

High resolution emission spectroscopy of the $E^2\Pi-X^2\Sigma^+$ transition of SrH and SrD

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ABSTRACT

Emission spectra of SrH and SrD have been studied at high resolution using a Fourier transform spectrometer. The molecules have been produced in a high temperature furnace from the reaction of strontium metal vapor with H_2/D_2 in the presence of a slow flow of Ar gas. The spectra observed in the 18000–19500 cm^{-1} region consist of the 0–0 and 1–1 bands of the $E^2\Pi-X^2\Sigma^+$ transition of the two isotopologues. A rotational analysis of these bands has been obtained by combining the present measurements with previously available pure rotation and vibration–rotation measurements for the ground state, and improved spectroscopic constants have been obtained for the $E^2\Pi$ state. The present analysis provides spectroscopic constants for the $E^2\Pi$ state as $\Delta G(\frac{1}{2}) = 1166.1011(15) cm^{-1}$, $B_e = 3.805503(32) cm^{-1}$, $\alpha_e = 0.098880(47) cm^{-1}$, $r_e = 2.1083727(89) \text{ \AA}$ for SrH, and $\Delta G(\frac{1}{2}) = 839.1283(23) cm^{-1}$, $B_e = 1.918564(15) cm^{-1}$, $\alpha_e = 0.034719(23) cm^{-1}$, $r_e = 2.1121943(83) \text{ \AA}$ for SrD.

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1. Introduction

Emission spectra of SrH have been known for several decades [1]. The first work on SrH was carried out by Watson and Fredrickson [1] by observation of two red systems, $^2\Pi-^2\Sigma^+$, and $^2\Sigma^+-^2\Sigma^+$ and preliminary effective rotational constants for the three low-lying electronic states were provided. The SrH bands were observed using a metallic Sr arc which was run in an atmosphere of hydrogen gas. The upper states of these transitions were later labeled as $A^2\Pi$ and $B^2\Sigma^+$ [2] by analogy with the corresponding states of CaH. There are other early reports published on the observation of several higher-lying electronic states, $C^2\Sigma^+$ [2,4,5], $D^2\Sigma^+$ [2,3,5] and $E^2\Pi$ [2]. Watson et al. [3] have reported the observation of the $B^2\Sigma^+$ and $C^2\Sigma^+$ states of SrD. The ultraviolet transitions of SrH and SrD were studied by Khan and coworkers [6–14].

As in the case of other alkaline earth metal hydrides, the characterization of low-lying states of SrH and SrD has been challenging because of strong interactions between the states, and the $A^2\Pi$ and $B^2\Sigma^+$ states have been the focus of several subsequent experimental [15,16] and theoretical [17–20] studies. The rotational structure of some $A^2\Pi-X^2\Sigma^+$ bands of SrD was reinvestigated by Appelblad and Barrow [15] and improved spectroscopic constants were reported. In another study Appelblad et al. [16] obtained a rotational analysis of several bands of the $A^2\Pi-X^2\Sigma^+$ and

$B^2\Sigma^+-X^2\Sigma^+$ transitions of SrH using spectra observed with a high resolution Fourier transform spectrometer using a King furnace. The $A^2\Pi$ and $B^2\Sigma^+$ interact with each other as well as possibly with an unobserved $^2\Delta$ state. In a recent theoretical calculation on the low-lying states of SrH, Leininger and Jeung [20] have computed the potential energy curves for the $X^2\Sigma^+$, $A^2\Pi$, $B^2\Sigma^+$ (with double minima) and $A^2\Delta$ states.

Among the alkaline earth metal hydrides MgH [21–24] and CaH [25–31] have been identified in the spectra of stars, sunspots and brown dwarfs. There is a possibility that SrH molecule may also be found. Because of possible astrophysical interest, Ramchandran et al. [32] calculated the Franck–Condon factors for a few transitions of SrH and SrD.

Berg et al. [33] applied the method of time-resolved laser spectroscopy to measure the lifetime of the $A^2\Pi$ state of SrH. A lifetime of 33.8 ± 1.9 ns was obtained for the $v=0$ vibrational level of the $A^2\Pi$ state. In a more recent study, Pauchard et al. [34] have measured lifetimes of 33.2 ± 3.2 ns and 33.7 ± 5.3 ns for the $v=0$ and 1 vibrational levels of the $A^2\Pi$ state and 48.4 ± 2.0 ns, and 50.5 ± 3.2 ns for the $v=0$ and 1 vibrational levels of the $B^2\Sigma^+$ state. Knight and Weltner [35] have measured the ground state hyperfine structure for SrH trapped in an Ar matrix while Steimle et al. [36] have measured the excited state hyperfine interaction in the $A^2\Pi_{1/2}$ state of SrH in the gas phase.

