6573	0.13665	1829.788
cc-pV5Z	3.6861	0.13647	1833.677	aug-cc-pV5Z	3.69119	0.13644	1834.949

In general, the PEC calculations of the $SD^+(X^3\Sigma^-)$ ion are carried out over the internuclear distance range from 0.09 to 2.46 nm. The *ab initio* calculation points are fitted to the analytic Murrell–Sorbie (M–S) function with the least-squares fitting method. Therefore, the dissociation energy D_e and the APEF are attained. These D_e results are also tabulated in Table 1. By careful comparison between the calculated D_e, R_e and ω_e values and the experimental findings,[7,8,10] we are certain that the aug-cc-pV5Z is an excellent basis set to calculate the spectroscopic parameters. Therefore, further investigations are performed by using the APEF obtained at the aug-cc-pV5Z basis set.

Based on the APEF obtained here, the force constants, quadratic f_2, cubic f_3 and quartic f_4, are determined. Then the rest spectroscopic parameters, $\omega_e\chi_e$, α_e and B_e, are derived. Thirdly, with the APEF obtained at the UCCSD(T)/aug-cc-pV5Z level of theory, the radial Schrödinger equation of nuclear motion is numerically solved to get all the vibrational states. And finally, the complete vibrational levels, the classical turning points, R_{min} and R_{max}, and the inertial rotation and centrifugal distortion constants are calculated when the rotational quantum number J is set to equal zero ($J = 0$).

Now, we briefly discuss the spin contamination at the self-consistent field level, which arises from the unrestricted *ab initio* calculations. The spin contamination comes about when the ground-state wavefunction mingles with the wavefunctions of some excited states. Generally, high spin contaminations will influence the molecular structure, especially the density of spin. The spin contamination can be validated by comparison between the total S_1 prospective value and the calculated one. S_1 is equal to $s(s+1)$, where the s is the total spin value of the $SD^+(X^3\Sigma^-)$ ion. In general, the result is acceptable if the deviation is not beyond 10%.

From Table 2, we can find that the prospective value of total spin is absolutely identical with the calculated result. It proves that no spin contamination exists at the present calculations.

Table 2. Spin contamination for the $SD^+(X^3\Sigma^-)$ ion at the UCCSD(T)/aug-cc-pV5Z level of theory.

multiplicity	state	expectance value S_1 of spin	calculation value S_1 of spin
3	$X^3\Sigma^-$	2.0	2.0

3. Results and discussion

3.1. APEF of the $SD^+(X^3\Sigma^-)$ radical ion

The M-S function is a widely-used potential energy function. It describes interaction potential energies of diatomic molecules well. The common M-S function[27] is

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

Where $\rho = R - R_e$, R is the internuclear distance of diatomic molecules. R_e is its equilibrium internuclear distance and is regarded as a fixed parameter in the fitting process. The dissociation energy D_e and the parameters a_i (i = 1, 2, 3, ..., n) are determined by fitting.

Fitting Eq.(1) by the least-squares method, we obtain the parameters a_i and D_e. In order to attain a satisfactory result, whose root means square error (ΔE_{RMSE}) is minimized and the extracted spectroscopic parameters are closest to the experiments[7,8,10] on the whole, we try it from n = 3 to n = 8. By comparison with the spectroscopic experimental values (R_e, ω_e, B_e, α_e and $\omega_e\chi_e$),[7,8,10] we find that the best results can be obtained at n = 6. The fitting results are tabulated in Table 3 together with the R_e for integrality. At the same time, the *ab initio* calculation points and the fitting results are both intuitively depicted in Fig.1.

Table 3. The parameters of the M-S APEF for the $SD^+(X^3\Sigma^-)$ ion at the UCCSD(T)/aug-cc- pV5Z level of theory.

