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Investigation of the FrH+ Alkali Hydride Cation: Analysis of Potential Energies, Dipole Functions, and Radiative Lifetimes

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Abstract: This paper presents an extensive *ab-initio* investigation of the structural and spectroscopic properties of the FrH^+ alkali hydride cation, utilizing non-empirical pseudo-potentials for Fr^+ core. We determine the potential energy curves for 19 electronic states with symmetries of $^2\Sigma^+$, $^2\Pi$, and $^2\Delta$, which exhibit dissociation up to Fr (8*p*) + H^+ and Fr^+ + H (3*d*). We identify and interpret avoided crossings between higher $^2\Sigma^+$ and $^2\Pi$ states. Additionally, we calculate the spectroscopic parameters, transition dipole functions, and vibrational energies associated with $1\text{-}3^2\Sigma^+$ states. Using accurate potential energies of $X^2\Sigma^+$ and $2^2\Sigma^+$ states, along with transition dipole functions between these states, we evaluate the radiative lifetimes for the vibrational states confined within the $2^2\Sigma^+$ state. As far as we are aware, no experimental or theoretical data concerning this system have been published to date. Therefore, we discuss and compare our findings with those of analogous systems. Consequently, this study presents the first theoretical results for the alkali hydride cation FrH^+.

Keywords: Alkali Hydride, Potential energy curves, Spectroscopic Parameters, Dipole Moments, Radiative lifetimes.

[1] Introduction

The interaction potentials of alkali hydride neutral systems XH (X=alkali atom) and their corresponding cations have been extensively investigated in various fields, including astrophysics, ultra-low temperature gases, interatomic forces, the formation of ultra-cold systems, and ultra-cold collisions [1-24]. These systems play a curcial role in ion-atom collisions, molecular ions, astrophysical phenomena such as interstellar clouds [25], as well as emerging areas like quantum information [26], precesion measurement [27], and chemical reactions in quantum regime [28]. Understanding the potential and its dissociation in the long-range region often requires a collaborative effort between theory and experiment. Hence, studying the structural and spectroscopic properties of electronic states for alkali hydride cations is of fundamental importance in the field of physics. In this regard, several theoretical studies have been conducted on the electronic properties of alkali hydride cations, including LiH^+ [14-16], NaH^+ [17-18], KH^+ [19-21], RbH^+ [22-24], and CsH^+ [23-24]. Building upon the previous findings of these systems, we expanded our investigation to specifically focus on the electronic structure of alkali hydride cations, through the detailed study of FrH^+.

The aim of this paper is to investigate the properties of the electronic states and spectroscopy of the FrH^+ alkali hydride cation. This includes analyzing potential energies, spectroscopic parameters, transition dipole functions, and radiative lifetimes. In the upcoming section, we will offer a concise overview of the the computational approach employed along in this study. Section 3 is subdivided into three distinct components: analysis of potential energies and their associated

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spectroscopic parameters, the examination of transition dipole functions pertaining to electronic states, and evaluation of the radiative lifetimes. Ultimately, our findings will be summarized in Section 4.

[2] Computational Method

Based on the methodology employed in our prior investigations [29-46], we utilize the non-empirical pseudopotential, specifically the semi-local form suggested by Barthelat et al. [47], to simulate the FrH^+ alkali hydride system. In this simulation the FrH^+ system is considered to have a single valence electron. Additionally, the interaction between the valence electron, the polarizable core Fr^+, and the hydrogen nucleus is introduced using the approach proposed by Müller et al. [48] through the polarization potential V_{CPP}:

$$V_{CPP} = -\frac{1}{2}\sum_{\lambda}\alpha_\lambda \vec{f}_\lambda \vec{f}_\lambda \qquad (1)$$

here $\vec{f}_\lambda$ is the electric field resulting from the combined effects of the valence electron and the other cores on the core λ, while α_λ symbolizes the dipole polarizability of the core λ. The electric field $\vec{f}_\lambda$ can be defined as follows:

$$\vec{f}_\lambda = \sum_i \frac{\vec{r}_{i\lambda}}{r_{i\lambda}^3} F(\vec{r}_{i\lambda}, \rho_\lambda) - \sum_{\lambda' \neq \lambda} \frac{\vec{R}_{\lambda'\lambda}}{r_{\lambda'\lambda}^3} Z_\lambda \qquad (2)$$

here $\vec{R}_{\lambda'\lambda}$ represents the core-core vector and $\vec{r}_{i\lambda}$ is the core-electron vector.