The vibration–rotation transitions in the $X^2\Sigma^+$ ground electronic state of SrH and SrD have been measured in the last decade using both diode laser and Fourier transform spectroscopy. The vibration–rotation spectra of the $1 \rightarrow 0$, $2 \rightarrow 1$ and $3 \rightarrow 2$ bands of SrH

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were measured by Magg et al. [37] while the same bands of SrD were measured by Birk et al. [38] using diode laser spectroscopy. Frum et al. [39] measured the $\nu = 1 \rightarrow 0$ vibration–rotation band of SrH in emission using a Fourier transform spectrometer. They have also measured the pure rotational spectra of SrH and SrD in the ground state using a millimeter-wave spectrometer [39]. In a more recent study, the vibration–rotation spectra of SrH and CaH were measured by Shayesteh et al. [40] for the $1 \rightarrow 0$ to $4 \rightarrow 3$ bands using a Fourier transform spectrometer.

Although some high resolution studies are available for the low-lying electronic states of SrH and SrD, most of the higher-lying electronic states of SrH are not well characterized. The $E^2\Pi$ state of SrH is known through the observation of the $E^2\Pi-X^2\Sigma^+$ transition by Fredrickson et al. [2] along with the $C^2\Sigma^+-X^2\Sigma^+$ and $D^2\Sigma^+-X^2\Sigma^+$ transitions. Preliminary spectroscopic constants for the $E^2\Pi$ state were reported from a rotational analysis of the 0–0 band. The observation of the corresponding transition for SrD has been lacking. In this paper, we report on the observation of high resolution spectra of the $E^2\Pi-X^2\Sigma^+$ transition of SrH and SrD using a Fourier transform spectrometer. We have obtained a rotational analysis of the 0–0 and 1–1 bands of the two isotopologues and obtained improved spectroscopic constants for the $E^2\Pi$ state.

2. Experimental

Molecules were produced in a high temperature source which is a combination of a high temperature furnace and an electrical discharge source. The electrical discharge was generated inside the furnace which was fitted with two tubular electrodes inserted in each end of the alumina tube. Strontium metal was placed in the middle of the alumina tube which was heated to a temperature of approximately 650 °C while maintaining a slow flow of Ar (20 Torr) and H_2/D_2 (1 Torr). When the metal started vaporizing, a continuous discharge was generated in the alumina tube by applying a 3 kV/330 mA DC discharge across the two electrodes. The two ends of the tube were sealed by quartz windows which were cooled by circulating cold water through copper cooling coils to avoid deposits on the windows. A quartz lens was used to focus the emitted light from the source onto the entrance aperture of the spectrometer. The spectra were recorded using a Bruker IFS 120 HR Fourier transform spectrometer. The spectrometer was equipped with visible quartz beam splitter and a photomultiplier detector. A total of five scans were coadded in both cases at a resolution of 0.06 cm^{-1} to record the spectra of SrH and SrD.

The spectral line positions were measured using a data reduction program called WSPECTRA written by M. Carleer of the Université Libre de Bruxelles. The peak positions were determined by fitting a Voigt line shape function to each spectral feature. The published measurements of Ar atomic lines [41], which were also present in the spectra, were used for calibration of the SrH and SrD molecular lines. The molecular lines appear with approximate widths of $\sim 0.07\text{ cm}^{-1}$ and a maximum signal-to-noise ratio of about 45:1 for the strongest Q lines of the 0–0 bands. The precision of measurements is expected to be of the order of $\pm 0.005\text{ cm}^{-1}$ or better for strong and unblended molecular lines.

