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DISSOCIATION ENERGIES, FRANCK-CONDON FACTORS AND R-CENTROIDS OF THE SULPHIDES OF METALS (LI AND NI)

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ABSTRACT

The experimental potential energy curves for the different electronic states of astrophysically important LiS^+ and NiS molecules are constructed by using Rydberg-Klein-Rees method as modified by Vanderslice et al. The ground state dissociation energies are determined by curve fitting techniques using the five parameters Hulburt-Hirschfelder (H-H) function. The estimated dissociation energies are 0.81 ± 0.02 and 3.56 ± 0.08 eV for LiS^+ , and NiS respectively. These values are in good agreement with the values reported in the earlier literature. The r-centroids and Franck-Condon factors (FC factors) for the bands of $3\Pi-X^3\Sigma^-$ system of LiS^+ and $A^3\Pi-X^3\Sigma^-$ system for NiS , molecules have been calculated. The Franck-Condon factors are evaluated by the approximated analytical methods of Jarmain and Fraser. The absence of the bands of these systems is explained.

Keywords: Diatomic molecules; Dissociation energies; Franck-Condon factors; r-centroids

I. INTRODUCTION

There has been considerable interest in spectroscopic studies of transition metal containing species because of their importance in chemistry, astrophysics, surface science and ab initio calculations. These compounds are widely used as catalysts in various chemical processes.

Theoretical calculations on these molecules often fail to predict the correct spectroscopic properties and energy ordering of electronic states. The spectroscopic studies of these molecules, therefore, have become important to gain insight into chemical bonding in simple

metal systems. Ram et al. [1] have mentioned that NiS might also be present in S-type stars.

There are several theoretical studies on the spectroscopic properties of low-lying electronic states of NiS . An experimental observation of NiS has been reported by Zheng et al. [2] in the 495-555nm regions. Ram et al. [1] have reported on the observation of NiS bands in the near IR region ($2500-7500 \text{ cm}^{-1}$). Molecular species containing sulphur atom are of astrophysical importance. Some of them have been definitely identified. Theoretical investigations of the SH^+ and LiS^+ cations have been pursued by Khadri et al. [3]. In view of their astrophysical / scientific importance, it is proposed to construct potential curves and evaluate dissociation energies. As no attempt has been made so far to evaluate dissociation energies, Franck-Condon factors (FC factors)

and r -centroids using spectroscopic data for LiS^+ and NiS molecules, the present authors have taken up this investigation.

II. THEORY & COMPUTATIONAL PROCEDURE

Potential energy curves

Experimental observed vibrational levels are used to construct the potential energy curve. The molecular constants required for the present study have been taken from the literature [1-4] and are listed in Table I. Many authors employed RKR method and constructed the potential energy curves [5-16]. The RKR [17-21] method is an improved form of RKR method, which makes use of Wentzel-Kramers-Brillouin (WKB) approximation from which we obtain reliable potential energy curves with the observed vibrational and rotational constants. The potential energy curves are constructed using the method of RKR [17-21] utilizing the molecular constants (listed in Table I) and the results are presented in Table II. The details of the said method were reported in literature, as such only the results of the present work are given Table I.

Dissociation energy

The RKR turning points are inserted into the five parameter Hulbert-Hirschfelder's [22-24] function and the potential energies $U(r)$ are calculated by varying the dissociation energy D_e values. An average percentage deviation is determined between the calculated $U(r)$ and the experimental $G(v)$ values. An accurate estimation of the dissociation energy (D_0) requires an empirical potential function, which provides the best reproduction of the experimental energy values. A critical evaluation of the importance of these functions was given by Steele et al. [24] and they have shown that the potential function of Hulbert-Hirschfelder (H-H) [22-24] fits well with the RKR curves of a large number of diatomic molecules. In the present investigation, it is

observed that the H-H function [22, 23] functions fits best and reproduces the experimental energy values (Table III). Different D_e values are used in the H-H function and the D_e value, for which the best fit of the energy values $U(r)$ is observed, which is taken as the dissociation energy (D_0) of the molecule.

r-Centroids and Franck-Condon factors

The Franck-Condon factors depend mainly on the shape and relative separation in the internuclear distance between the upper and lower potentials involved. These factors control the form of the wave function $\psi_{v'}$, $\psi_{v''}$ and their overlap. In order to calculate Franck-Condon factors, one has to evaluate the integral $\int \psi_{v'} \psi_{v''} dr$. In the absence of exact expression for $\psi_{v'}$, one may use the eigen functions derived from same approximate potential functions. Therefore, the methods for calculating Franck-Condon factors depend on the choice of approximate eigen functions $\psi_{v'}$ obtained by solving Schroedinger equations with approximate potential functions.