Based on the formalism introduced by Foucrault et al. [49], the selection of the cut-off function depends on the value of *l*, allowing for differentiation in the interaction between valence electrons with different spatial symmetries and core electrons.

$$F(\vec{r}_{i\lambda}, \rho_\lambda) = \sum_{l=0}^{\infty}\sum_{m=-l}^{+l} F_l(r_{i\lambda}, \rho_\lambda^l) |lm\lambda\rangle\langle lm\lambda|$$

(3)

where $|lm\lambda\rangle$ represents the spherical harmonic centred on λ, while $F_l(r_{i\lambda}, \rho_\lambda^l)$ denotes the cut-off operator, defined as a step function following the formalism of Foucrault et al. [49]:

$$F_l(r_{i\lambda}, \rho_\lambda^l) = \begin{cases} 0, r_{i\lambda} < \rho_\lambda \\ 1, r_{i\lambda} > \rho_\lambda \end{cases} \qquad (4)$$

In the formalism introduced by Müller et al. [48], the cut-off function excludes the valence electrons from the core region when computation of the electric field. This cut-off function is specific to each atom, and its adjustments are commonly made to accurately replicate the atomic energy levels corresponding to the lowest states of the lowest states within each symmetry. For the francium, we utilized a dipole polarizability of 20.38 a_0^3 and cut-off radii of 3.16372, 3.045 and 3.1343 atomic units for the lowest valence *s*, *p*, and *d* one-electron states, respectively. The extended basis sets used for the francium and hydrogen atoms are (9*s*9*p*9*d*) [50] and (9*s*5*p*3*d*1*f*/7*s*5*p*3*d*1*f*) [17], respectively. The calculated energies (in cm^{-1}) for H (1*s*, 2*s*, 2*p*, 3*s*, 3*p*, and 3*d*) and Fr (7*s*, 7*p*, 6*d*, 8*s*, and 8*p*) atomic levels exhibit excellent agreement with experimental [51] values. The results, including the difference (ΔE) between our findings and the experimental energies, are presented in table 1.

3.Results and discussion

2.1. Potential energies and spectroscopic parameters

The potential energies were computed for 19 electronic states with symmetries of $^2\Sigma^+$, $^2\Pi$, and $^2\Delta$ for the alkali hydride cation FrH^+ dissociating up to Fr(8*p*) + H^+ and Fr^+ + H (3*d*). These energies were obtained over a wide range of distances, spanning from 2.80 to 150 atomic units (a. u.). Figure 1 displays the potential energy curves for the 1-10$^2\Sigma^+$ states, whereas Figure 2 shows the results for the $^2\Pi$ and $^2\Delta$ symmetries. These curves showcase characteristics that are comparable to those of other alkali hydride cations (XH^+, where X represents an alkali atom). In fact, except for the LiH^+ [14] system, the ground states of these cations exhibit a weak bonds with depths of several tens or hundreds of cm^{-1}, and these depths increase from the heaviest cation to the lightest one. The ground state of FrH^+ demonstrates a slight well depth (10 cm^{-1}), in contrast to LiH^+ [14] (1229 cm^{-1}), NaH^+ [17] (458 cm^{-1}), KH^+ [19] (384 cm^{-1}), RbH^+ [23] (347 cm^{-1}), and CsH^+ [23] (282 cm^{-1}). Additionally, the $2^2\Sigma^+$ state exhibits the most profound potential well when compared to the other higher states or alternative symmetries. The equilibrium position for this state is 9.43 atomic units, with a corresponding potential well measuring 5129 cm^{-1}. Moreover, the excited states of $^2\Sigma^+$ and $^2\Pi$ symmetries are characterized, at both short and large distances, by the presence of several avoided crossing. Previous investigations [17, 30-31, 33, 35, 37] have documented comparable behavior in charged diatomic systems. We found the avoided crossings between the electronic states $4^2\Sigma^+/5^2\Sigma^+$, $5^2\Sigma^+/6^2\Sigma^+$, $7^2\Sigma^+/8^2\Sigma^+$, $8^2\Sigma^+/9^2\Sigma^+$, $9^2\Sigma^+/10^2\Sigma^+$, $2^2\Pi/3^2\Pi$ and $5^2\Pi/6^2\Pi$ at distances of 4.74, 11.97, 48.81, 25.90, 18.76, 7.19 and 7.04 a.u.. respectively. Some of these avoided crossings are attributed to the interaction between the energy curves, whereas others arise from charge transfer processes involving the hydrogen and francuim atoms.

