



# New Fourier transform infrared emission spectra of CaH and SrH: combined isotopomer analyses with CaD and SrD

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## Abstract

In a search for the infrared spectra of gaseous CaH<sub>2</sub> and SrH<sub>2</sub>, we obtained new Fourier transform infrared emission spectra of CaH and SrH, but no evidence of the metal dihydrides. The vibration-rotation bands from  $\nu = 1 \rightarrow 0$  to  $\nu = 4 \rightarrow 3$  of <sup>40</sup>CaH and <sup>88</sup>SrH, and the  $\nu = 1 \rightarrow 0$  band of <sup>87</sup>SrH and <sup>86</sup>SrH were observed in the X<sup>2</sup>Σ<sup>+</sup> ground electronic states. The new data were combined with the previous ground state data, obtained from diode laser infrared and pure rotational spectra, and the spectroscopic constants for  $\nu = 0$  to 4 of <sup>40</sup>CaH and <sup>88</sup>SrH were determined. In addition, the Dunham constants and the Born–Oppenheimer breakdown correction parameters were obtained using the previous ground state data for CaD and SrD in combined isotopomer fits. The equilibrium vibrational constants ( $\omega_e$ ) for CaH and SrH were found to be 1298.400(1) and 1207.035(1) cm<sup>-1</sup>, respectively, while the equilibrium rotational constants ( $B_e$ ) are 4.277043(4) and 3.673495(4) cm<sup>-1</sup>. The equilibrium bond distances ( $r_e$ ) were determined to be 2.0023603(9) Å for CaH and 2.1460574(10) Å for SrH.

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## 1. Introduction

We have recently undertaken a search for the infrared spectra of gas phase alkaline earth dihydride molecules using Fourier transform emission spectroscopy. Laboratory measurements of these species are of interest because theoretical calculations have predicted that the dihydrides of the heavier alkaline earth atoms may have bent structures whereas those for the lighter metal atoms are linear [1–5].

Our investigation started with the discovery of gaseous BeH<sub>2</sub> [6,7] while recording the infrared emission spectrum of BeH [8]. Following this, a search was conducted for MgH<sub>2</sub> and its vibration–rotation spectrum was observed [9]. In these studies, both BeH<sub>2</sub> and MgH<sub>2</sub> were found to have linear geometries. Subsequent experiments were carried out to search for the dihydrides of Ca, Sr and Ba, but proved unsuccessful. However, in the course of these measurements, new infrared emission spectra were obtained

for calcium monohydride and strontium monohydride, which are described in this paper.

Most of the previous experimental work on the spectroscopy of calcium monohydride has focused on its electronic transitions. CaH was first observed in sunspot spectra and was identified via its electronic spectrum [10, 11]. Early laboratory measurements, in the 1920s and 30s, focused on emission spectroscopy from low-lying excited electronic states [12–19]. During the 1960s and 70s, these measurements were extended to include transitions in the ultraviolet region, which led to the identification of several Rydberg complexes [20–29]. Transitions involving the low-lying excited states were reinvestigated in order to examine perturbations which had been seen in earlier spectra [30–39]. Most recently, CaH has been studied by Zeeman [40,41] and REMPI [42] spectroscopy techniques.

The work on the electronic spectroscopy of strontium monohydride parallels that of CaH, however, SrH has been the subject of fewer studies. In the 1930s, the first band systems of SrH to be studied were the electronic transitions involving the low-lying excited electronic states [43–47]. Investigations involving higher energy excited electronic

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states followed in the 1960s and 70s [48–57]. More recently, there have been two studies which re-examined transitions between low-lying electronic states and the ground state using a Fourier transform spectrometer (FTS) [58,59].

Ground state hyperfine interactions have been measured for CaH and SrH trapped in an Ar matrix [60] and the excited state hyperfine interactions, in the  $B^2\Sigma^+$  state of CaH and the  $A^2\Pi_{1/2}$  state of SrH, have been investigated in the gas phase [61]. Several calculations of potential energy curves and molecular parameters have been made for CaH [1,62–79] and SrH [1,69,76,80].

It is only in the last decade that the vibration–rotation transitions in the  $X^2\Sigma^+$  ground electronic state of calcium and strontium monohydride have been measured. The first infrared study of CaH and CaD was done by Petitprez et al. using a diode laser spectrometer [81]. They measured transitions in four vibration–rotation bands, from  $\nu = 1 \leftarrow 0$  to  $\nu = 4 \leftarrow 3$ , however, the number of lines within each band was limited by the spectral ranges of the diodes available. Frum and Pickett [82] re-measured the fundamental and the first hot band of CaH in emission using a FTS. In both cases, a furnace source with a dc discharge was used to generate the molecules. The pure rotational spectra of CaH and CaD were investigated by both Frum et al. [83] and Barclay et al. [84].

Both diode laser and Fourier transform spectroscopy have also been used to study the infrared spectra of SrH and SrD. Three vibration–rotation bands ( $\nu = 1 \leftarrow 0$  to  $\nu = 3 \leftarrow 2$ ) of SrH and SrD were recorded by Magg et al. [85] and Birk et al. [86], respectively, using a diode laser spectrometer. Frum et al. [87] recorded the  $\nu = 1 \rightarrow 0$  band of SrH in emission using a FTS. As was done for CaH, the gas phase molecules were produced in a furnace coupled with a dc discharge. Frum et al. [87] also measured pure rotational spectra of SrH and SrD using the same source and a millimeter-wave spectrometer.

We report here new Fourier transform infrared emission spectra of CaH and SrH containing four vibration–rotation bands in their  $X^2\Sigma^+$  ground electronic states. Analyses of the new spectra have provided improved molecular constants for these species. We also used the available CaD and SrD data to study the Born–Oppenheimer breakdown effects.

## 2. Experimental

An emission source that combines an electrical discharge with a high temperature furnace was used to generate the CaH and SrH molecules. About 50 g of calcium metal was placed inside the central part of an alumina tube (120 cm long and 5 cm diameter), and heated by a CM Rapid Temp furnace. Two stainless steel tube electrodes were placed inside the two ends of the tube, which were cooled by water and sealed with BaF<sub>2</sub> windows. The central part of the tube

was heated to 780 °C in order to produce about 1 Torr vapor pressure of calcium metal. About 1 Torr of hydrogen was flowed through the cell, and a dc discharge (3 kV, 333 mA) was struck between the electrodes. At intermediate temperatures, from 650 to 750 °C, the hot metal absorbed hydrogen and probably formed the solid metal dihydride (CaH<sub>2</sub>). We had to keep the temperature at 780 °C to avoid the hydrogen absorption process. The same experimental setup was used for strontium, and a similar hydrogen absorption reaction was observed, but the optimal temperature for strontium was 850 °C. A BaF<sub>2</sub> lens was used to focus the emission from CaH and SrH molecules onto the entrance aperture of a Bruker IFS HR 120 FTS. The spectra were recorded using a KBr beamsplitter and a liquid nitrogen-cooled HgCdTe (MCT) detector at an instrumental resolution of 0.01 cm<sup>-1</sup>. The spectral region was limited to 800–1700 cm<sup>-1</sup> by the detector response, the BaF<sub>2</sub> lens, and a 1700 cm<sup>-1</sup> longwave pass filter. The spectra contained CaH and SrH emission lines, as well as blackbody emission from the hot tube and absorption lines from atmospheric water vapor. Hundreds of scans were co-added in order to improve the signal-to-noise ratios (600 scans for CaH and 300 scans for SrH), and the achieved signal-to-noise ratios for the strongest emission lines of CaH and SrH were 50 and 25, respectively.

