Rotation-vibration spectra for ground state of NaH and its isotopes with explicitly multireference configuration interaction method

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Abstract. High-level *ab initio* calculations utilizing explicitly correlated multi-reference configuration interaction method (MRCI-F12), considering Davidson modification(Q), core-valence correlation correction(CV) and scalar relativistic correction(SR), were performed to compute the Born-Oppenheimer potential energy curve (PEC) of the ground state $X^1\Sigma^+$ of NaH. On the base of the PEC, we obtained vibrational and rotational energy levels information of the ground state $X^1\Sigma^+$. The vibrational and rotational spectroscopic constants of $X^1\Sigma^+$ were compared with the available experimental values. We also report rotation-vibration spectra of the ground state for the isotopes of NaH, NaD and NaT molecules. The equilibrium internuclear distances R_e and dissociation energies D_e were calculated to be 1.8865Å and 15823.29cm^{-1} for the ground state $X^1\Sigma^+$ of NaH, which are in good agreement with the experimental results of 1.8859Å and 15815±5cm^{-1}.

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Key words: MRCI-F12, NaH, rotational-vibration constants

1 Introduction

Due to its important role in regulating the fractional ionization in molecular clouds, astrophysicists are interested in sodium chemistry which strongly influences ion-molecule dynamics in the interstellar space [1]. Astronomers suppose interstellar sodium is in the form of gas-phase NaH [2, 3]. And it is important to know the abundance information of sodium hydride in the interstellar medium for a better understanding of interstellar sodium chemistry. The investigations on the rotation-vibration spectrum for the ground state $X^1\Sigma^+$ of NaH are motivated by its astrophysical significance.

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Since the early 1930s, several experimental [4-15] and theoretical computational [16-27] studies on the spectra and interactions of NaH have been reported. In the aspect of the experiment, NaH was the first studied in 1930 by Hori, who observed and analyzed $X^1\Sigma^+$-$A^1\Sigma^+$ bands in absorption [4]. Next year, Hori reported the emission spectrum of $X^1\Sigma^+$l-$A^1\Sigma^+$ bands for NaH [5]. In 1934, Olsson [6] reported the new NaH measurements together with the NaD data of absorption spectroscopy in the spectral region of 358 nm $\leq \lambda \leq$ 445 nm cover vibrational levels in the range $0 \leq v'' \leq 3$ and $1 \leq v'' \leq 20$. In 1948, Panhhurst observed on the spectrum of NaH and extended it to longer wavelengths (from 4600 Å to 6450 Å) [7]. After 30 years, in 1988 Magg and Jones used a tunable diode laser spectrometer to measure the first infrared vibrational for NaH [9]. One year later, Maki and Olson measured the infrared spectrum of NaH using a Fourier transform spectrometer [10]. In 1993, Rafi *et al.* [11] reported new band origins and $A^1\Sigma^+$ state B_v and D_v rotational constants of $v''(X^1\Sigma^+)$ = 0 bands for $v'(A^1\Sigma^+)$ = 13-22 and of $v''(X^1\Sigma^+)$=1 bands for $v'(A^1\Sigma^+)$=12-25. In 1996, Lochbrunner *et al.* [12] reported NaH band absorption from $v''(X^1\Sigma^+)$ = 0-3 into $v'(A^1\Sigma^+)$ = 2-15 and NaD bands from $v''(X^1\Sigma^+)$ = 0-2 into $v'(A^1\Sigma^+)$ = 5-17. In 2000, Pesl *et al.* [13] measured high-resolution spectroscopy data for the $A^1\Sigma^+$-$X^1\Sigma^+$ transition. Most recently, Huang *et al.* [14, 15] observed vibrational quantum numbers of up to v''=21 in the ground state of NaH.