3. Results and discussion

The $E^2\Pi-X^2\Sigma^+$ transition of SrH and SrD is located in the $18000\text{--}19500\text{ cm}^{-1}$ region and the spectra of the two isotopologues are very similar in appearance. The observed spectra consist of only $\Delta\nu = 0$ sequence bands. A compressed portion of the spectrum of the $\Delta\nu = 0$ sequence of SrD is presented in Fig. 1, in which the bands belonging to the $^2\Pi_{1/2}-^2\Sigma^+$ and $^2\Pi_{3/2}-^2\Sigma^+$ subbands have been marked. The $\Delta\nu = 0$ sequence consists of only the 0–0 and 1–1

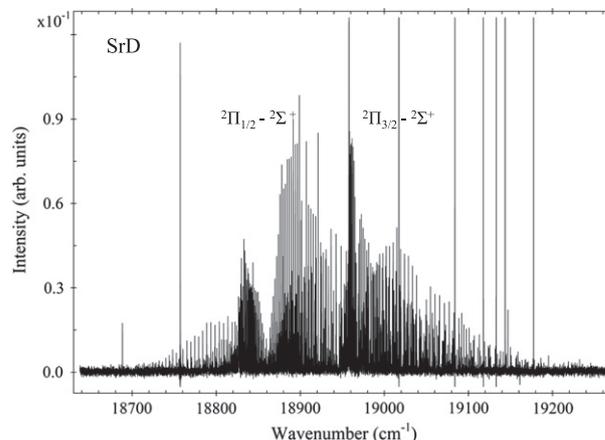


Fig. 1. A compressed view of the $\Delta\nu = 0$ sequence, marking the two subbands of the $E^2\Pi-X^2\Sigma^+$ transition of SrD.

bands with the 1–1 band being about 20% of the intensity of the 0–0 band. The rotational structure of both these bands has been measured and rotationally analyzed.

In a $^2\Pi-^2\Sigma^+$ transition, six main branches, P_1 , Q_1 , R_1 , P_2 , Q_2 , R_2 and six satellite branches R_{12} , Q_{12} , P_{12} , R_{21} , Q_{21} , P_{21} , R_{21} , are expected to be present for a $^2\Pi$ state that has Hund's case (a) coupling. Most of these branches have been identified in the 0–0 band of SrH and SrD. This observation is in contrast to the $E^2\Pi-X^2\Sigma^+$ transition of CaH and CaD where only the six main branches were observed in the spectra [42]. The reason is that the $E^2\Pi$ state of CaH is closer to Hund's case (b) coupling with $A \approx 15\text{ cm}^{-1}$, whereas for SrH this state is closer to a case (a) state with $A \approx 112\text{ cm}^{-1}$. In the 0–0 band of SrH all of the allowed branches have been identified but in the 1–1 band some of the branches could not be identified because of their weaker intensity and overlapping from other stronger molecular lines present in the same region. Some of the satellite branches of SrD were also not identified because of their very weak intensity. The precision of our Fourier transform measurements is greater than those of Fredrickson et al. [2]; therefore considerable improvement is expected in the derived spectroscopic constants.

A part of the spectrum of SrH showing some rotational lines of the 0–0 band is presented in Fig. 2. We have identified rotational lines up to $J = 29.5$ and 24.5 in the strongest branches of the 0–0 and 1–1 bands of SrH. We have observed perturbations in the $^2\Pi_{1/2}$ spin component at about $J = 10.5$ and 25.5 , and in the $^2\Pi_{3/2}$

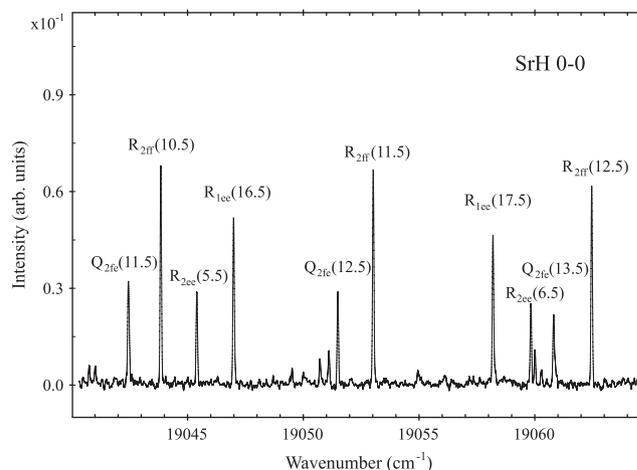


Fig. 2. An expanded portion of SrH spectrum with some rotational lines of the 0–0 band marked.

spin component at $J = 28.5$ levels of the $v = 0$ vibrational level of SrH. For the $v = 1$ vibrational level of SrH, the $^2\Pi_{1/2}$ spin component is perturbed near $J = 16.5$ but the $^2\Pi_{3/2}$ spin component is not perturbed.