## 3. Results and analyses

The infrared emission spectrum of CaH contained vibration–rotation bands in the ground electronic state of the most abundant isotopomer (<sup>40</sup>CaH, 96.9%). The lines from  $\nu = 1 \rightarrow 0$  to  $\nu = 4 \rightarrow 3$  transitions were found and analyzed. The SrH spectrum contained vibration–rotation bands of three isotopomers in the ground electronic state: The  $\nu = 1 \rightarrow 0$  to  $\nu = 4 \rightarrow 3$  bands of <sup>88</sup>SrH (82.6%), and the  $\nu = 1 \rightarrow 0$  band of <sup>87</sup>SrH (7.0%) and <sup>86</sup>SrH (9.9%). The blackbody emission from the hot tube was significant, and in order to display the bands clearly, we corrected the baselines of the spectra using the Bruker OPUS program. The overviews of CaH and SrH spectra (after baseline correction) are shown in Figs. 1 and 2. The ground electronic states of CaH and SrH are  $X^2\Sigma^+$ , and the spin-rotation interaction splits the  $e(F_1)$  and  $f(F_2)$  parity levels. An expanded view of the CaH spectrum in Fig. 3 shows the splitting in all the bands. The lines from three isotopomers of SrH were also resolved, and their intensity ratios are consistent with their natural abundances, as shown in Fig. 4.

The program WSPECTRA [88] written by Carleer was used to determine the line positions in the spectra. Both CaH and SrH spectra were calibrated using the line lists of the previous diode laser infrared measurements [81,85], and the absolute accuracy of the calibrated lines is about 0.001 cm<sup>-1</sup>. We assigned the experimental uncertainty of 0.001 cm<sup>-1</sup> to strong unblended lines. For very weak bands, i.e. the  $\nu = 4 \rightarrow 3$  band of both molecules and the  $\nu = 1 \rightarrow 0$

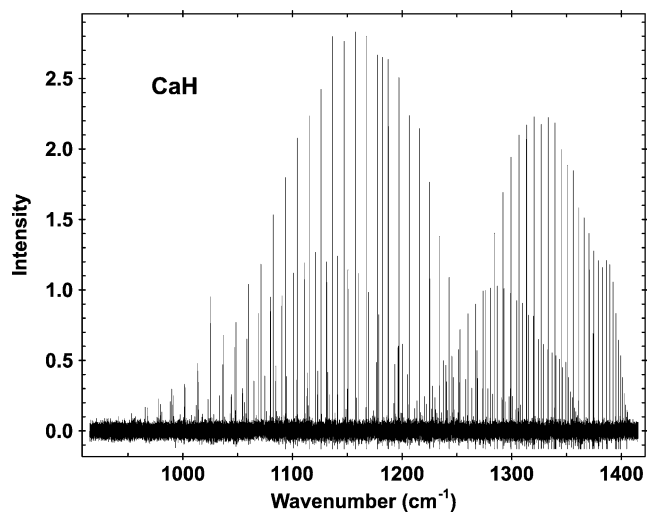


Fig. 1. An overview of the infrared emission spectrum of CaH after baseline correction.

band of  $^{87}\text{SrH}$  and  $^{86}\text{SrH}$ , the uncertainty of  $0.002\text{ cm}^{-1}$  was used. The bands were found and assigned using a color Loomis-Wood program.

The available diode laser infrared spectra of CaH and SrH contain four vibration–rotation bands of  $^{40}\text{CaH/D}$  [81] and three bands of  $^{88}\text{SrH/D}$  [85,86], but there are only a few lines in each band, and in some bands there are lines from one branch (P or R) only. We found that for the R(9) and R(10) rotational lines of the  $^{40}\text{CaH } \nu = 4 \leftarrow 3$  band reported by Petitprez et al. [81], the *e* and *f* parity labels had to be switched. This was also mentioned by Uehara [89]. We included all the diode laser infrared lines in our data set, as well as all the pure rotational data for  $^{40}\text{CaH/D}$  [83,84],  $^{88}\text{SrH/D}$ , and  $^{86}\text{SrH/D}$  [87]. For the pure rotational transitions, we removed the hyperfine structure by using the reported rotational and spin-rotation interaction

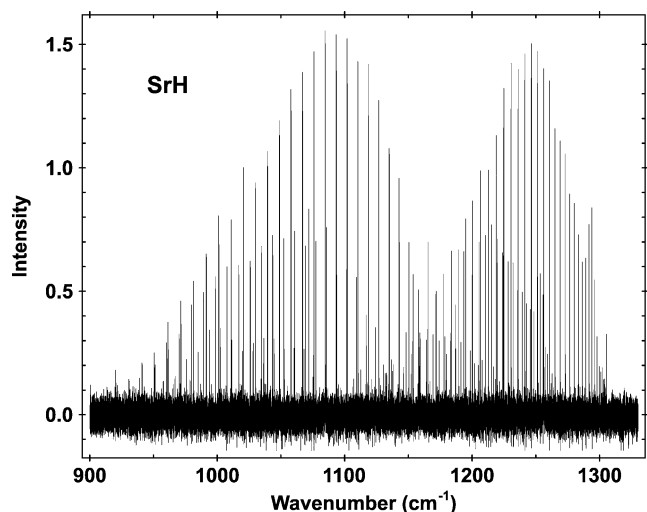


Fig. 2. An overview of the infrared emission spectrum of SrH after baseline correction.

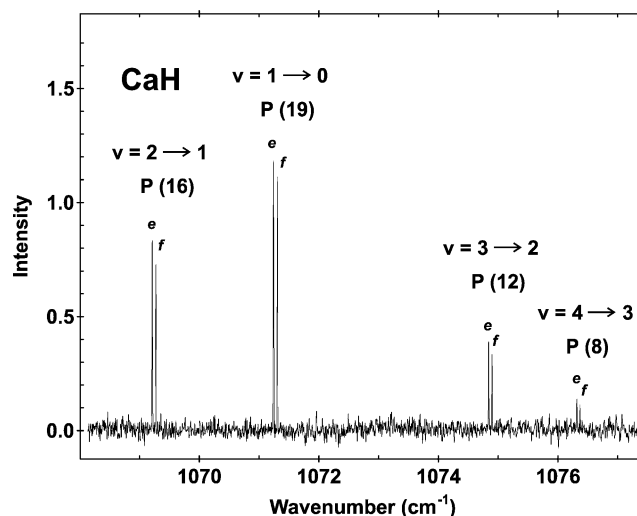


Fig. 3. An expanded view of the CaH spectrum showing the spin-splitting in all the vibration–rotation bands.

constants to compute the hyperfine-free line positions. The previous Fourier transform infrared spectra of Frum et al. [82,87] contained two bands of  $^{40}\text{CaH}$  and one band of  $^{88}\text{SrH}$ , but we did not use their data because the signal-to-noise ratios of our spectra are better. A complete list of the line positions and assignments is in Table 1.

The Hamiltonian operator which includes the spin-rotation interaction,

$$\hat{H}_{\text{rfs}} = B\hat{N}^2 - D\hat{N}^4 + H\hat{N}^6 + L\hat{N}^8 + \hat{N} \cdot \hat{S}(\gamma + \gamma_D \hat{N}^2) \quad (1)$$

was used to obtain the rotational energy levels. The data for  $\nu = 0$  to  $\nu = 4$  of  $^{40}\text{CaH}$  and  $^{88}\text{SrH}$  were fitted to the analytical expression for the levels obtained from the above Hamiltonian using the DPARFIT program [90] written by Le Roy, and the band constants of Tables 2 and 3 were

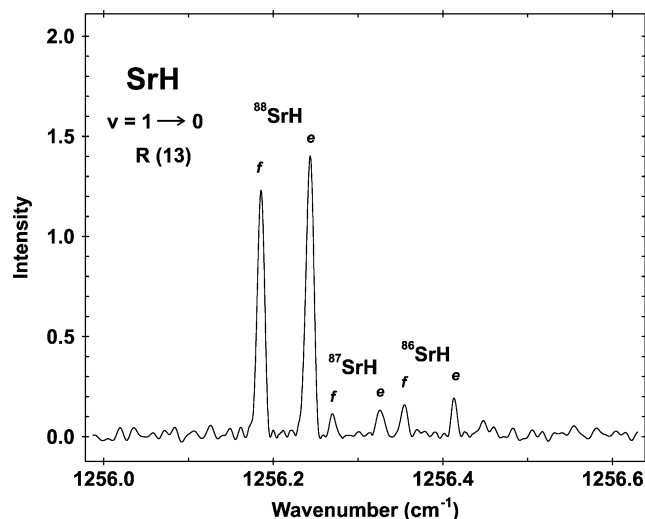


Fig. 4. An expanded view of the SrH spectrum showing lines from three isotopomers of strontium monohydride.