Theoretically, first computational work was reported in 1975, Sachs and Hinze used multiconfigurational method to calculate first six states of NaH [16], Sachs and Hinze published the transition moments, band strengths and line strengths for NaH [18] and reported the rotation-vibrational analysis for three low-lying states of NaH and NaD [17] . Since then, lots of computational works [19-24] were engaged in the electronic states information of NaH. In 2004, Brian and Philip R [25] used basis set extrapolation technique in combination with highly correlated *ab initio* calculations obtained nearly exact properties for the $X^1\Sigma^+$ electronic ground state of the NaH and NaD molecule, and found 20 vibrational levels for NaH. In 2004, Yang *et al.* [26] utilized MRCI method with Davidson correction calculated PECs and obtained spectroscopic parameters of first few electronic states of NaH. More recently, Sadru-Dean *et al.* [27] summarized previous experimental and theoretical reports, analyzed the dissociation energies and potential energy functions for the ground $X^1\Sigma^+$ and "avoided-crossing" $A^1\Sigma^+$ states of NaH.

In this work, we performed the explicitly correlated multireference configuration interaction method for the lowest $X^1\Sigma^+$ state of the sodium hydride with Davidson correction (+Q), core-valence (CV) effect and scalar relativistic (SR) effect. Based on computed adiabatic PEC of the $X^1\Sigma^+$, the vibrational energy spacings $G_{v+1/2}$, vibrational energy terms Gv, the vibration-dependent rotational constant Bv, and centrifugal distortion constant Dv of ground state were also obtained by numerically solving the ro-vibrational Schrödinger equations. The vibrational and rotational constants of the $X^1\Sigma^+$ state for NaD and NaT are also presented in this work.

2   Computational methods

All electronic structure calculations were performed with Molpro 2012 package [28, 29]. The symmetry point group of NaH constrained into C_{2v} in the present calculation. The C_{2v} point group holds A1/B1/B2/A2 irreducible representations, and the corresponding relationships between the C_{2v} and $C_{\infty v}$ point group are $\Sigma^+=A_1$, $\Pi=B_1+B_2$, $\Delta=A_1+A_2$, and $\Sigma^-=A_2$. For the NaH, $5a_1$, $3b_1$, $3b_2$, and $1a_2$ symmetry molecular orbitals (MOs) were determined as the active space, corresponding to the atomic orbitals 3s3p4s3d4p for Na and 1s for H. The outermost $3s^1$ electrons of the Na atom and $1s^1$ electron of the H atom were placed in the active space. And electrons in n=2 shells were correlated in subsequent MRCI-F12 computations. That is, there were total of 6 electrons of the NaH used in the calculation of electronic correlation energy. The adiabatic PEC of the ground state of NaH, were constructed from 68 single-point energies in the range of internuclear distances from 1.0Å to 10.0Å. In these calculations, the Gaussian-type contracted basis sets cc-pCVQZ-F12 [30, 31] were selected for Na atom and H atom. The calculations were performed via the following three steps: the single-configuration wavefunction of the ground state for the NaH was firstly calculated with the restricted Hartree-Fock (RHF) method; then, the single-root complete active space self-consistent field (CASSCF) method [32, 33] was used to construct the multi-configuration wavefunction; finally, the explicitly correlated multireference configuration interaction (MRCI-F12) [34] approach was employed to treatment the dynamical correlation of the electrons. In addition, the size-consistency correction was taken into account through Davidson correction [35]. The core-valence correlation correction calculations [36] induced by the n=2 shell of Na atom were estimated by MRCI-F12 method and the 1s orbit of Na was excluded in the CV calculations. And we also considered the scalar relativistic effect into our study utilizing second-order Douglas-Kroll [37] and Hess (DKH) [15, 34] one-electron integrals with MRCI method in combination with uncontacted aug-cc-pVQZ basis set [38]. Finally, on the basis of the PEC, we obtained the rotational-vibration constants of the $X^1\Sigma^+$ of the NaH by solving the nuclear Schrödinger equations utilizing numerical integration LEVEL procedure [39]. In this work, similar computational strategy was employed in PEC calculations [40, 41]. And the present computational strategy shows good extensibility, which is expected having extensive applications to other diatomic system.