Table 1. Theoretical atomic energies of hydrogen and francium atoms (in cm^{-1}) compared with experimental values. ΔE represents the difference between theoretical and experimental energies.

Atoms	Levels	This work	Experimental [51]	ΔE
H	1s	-109726.52	-109737.31	10.79
	2s	-27432.39	-27434.33	1.94
	2p	-27427.57	-27434.33	6.76
	3s	-12187.00	-12193.03	6.03
	3p	-12156.06	-12193.03	36.97
	3d	-12138.50	-12193.03	54.53
Fr	7s	-32848.82	-32848.87	0.05
	7p	-19487.18	-19487.07	0.11
	6d	-16470.94	-16471.25	0.31
	8s	-13136.89	-13116.39	20.50
	8p	-9424.91	-9372.35	52.56

Table 2: Spectroscopic parameters of the attractive $^2\Sigma^+$ and $^2\Pi$ electronic states of the FrH^+ alkali hydride cation.

State	R_e(a.u.)	D_e(cm^{-1})	ω_e(cm^{-1})	$\omega_e x_e$(cm^{-1})	B_e(cm^{-1})
$1^2\Sigma^+$	13.86	10	5.61	0.15	0.309106
$2^2\Sigma^+$	9.43	5129	285.08	4.87	0.674215
$3^2\Sigma^+$	16.46	2523	135.05	2.07	0.221353
$5^2\Sigma^+$	20.56	1585	91.89	2.00	0.141860
$6^2\Sigma^+$	73.86	12	1.60	0.65	0.010842
$7^2\Sigma^+$	27.76	2171	70.01	0.37	0.077882
$8^2\Sigma^+$	43.46	1021	13.66	63.55	0.032734
$11^2\Sigma^+$	43.93	921	37.40	0.16	0.609766
$1^2\Pi$ Hump	9.87 16.95	193 81	112.29	32.73	0.609766
$2^2\Pi$	15.62	638	88.19	10.59	0.249566
$4^2\Pi$	24.20	1224	60.76	3.42	0.102343
$6^2\Pi$	35.45	459	31.70	49.91	0.046993

To date, no spectroscopic parameters for the FrH^+ alkali hydride cation have been reported in literature, making it impossible for us to conduct further parameter comparisons for this system. However, our work can be regarded as the first to present theoretical results on the fundamental properties of FrH^+. In Table 2, we list the spectroscopic parameters of the FrH^+ alkali hydride cation, including the equilibrium distance (R_e), well depth (D_e), harmonic frequency (ω_e), anharmonicity constant ($\omega_e\chi_e$), and rotational constant (B_e). To analyze our findings, we qualitatively compare the spectroscopic parameters for the ground state of FrH^+ with those of similar systems involving hydrogen and other alkali atoms [14, 17, 19, 23]. The equilibrium position of FrH^+ in its ground state is 13.86 a.u., with a corresponding potential well measuring 10 cm^{-1}. When comparing these results with previous studies on alkali hydride cations, LiH^+ [14] exhibits the deepest well (1229 $cm^{-}1$) and the smallest equilibrium distance (4.12 a.u.). The well depths of the ground states for NaH^+ [17], KH^+ [19], RbH^+ [23], and CsH^+ [23] are 458, 384, 347 cm^{-1}, and 282 cm^{-1}, respectively, with equilibrium positions at 5.09, 5.52, 5.83, and 6.14 a.u.. We observe a systematic decrease in well depths with increasing alkali atom mass, while equilibrium distances increase. On the other hand, among the excited states, the $2^2\Sigma^+$ state, possesses the most profound well (D_e=5129 cm^{-1}). It is worth noting that the $4^2\Sigma^+$, $9\text{-}10^2\Sigma^+$, $3^2\Pi$, $5^2\Pi$, and $1\text{-}2^2\Delta$ states exhibit repulsive behavior among the other higher electronic states. Conversely, all the remaining electronic states demonstrate attractive characteristics, with potential well depths ranging in the several hundreds of cm^{-1} range, except for the $2\text{-}3^2\Sigma^+$ and $7^2\Sigma^+$ states. The well depths of the $2\text{-}3^2\Sigma^+$ and $7^2\Sigma^+$ states are 5129, 2523, and 2171 cm^{-1}, respectively, located respectively 9.43, 16.46, and 27.76 a. u.