Table 1  
Line positions of CaH and SrH (in cm<sup>-1</sup>)

Line	Wavenumber	Line	Wavenumber	Line	Wavenumber	Line	Wavenumber	Line	Wavenumber
<sup>40</sup> CaH $v = 1 - 0$									
R(32)e	1405.4657(-7) <sup>a</sup>	R(15)f	1366.0865(-3)	P(6)e	1206.6091(0)	P(8)e	1187.3911(-5) <sup>b</sup>	P(20)f	1059.9907(-1)
R(31)e	1405.5390(-35)	R(14)f	1361.2502(-1)	P(7)e	1197.0813(0)	P(9)e	1177.5413(-1) <sup>b</sup>	P(21)f	1048.5600(0)
R(30)e	1405.2964(-36)	R(13)f	1356.1567(0)	P(8)e	1187.3906(0)	P(10)e	1167.5371(3) <sup>b</sup>	P(22)f	1037.0229(-2)
R(29)e	1404.7434(-40)	R(12)f	1350.8097(0)	P(9)e	1177.5410(2)	P(11)e	1157.3844(-8) <sup>b</sup>	P(23)f	1025.3812(10)
R(18)e	1379.0237(-13)	R(11)f	1345.2131(1)	P(10)e	1167.5373(1)	P(12)e	1147.0832(6) <sup>b</sup>	P(24)f	1013.6422(-5)
R(17)e	1374.9825(6)	R(10)f	1339.3713(0)	P(11)e	1157.3835(1)	P(14)e	1126.0638(-3) <sup>b</sup>	P(25)f	1001.8045(2)
R(16)e	1370.6750(1)	R(9)f	1333.2879(1)	P(12)e	1147.0837(1)	P(20)e	1059.9250(-2) <sup>b</sup>	P(26)f	989.8742(2)
R(15)e	1366.1022(-1)	R(8)f	1326.9673(0)	P(13)e	1136.6424(0)	P(23)e	1025.3145(-5) <sup>b</sup>	P(27)f	977.8547(-8)
R(14)e	1361.2676(3)	R(7)f	1320.4134(1)	P(14)e	1126.0635(0)	P(25)e	1001.7354(-3) <sup>b</sup>	P(28)f	965.7478(-14)
R(13)e	1356.1762(2)	R(6)f	1313.6306(2)	P(15)e	1115.3511(-1)	P(26)e	989.8040(1) <sup>b</sup>	P(29)f	953.5564(-15)
R(12)e	1350.8310(2)	R(5)f	1306.6235(1)	P(16)e	1104.5091(0)	P(28)e	965.6750(0) <sup>b</sup>	P(30)f	941.2826(-5)
R(11)e	1345.2365(2)	R(4)f	1299.3959(2)	P(17)e	1093.5415(1)	P(30)e	941.2093(2) <sup>b</sup>	P(31)f	928.9289(20)
R(10)e	1339.3961(3)	R(3)f	1291.9524(2)	P(18)e	1082.4525(1)	P(2)f	1243.0481(0)	P(5)f	1216.0194(-2) <sup>b</sup>
R(9)e	1333.3146(3)	R(2)f	1284.2977(-2)	P(19)e	1071.2455(2)	P(3)f	1234.2175(1)	P(6)f	1206.6600(1) <sup>b</sup>
R(8)e	1326.9955(4)	R(1)f	1276.4347(4)	P(20)e	1059.9247(2)	P(4)f	1225.2065(0)	P(7)f	1197.1344(-8) <sup>b</sup>
R(7)e	1320.4435(3)	R(28)	1403.8818(22)	P(21)e	1048.4932(3)	P(5)f	1216.0190(1)	P(8)f	1187.4451(-11) <sup>b</sup>
R(6)e	1313.6624(5)	R(27)	1402.7157(17)	P(22)e	1036.9555(-1)	P(6)f	1206.6600(0)	P(9)f	1177.5950(8) <sup>b</sup>
R(5)e	1306.6572(1)	R(26)	1401.2483(9)	P(23)e	1025.3144(-4)	P(7)f	1197.1336(0)	P(10)f	1167.5943(-11) <sup>b</sup>
R(4)e	1299.4313(1)	R(25)	1399.4823(-1)	P(24)e	1013.5729(-1)	P(8)f	1187.4441(-1)	P(11)f	1157.4413(-8) <sup>b</sup>
R(3)e	1291.9892(2)	R(24)	1397.4195(1)	P(25)e	1001.7350(1)	P(9)f	1177.5958(0)	P(12)f	1147.1412(6) <sup>b</sup>
R(2)e	1284.3356(3)	R(23)	1395.0647(0)	P(26)e	989.8042(-1)	P(10)f	1167.5934(-2)	P(14)f	1126.1232(4) <sup>b</sup>
R(1)e	1276.4749(2)	R(22)	1392.4205(-1)	P(27)e	977.7834(-4)	P(11)f	1157.4407(-2)	P(20)f	1059.9902(3) <sup>b</sup>
R(0)e	1268.4113(2)	R(21)	1389.4903(-1)	P(28)e	965.6750(0)	P(12)f	1147.1419(-1)	P(23)f	1025.3810(11) <sup>b</sup>
R(32)f	1405.4860(1)	R(20)	1386.2773(-1)	P(29)e	953.4820(8)	P(13)f	1136.7016(-1)	P(25)f	1001.8048(-2) <sup>b</sup>
R(31)f	1405.5503(39)	R(19)	1382.7844(6)	P(30)e	941.2087(8)	P(14)f	1126.1236(-1)	P(26)f	989.8739(4) <sup>b</sup>
R(30)f	1405.3090(0)	P(1)e	1251.6494(-2)	P(31)e	928.8594(-17)	P(15)f	1115.4122(-1)	P(28)f	965.7460(4) <sup>b</sup>
R(29)f	1404.7533(1)	P(2)e	1243.0022(2)	P(32)e	916.4304(-2)	P(16)f	1104.5713(-1)	P(30)f	941.2804(17) <sup>b</sup>
R(18)f	1379.0133(-10)	P(3)e	1234.1706(0)	P(5)e	1215.9698(-3) <sup>b</sup>	P(17)f	1093.6048(-1)		
R(17)f	1374.9716(-6)	P(4)e	1225.1580(1)	P(6)e	1206.6085(6) <sup>b</sup>	P(18)f	1082.5167(-1)		
R(16)f	1370.6616(-5)	P(5)e	1215.9694(0)	P(7)e	1197.0826(-13) <sup>b</sup>	P(19)f	1071.3108(-2)		
<sup>40</sup> CaH $v = 2 - 1$									
R(29)e	1359.9770(9)	R(6)e	1274.0187(3)	R(13)f	1315.0713(-3)	R(27)	1358.4630(-9)	P(4)e	1187.6720(-2)
R(28)e	1359.3747(-26)	R(5)e	1267.2145(2)	R(12)f	1309.9343(1)	R(26)	1357.2342(56)	P(5)e	1178.6730(-1)
R(17)e	1333.0401(-20)	R(4)e	1260.1886(4)	R(11)f	1304.5465(2)	R(25)	1355.7135(14)	P(6)e	1169.5011(1)
R(16)e	1328.9473(0)	R(3)e	1252.9457(4)	R(10)f	1298.9120(1)	R(24)	1353.8907(-1)	P(7)e	1160.1608(1)
R(15)e	1324.5897(-2)	R(2)e	1245.4905(2)	R(9)f	1293.0346(2)	R(23)	1351.7709(-6)	P(8)e	1150.6566(-1)
R(14)e	1319.9690(-3)	R(1)e	1237.8271(-2)	R(8)f	1286.9189(0)	R(22)	1349.3578(0)	P(9)e	1140.9924(-2)
R(13)e	1315.0890(0)	R(0)e	1229.9583(10)	R(7)f	1280.5686(2)	R(21)	1346.6563(0)	P(10)e	1131.1725(-2)
R(12)e	1309.9543(-1)	R(29)f	1359.9933(5)	R(6)f	1273.9886(0)	R(20)	1343.6693(0)	P(11)e	1121.2010(0)
R(11)e	1304.5683(0)	R(28)f	1359.3883(-26)	R(5)f	1267.1823(3)	R(19)	1340.4011(-4)	P(12)e	1111.0827(-1)
R(10)e	1298.9356(0)	R(17)f	1333.0292(-13)	R(4)f	1260.1549(4)	R(18)	1336.8536(2)	P(13)e	1100.8210(0)
R(9)e	1293.0600(1)	R(16)f	1328.9351(0)	R(3)f	1252.9106(3)	P(1)e	1213.5878(-3)	P(14)e	1090.4205(-2)
R(8)e	1286.9460(0)	R(15)f	1324.5752(1)	R(2)f	1245.4536(2)	P(2)e	1205.1336(0)	P(15)e	1079.8849(-4)