D_e/eV	R_e/nm	a_1/nm^{-1}	a_2/nm^{-2}	a_3/nm^{-3}	a_4/nm^{-4}	a_5/nm^{-5}	a_6/nm^{-6}	ΔE_{RMSE}/eV
3.6912	0.13644	33.2629	244.6847	1368.167	–7246.259	–98224.07	500397.38	0.00336

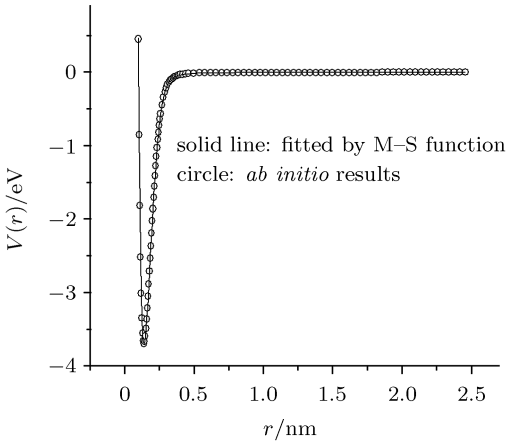


Fig.1. PEC of the ground state for SD^+ion.

In order to evaluate the fitting quality of PEC, we calculate the ΔE_{RMSE} in the fitting process,

$$\Delta E_{\mathrm{RMSE}} = \sqrt{\frac{1}{N}\left[\sum_{i=1}^{N}(V_{\mathrm{APEF}} - V_{ab\ initio})^2\right]}. \qquad (2)$$

Where V_{APEF} and $V_{ab\ initio}$ are energies attained by the fitting and by the *ab initio* calculations, respectively. N is the number of fitting points (here N = 100). The present ΔE_{RMSE} is of only 0.00336 eV (about 0.0776 Kcal/mol). Obviously, our fitting accuracy about the APEF is greatly superior to the chemical accuracy (1.0 Kcal/mol).[28] It shows that the analytic M-S function is very suitable for reproducing the PEC of this state, and the fitting process is of high quality. Therefore, the present APEF collected in Table 3 should be accurate and can be employed to perform the spectroscopic and vibrational manifold calculations, such as the spectroscopic parameters, the vibrational levels, the classical turning points, the inertial rotation and the centrifugal distortion constants, etc.

3.2. Spectroscopic parameters (B_e, α_e and ω_e χ_e)

Now, we calculate the rest spectroscopic parameters (B_e, α_e and $\omega_e\chi_e$) of the $SD^+(X^3\Sigma^-)$ ion according to the APEF tabulated in Table 3. Using Eq.(1), we can derive the expressions of the force constants, quadratic f_2, cubic f_3 and quartic f_4, at the equilibrium position as follows:[24,25]

$$f_2 = D_e(a_1^2 - 2a_2), \qquad (3)$$

$$f_3 = -6D_e(a_3 - a_1a_2 + a_1^3/3), \quad (4)$$

$$f_4 = D_e(3a_1^4 - 12a_1^2a_2 + 24a_1a_3). \quad (5)$$

Then the spectroscopic parameters B_e, α_e and $\omega_e\chi_e$ can be determined according to the following Eqs.(6)–(8),

$$B_e = \frac{h}{8\pi c\mu R_e^2}, \quad (6)$$

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

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

The present B_e, α_e and $\omega_e\chi_e$ results are tabulated in Table 4. In order to be convenient for further comparisons, we also collect the available experimental[7,8,10] and theoretical[11] data in Table 4.

Table 4. Spectroscopic parameter comparisons with the measurements and other theories for the $SD^+(X^3\ \Sigma^-)$ ion at the UCCSD(T)/aug-cc-pV5Z level of theory.

source	D_e/eV	R_e/nm	ω_e/cm^{-1}	B_e/cm^{-1}	α_e/cm^{-1}	$\omega_e\chi_e$/cm^{-1}
this work	3.69119	0.13644	1834.949	4.7778	0.1068	25.6208
exp.[7]	-	0.13635	1829.5	4.7856	0.1056	25.4
exp.[8]	-	-	1829.543	4.7856	0.10540	25.400
exp.[10]	-	0.13636	1829.096	4.78336	0.10596	25.3096
theory[11]	-	-	1835.5	4.786	0.106	25.79