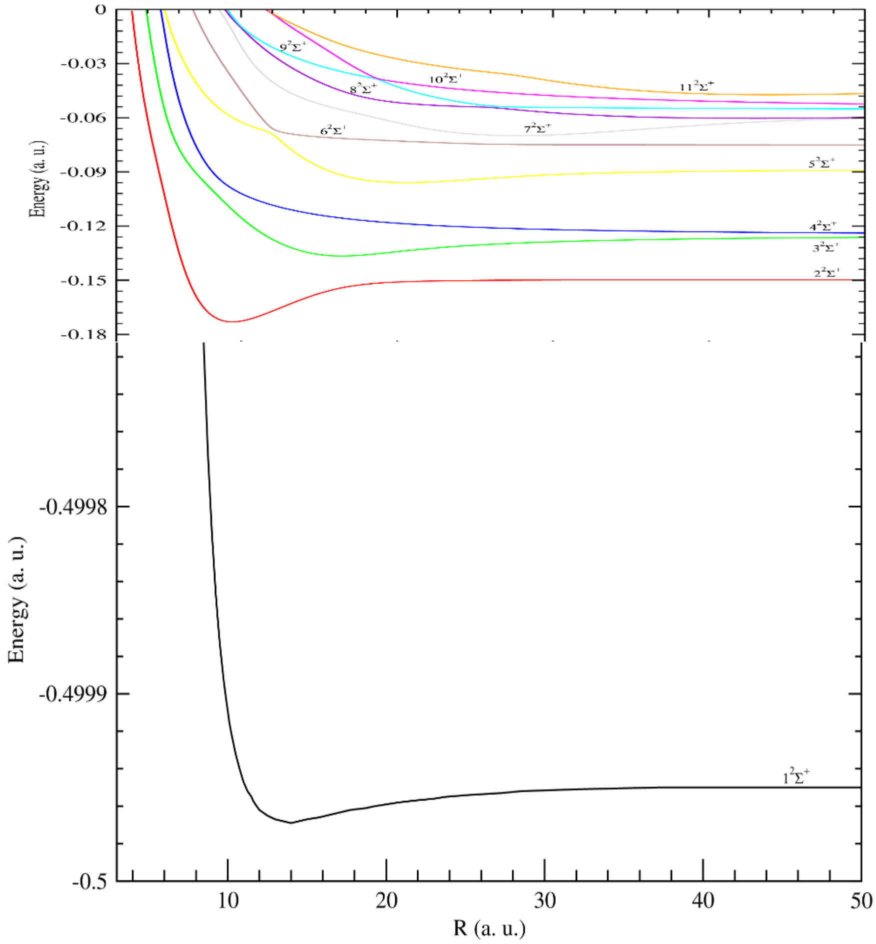

Figure 1: Potential energy curves for the the $1\text{-}11^2\Sigma^+$ states of the FrH^+ alkali hydride cation.