<i>R</i> (7) <i>e</i>	1280.5972(3)	<i>R</i> (14) <i>f</i>	1319.9531(−4)	<i>R</i> (1) <i>f</i>	1237.7887(−2)	<i>P</i> (3) <i>e</i>	1196.4933(2)	<i>P</i> (16) <i>e</i>	1069.2178(−2)
<i>P</i> (17) <i>e</i>	1058.4238(−3)	<i>P</i> (3) <i>e</i>	1196.4933(2) <sup>b</sup>	<i>P</i> (4) <i>f</i>	1187.7188(0)	<i>P</i> (16) <i>f</i>	1069.2787(−1)	<i>P</i> (3) <i>f</i>	1196.5394(−2) <sup>b</sup>
<i>P</i> (18) <i>e</i>	1047.5061(−3)	<i>P</i> (4) <i>e</i>	1187.6717(2) <sup>b</sup>	<i>P</i> (5) <i>f</i>	1178.7213(0)	<i>P</i> (17) <i>f</i>	1058.4853(2)	<i>P</i> (4) <i>f</i>	1187.7193(−5) <sup>b</sup>
<i>P</i> (19) <i>e</i>	1036.4684(0)	<i>P</i> (6) <i>e</i>	1169.5016(−4) <sup>b</sup>	<i>P</i> (6) <i>f</i>	1169.5508(0)	<i>P</i> (18) <i>f</i>	1047.5688(−1)	<i>P</i> (6) <i>f</i>	1169.5510(−2) <sup>b</sup>
<i>P</i> (21) <i>e</i>	1014.0486(−2)	<i>P</i> (10) <i>e</i>	1131.1729(−6) <sup>b</sup>	<i>P</i> (7) <i>f</i>	1160.2118(0)	<i>P</i> (19) <i>f</i>	1036.5322(−1)	<i>P</i> (10) <i>f</i>	1131.2271(−3) <sup>b</sup>
<i>P</i> (22) <i>e</i>	1002.6731(−3)	<i>P</i> (18) <i>e</i>	1047.5055(3) <sup>b</sup>	<i>P</i> (8) <i>f</i>	1150.7088(−2)	<i>P</i> (21) <i>f</i>	1014.1139(−1)	<i>P</i> (19) <i>f</i>	1036.5318(3) <sup>b</sup>
<i>P</i> (23) <i>e</i>	991.1912(2)	<i>P</i> (19) <i>e</i>	1036.4682(2) <sup>b</sup>	<i>P</i> (9) <i>f</i>	1141.0455(0)	<i>P</i> (22) <i>f</i>	1002.7388(3)	<i>P</i> (22) <i>f</i>	1002.7380(11) <sup>b</sup>
<i>P</i> (24) <i>e</i>	979.6070(2)	<i>P</i> (22) <i>e</i>	1002.6730(−2) <sup>b</sup>	<i>P</i> (10) <i>f</i>	1131.2270(−2)	<i>P</i> (23) <i>f</i>	991.2585(−1)	<i>P</i> (23) <i>f</i>	991.2582(2) <sup>b</sup>
<i>P</i> (25) <i>e</i>	967.9244(−8)	<i>P</i> (23) <i>e</i>	991.1915(−2) <sup>b</sup>	<i>P</i> (11) <i>f</i>	1121.2571(−4)	<i>P</i> (24) <i>f</i>	979.6749(2)	<i>P</i> (24) <i>f</i>	979.6730(21) <sup>b</sup>
<i>P</i> (26) <i>e</i>	956.1445(−9)	<i>P</i> (24) <i>e</i>	979.6064(8) <sup>b</sup>	<i>P</i> (12) <i>f</i>	1111.1396(−3)	<i>P</i> (25) <i>f</i>	967.9924(−2)		
<i>P</i> (27) <i>e</i>	944.2694(6)	<i>P</i> (25) <i>e</i>	967.9237(−1) <sup>b</sup>	<i>P</i> (13) <i>f</i>	1100.8791(−3)	<i>P</i> (26) <i>f</i>	956.2125(3)		
<i>P</i> (28) <i>e</i>	932.3056(0)	<i>P</i> (2) <i>f</i>	1205.1768(10)	<i>P</i> (14) <i>f</i>	1090.4795(−3)	<i>P</i> (27) <i>f</i>	944.3416(−17)		
<i>P</i> (1) <i>e</i>	1213.5877(−2) <sup>b</sup>	<i>P</i> (3) <i>f</i>	1196.5393(−1)	<i>P</i> (15) <i>f</i>	1079.9447(−2)	<i>P</i> (28) <i>f</i>	932.3756(6)		
<sup>40</sup> CaH $v = 3 - 2$									
<i>R</i> (25) <i>e</i>	1311.3740(6)	<i>R</i> (14) <i>f</i>	1278.3421(4)	<i>P</i> (1) <i>e</i>	1175.3310(−41)	<i>P</i> (24) <i>e</i>	945.2408(−27)	<i>P</i> (14) <i>f</i>	1054.5812(4)
<i>R</i> (16) <i>e</i>	1286.8741(2)	<i>R</i> (13) <i>f</i>	1273.6863(7)	<i>P</i> (2) <i>e</i>	1167.0656(6)	<i>P</i> (25) <i>e</i>	933.6918(−52)	<i>P</i> (15) <i>f</i>	1044.2133(3)
<i>R</i> (15) <i>e</i>	1282.7493(−7)	<i>R</i> (12) <i>f</i>	1268.7736(2)	<i>P</i> (3) <i>e</i>	1158.6182(−6)	<i>P</i> (1) <i>e</i>	1175.3271(−2) <sup>b</sup>	<i>P</i> (16) <i>f</i>	1033.7121(−4)
<i>R</i> (14) <i>e</i>	1278.3562(7)	<i>R</i> (11) <i>f</i>	1263.6061(8)	<i>P</i> (4) <i>e</i>	1149.9858(−2)	<i>P</i> (2) <i>e</i>	1167.0667(−6) <sup>b</sup>	<i>P</i> (17) <i>f</i>	1023.0795(3)
<i>R</i> (13) <i>e</i>	1273.7031(3)	<i>R</i> (10) <i>f</i>	1258.1909(−1)	<i>P</i> (5) <i>e</i>	1141.1745(0)	<i>P</i> (4) <i>e</i>	1149.9850(6) <sup>b</sup>	<i>P</i> (18) <i>f</i>	1012.3203(10)
<i>R</i> (12) <i>e</i>	1268.7921(−1)	<i>R</i> (9) <i>f</i>	1252.5291(4)	<i>P</i> (6) <i>e</i>	1132.1890(−2)	<i>P</i> (6) <i>e</i>	1132.1888(1) <sup>b</sup>	<i>P</i> (19) <i>f</i>	1001.4404(−4)
<i>R</i> (11) <i>e</i>	1263.6270(0)	<i>R</i> (8) <i>f</i>	1246.6271(4)	<i>P</i> (7) <i>e</i>	1123.0332(−4)	<i>P</i> (13) <i>e</i>	1064.7557(−4) <sup>b</sup>	<i>P</i> (20) <i>f</i>	990.4375(15)
<i>R</i> (10) <i>e</i>	1258.2128(−2)	<i>R</i> (7) <i>f</i>	1240.4893(−2)	<i>P</i> (8) <i>e</i>	1113.7107(−1)	<i>P</i> (15) <i>e</i>	1044.1546(2) <sup>b</sup>	<i>P</i> (21) <i>f</i>	979.3237(−19)
<i>R</i> (9) <i>e</i>	1252.5530(2)	<i>R</i> (6) <i>f</i>	1234.1185(0)	<i>P</i> (9) <i>e</i>	1104.2264(2)	<i>P</i> (18) <i>e</i>	1012.2592(4) <sup>b</sup>	<i>P</i> (22) <i>f</i>	968.0962(−44)