Fraser and Jarman [25] introduced the method of average ' α ' Morse constant, which allows analytic integration of the integral

$$q_{v',v''} = \int_0^{\infty} \psi_{v'} r^n \psi_{v''} dr \quad (1)$$

where $n=0,1,2$. The above integral becomes Franck-Condon factor when $n=0$. This method successfully replaces cumbersome numerical integration for many band systems. The details of the method are described elsewhere [9, 10, 15, 25, 26]. The method yields accurate Franck-Condon factor especially when vibrational quantum numbers are low. The r -Centroids $r_{v',v''}$ represent the characteristic internuclear separation of a $v' \rightarrow v''$ transition in a diatomic molecule band system and are defined by

$$r_{v',v''} = \frac{\int \psi_{v'} \cdot r \psi_{v''} dr}{\int \psi_{v'} \psi_{v''} dr} \quad (2)$$

By use of the quadratic equation method of Nicholls and Jarman [26] and Fraser and Jarman [25, 26], r-Centroids are estimated for different bands.

III. RESULTS AND DISCUSSION

The inherent error in the H-H function given by Steele et al [24] is 2%. The error involved in the evaluation of D_e is minimum average percentage deviation plus the inherent error in the potential function. The D_0 values are found to be 0.79 ± 0.02 and 3.52 ± 0.08 eV LiS^+ and NiS respectively. Here $D_0 = D_e - G(0)$. The turning points obtained from RKR [17-21] method are inserted in H-H [22-24,27] function and evaluated $U(r)$ values. The relevant $U(r)$ values for the selected D_e values are given in Table III. The estimated D_0 value for LiS^+ (0.79 ± 0.02 eV) is in good agreement with the value (0.83 eV) recommended by Boldrev et al. [28]. The dissociation energy for the ground state of NiS (3.52 ± 0.08 eV) is in close agreement with the value 3.53 eV quoted by Huber and Herzberg [29] and also the value (3.58 eV) listed by Lide [30].

The vibrational sum rule is satisfied for v' and v'' progressions in the case of ${}^1\Pi-X^3\Sigma^-$ transition of LiS^+ . (1,1),(3,2) and (5,0) bands are found to be small in magnitude, which indicates that the bands are not experimentally be observed. From the magnitudes of the F-C factors of the ${}^1\Pi-X^3\Sigma^-$ system of LiS^+ , one may conclude that in the v' progression with $v'=0$ with $v'' \geq 5$ and v'' progression with $v'=0$ $v'' \geq 5$ would not be observed. As seen from Table IV, for ${}^1\Pi-X^3\Sigma^-$ the order of magnitude of the F-C factors for the bands (1,3),(3,1) and also (0,2),(2,0) are equal which suggest that bands are of nearly equal intensity.

Keen observation of the Table IV reveals that in the case of $2^1\Sigma^- - X^3\Sigma^-$ system of LiS^+ that the vibrational sum rule is not satisfied for v' and

v'' progressions as far as the bands are observed. Therefore, it is suggested that if more experimental work is done on the above system, it would definitely yields more new bands. Among all bands observed in this system (5, 0) band is found to be the strongest. The magnitude of the F-C factors in the case of A-X and ${}^1\Pi-X$ systems of NiS beyond (0,3) and (3,0) are very small in comparison with the other values and hence they may not be observed experimentally [25].

The F-C factor for (0,0) band is strongest in A-X system of NiS among all the bands observed. (0,1),(1,0) and also (1,1),(2,1) bands of F-C factor values in A-X system of NiS are appears to have equal intensity.