2.2. Transition dipole functions

To further investigate the electronic properties of the FrH^+ alkali hydride cation, we conducted calculations on the dipole functions between states characterized by $^2\Sigma^+$ and $^2\Pi$ symmetries. These dipole functions are crucial for understanding the electric and optical properties of these molecules, including spontaneous and stimulated emissions, radiative charge exchange, and photo-association. Figure 3 illustrates the dipole functions across various electronic states: $1^2\Sigma^+$ to $2^2\Sigma^+$, $1^2\Sigma^+$ to $3^2\Sigma^+$, $1^2\Sigma^+$ to $4^2\Sigma^+$, $1^2\Sigma^+$ to $5^2\Sigma^+$, $1^2\Sigma^+$ to $1^2\Pi$, $1^2\Sigma^+$ to $2^2\Pi$, $2^2\Sigma^+$ to $3^2\Sigma^+$, $2^2\Sigma^+$ to $4^2\Sigma^+$, $2^2\Sigma^+$ to $5^2\Sigma^+$, $2^2\Sigma^+$ to $1^2\Pi$, and $2^2\Sigma^+$ to $2^2\Pi$ of the FrH^+ alkali hydride cation. These dipole functions exhibit comparable patterns to those identified in earlier previous studies [17, 30-31, 33, 35, 37].

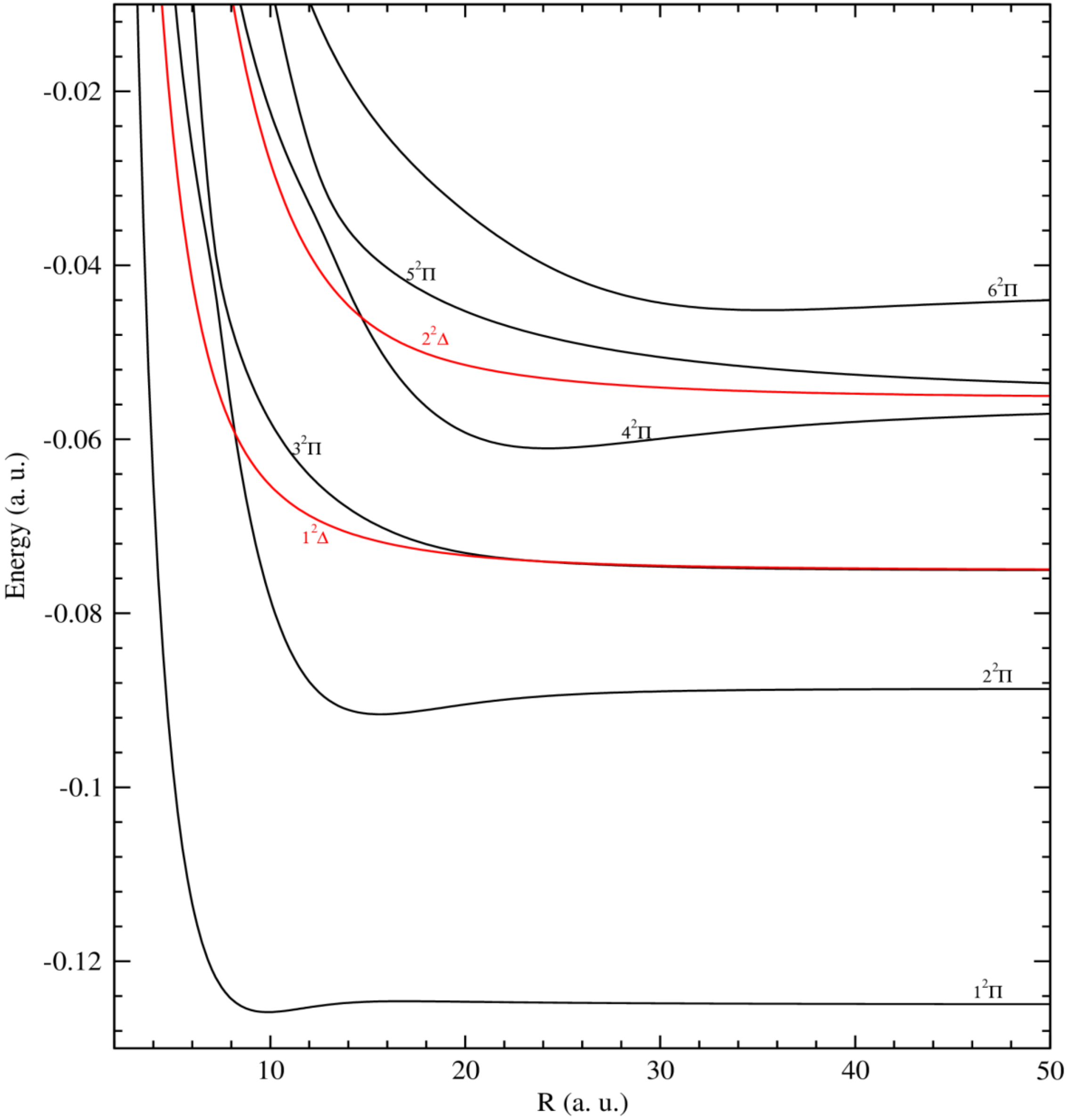

Figure 2: Potential energy curves for the 1-$6^2\Pi$ (black line) and 1-$2^2\Delta$ (red line) states of the FrH^+ alkali hydride cation.