<i>R</i> (8) <i>e</i>	1246.6530(−1)	<i>R</i> (5) <i>f</i>	1227.5198(3)	<i>P</i> (10) <i>e</i>	1094.5850(0)	<i>P</i> (20) <i>e</i>	990.3744(11) <sup>b</sup>	<i>P</i> (23) <i>f</i>	956.7519(−2)
<i>R</i> (7) <i>e</i>	1240.5161(0)	<i>R</i> (4) <i>f</i>	1220.6984(1)	<i>P</i> (11) <i>e</i>	1084.7896(2)	<i>P</i> (23) <i>e</i>	956.6852(6) <sup>b</sup>	<i>P</i> (24) <i>f</i>	945.3041(9)
<i>R</i> (6) <i>e</i>	1234.1471(2)	<i>R</i> (3) <i>f</i>	1213.6559(20)	<i>P</i> (12) <i>e</i>	1074.8456(−3)	<i>P</i> (2) <i>f</i>	1167.1097(−7)	<i>P</i> (25) <i>f</i>	933.7569(−27)
<i>R</i> (5) <i>e</i>	1227.5504(2)	<i>R</i> (2) <i>f</i>	1206.4031(−2)	<i>P</i> (13) <i>e</i>	1064.7548(6)	<i>P</i> (3) <i>f</i>	1158.6623(−5)	<i>P</i> (2) <i>f</i>	1167.1093(−3) <sup>b</sup>
<i>R</i> (4) <i>e</i>	1220.7303(3)	<i>R</i> (3) <i>f</i>	1213.6584(−5) <sup>b</sup>	<i>P</i> (14) <i>e</i>	1054.5241(−2)	<i>P</i> (4) <i>f</i>	1150.0308(4)	<i>P</i> (4) <i>f</i>	1150.0307(5) <sup>b</sup>
<i>R</i> (3) <i>e</i>	1213.6924(−8)	<i>R</i> (1) <i>f</i>	1198.9389(−11) <sup>b</sup>	<i>P</i> (15) <i>e</i>	1044.1541(7)	<i>P</i> (5) <i>f</i>	1141.2211(4)	<i>P</i> (6) <i>f</i>	1132.2368(3) <sup>b</sup>
<i>R</i> (2) <i>e</i>	1206.4390(−7)	<i>R</i> (24)	1309.8264(−16)	<i>P</i> (16) <i>e</i>	1033.6519(1)	<i>P</i> (6) <i>f</i>	1132.2370(1)	<i>P</i> (13) <i>f</i>	1064.8115(4) <sup>b</sup>
<i>R</i> (1) <i>e</i>	1198.9726(22)	<i>R</i> (23)	1307.9702(−5)	<i>P</i> (17) <i>e</i>	1023.0186(4)	<i>P</i> (7) <i>f</i>	1123.0825(−2)	<i>P</i> (15) <i>f</i>	1044.2128(7) <sup>b</sup>
<i>R</i> (3) <i>e</i>	1213.6926(−9) <sup>b</sup>	<i>R</i> (22)	1305.8162(8)	<i>P</i> (18) <i>e</i>	1012.2595(2)	<i>P</i> (8) <i>f</i>	1113.7617(−3)	<i>P</i> (18) <i>f</i>	1012.3210(3) <sup>b</sup>
<i>R</i> (1) <i>e</i>	1198.9756(−9) <sup>b</sup>	<i>R</i> (21)	1303.3685(21)	<i>P</i> (19) <i>e</i>	1001.3777(−4)	<i>P</i> (9) <i>f</i>	1104.2784(3)	<i>P</i> (20) <i>f</i>	990.4395(−5) <sup>b</sup>
<i>R</i> (0) <i>e</i>	1191.3046(10) <sup>b</sup>	<i>R</i> (20)	1300.6336(7)	<i>P</i> (20) <i>e</i>	990.3755(0)	<i>P</i> (10) <i>f</i>	1094.6381(1)	<i>P</i> (23) <i>f</i>	956.7527(−9) <sup>b</sup>
<i>R</i> (25) <i>f</i>	1311.3844(−11)	<i>R</i> (19)	1297.6113(7)	<i>P</i> (21) <i>e</i>	979.2582(−7)	<i>P</i> (11) <i>f</i>	1084.8440(3)		
<i>R</i> (16) <i>f</i>	1286.8640(−2)	<i>R</i> (18)	1294.3086(−10)	<i>P</i> (22) <i>e</i>	968.0273(−8)	<i>P</i> (12) <i>f</i>	1074.9006(2)		
<i>R</i> (15) <i>f</i>	1282.7353(9)	<i>R</i> (17)	1290.7253(−1)	<i>P</i> (23) <i>e</i>	956.6885(−27)	<i>P</i> (13) <i>f</i>	1064.8118(1)		
<sup>40</sup> CaH $v = 4 - 3$									
<i>R</i> (15) <i>e</i>	1240.2913(−7)	<i>R</i> (8) <i>e</i>	1205.8689(−15)	<i>R</i> (5) <i>e</i>	1187.4255(13) <sup>b</sup>	<i>R</i> (12) <i>f</i>	1227.0597(−11)	<i>R</i> (4) <i>f</i>	1180.7897(7)
<i>R</i> (14) <i>e</i>	1236.1490(14)	<i>R</i> (7) <i>e</i>	1199.9549(−4)	<i>R</i> (3) <i>e</i>	1173.9933(−1) <sup>b</sup>	<i>R</i> (11) <i>f</i>	1222.1295(8)	<i>R</i> (3) <i>f</i>	1173.9604(6)
<i>R</i> (13) <i>e</i>	1231.7456(−19)	<i>R</i> (6) <i>e</i>	1193.8051(10)	<i>R</i> (1) <i>e</i>	1159.6893(4) <sup>b</sup>	<i>R</i> (10) <i>f</i>	1216.9489(−2)	<i>R</i> (10) <i>f</i>	1216.9498(−11) <sup>b</sup>
<i>R</i> (12) <i>e</i>	1227.0723(27)	<i>R</i> (4) <i>e</i>	1180.8205(5)	<i>R</i> (0) <i>e</i>	1152.2230(0) <sup>b</sup>	<i>R</i> (9) <i>f</i>	1211.5173(11)	<i>R</i> (9) <i>f</i>	1211.5187(−3) <sup>b</sup>
<i>R</i> (11) <i>e</i>	1222.1476(10)	<i>R</i> (3) <i>e</i>	1173.9909(24)	<i>R</i> (15) <i>f</i>	1240.2790(10)	<i>R</i> (8) <i>f</i>	1205.8425(11)	<i>R</i> (3) <i>f</i>	1173.9609(1) <sup>b</sup>
<i>R</i> (10) <i>e</i>	1216.9703(−14)	<i>R</i> (10) <i>e</i>	1216.9702(−13) <sup>b</sup>	<i>R</i> (14) <i>f</i>	1236.1370(8)	<i>R</i> (7) <i>f</i>	1199.9303(−12)	<i>R</i> (1) <i>f</i>	1159.6539(4) <sup>b</sup>
<i>R</i> (9) <i>e</i>	1211.5420(−16)	<i>R</i> (9) <i>e</i>	1211.5408(−5) <sup>b</sup>	<i>R</i> (13) <i>f</i>	1231.7289(3)	<i>R</i> (6) <i>f</i>	1193.7787(3)	<i>R</i> (21)	1259.2923(20)
<i>R</i> (20)	1256.8427(−2)	<i>P</i> (9) <i>e</i>	1067.0129(−6)	<i>P</i> (20) <i>e</i>	954.8304(14)	<i>P</i> (8) <i>f</i>	1076.3726(−3)	<i>P</i> (18) <i>f</i>	976.5125(−28)
<i>R</i> (19)	1254.0993(−9)	<i>P</i> (10) <i>e</i>	1057.5419(−10)	<i>P</i> (21) <i>e</i>	943.8374(24)	<i>P</i> (9) <i>f</i>	1067.0628(2)	<i>P</i> (19) <i>f</i>	965.7643(−2)