From Table 4, we can see that the present R_e and ω_e values are in excellent agreement with the recent experimental findings,[10] and the deviations are within 0.059% for R_e and 0.320% for ω_e, respectively. At the same time, we find that the present R_e and ω_e results are also in good accord with the experiments,[7] and the differences between them are of only 0.066% and 0.298%, respectively. The rest spectroscopic parameters B_e, α_e and $\omega_e\chi_e$ reproduced from the APEF are favourite well with the measurements,[7,8,10] too. According to these, we conclude that the D_e value obtained at the UCCSD(T)/aug-cc-pV5Z level of theory should be accurate, and that the APEF fitted here should be credible.

Very recently, Khadri *et al*[11] used the full valence complete active space self-consistent field method followed by the internally contracted multireference configuration interaction approach to perform the spectroscopic parameter calculations of the $SD^+(X^3\Sigma^-)$ ion. In their calculations, the spdfg(h) cc-pV5Z basis sets of Dunning and co-workers for sulfur and hydrogen atoms were used. From Table 4, one can easily find that there is a very close similarity between the present calculations and their results. Unfortunately, on the one hand, they did not calculate the D_e and R_e values; on the other hand, they did not give the expression of the APEF, and either did not calculate the vibrational levels, classical turning points and inertial rotation and centrifugal distortion constants, which are very useful in the theoretical rovibrational transition calculations.

From above discussion, one can see that the present spectroscopic parameters, R_e, ω_e, B_e, α_e and $\omega_e\chi_e$, which are obtained from the UCCSD(T)/aug-cc-pV5Z level of theory, are in excellent agreement with the measurements.[7,8,10] Therefore, we can employ the APEF tabulated in Table 3 to carry out the vibrational manifold calculations.

3.3. Vibrational manifolds

In order to obtain the vibrational states, we must solve the radial Schrödinger equation of nuclear motion. In the adiabatic approximation, the radial Schrödinger equation of nuclear motion can be written as

$$\left[-\frac{\hbar^2}{2\mu}\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{\hbar^2}{2\mu r^2}J(J+1) + V(r)\right]\Psi_{\nu,J}(r) = E_{\nu,J}\,\Psi_{\nu,J}(r). \quad (9)$$

Where $V(r)$ is the adiabatic rotationless APEF tabulated in Table 3, r is the internuclear distance of the two atoms, μ is the reduced mass of the SD^+ ion, υ and J are the vibrational and the rotational quantum numbers, respectively, $E_{\nu,J}$ and $\Psi_{\nu,J}(r)$ are the eigenvalues and eigenfunctions of the potential $J(J+1)\cdot\hbar^2/2\mu r^2 + V(r)$, respectively. The rotational sublevel of a given vibrational level is represented by the following power series,[29]

$$E_{\nu,J} = G(\nu) + B_\nu[J(J+1)] - D_\nu[J(J+1)]^2$$

$$+H_\nu[J(J+1)]^3 + L_\nu[J(J+1)]^4 + M_\nu[J(J+1)]^5 + N_\nu[J(J+1)]^6 + O_\nu[J(J+1)]^7. \quad (10)$$

Where $G(\upsilon)$ is the vibrational level, B_υ is the inertial rotation constant, D_υ, H_υ, L_υ, M_υ, N_υ and O_υ are the centrifugal distortion constants. Solving Eq.(9) numerically, we have obtained a total of 29 vibrational states for $SD^+(X^3\Sigma^-)$ ion when the rotational quantum number J is set to equal zero. For each vibrational state, we obtain 1 vibrational level, 1 inertial rotation constant and 6 centrifugal distortion constants. The vibrational levels, the classical turning points and the inertial rotation constants are all collected in Table 5, and the centrifugal distortion constants are all collected in Table 6.

Table 5. Vibrational levels and classical turning points for the $SD^+(X^3\Sigma^-)$ ion at the UCCSD(T)/ aug-cc-pV5Z level of theory when $J = 0$.