Analysis of the data reveals significant transition dipole functions occurring from $1^2\Sigma^+$ to $2^2\Sigma^+$ and from $2^2\Sigma^+$ to $4^2\Sigma^+$, which exhibit large magnitudes at short and intermediate distances, which gradually decrease toward zero at large distances. These signify forbidden transitions between two different species, H(1*s*) and Fr(7*s*), for the $1^2\Sigma^+$ to $2^2\Sigma^+$ transition, and Fr(7s) and H(2s) for the $2^2\Sigma^+$ to $3^2\Sigma^+$ transition. Additionally, the transitions from $1^2\Sigma^+$ to $3^2\Sigma^+$, $1^2\Sigma^+$ to $4^2\Sigma^+$, and $1^2\Sigma^+$ to $1^2\Pi$ converge to constants of, 0.527, 0.527, and 0.745 a. u., respectively at large distances. These values align with the H(1*s*)-H(2*s*), H(1*s*)-H(2*p*), and H(1*s*)-H(3*p*) atomic transitions. Furthermore, the transitions from $2^2\Sigma^+$ to $5^2\Sigma^+$ and $2^2\Sigma^+$ to $2^2\Pi$ initiate with modest values, then undergo a rapid increase, and eventually converge to the precise value of 2.74 atomic units (a.u.), which corresponds to the Fr(7*s*)-Fr(7*p*) atomic transition. Lastly, it is observed that the remaining transitions have lesser significance, approaching zero in cases where atomic transitions are forbidden, and attaining precise values when the transitions are allowed.

This alignment with the pure atomic transition occurs at larger internuclear distances.

2.3. Vibrational states and radiative lifetimes

We utilized a Fortran program employing the Numerov algorithm to compute the vibrational states of the electronic states of the FrH$^+$ alkali hydride cation. The necessary inputs included the minimum and maximum interatomic distances, atomic mass values, the specific number of data points, and the potential energies corresponding to the considered states. Table 3 presents the calculated vibrational level spacings (E_{v+1}- E_v) for the 1-3$^2\Sigma^+$, 5$^2\Sigma^+$ and 1-2$^2\Pi$ states of the FrH$^+$ alkali hydride cation. These states encompass 3, 49, 35, 34 and 16 confined vibrational levels, respectively.