(continued on next page)

Table 1 (continued)

Line	Wavenumber	Line	Wavenumber	Line	Wavenumber	Line	Wavenumber	Line	Wavenumber				
R(18)	1251.0679(−15)	P(11)e	1047.9133(−6)	P(22)e	932.7271(25)	P(10)f	1057.5935(−7)	P(20)f	954.8942(0)				
R(17)	1247.7517(−11)	P(12)e	1038.1329(−11)	P(10)e	1057.5412(−3) <sup>b</sup>	P(11)f	1047.9657(1)	P(21)f	943.8988(42)				
R(16)	1244.1566(−14)	P(13)e	1028.2019(0)	P(15)e	1007.9109(−2) <sup>b</sup>	P(12)f	1038.1856(5)	P(22)f	932.7951(−14)				
P(3)e	1120.3195(−19)	P(14)e	1018.1285(−15)	P(19)e	965.7020(6) <sup>b</sup>	P(13)f	1028.2551(22)	P(10)f	1057.5937(−9) <sup>b</sup>				
P(4)e	1111.8736(3)	P(15)e	1007.9123(−16)	P(3)f	1120.3573(32)	P(14)f	1018.1841(−7)	P(15)f	1007.9689(−7) <sup>b</sup>				
P(6)e	1094.4442(8)	P(16)e	997.5575(−9)	P(4)f	1111.9175(5)	P(15)f	1007.9674(8)	P(19)f	965.7639(2) <sup>b</sup>				
P(7)e	1085.4669(15)	P(17)e	987.0671(12)	P(6)f	1094.4911(7)	P(16)f	997.6165(−13)						
P(8)e	1076.3223(5)	P(18)e	976.4490(3)	P(7)f	1085.5165(1)	P(17)f	987.1291(−12)						
<sup>40</sup> CaH													
v'	N'	p'	v''	N''	p''	v'	N'	p'	v''	N''	p''		
0	1	e	0	0	e	8.4784175(−3) <sup>c</sup>	1	1	f	0	0	e	1268.3474(9)
0	1	f	0	0	e	8.4130846(−2) <sup>c</sup>	1	0	e	0	1	f	1251.7135(11)
0	1	e	0	0	e	8.478417(0) <sup>d</sup>	2	1	f	1	0	e	1229.8984(−1)
0	2	e	0	1	e	16.930598(−3) <sup>d</sup>	2	0	e	1	1	f	1213.6559(−52)
0	1	f	0	0	e	8.413082(3) <sup>d</sup>	3	1	f	2	0	e	1191.2469(−1) <sup>b</sup>
0	2	f	0	1	f	16.887089(0) <sup>d</sup>	3	0	e	2	1	f	1175.3907(−28) <sup>b</sup>
							4	1	f	3	0	e	1152.1658(6) <sup>b</sup>
<sup>40</sup> CaD													
v'	N'	p'	v''	N''	p''	v'	N'	p'	v''	N''	p''		
0	1	e	0	0	e	4.3649077(65) <sup>c</sup>	0	5	e	0	4	e	21.756254(−11) <sup>d</sup>
0	2	e	0	1	e	8.7174326(13) <sup>c</sup>	0	3	f	0	2	f	13.045170(34) <sup>d</sup>
0	2	f	0	1	f	8.6950164(−59) <sup>c</sup>	0	4	f	0	3	f	17.391882(9) <sup>d</sup>
0	3	e	0	2	e	13.0676078(−1) <sup>c</sup>	0	5	f	0	4	f	21.733903(0) <sup>d</sup>
0	3	e	0	2	e	13.067636(−28) <sup>d</sup>	2	1	f	1	0	e	894.8975(0) <sup>b</sup>
0	4	e	0	3	e	17.414282(−16) <sup>d</sup>							
<sup>40</sup> CaD v = 1 − 0													
R(26)e	997.2249(1) <sup>b</sup>	R(3)e	927.0018(0) <sup>b</sup>	R(5)f	934.8770(10) <sup>b</sup>	P(5)e	887.8300(13) <sup>b</sup>	P(5)f	887.8560(0) <sup>b</sup>				
R(25)e	995.1867(5) <sup>b</sup>	R(1)e	918.8041(−7) <sup>b</sup>	R(4)f	930.9677(7) <sup>b</sup>	P(7)e	878.3832(−2) <sup>b</sup>	P(7)f	878.4084(3) <sup>b</sup>				
R(24)e	993.0504(−4) <sup>b</sup>	R(26)f	997.2208(−8) <sup>b</sup>	R(3)f	926.9829(−11) <sup>b</sup>	P(8)e	873.5634(5) <sup>b</sup>	P(8)f	873.5903(−3) <sup>b</sup>				
R(22)e	988.4799(12) <sup>b</sup>	R(25)f	995.1818(−4) <sup>b</sup>	R(1)f	918.7831(−8) <sup>b</sup>	P(10)e	863.7413(0) <sup>b</sup>	P(10)f	863.7687(−3) <sup>b</sup>				
R(20)e	983.5253(9) <sup>b</sup>	R(24)f	993.0440(−5) <sup>b</sup>	R(36)	1011.9381(−3) <sup>b</sup>	P(11)e	858.7403(0) <sup>b</sup>	P(11)f	858.7675(3) <sup>b</sup>				
R(13)e	963.2602(7) <sup>b</sup>	R(22)f	988.4718(14) <sup>b</sup>	R(32)	1007.3130(−6) <sup>b</sup>	P(12)e	853.6813(−4) <sup>b</sup>	P(12)f	853.7100(−12) <sup>b</sup>				
R(9)e	949.7417(−13) <sup>b</sup>	R(20)f	983.5162(6) <sup>b</sup>	R(30)	1004.3619(6) <sup>b</sup>	P(13)e	848.5642(0) <sup>b</sup>	P(13)f	848.5928(−2) <sup>b</sup>				
R(8)e	946.1496(11) <sup>b</sup>	R(13)f	963.2462(7) <sup>b</sup>	R(27)	999.1603(−1) <sup>b</sup>	P(16)e	832.8828(−3) <sup>b</sup>	P(16)f	832.9127(−6) <sup>b</sup>				
R(7)e	942.4795(0) <sup>b</sup>	R(9)f	949.7249(−10) <sup>b</sup>	P(1)e	905.9359(−9) <sup>b</sup>	P(17)e	827.5482(1) <sup>b</sup>	P(17)f	827.5788(−5) <sup>b</sup>				
R(5)e	934.8964(5) <sup>b</sup>	R(8)f	946.1334(2) <sup>b</sup>	P(2)e	901.5119(−8) <sup>b</sup>	P(2)f	901.5348(−5) <sup>b</sup>						
R(4)e	930.9868(10) <sup>b</sup>	R(7)f	942.4620(−2) <sup>b</sup>	P(4)e	892.4578(3) <sup>b</sup>	P(4)f	892.4812(11) <sup>b</sup>						
<sup>40</sup> CaD v = 2 − 1													
R(16)e	951.6542(3) <sup>b</sup>	R(10)e	932.8581(−2) <sup>b</sup>	R(4)e	911.0355(8) <sup>b</sup>	R(16)f	951.6429(1) <sup>b</sup>	R(10)f	932.8428(−2) <sup>b</sup>				
R(14)e	945.7399(1) <sup>b</sup>	R(8)e	925.9082(−1) <sup>b</sup>	R(3)e	907.1191(34) <sup>b</sup>	R(14)f	945.7274(−2) <sup>b</sup>	R(8)f	925.8916(0) <sup>b</sup>				
R(13)e	942.6510(−16) <sup>b</sup>	R(6)e	918.6311(1) <sup>b</sup>	R(2)e	903.1315(11) <sup>b</sup>	R(13)f	942.6376(−16) <sup>b</sup>	R(6)f	918.6131(4) <sup>b</sup>				
R(12)e	939.4711(4) <sup>b</sup>	R(5)e	914.8734(−5) <sup>b</sup>	R(0)e	894.9295(0) <sup>b</sup>	R(12)f	939.4577(−3) <sup>b</sup>	R(5)f	914.8549(−3) <sup>b</sup>				
R(4)f	911.0172(2) <sup>b</sup>	P(4)e	873.1489(4) <sup>b</sup>	P(11)e	839.9187(−2) <sup>b</sup>	P(8)f	854.5621(−17) <sup>b</sup>						
R(3)f	907.1028(2) <sup>b</sup>	P(6)e	863.9712(−5) <sup>b</sup>	P(4)f	873.1726(4) <sup>b</sup>	P(11)f	839.9450(5) <sup>b</sup>						