3   Results and discussion

3.1   Rotation-vibration spectrum for NaH

The calculation of rotational and vibrational energy levels E_{vJ}, where v and J are the vibrational and rotational quantum numbers, respectively, requires the solution of the nuclear Schrödinger equation. Following spectroscopic conventions, we express the rotational-

vibrational energy levels in the form

$$E_{vJ} = V_{eq} + G_v + F_v(J) \tag{1}$$

Where V_{eq} is the minimum value of the potential at equilibrium distance R_{eq}, and v and J are the vibrational and rotational quantum numbers, G_v is the pure vibrational term and $F_v(J)$ is the rotational term. Since the rotational energy is very small compared to the vibrational energy, the $F_v(J)$ can be expanded as

$$F_v(J) = B_v[J(J+1)] - D_v[J(J+1)]^2 + \cdots \tag{2}$$

Where B_v is the rotational constant, D_v is the centrifugal constant.

On the base of the adiabatic PEC deduced from the MRCI-F12+CV+SR+Q computations, our fitted equilibrium internuclear distances R_e is 1.8865Å, which is only 0.0006Å deviated from experimental value 1.8859Å [15], the relative error is less than 0.05%. Our computed dissociation energies D_e is 15823.29cm^{-1} and only few cm^{-1} overestimated comparing to the experimental value [15]. The present R_e and D_e values are significantly improved by comparing with recent theoretical values of 1.8870Å and 15797.4cm^{-1} [27]. By the solution of nuclear motion Schrödinger equation, we obtained vibrational and rotational information of the $X^1\Sigma^+$. Total 21 vibrational levels for the $X^1\Sigma^+$ are found and all the vibrational and rotational constants are listed in Table 1 and Table 2, respectively. As listed in Table 1, the recently experimental spectroscopic data [15] are represented in terms of vibrational energy G_v and the vibrational energy spacings $G_{v+1/2} = G_{v+1} - G_v$, which are reported in column 2 and 5 in Table 1. In the subsequent columns of Table 1, we list the G_v and $G_{v+1/2}$ that we obtained from *ab initio* potentials, the theoretical values in the third and sixth column were obtained from MRCI-F12+SR potential, while the values in the fourth and seventh column were obtained from MRCI-F12+SR+Q potential. The row below $v = 20$ lists the mean absolute deviation (MAD) for each column. Comparing the MAD for each column values, we can find that Davidson correction plays a significant role in the determination of the vibrational constants. Therefore, we adopted MRCI-F12+SR+Q potential to compute rotational and vibrational spectra in present work. For the $v=0\sim13$ vibrational levels, the G_v values deviations between present work and experiment results [15] are within 10cm^{-1}; for the $v=14\sim20$ level, our computed values differ in the range of $10\sim28$cm^{-1} from experimental ones [15]. While the relative errors for all available energy levels are all less than 0.2%. For some certain vibrational levels, such as $v=2\sim7$, 14 and 16, the deviations of $G_{v+1/2}$ values are less than 1cm^{-1}. Comparing to the latest experiment [15], the MADs for presently computed G_v and $G_{v+1/2}$ values are 9.22 cm^{-1} and 2.03cm^{-1}, respectively.

For each vibrational quantum number v, there are many rotational levels labeled by J. We calculated the spectroscopic constants of levels J=0 for each vibrational level v. The computational results for B_v and D_v are reported in Table 2. The experimental data for B_v are taken from Ref. [15] for $v=0\sim20$ and recent theoretical values for D_v are brought from Ref. [25] for $v=0\sim10$. The deviations of our theoretical results from the experimental data and recent theoretical values are listed in column 4 for B_v and in column 7

Table 1: Comparisons of theoretical spectroscopic vibration levels G_ν and vibrational energy spacings $\Delta G_{\nu+1/2} = G_{\nu+1} - G\nu$ for NaH with the experimental values. Energies are in cm^{-1}.