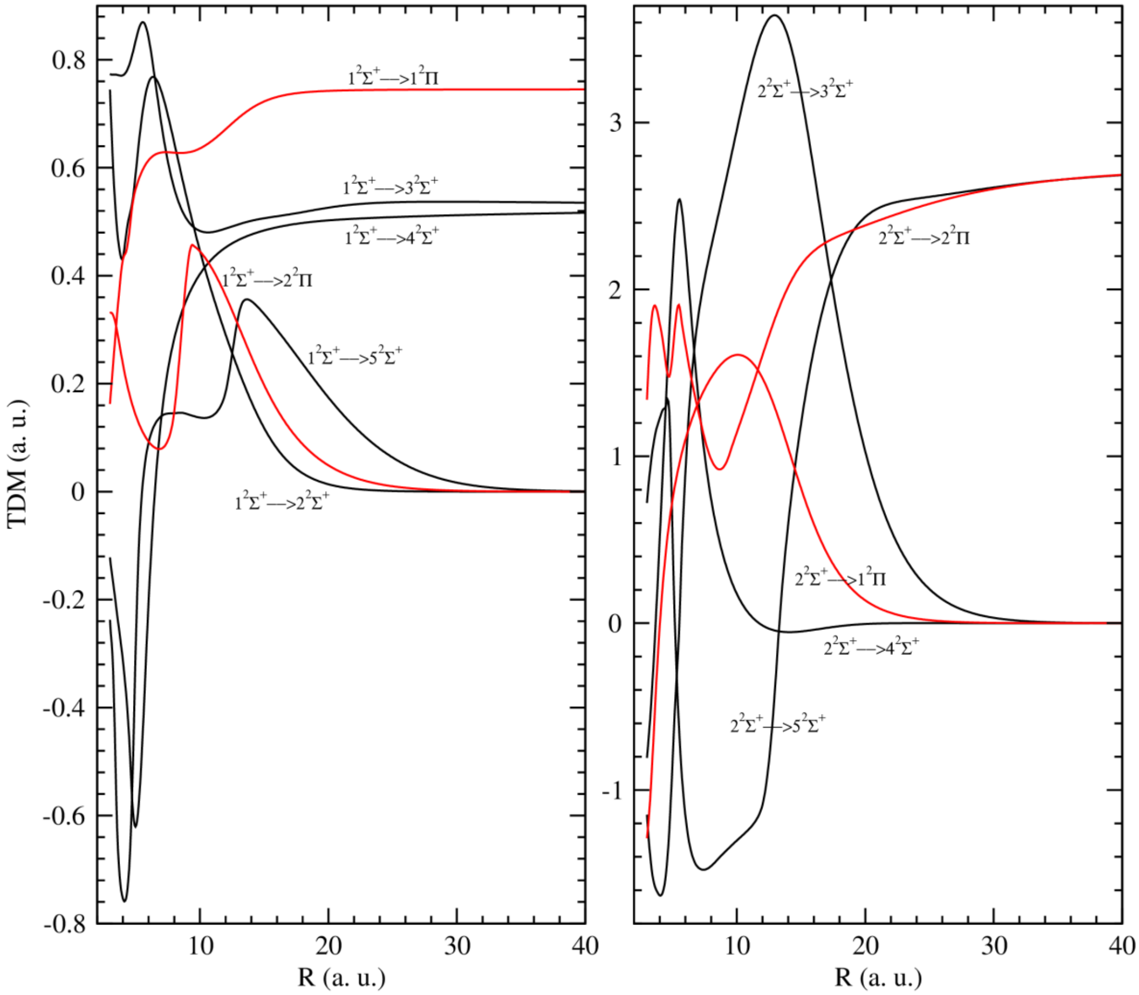

Figure 3: Transition dipole moments from the ground and the first excited states to higher excited states of $^2\Sigma^+$ and $^2\Pi$ symmetries in the FrH$^+$ alkali hydride cation.

Table 3: Vibrational energy spacing (E_v-E_{v+1}) (in cm^{-1}) for the 1-3$^2\Sigma^+$, 3$^2\Sigma^+$ and 1-2$^2\Pi$ states of the FrH$^+$ alkali hydride cation.

v	X$^2\Sigma^+$	2$^2\Sigma^+$	3$^2\Sigma^+$	5$^2\Sigma^+$	1$^2\Pi$	2$^2\Pi$
1	1.114	279.159	127.375	88.800	97.464	79.410
2	0.076	273.394	122.751	86.744	40.286	73.925
3		267.620	118.074	84.659		68.341
4		261.877	113.418	82.406		62.569
5		256.065	108.659	80.062		56.558
6		250.213	103.931	77.575		50.369
7		244.279	99.216	75.001		44.058

8		238.273	94.566	72.259		37.755
9		232.172	89.937	69.489		31.602
10		225.840	85.430	66.500		25.792
11		219.346	81.007	63.412		20.379
12		212.623	76.747	60.240		15.515
13		205.576	72.595	56.936		11.135
14		198.146	68.612	53.597		7.248
15		190.287	64.771	50.175		3.749
16		181.794	61.102	46.770		
17		172.623	57.618	43.346		
18		162.578	54.285	40.010		
19		151.485	51.147	36.712		
20		139.074	48.156	33.606		
21		125.249	45.364	30.609		
22		109.852	42.699	27.761		
23		93.176	40.208	25.104		
24		75.944	37.839	22.660		
25		59.395	35.613	20.347		
26		44.864	33.485	18.191		
27		33.137	31.570	16.227		
28		23.982	29.672	14.418		
29		16.986	27.924	12.756		
30		11.635	26.295	11.237		
31		7.615	24.762	9.828		
32		4.742	23.280	8.594		
33		2.717	21.921	7.466		
34		20.616	6.418			
35		19.431				
36		18.282				
37		17.184				
38		16.174				
39		15.237				
40		14.344				
41		13.502				
42		12.703				
43		11.959				
44		11.265				
45		10.588				
46		9.949				
47		9.413				
48		8.856				