$R(2)f$	903.1080(46) <sup>b</sup>	$P(8)e$	854.5362(-14) <sup>b</sup>	$P(6)f$	863.9953(1) <sup>b</sup>				
$^{40}\text{CaD } v = 3 - 2$									
$R(17)e$	933.5079(2) <sup>b</sup>	$R(10)e$	912.4248(1) <sup>b</sup>	$R(16)f$	930.7533(-2) <sup>b</sup>	$R(7)f$	902.0846(-5) <sup>b</sup>	$P(7)e$	840.1543(-37) <sup>b</sup>
$R(16)e$	930.7643(-3) <sup>b</sup>	$R(7)e$	902.1007(0) <sup>b</sup>	$R(15)f$	927.9166(6) <sup>b</sup>	$R(6)f$	898.4787(-1) <sup>b</sup>	$P(4)f$	853.8293(1) <sup>b</sup>
$R(15)e$	927.9269(18) <sup>b</sup>	$R(6)e$	898.4956(2) <sup>b</sup>	$R(13)f$	921.9767(-1) <sup>b</sup>	$R(5)f$	894.7923(10) <sup>b</sup>	$P(5)f$	849.3431(4) <sup>b</sup>
$R(13)e$	921.9901(-7) <sup>b</sup>	$R(5)e$	894.8111(0) <sup>b</sup>	$R(12)f$	918.8741(0) <sup>b</sup>	$P(4)e$	853.8065(-3) <sup>b</sup>		
$R(12)e$	918.8876(-1) <sup>b</sup>	$R(17)f$	933.4979(1) <sup>b</sup>	$R(10)f$	912.4119(-18) <sup>b</sup>	$P(5)e$	849.3189(9) <sup>b</sup>		
$^{40}\text{CaD } v = 4 - 3$									
$R(15)e$	907.0060(2) <sup>b</sup>	$R(10)e$	891.8955(-1) <sup>b</sup>	$R(15)f$	906.9957(-4) <sup>b</sup>	$R(10)f$	891.8834(-21) <sup>b</sup>		
$R(14)e$	904.1610(-2) <sup>b</sup>	$R(8)e$	885.2468(17) <sup>b</sup>	$R(14)f$	904.1493(-1) <sup>b</sup>	$R(8)f$	885.2333(-2) <sup>b</sup>		
$R(12)e$	898.2017(8) <sup>b</sup>	$R(6)e$	878.2718(-8) <sup>b</sup>	$R(12)f$	898.1886(11) <sup>b</sup>	$R(6)f$	878.2561(-16) <sup>b</sup>		
$R(11)e$	895.0918(2) <sup>b</sup>	$R(5)e$	874.6611(2) <sup>b</sup>	$R(11)f$	895.0786(-1) <sup>b</sup>	$R(5)f$	874.6444(-3) <sup>b</sup>		
$^{88}\text{SrH } v = 1 - 0$									
$R(35)e$	1303.8152(-2)	$R(7)e$	1224.9277(5)	$R(20)f$	1283.4341(-2)	$P(4)e$	1142.7394(-1)	$P(8)e$	1110.3763(-3) <sup>c</sup>
$R(34)e$	1304.1852(-18)	$R(6)e$	1219.0387(0)	$R(19)f$	1280.1917(-3)	$P(5)e$	1134.8616(0)	$P(9)e$	1101.9400(8) <sup>c</sup>
$R(33)e$	1304.2958(-1)	$R(5)e$	1212.9657(3)	$R(18)f$	1276.7279(-1)	$P(6)e$	1126.8398(-2)	$P(11)e$	1084.6805(-9) <sup>c</sup>
$R(32)e$	1304.1538(4)	$R(4)e$	1206.7134(2)	$R(17)f$	1273.0461(-2)	$P(7)e$	1118.6767(0)	$P(2)f$	1158.1783(10)
$R(31)e$	1303.7593(16)	$R(3)e$	1200.2831(14)	$R(16)f$	1269.1486(-1)	$P(8)e$	1110.3762(-1)	$P(3)f$	1150.6041(-5)
$R(30)e$	1303.1187(-7)	$R(2)e$	1193.6814(3)	$R(15)f$	1265.0383(0)	$P(9)e$	1101.9409(-1)	$P(4)f$	1142.8775(-4)
$R(29)e$	1302.2274(3)	$R(1)e$	1186.9088(1)	$R(14)f$	1260.7179(1)	$P(10)e$	1093.3744(-1)	$P(5)f$	1135.0028(4)
$R(28)e$	1301.0921(1)	$R(0)e$	1179.9687(2)	$R(13)f$	1256.1907(0)	$P(11)e$	1084.6798(-2)	$P(6)f$	1126.9847(2)
$R(27)e$	1299.7137(0)	$R(13)e$	1256.2493(-5) <sup>c</sup>	$R(12)f$	1251.4591(-1)	$P(12)e$	1075.8598(1)	$P(7)f$	1118.8259(-2)
$R(26)e$	1298.0953(-10)	$R(8)e$	1230.6317(0) <sup>c</sup>	$R(11)f$	1246.5261(0)	$P(13)e$	1066.9186(-2)	$P(8)f$	1110.5283(3)
$R(25)e$	1296.2385(-18)	$R(6)e$	1219.0384(3) <sup>c</sup>	$R(10)f$	1241.3947(2)	$P(14)e$	1057.8581(-1)	$P(9)f$	1102.0970(-1)
$R(24)e$	1294.1428(1)	$R(5)e$	1212.9656(5) <sup>c</sup>	$R(9)f$	1236.0679(4)	$P(15)e$	1048.6821(0)	$P(10)f$	1093.5339(0)
$R(23)e$	1291.8127(29)	$R(2)e$	1193.6814(4) <sup>c</sup>	$R(8)f$	1230.5494(0)	$P(16)e$	1039.3934(0)	$P(11)f$	1084.8425(0)
$R(22)e$	1289.2553(15)	$R(35)f$	1303.8753(36)	$R(7)f$	1224.8414(-1)	$P(17)e$	1029.9951(-1)	$P(12)f$	1076.0260(2)
$R(21)e$	1286.4692(2)	$R(34)f$	1304.2403(9)	$R(6)f$	1218.9470(1)	$P(18)e$	1020.4900(-1)	$P(13)f$	1067.0877(1)
$R(20)e$	1283.4558(1)	$R(33)f$	1304.3487(-11)	$R(5)f$	1212.8701(-1)	$P(19)e$	1010.8810(2)	$P(14)f$	1058.0305(1)
$R(19)e$	1280.2184(2)	$R(32)f$	1304.2003(-1)	$R(4)f$	1206.6130(0)	$P(20)e$	1001.1714(1)	$P(15)f$	1048.8576(0)
$R(18)e$	1276.7601(2)	$R(31)f$	1303.7998(12)	$R(3)f$	1200.1796(-2)	$P(21)e$	991.3636(0)	$P(16)f$	1039.5720(-1)
$R(17)e$	1273.0835(2)	$R(30)f$	1303.1528(-6)	$R(2)f$	1193.5726(-2)	$P(22)e$	981.4605(1)	$P(17)f$	1030.1763(2)
$R(16)e$	1269.1913(1)	$R(29)f$	1302.2558(3)	$R(1)f$	1186.7950(3)	$P(23)e$	971.4647(2)	$P(18)f$	1020.6740(2)
$R(15)e$	1265.0858(5)	$R(28)f$	1301.1148(0)	$R(13)f$	1256.1906(1) <sup>c</sup>	$P(24)e$	961.3789(5)	$P(19)f$	1011.0677(4)
$R(14)e$	1260.7709(2)	$R(27)f$	1299.7294(11)	$R(8)f$	1230.5500(-6) <sup>c</sup>	$P(25)e$	951.2055(11)	$P(20)f$	1001.3608(2)
$R(13)e$	1256.2486(2)	$R(26)f$	1298.1050(5)	$R(6)f$	1218.9469(2) <sup>c</sup>	$P(26)e$	940.9488(3)	$P(21)f$	991.5557(1)
$R(12)e$	1251.5220(1)	$R(25)f$	1296.2385(38)	$R(5)f$	1212.8698(2) <sup>c</sup>	$P(27)e$	930.6094(1)	$P(22)f$	981.6553(-1)
$R(11)e$	1246.5940(0)	$R(24)f$	1294.1428(1)	$R(2)f$	1193.5715(10) <sup>c</sup>	$P(28)e$	920.1938(-38)	$P(23)f$	971.6621(-1)
$R(10)e$	1241.4676(0)	$R(23)f$	1291.8127(-27)	$P(1)e$	1165.4772(-24)	$P(3)e$	1150.4691(5) <sup>c</sup>	$P(24)f$	961.5796(-8)
$R(9)e$	1236.1457(1)	$R(22)f$	1289.2470(-11)	$P(2)e$	1158.0489(3)	$P(4)e$	1142.7403(-10) <sup>c</sup>	$P(25)f$	951.4086(-4)
$R(8)e$	1230.6315(1)	$R(21)f$	1286.4530(0)	$P(3)e$	1150.4698(-1)	$P(7)e$	1118.6767(0) <sup>c</sup>	$P(26)f$	941.1541(-13)
$P(27)f$	930.8169(-17)	$P(30)f$	899.3316(10)	$P(4)f$	1142.8788(-16) <sup>c</sup>	$P(8)f$	1110.5286(0) <sup>c</sup>	$P(11)f$	1084.8427(-2) <sup>c</sup>
$P(28)f$	920.3980(-3)	$P(3)f$	1150.6037(-1) <sup>c</sup>	$P(7)f$	1118.8257(0) <sup>c</sup>	$P(9)f$	1102.0962(7) <sup>c</sup>		
$^{88}\text{SrH } v = 2 - 1$									
$R(29)e$	1262.8801(4)	$R(3)e$	1165.4772(12)	$R(13)f$	1219.7236(-2)	$P(8)e$	1077.4889(-3)	$P(6)f$	1093.7806(2)
$R(28)e$	1261.9373(5)	$R(2)e$	1159.0389(-2)	$R(12)f$	1215.1616(0)	$P(9)e$	1069.2092(-5)	$P(7)f$	1085.7786(-5)