| ν | G_ν | | | $\Delta G_{\nu+1/2}$ | | |
	Expt.[a]	This work[b]	This work[c]	Expt.[a]	This work[b]	This work[c]
0	581.09	-2.05	-1.16	1133.10	-5.45	-2.42
1	1714.18	-7.50	-3.58	1095.08	-4.45	-1.34
2	2809.26	-11.95	-4.91	1057.79	-3.48	-0.66
3	3867.05	-15.43	-5.58	1021.08	-3.01	-0.10
4	4888.13	-18.44	-5.68	984.78	-2.95	-0.19
5	5872.91	-21.40	-5.87	948.75	-2.22	0.42
6	6821.66	-23.62	-5.44	912.82	-1.61	0.75
7	7734.48	-25.23	-4.69	876.84	-1.30	0.76
8	8611.32	-26.52	-3.93	840.55	-1.35	1.24
9	9451.86	-27.88	-2.69	802.82	0.16	2.45
10	10254.69	-27.72	-0.24	764.02	1.66	3.64
11	11018.71	-26.06	3.40	723.72	3.47	5.45
12	11742.43	-22.59	8.85	688.80	-2.76	-1.05
13	12431.23	-25.35	7.80	641.20	1.23	2.99
14	13072.42	-24.13	10.79	595.80	-1.28	0.33
15	13668.22	-25.41	11.12	537.44	4.16	5.49
16	14205.66	-21.24	16.61	481.44	-0.36	0.64
17	14687.10	-21.60	17.25	408.55	3.03	4.41
18	15095.64	-18.57	21.65	328.30	1.62	2.85
19	15423.94	-16.95	24.50	231.30	3.91	3.39
20	15655.25	-13.03	27.89			
MAD		20.13	9.22		2.47	2.03
D_e	15815±5	15784.32	15823.29			
R_e(Å)	1.88586	1.8895	1.8865			

[a] Ref [15].
[b] deviations of MRCI-F12+SR values from experiment.
[c] deviations of MRCI-F12+Q+SR values from experiment.

for D_ν. For the $\nu=0\sim3$ and $10\sim20$ vibrational levels, the experimental values for B_ν are slightly larger than our theoretical values; for the $\nu=4\sim9$, the B_ν values deviations between present work and experiment results [15] are less than 0.0050cm^{-1}. Unfortunately, no experiment values of D_ν are available for comparison with our present work. For the $\nu=0\sim10$ vibrational levels, our calculated the theoretical values of D_ν are close to the theoretical values [25]. Tables 1 and 2 reveals excellent agreement between theory and experiment for the vibrational and rotational constants. It is worth noting that only 21 vibrational levels ($\nu=0\sim20$) are found in present theoretical work, though an additional vibrational level ($\nu=20$) is found, one vibrational level ($\nu=21$) observed in experiment is still absent using presently best-estimated adiabatic potential. Further inclusions of diagonal Born-Oppenheimer correction (DBOC), and nonadiabatic effect are expected to improve the potential. We note recent theoretical analysis considered the coupling between ground state and first excited electronic state, especially in the avoided-crossing

Table 2: Rotational constants (in cm^{-1}) of the ground state of NaH.

ν	B_ν			$10^4 D_\nu$		
	Expt.[a]	This work[b]	δ^c	Theory[d]	This work[b]	δ^c
0	4.8350	4.8346	-0.0004	3.4189	3.4233	0.0044
1	4.7000	4.6990	-0.001	3.3611	3.3638	0.0027
2	4.5670	4.5666	-0.0004	3.3118	3.3143	0.0025
3	4.4365	4.4356	-0.0009	3.2685	3.2705	0.002
4	4.3050	4.3076	0.0026	3.2295	3.2426	0.0131
5	4.1777	4.1784	0.0007	3.1944	3.1866	-0.0078
6	4.0486	4.0522	0.0036	3.1648	3.1682	0.0034
7	3.9214	3.9247	0.0033	3.1436	3.1437	0.0001
8	3.7928	3.7960	0.0032	3.1319	3.1130	-0.0189
9	3.6634	3.6680	0.0046	3.1215	3.1184	-0.0031
10	3.6597	3.5364	-0.1233	3.1094	3.1400	0.0306
11	3.5017	3.4029	-0.0988		3.1351	
12	3.3988	3.2614	-0.1374		3.2574	
13	3.3203	3.1150	-0.2053		3.3337	
14	3.0839	2.9559	-0.128		3.5231	
15	2.9531	2.7806	-0.1725		3.7669	
16	2.7799	2.5834	-0.1965		4.2171	
17	2.6117	2.3555	-0.2562		4.7479	
18	2.3473	2.0866	-0.2607		5.7695	
19	2.0736	1.7529	-0.3207		7.3350	
20	1.7050	1.3288	-0.3762		10.288	
MAD			0.1093			0.0081