In the case of SrD, we have identified rotational lines up to $J = 41.5$ and $J = 34.5$ in the strong branches of the 0–0 and 1–1 bands. The excited state vibrational levels of SrD are also affected by perturbations as in the case of SrH. The $v = 0$ level is perturbed near $J = 18.5$ of the $^2\Pi_{1/2}$ spin component and near $J = 19.5$ of the $^2\Pi_{3/2}$ spin component. For the $v = 1$ vibrational level of SrD, the $^2\Pi_{1/2}$ spin component is not perturbed whereas for the $^2\Pi_{3/2}$ spin component, the rotational lines with $J < 10.5$ and $J > 29.5$ have to be deweighted for both parity levels. A number of rotational lines in the perturbed regions could not be identified with certainty because of the dense rotational structure in the vicinity. The lines affected by perturbations were given lower weights or were deweighted completely. A portion of the spectrum of SrD with some rotational lines of the P_{1e} and Q_{1f} branches in the 0–0 and 1–1 bands marked is presented in Fig. 3.

In order to determine the rotational constants, the observed rotational line positions of two bands were fitted with the effective N^2 Hamiltonian of Brown et al. [43]. The $^2\Pi$ and $^2\Sigma^+$ matrix elements of this Hamiltonian are provided by Douay et al. [44] and Amiot et al. [45], respectively. The lines in each vibrational band were initially fitted separately using a nonlinear least-squares procedure. In the final fit the infrared vibration–rotation measurements and the pure rotational transition frequencies in the ground state [37–40] were combined with the present measurements. These infrared and millimeter wave frequencies were weighted by the estimated uncertainties provided in the original papers. The weights for the weaker and blended lines were chosen according to the signal-to-noise ratio and extent of blending. The spectroscopic parameters T_v , A_v , γ_v , γ_{Dv} , B_v , D_v , H_v , L_v , q_v , q_{Dv} , q_{Hv} , p_v , p_{Dv} and p_{Hv} were determined for the $E^2\Pi$ state. For the ground state, the constants T_v (except $v = 0$), B_v , D_v , H_v , L_v , γ_v and γ_{Dv} were determined.

A list of measured rotational lines of SrH and SrD bands used in the determination of the final spectroscopic constants, along with their obs.–calc. residuals is available as Supplement 1 on ScienceDirect (www.sciencedirect.com) and as part of the Ohio State University Molecular Spectroscopy Archives (http://msa.lib.ohio-state.edu/jmsa_hp.htm). The term values for the observed vibrational levels of the $E^2\Pi$ and $X^2\Sigma^+$ states were calculated using the spectroscopic constants obtained in the final fit. A list of term values is provided in Supplement 2. The spectroscopic constants for SrH and SrD obtained from this fit are provided in Table 1.

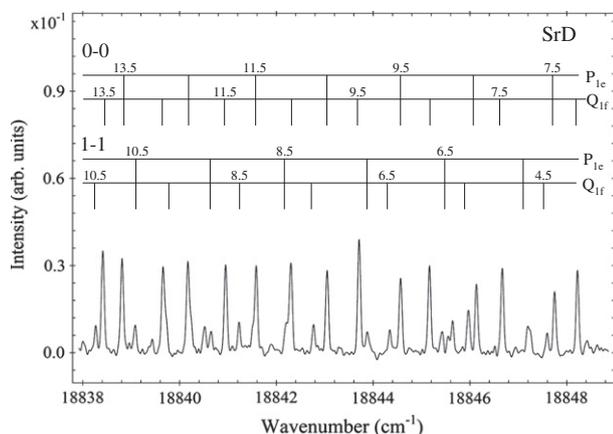


Fig. 3. An expanded portion of SrD spectrum with some rotational lines of the 0–0 and 1–1 bands marked.

The inclusion of high- J transitions from this work compared to the available infrared transitions [37–40] is expected to improve the centrifugal distortion and other higher order constants especially for the ground state of SrD. The present ground state values are in excellent agreement with the previously reported values [37–40], partly because of the inclusion of all the previous infrared measurements. Since the ground state molecular parameters are known with excellent precision from the previous infrared studies [37–40], the main purpose of the present study was to improve the molecular constants for the excited $E^2\Pi$ state. It is therefore interesting to compare the present excited state constants for the $E^2\Pi$ state of SrH with the values obtained previously by Fredrickson et al. [2]. For $v = 0$ vibrational level of the $E^2\Pi$ state, our analysis provides $T_0 = 18912.17974(92)$ cm^{-1} , $A_0 = 111.4908(14)$ cm^{-1} , $B_0 = 3.756063(21)$ cm^{-1} and $D_0 = 1.6262(12) \times 10^{-4}$ cm^{-1} . Fredrickson et al. [2] did not report their T_0 value (band origin) but reported $A_0 = 117$ cm^{-1} which agrees poorly with our present value of $A_0 = 111.4908(14)$ cm^{-1} . Also they did not report a single value for the rotational and distortion constants since they treated the $^2\Pi_{1/2}$ and $^2\Pi_{3/2}$ components separately. For comparison purposes we took the average of the values of two components. This provided their $B_0 = 3.7538$ cm^{-1} and $D_0 = 1.49 \times 10^{-4}$ cm^{-1} which compares reasonably well with our values of $B_0 = 3.756063(21)$ cm^{-1} and $D_0 = 1.6262(12) \times 10^{-4}$ cm^{-1} .