To understand the physical conditions of the emitter from the relative intensities of the bands of a molecule. One must have a theoretical knowledge of the corresponding r-Centroids and vibrational transition probabilities for the respective band heads in a band system. In the present study, the r-Centroids for the ${}^3\Pi - X^3\Sigma^-$ and $2^1\Sigma^- - X^3\Sigma^-$ systems of LiS^+ are calculated by the quadratic equation method of Nicholls and Jarman [26] are presented in Table IV. It is of interest to note that $\bar{r}_{0,0}$ is greater than $(r_{e1}+r_{e2})/2$ in the case of $2^1\Sigma^- - X^3\Sigma^-$ which shows that the potential functions are not very anharmonic. The $\Delta \bar{r}$ values for the band system A-X of LiS^+ is greater than 0.01 \AA^0 , which indicates that the potentials are wide. The sequence difference $\Delta \bar{r} = \bar{r}_{v'+1, v''+1} - \bar{r}_{v', v''}$ has been found to be constant in accordance with the observations of Nicholls and Jarman [26]. Since $r_{e1} > r_{e2}$ in all cases of LiS^+ band systems. r-Centroids estimates are expected to increase with wavelength, which is the trend observed in a red-degraded band system.

The values of r-Centroids of NiS molecule are estimated and presented in the Table IV. The

value of $\bar{r}_{v',v''}$ (r-Centroids) was found to increase with the increase of the $\lambda_{v',v''}$ value as has been observed by Nicholls and Jarman [26]. The internuclear distance of the upper state is greater than the ground state ($r_{e1} > r_{e2}$) in all cases, r-Centroids estimates are expected to increase with wave lengths which is the trend observed in red-degraded band systems of NiS molecule. The sequence difference $\Delta \bar{r} = \bar{r}_{v'+1, v''+1} - \bar{r}_{v', v''}$ for this system is found to be a constant ($0.007A^0$). It is seen that $\Delta \bar{r}$ is less than $0.01A^0$ for this system suggesting that the potentials are not wide. In the case of $A^3 \Pi_1 - X^3 \Sigma^-$ and $[5.8]^1\Pi - X^3 \Sigma^-$ system of NiS, $r_{0,0}$ is found to be slightly greater than $(r_{e1} + r_{e2})/2$ indicating there by that the potentials are not very anharmonic [9,10]

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Table I: Molecular constants for different electronic states of LiS⁺ and NiS

Molecule	μ	State	T_e (cm ⁻¹)	ω_e (cm ⁻¹)	$\omega_e x_e$ (cm ⁻¹)	B_e (cm ⁻¹)	α_e (cm ⁻¹)	r_e (Å)	Reference
LiS ⁺	5.7059	X ³ Σ ⁻	0	376.1	4.50	0.562	0.011	2.43	Khadri et al. ⁸
		3Π	5597.5	226.4	9.63	0.496	0.021	2.59	
		1Δ	8904.5	385.5	4.62	0.566	0.008	2.42	
		1 ¹ Σ ⁺	14171.43	322.3	16.19	0.546	0.015	2.47	
		1Π	14518.26	210.9	4.17	0.480	0.023	2.63	
		2 ¹ Σ	27479.8	156.3	3.98	0.385	0.007	2.94	
NiS	20.602	X ³ Σ ⁻	0	512.68	3.61	0.212	0.00118	1.962	Ram et al. ¹
		A ³ Π _i	3864.56	466.69	1.1515	0.202	0.000728	2.012	
		[5.8] ¹ π	5837.58	427.66	3.329	0.1956	0.001194	2.045	

Table II: The turning points of the potential energy curves for the different electronic states of LiS⁺ and NiS, molecules.