[a] Ref [15].
[b] deviations of MRCI-F12+Q+SR values from experiment.
[c] δ, differences between present MRCI-F12+Q+SR values and experimental ones.
[d] Ref [25].

region, and deduced accurate vibration-rotation information.

3.2 Rotation-Vibration Spectrum For NaD And NaT

The values of G_ν and $G_{\nu+1/2}$ for NaD and NaT are listed in the Table 3. Total 30(ν=0~29) vibrational levels for the $X^1\Sigma^+$ of NaD are found. Similar to the case for NaH, the highest vibrational level (ν=30) in NaD predicted in experimental analysis [27] is absent in this work. The differences for the ν=0~18 between our calculated values and the existing experimental values [8] are merely less than 2.3cm^{-1} for $G_{\nu+1/2}$ values. The highest vibrational level of ground state for NaT is ν=35 in this work. The rotational constants for NaD and NaT are listed in Table 4. For the ν=0~20 vibrational levels, the B_ν values of NaD deviations between present work and experiment results [8] are in the range of 0~0.020cm^{-1}. Both vibrational and rotational constants for NaT are unavailable in previous experimental and theoretical works. We expect our computed vibrational and rotational constants for NaT are helpful in further spectroscopy investigations.

Table 3: Theoretical spectroscopic vibration levels Gν and spacings $\Delta G_{\nu+1/2}$ for NaD and NaT. Energies are in cm^{-1}.

| | | NaD | | | | NaT | |
| | | | $\Delta G_{\nu+1/2}$ | | | | |
ν	Gν	Expt.[a]	This work[b]	δ^c		Gν	$\Delta G_{\nu+1/2}$
0	419.5	825.3	824.0	-1.3		349.8	689.5
1	1243.4	806.0	804.5	-1.5		1039.3	675.7
2	2047.9	787.8	785.6	-2.2		1715.0	662.9
3	2833.5	766.2	766.0	-0.2		2377.9	648.9
4	3599.5	747.1	747.6	0.5		3026.8	636.1
5	4347.1	729.7	728.3	-1.4		3662.9	622.8
6	5075.4	708.2	709.5	1.3		4285.7	609.8
7	5784.9	690.9	691.1	0.2		4895.5	596.4
8	6476.1	673.0	672.6	-0.4		5491.9	583.6
9	7148.6	653.4	654.0	0.6		6075.5	570.8
10	7802.7	634.3	635.0	0.7		6646.3	558.2
11	8437.7	616.5	616.8	0.3		7204.5	544.8
12	9054.5	597.4	597.6	0.2		7749.3	531.9
13	9652.1	578.4	578.4	0		8281.2	519.2
14	10230.5	557.0	559.2	2.2		8800.4	506
15	10789.8	538.0	539.2	1.2		9306.4	492.7
16	11329.0	518.4	518.2	-0.2		9799.1	479.4
17	11847.2	494.8	497.0	2.2		10278.5	466.2
18	12344.2	473.1	474.3	1.2		10744.7	452.1
19	12818.6	455.3	450.3	-5		11196.8	437.7
20	13268.8		424.7			11634.5	423.2
21	13693.5		396.8			12057.7	408.1
22	14090.3		366.0			12465.8	392
23	14456.3		332.7			12857.8	375.2
24	14789.0		295.5			13233.0	357.7
25	15084.5		253.5			13590.7	339.1
26	15338.1		206.2			13929.8	317.7
27	15544.2		152.8			14247.5	295.9
28	15697.0		95.0			14543.4	272.5
29	15792.0					14815.9	246.2
30						15062.1	217.4
31						15279.5	185.5
32						15465.0	150
33						15615.0	111.7
34						15726.7	70.5
35						15797.2	
36							
MAD			1.1				

[a] Ref [27].
[b] deviations of MRCI-F12+Q+SR values from experiment.
[c] δ, differences between present MRCI-F12+Q+SR values and experimental ones.