The molecular constants of the $v = 0$ and $v = 1$ vibrational levels (Table 1) have been used to determine the equilibrium constants for SrH and SrD from an exact fit. These constants are listed in Table 2. Since we observed only the $v = 0$ and 1 vibrational levels, we could not determine the equilibrium vibrational constants for the excited state, although our analysis provides the excited state vibrational interval of $\Delta G(\frac{1}{2}) = 1166.1011(15)$ cm^{-1} . The excited state equilibrium rotational constants obtained from this work are $B'_e = 3.805503(32)$ cm^{-1} , $\alpha_e = 0.098880(47)$ cm^{-1} for SrH and $B'_e = 1.918564(15)$ cm^{-1} , $\alpha_e = 0.034719(23)$ cm^{-1} for SrD. The values reported in parentheses are estimated uncertainties in the last two digits. Since these values have been estimated by the propagation of errors, the actual uncertainties in these values are expected to be much higher than the quoted values. The equilibrium bond lengths for the excited $E^2\Pi$ state of SrH and SrD were determined using the derived equilibrium constants which are 2.1083727 (89) Å for SrH and 2.1121943(83) Å for SrD.

In a theoretical study on SrH, Leininger and Jeung [20] have predicted the spectroscopic properties of the four low-lying electronic states $X^2\Sigma^+$, $A^2\Pi$, $B^2\Sigma^+$ and $(1)^2\Delta$ states. The spectroscopic properties of other higher-lying excited electronic states have not been calculated theoretically. Out of these states the ground $X^2\Sigma^+$ state dissociates to the $[\text{Sr}(5s^2, ^1S) + \text{H}(^2S)]$ atomic limit and the $A^2\Pi$ and $B^2\Sigma^+$ states correlate to $[\text{Sr}(5s5p, ^3P) + \text{H}(^2S)]$. The calculated $(1)^2\Delta$ state which has not been observed experimentally, correlates to the next excited atomic limit $[\text{Sr}(5s4d, ^3D) + \text{H}(^2S)]$. As was found in the case of CaH [46], the $E^2\Pi$ state will also correlate to the $[\text{Sr}(5s4d, ^3D) + \text{H}(^2S)]$ atomic limit although its spectroscopic properties have not yet been calculated.

As in the case of other alkaline earth hydrides, the low-lying excited electronic states of SrH, particularly the $A^2\Pi$ and $B^2\Sigma^+$ states lie very close in energy, and interact strongly. The mutual interaction can become so severe that their characterization becomes difficult using the usual spectroscopic methods and a perturbation treatment becomes necessary. For the $E^2\Pi$ state, there has been no high resolution study made since the first observation in 1935 by Fredrickson et al. [2]. The analysis of this state shows that the spectra of both SrH and SrD are affected by perturbations from close-lying electronic states. The definite assignment of the perturbing state (or states) is only possible after the characterization of other electronic states located in the same energy range. The available experimental results on SrH [47] suggest that the $D^2\Sigma^+$

Table 1
Spectroscopic constants (in cm^{-1}) of the observed vibrational levels of the $E^2\Pi$ and $X^2\Sigma^+$ electronic states of SrH and SrD.