LiS ⁺ molecule															
v	X ³ Σ ⁻ State, T _e = 0			3Π state, T _e = 5597.59 cm ⁻¹			1Δ state, T _e = 8904.5 cm ⁻¹			1 ¹ Σ ⁺ state, T _e = 14171.43 cm ⁻¹			2 ¹ Σ State, T _e = 27479.8cm ⁻¹		
	U (cm ⁻¹)	r _{max} (Å)	r _{min} (Å)	U (cm ⁻¹)	r _{max} (Å)	r _{min} (Å)	U (cm ⁻¹)	r _{max} (Å)	r _{min} (Å)	U (cm ⁻¹)	r _{max} (Å)	r _{min} (Å)	U (cm ⁻¹)	r _{max} (Å)	r _{min} (Å)
0	186.92	2.575	2.308	110.94	2.788	2.440	191.59	2.561	2.298	157.10	2.633	2.339	77.15	3.165	2.747
1	554.02	2.699	2.232	318.38	2.972	2.352	567.85	2.679	2.218	447.02	2.785	2.253	225.49	3.359	2.620
2	912.12	2.794	2.185	506.56	3.143	2.298	933.87	2.783	2.167	704.56	2.917	2.193	365.87	3.513	2.537
3	1261.22	2.879	2.150	675.48	3.303	2.257	1292.65	2.847	2.127	929.72	3.048	2.141	498.29	3.654	2.470
4	1601.32	2.957	2.122	825.14	3.469	2.221	1641.19	2.920	2.095	1122.50	3.188	2.090	622.75	3.790	2.410
5	1932.42	3.033	2.099	955.54	3.648	2.187	1980.49	2.989	2.669	1282.90	3.344	2.035	739.25	3.925	2.360
6	2254.52	3.106	2.079	1066.68	3.847	2.151	2310	3.056	2.042	1410.92	3.532	1.972	847.79	4.063	2.3119

NiS molecule									
v	$X^3 \Sigma^-, T_e = 0$			$A^3 \Pi_i, T_e = 3864.56 \text{ cm}^{-1}$			$[5.8]^1 \Pi, T_e = 5837 \text{ cm}^{-1}$		
	U (cm ⁻¹)	r _{max} (Å)	r _{min} (Å)	U (cm ⁻¹)	r _{max} (Å)	r _{min} (Å)	U (cm ⁻¹)	r _{max} (Å)	r _{min} (Å)
0	255.43	2.021	1.908	233.06	2.073	1.955	213.00	2.110	1.985
1	760.89	2.069	1.871	697.45	2.121	1.915	634.01	2.162	1.945
2	1259.13	2.104	1.847	1159.54	2.156	1.889	1048.36	2.200	1.919
3	1750.15	2.133	1.828	1619.33	2.184	1.869	1456.06	2.234	1.899
4	2233.95	2.160	1.812	2076.81	2.210	1.852	1857.09	2.264	1.881
5	27110.53	2.186	1.798	2532.00	2.23	1.837	2251.47	2.292	1.866
6	3179.89	2.209	1.786	2984.87	2.256	1.823	2639.19	2.318	1.852

Table III: Energy values using Hulbert – Hirschfelder (H-H) function for the $X^3 \Sigma^-$ electronic state of LiS^+ molecule

r (A°)	U (cm ⁻¹)	Calculated U(r) in cm ⁻¹		
		D _e =6344 cm ⁻¹	D _e =6544 cm ⁻¹	D _e =6744 cm ⁻¹
2.575	186.9	182.01	187.74	193.48
2.698	554.0	539.57	556.58	573.59
2.794	912.1	888.24	916.24	944.24
2.878	1261.2	1227.61	1266.31	1305.01
2.957	1601.3	1557.25	1606.34	1655.44
3.032	1932.4	1876.75	1935.91	1995.08
3.105	2254.0	2185.66	2254.57	2323.47
2.308	186.9	181.95	187.22	193.48
2.231	554.0	538.59	555.57	572.55
2.184	912.1	884.90	912.80	940.69
2.149	1261.2	1220.27	1258.74	1297.21
2.121	1601.3	1544.20	1592.88	1641.56
2.098	1932.4	1856.29	1914.81	1973.33
2.078	2254.0	2156.25	2224.23	2292.21
Average percentage deviation		3.05	0.43	3.06