The Golden Rule approximation serves as the basis for the calculation method employed to determine the radiative lifetimes. In the case of a specific vibrational within an excited electronic state (e.g., $2^2\Sigma^+$), two distinct types of transitions are possible: bound-free and bound-bound transitions. The contribution bound-free transitions to the lifetime was precisely calculated by Franck-Condon approximation. Further details about the calculation procedure can be found in Ref. 52. To calculate the radiative lifetimes for a vibrational state of $2^2\Sigma^+$ state, we utilized the potential energies of the $1^2\Sigma^+$ and $2^2\Sigma^+$ states, as well as the dipole functions connecting these two states. Previously, we conducted evaluations of radiative lifetimes for vibrational states of $2^2\Sigma^+$ of NaH^+ [17] and LiY^+ (Y=K, Rb, and Cs) [53] ionic molecules. Table 4 presents the bound-free and bound-bound contributions, as well as the radiative lifetimes, of vibrational states confined within the $2^2\Sigma^+$ state for the FrH^+ system. As far as we are aware, these radiative lifetimes have not been previously determined, either through theoretically calculations or experimental investigations. Hence, our study offers the first evaluation of these lifetimes. The computation of the bound-free term has been performed and integrated into the overall calculation of the radiative lifetime. Notably, the bound-free contributions hold greater significance compared to the bound-bound contributions. It is important to mention that the radiative lifetimes for all vibrational states confined within the $2^2\Sigma^+$ state of FrH^+ are on the order of nanoseconds. These findings align reasonably well with the previous calculations for NaH^+ [17], NaLi [52], and LiY^+ (Y=K, Rb, and Cs) [53].

Table 4: Radiative lifetimes of the vibrational levels of the $^2\Sigma^+$ state of FrH^+

v	Bound-bound ($\times 10^6$ s^{-1})	Bound-free ($\times 10^6$ s^{-1})	Total exact (ns)
0	0.60	871.15	1.15
1	0.25	868.02	1.15
2	0.49	857.06	1.17
3	0.37	841.44	1.19
4	0.50	825.40	1.21
5	0.43	811.62	1.23
6	0.50	797.42	1.25
7	0.44	780.26	1.28
8	0.47	758.87	1.32
9	0.42	740.21	1.35
10	0.41	721.06	1.39
11	0.36	698.49	1.43
12	0.35	675.88	1.48
13	0.30	653.77	1.53
14	0.27	626.85	1.59
15	0.22	600.43	1.66
16	0.19	572.94	1.74
17	0.15	540.92	1.85
18	0.13	505.08	1.98
19	0.09	465.63	2.15
20	0.07	419.23	2.38

[3] Conclusions

In this study, our primary objective was to investigate the electronic properties of the FrH^+ alkali hydride cation dissociating up to Fr(9*s*) + H^+ and Fr^+ + H(3*d*). Employing the pseudopotential method, we successfully computed potential energies and spectroscopic parameters for a total of 18 electronic states characterized by of $^2\Sigma^+$, $^2\Pi$, and $^2\Delta$ symmetries. Furthermore, we identified and comprehensively interpreted the avoided crossings that are characteristic of the excited electronic states possessing $^2\Sigma^+$ and $^2\Pi$ symmetries. Additionally, we calculated the transition dipole functions between electronic states characterized by $^2\Sigma^+$ and $^2\Pi$ symmetries. Moreover, we utilized the precise potential energies of the $X^2\Sigma^+$ and $2^2\Sigma^+$ states, along with the transition dipole functions between these states, to determine the radiative lifetimes of the vibrational states trapped within the $2^2\Sigma^+$ state. Given the absence of experimental investigations or theoretical calculations specifically on FrH^+ specie, we conducted a comparative analysis with findings obtained from analogous systems.

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