Constants	$X^2\Sigma^+$		$E^2\Pi$	
	$v = 0$	$v = 1$	$v = 0$	$v = 1$
<i>SrH</i>				
T_v	0.0	1172.802866(93)	18912.17974(92)	20078.2808(12)
A_v	–	–	111.4908(14)	115.1416(14)
B_v	3.63344253(60)	3.55318277(65)	3.756063(21)	3.657183(42)
$D_v \times 10^4$	1.355128(72)	1.352948(66)	1.6262(12)	1.6310(43)
$H_v \times 10^8$	0.36189(89)	0.36469(52)	1.513(23)	1.19(14)
$L_v \times 10^{11}$	0.00537(40)	–	–0.508(14)	–1.46(15)
$\gamma'_v \times 10^1$	1.239888(31)	1.198732(51)	–4.5668(31)	–4.7506(50)
$\gamma'_{Dv} \times 10^4$	–0.11201(93)	–0.11082(88)	0.6066(81)	1.264(17)
$q_v \times 10^3$	–	–	8.091(21)	6.806(70)
$q_{Dv} \times 10^6$	–	–	–0.880(77)	4.34(57)
$q_{Hv} \times 10^8$	–	–	–0.0556(69)	–1.96(11)
$p_v \times 10^2$	–	–	7.811(52)	5.796(26)
$p_{Dv} \times 10^5$	–	–	–4.24(23)	–2.54(15)
$p_{Hv} \times 10^8$	–	–	2.35(27)	–
<i>SrD</i>				
T_v	0.0	841.57492(21)	18913.26195(66)	19752.3902(22)
A_v	–	–	110.59501(84)	113.4192(24)
B_v	1.8462442(12)	1.8173562(41)	1.901204(10)	1.866485(21)
$D_v \times 10^5$	3.4770(30)	3.4657(49)	3.7379(40)	3.9761(79)
$H_v \times 10^9$	0.466(25)	0.364(64)	–0.472(35)	1.571(96)
$L_v \times 10^{13}$	–	–	2.192(91)	–5.35(38)
$\gamma'_v \times 10^1$	0.63053(11)	0.61566(54)	–2.6084(34)	–2.5007(20)
$\gamma'_{Dv} \times 10^6$	–3.050(57)	–2.79(20)	7.77(32)	–
$q_v \times 10^3$	–	–	1.8735(56)	1.934(14)
$q_{Dv} \times 10^7$	–	–	–	–1.52(22)
$p_v \times 10^2$	–	–	3.729(13)	3.343(13)
$p_{Dv} \times 10^6$	–	–	–4.87(24)	–5.95(27)

Note: Numbers in parentheses are one standard deviation in the last digits quoted.

Table 2
Equilibrium constants (in cm^{-1}) of the $E^2\Pi$ state of SrH and SrD.

Constants	SrH	SrD
$\Delta G(1/2)$	1166.1011(15)	839.1283(23)
B_e	3.805503(32)	1.918564(15)
α_e	0.098880(47)	0.034719(23)
r_e (Å)	2.1083727(89)	2.1121943(83)

Note: Numbers in parentheses are one standard deviation in the last digits quoted.

state is only 1840 cm^{-1} higher than the $E^2\Pi$ state. Although the spectroscopic constants for the $D^2\Sigma^+$ state are not known accurately, a plot of the calculated term values of the $D^2\Sigma^+$ and the $E^2\Pi$ states indicates interaction between the two states for higher J values ($J > 15.5$) of the $v = 0$ and 1 vibrational levels. As mentioned earlier we have also observed local perturbations near $J = 10.5$ of the $v = 0$ vibrational level of the $E^2\Pi$ state which could not be explained as due to interaction with the $D^2\Sigma^+$ state. This perturbation is likely caused by interaction with higher vibrational levels of the lower-lying $B^2\Sigma^+$ state.

4. Conclusion

The emission spectra of the $E^2\Pi$ – $X^2\Sigma^+$ electronic transition of SrH and SrD have been observed at high resolution using a Fourier transform spectrometer. The rotational structure of the 0–0 and 1–1 bands has been measured and improved spectroscopic constants obtained. The equilibrium bond lengths of the $E^2\Pi$ state of SrH and SrD derived from the present analysis are $2.1083727(89) \text{ \AA}$ and $2.1121943(83) \text{ \AA}$, respectively. The observed perturbations in the $E^2\Pi$ state of the two isotopologues are likely caused by the interaction with the close-lying $D^2\Sigma^+$ state and higher vibrational levels of the lower-lying $B^2\Sigma^+$ state.

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Appendix A. Supplementary material

Supplementary data for this article are available on ScienceDirect (www.sciencedirect.com) and as part of the Ohio State University Molecular Spectroscopy Archives (http://library.osu.edu/sites/msa/jmsa_hp.htm). Supplementary data associated with this article can be found, in the online version, at [doi:10.1016/j.jms.2011.11.001](https://doi.org/10.1016/j.jms.2011.11.001).

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