υ	$G(\upsilon)/\mathrm{cm}^{-1}$	$R_{\min}$/nm	$R_{\max}$/nm	$B_\upsilon/\mathrm{cm}^{-1}$
0	899.980	0.12734	0.14730	4.725323
1	2663.712	0.12164	0.15659	4.619619
2	4383.341	0.11812	0.16366	4.516108
3	6059.128	0.11548	0.16995	4.414248
4	7691.081	0.11334	0.17579	4.313530
5	9278.986	0.11155	0.18138	4.213475
6	10822.429	0.11000	0.18681	4.113623
7	12320.809	0.10864	0.19216	4.013529
8	13773.347	0.10744	0.19748	3.912748
9	15179.090	0.10635	0.20282	3.810832
10	16536.907	0.10537	0.20822	3.707314
11	17845.482	0.10448	0.21372	3.601696
12	19103.305	0.10367	0.21935	3.493432
13	20308.643	0.10293	0.22517	3.381910
14	21459.520	0.10226	0.23122	3.266422
15	22553.673	0.10164	0.23758	3.146129
16	23588.496	0.10107	0.24430	3.020009
17	24560.967	0.10056	0.25150	2.886774
18	25467.541	0.10009	0.25931	2.744760
19	26303.996	0.09968	0.26791	2.591725
20	27065.215	0.09930	0.27757	2.424539
21	27744.851	0.09898	0.28874	2.238607
22	28334.809	0.09870	0.30215	2.026827
23	28824.509	0.09847	0.31925	1.777732
24	29200.352	0.09830	0.34329	1.474374
25	29450.748	0.09819	0.38185	1.121196
26	29596.825	0.09812	0.43578	0.848427
27	29693.648	0.09808	0.49352	0.684440
28	29759.654	0.09805	0.56991	0.510122

In experiment, the inertial rotation constant (B_υ) and centrifugal distortion constant (D_υ) can be found in the literature[7] only when the energy level is lower than three. In order to keep clarity of Tables 5 and 6, we separately tabulate these data in Table 7. From the B_υ comparison between our theories and experiments,[7] we find that the largest relative deviation does not exceed 0.13%. In addition, by comparison with the centrifugal distortion constant, D_υ, tabulated in Tables 6 and 7, we also find that there is excellent agreement between them.

Table 6. The centrifugal distortion constants for the $SD^+(X^3\Sigma^-)$ ion at the UCCSD(T)/aug-cc- pV5Z level of theory when $J = 0$.

v	$D_v/10^{-4}\,cm^{-1}$	$H_v/10^{-9}\,cm^{-1}$	$L_v/10^{-13}\,cm^{-1}$	$M_v/10^{-18}\,cm^{-1}$	$N_v/10^{-21}\,cm^{-1}$	$O_v/10^{-27}\,cm^{-1}$
0	1.321116	2.116916	−0.249537	0.515257	−0.149552	1.494496
1	1.295009	2.080481	−0.387468	0.425896	−0.125079	1.906589
2	1.272401	2.016242	−0.509681	0.406325	−0.117748	1.132089
3	1.253348	1.929156	−0.620305	0.373693	−0.126502	−0.414560
4	1.237886	1.822206	−0.724441	0.264281	−0.150885	−2.728802
5	1.226051	1.696591	−0.827872	0.022124	−0.192209	−6.150492
6	1.217909	1.551849	−0.937114	−0.412343	−0.254518	−11.39142
7	1.213571	1.385868	−1.059778	−1.114638	−0.345847	−19.69040
8	1.213217	1.194751	−1.205224	−2.191849	−0.480332	−33.16341
9	1.217118	0.972496	−1.385630	−3.805292	−0.682010	−55.50069
10	1.225660	0.710422	−1.617667	−6.206750	−0.991829	−93.34264
11	1.239386	0.396205	−1.925184	−9.800239	−1.480907	−159.0623
12	1.259045	0.012339	−2.343644	−15.25231	−2.276415	−276.6222
13	1.285668	−0.466369	−2.927714	−23.69757	−3.614193	−494.4990
14	1.320682	−1.076943	−3.764780	−37.13921	−5.950882	−915.7806
15	1.366083	−1.875291	−5.000088	−59.26891	−10.21660	−1772.818
16	1.424719	−2.948709	−6.885916	−97.24494	−18.42269	−3626.545
17	1.500759	−4.439111	−9.883497	−165.8162	−35.24036	−7947.013
18	1.600503	−6.588662	−14.88925	−297.6835	−72.49635	−18989.84
19	1.733882	−9.835695	−23.77960	−572.1526	−163.4755	−50677.33
20	1.917387	−15.03300	−40.85714	−1204.083	−414.9740	−156031.9
21	2.180218	−23.99221	−77.15151	−2860.390	−1229.666	−578634.5
22	2.578036	−40.96749	−164.7550	−7955.505	−4428.099	−2698285.8
23	3.222862	−76.61504	−403.7951	−25855.43	−18759.33	-1.468593×10^7
24	4.292234	−146.7131	−892.6165	−54966.65	−24153.09	1.012014×10^7
25	5.210602	−94.53676	1123.8958	227160.2	132808.55	-2.473496×10^8
26	3.824060	71.76061	−989.5322	−407409.7	−327641.97	3.614127×10^7
27	3.586915	−187.1040	−4350.173	−878947.7	−2494003.6	-7.328832×10^9
28	5.611998	−1069.482	−47500.16	2.804705×10^7	-2.000844×10^8	-1.614267×10^{12}