4　Conclusions

High-level MRCI-F12+CV+SR+Q calculations have been performed to calculate the PEC of the ground state $X^1\Sigma^+$ of NaH. Our results of equilibrium internuclear distances R_e

Table 4: Theoretical rotational constants (in cm^{-1}) of the ground state of NaD and NaT.

	NaD				NaT	
		B_v				
v	Expt.[a]	This work[b]	δ^c	$10^5 D_v$	B_v	$10^5 D_v$
0	2.522	2.531	0.009	9.3270	1.761	4.5026
1	2.480	2.479	-0.001	9.2101	1.731	4.4557
2	2.426	2.429	0.003	9.0788	1.701	4.4099
3	2.376	2.379	0.003	9.0456	1.672	4.3735
4	2.324	2.330	0.006	8.8724	1.643	4.3217
5	2.277	2.281	0.004	8.8946	1.616	4.3235
6	2.234	2.233	-0.001	8.7705	1.587	4.2428
7	2.190	2.184	-0.006	8.6680	1.559	4.2657
8	2.147	2.137	-0.01	8.6452	1.531	4.2053
9	2.089	2.089	0	8.5382	1.503	4.1723
10	2.040	2.040	0	8.5845	1.476	4.1368
11	1.992	1.992	0	8.3945	1.448	4.1529
12	1.941	1.944	0.003	8.5606	1.420	4.1220
13	1.887	1.895	0.008	8.4914	1.392	4.0848
14	1.831	1.846	0.015	8.4332	1.365	4.1114
15	1.783	1.796	0.013	8.5628	1.336	4.0825
16	1.737	1.744	0.007	8.7372	1.308	4.1113
17	1.672	1.691	0.019	8.7129	1.280	4.0631
18	1.629	1.635	0.006	9.0694	1.250	4.1167
19	1.572	1.577	0.005	9.3341	1.220	4.1925
20	1.508	1.514	0.006	9.7148	1.190	4.1965
21		1.448		1.0.284	1.158	4.2964
22		1.374		11.1943	1.126	4.3743
23		1.293		11.9680	1.091	4.5533
24		1.204		13.3823	1.055	4.6533
25		1.101		15.4426	1.018	4.8835
26		0.983		18.1316	0.976	5.2090
27		0.841		22.2942	0.931	5.5473
28		0.674		28.2696	0.884	5.9435
29		0.462		47.6966	0.830	6.5728
30					0.771	7.2712
31					0.704	8.3577
32					0.627	9.8095
33					0.537	11.8307
34					0.436	15.6954
35					0.305	23.5968
MAD			0.006			

[a] Ref [27].
[b] deviations of MRCI-F12+Q+SR values from experiment.
[c] δ differences between present MRCI-F12+Q+SR values and experimental ones.

and dissociation energies D_e for the ground state $X^1\Sigma^+$ of NaH are 1.8865Å and 15823.29 cm^{-1}, which are in excellent agreement with the experimental values [15] of 1.8859Å and 15815±5cm^{-1}. From the computed PECs, the vibrational and rotational constants of NaH and its Isotopes, NaD and NaT, are determined, good agreement with available

experimental measurements is found. Total 21, 30 and 36 vibrational levels are found for NaH, NaD, and NaT, respectively. And additional one vibrational level is found for NaH and NaD compared to previous theoretical work. Some spectroscopic constants absent in experiments are presented in this work and are expected to be helpful in further experimental spectroscopy investigations.

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