Energy values using Hulbert – Hirschfelder (H-H) function for the $X^3 \Sigma^-$ electronic state of NiS molecule

r (A°)	U (cm ⁻¹)	Calculated U(r) in cm ⁻¹		
		D _e =25522 cm ⁻¹	D _e =28722 cm ⁻¹	D _e =28922 cm ⁻¹
2.021	255.43	253.33	255.11	256.88
2.069	760.89	754.21	759.50	764.79
2.104	1259.13	1248.59	1257.34	1266.10
2.133	1750.15	1732.16	1744.31	1756.45
2.160	2233.95	2209.12	2224.61	2240.10
2.186	2710.53	2678.14	2696.92	2715.70
2.209	3179.89	3139.27	3161.28	3183.29
1.908	255.43	255.11	255.20	256.98
1.871	760.89	759.50	760.82	766.12
1.847	1259.13	1257.34	1260.62	1269.40
1.828	1750.15	1744.31	1755.04	1767.26
1.812	2233.95	2224.61	2244.56	2260.20
1.798	2710.53	2696.92	2729.57	2748.57
1.786	3179.89	3161.28	3210.39	3232.75
Average percentage deviation		0.68	0.35	0.71

Table IV: Franck-Condon factors and r-centroids for the $^3\Pi - X^3\Sigma^-$ transition of LiS^+ molecule

(v',v'')	FC factor	r-centroids
(0,0)	0.495	2.528
(0,1)	0.334	2.678
(0,2)	0.132	2.813
(0,3)	0.033	2.948
(0,4)	0.005	3.088
(1,0)	0.328	2.422
(1,1)	0.029	2.592
(1,2)	0.253	2.731
(1,3)	0.247	2.862
(1,4)	0.109	2.994
(1,5)	0.027	3.132

Franck-Condon factors and r-centroids for the $2^1\Sigma^- - X^3\Sigma^-$ transition of LiS^+ molecule

(v',v'')	FC factor	r-centroids
(0,0)	0.004	2.696
(0,1)	0.024	2.739
(0,2)	0.070	2.780
(0,3)	0.132	2.821
(0,4)	0.183	2.861
(0,5)	0.197	2.902
(1,0)	0.016	2.679
(1,1)	0.067	2.722
(1,2)	0.123	2.763
(1,3)	0.123	2.804
(1,4)	0.060	2.844
(1,5)	0.004	2.844
(2,0)	0.035	2.662
(2,1)	0.099	2.706
(2,2)	0.103	2.747
(3,0)	0.055	2.646
(3,1)	0.102	2.690
(3,2)	0.048	2.732
(4,0)	0.012	2.631
(4,1)	0.082	2.676
(5,0)	0.819	2.616
(5,1)	0.053	2.662
(5,2)	---	2.705
(5,3)	0.068	2.745

Franck-Condon factors and r-centroids for the $A^3\Pi_i - X^3\Sigma^-$ transition of NiS molecule

(v',v'')	FC factor	r-centroids
(0,0)	0.710	1.990
(0,1)	0.249	2.063
(0,2)	0.036	2.142
(0,3)	0.003	2.230
(0,4)	--	2.328
(0,5)	0.002	2.441
(1,0)	0.230	1.929
(1,1)	0.306	1.996

(1,2)	0.357	2.069
(1,4)	0.002	2.236
(1,5)	0.095	2.334
(2,0)	0.046	1.872
(2,1)	0.310	1.935
(2,2)	0.103	2.003
(3,0)	0.007	1.819
(3,1)	0.108	1.879
(3,2)	0.579	1.942
(4,0)	0.009	1.377
(4,1)	0.032	1.825

Franck-Condon factors and r-centroids for the $[5.8]^1\Pi - X^3\Sigma^-$ transition of NiS molecule

(v',v'')	FC factor	r-centroids
(0,0)	0.409	2.006
(0,1)	0.389	2.053
(0,2)	0.158	2.005
(0,3)	0.036	2.161
(0,4)	0.005	2.223
(0,5)	0.001	2.292
(1,0)	0.336	2.969
(1,1)	0.004	2.013
(1,2)	0.265	2.061
(1,3)	0.268	2.113
(1,4)	0.093	2.169
(1,5)	--	2.231
(2,0)	0.163	1.935
(2,1)	0.176	1.977
(2,2)	0.065	2.021
(3,0)	0.062	1.902
(3,1)	0.206	1.943
(3,2)	0.027	1.985
(3,3)	0.013	2.029
(4,0)	0.020	1.873
(4,1)	0.135	1.911
(4,2)	0.530	1.951