Table 7. The experimental B_v and D_v centrifugal distortion constants[7] from $v = 0$ to $v = 2$ for the $SD^+(X^3\Sigma^-)$ ion when $J = 0$.

	$v = 0$	$v = 1$	$v = 2$
B_v/cm^{-1}	4.73298	4.62711	4.52178
$D_v/10^{-4}cm^{-1}$	1.2891	1.2795	1.2688

By the way, we have used the present program codes to calculate the vibrational level, inertial rotation and centrifugal distortion constants of the $NH(X^3\Sigma^-)$,[23] $CH(X^2\Pi)$,[24] and $ND(X^3\Sigma^-)$[25] radicals and the $^7Li_2(X^1\Sigma_g^+)$ dimer.[30] Favourable agreement has been obtained when compared with the available Rydberg–Klein–Rees (RKR) data. These investigations[23−25,30] show that the present method is reliable and accurate.

Unfortunately, to the best of our knowledge, no experiments and theories exist in the literature about the vibrational levels and classical turning points, and no inertial rotation constants and centrifugal distortion constants can be found when the vibrational level is higher than two in the literature. Thus we cannot make any direct comparison among them. But according to the high-quality fitting process of the APEF, we have the good accord between the present spectroscopic parameters and the measurements[7,8,10] and the excellent agreement of the inertial rotation constants and centrifugal distortion constants between theory and experiment,[7] we conclude that the results collected in Tables 5 and 6 must be reliable and accurate. Therefore, we can say that the present APEF obtained at the UCCSD(T)/aug-cc-pV5Z level of theory can well describe the $SD^+(X^3\Sigma^-)$ ion.

4. Conclusions

In this paper, we report the equilibrium internuclear distance, the dissociation energy and the harmonic frequency for the ground state of the SD^+ ion at the UCCSD(T) level of theory in combination with the largest correlation-consistent quintuple basis set, aug-cc-pV5Z, for the S atom in the valence range. Favourable agreement has been found in comparison with the recent experimental findings. Employing the interaction potential obtained at the UCCSD(T)/aug-cc-pV5Z level of theory, we accurately determine the spectroscopic parameters (D_e, $\omega_e\chi_e$, α_e and B_e) are accurately determined. The total of 29 vibrational states has been predicted by numerically solving the radial Schrödinger equation of nuclear motion. For each vibrational state, the vibrational level, classical turning points, inertial rotation and centrifugal distortion constants are also calculated when $J = 0$. As a whole, the present results provide more complete investigations on the molecular ion properties of the $SD^+(X^3\Sigma^-)$ ion.

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