(continued on next page)

Table 1 (continued)

Line	Wavenumber	Line	Wavenumber	Line	Wavenumber	Line	Wavenumber	Line	Wavenumber
<i>R</i> (27) <i>e</i>	1260.7474(23)	<i>R</i> (1) <i>e</i>	1152.4284(−3)	<i>R</i> (11) <i>f</i>	1210.3976(0)	<i>P</i> (10) <i>e</i>	1060.7973(−7)	<i>P</i> (8) <i>f</i>	1077.6368(2)
<i>R</i> (26) <i>e</i>	1259.3197(−10)	<i>R</i> (0) <i>e</i>	1145.6492(8)	<i>R</i> (10) <i>f</i>	1205.4341(4)	<i>P</i> (11) <i>e</i>	1052.2556(1)	<i>P</i> (9) <i>f</i>	1069.3606(0)
<i>R</i> (25) <i>e</i>	1257.6501(−30)	<i>R</i> (13) <i>e</i>	1219.7788(−11) <sup>c</sup>	<i>R</i> (9) <i>f</i>	1200.2746(8)	<i>P</i> (12) <i>e</i>	1043.5891(−2)	<i>P</i> (10) <i>f</i>	1060.9519(1)
<i>R</i> (24) <i>e</i>	1255.7388(−12)	<i>R</i> (11) <i>e</i>	1210.4621(−4) <sup>c</sup>	<i>R</i> (8) <i>f</i>	1194.9229(4)	<i>P</i> (13) <i>e</i>	1034.8001(−6)	<i>P</i> (11) <i>f</i>	1052.4143(1)
<i>R</i> (23) <i>e</i>	1253.5912(14)	<i>R</i> (10) <i>e</i>	1205.5037(−3) <sup>c</sup>	<i>R</i> (7) <i>f</i>	1189.3808(5)	<i>P</i> (14) <i>e</i>	1025.8907(−3)	<i>P</i> (12) <i>f</i>	1043.7512(−3)
<i>R</i> (22) <i>e</i>	1251.2100(48)	<i>R</i> (6) <i>e</i>	1183.7407(−5) <sup>c</sup>	<i>R</i> (6) <i>f</i>	1183.6522(4)	<i>P</i> (15) <i>e</i>	1016.8650(−3)	<i>P</i> (13) <i>f</i>	1034.9647(−1)
<i>R</i> (21) <i>e</i>	1248.6066(1)	<i>R</i> (4) <i>e</i>	1171.7443(−2) <sup>c</sup>	<i>R</i> (5) <i>f</i>	1177.7404(−2)	<i>P</i> (16) <i>e</i>	1007.7257(−4)	<i>P</i> (14) <i>f</i>	1026.0586(0)
<i>R</i> (20) <i>e</i>	1245.7703(6)	<i>R</i> (3) <i>e</i>	1165.4776(9) <sup>c</sup>	<i>R</i> (4) <i>f</i>	1171.6472(3)	<i>P</i> (17) <i>e</i>	998.4754(0)	<i>P</i> (15) <i>f</i>	1017.0361(−2)
<i>R</i> (19) <i>e</i>	1242.7099(4)	<i>R</i> (30) <i>f</i>	1263.6122(4)	<i>R</i> (3) <i>f</i>	1165.3776(−1)	<i>P</i> (18) <i>e</i>	989.1179(−3)	<i>P</i> (16) <i>f</i>	1007.8994(2)
<i>R</i> (18) <i>e</i>	1239.4276(−1)	<i>R</i> (29) <i>f</i>	1262.9115(5)	<i>R</i> (2) <i>f</i>	1158.9344(−9)	<i>P</i> (19) <i>e</i>	979.6546(3)	<i>P</i> (17) <i>f</i>	998.6520(5)
<i>R</i> (17) <i>e</i>	1235.9248(4)	<i>R</i> (28) <i>f</i>	1261.9639(−1)	<i>R</i> (1) <i>f</i>	1152.3193(−7)	<i>P</i> (20) <i>e</i>	970.0903(−3)	<i>P</i> (18) <i>f</i>	989.2975(0)
<i>R</i> (16) <i>e</i>	1232.2061(1)	<i>R</i> (27) <i>f</i>	1260.7709(−9)	<i>R</i> (13) <i>f</i>	1219.7244(−10) <sup>e</sup>	<i>P</i> (21) <i>e</i>	960.4261(−2)	<i>P</i> (19) <i>f</i>	979.8375(1)
<i>R</i> (15) <i>e</i>	1228.2734(0)	<i>R</i> (26) <i>f</i>	1259.3341(−9)	<i>R</i> (11) <i>f</i>	1210.3980(−4) <sup>c</sup>	<i>P</i> (22) <i>e</i>	950.6656(−5)	<i>P</i> (20) <i>f</i>	970.2749(5)
<i>R</i> (14) <i>e</i>	1224.1297(−1)	<i>R</i> (24) <i>f</i>	1255.7388(22)	<i>R</i> (10) <i>f</i>	1205.4341(4) <sup>c</sup>	<i>P</i> (23) <i>e</i>	940.8100(3)	<i>P</i> (21) <i>f</i>	960.6134(4)
<i>R</i> (13) <i>e</i>	1219.7775(2)	<i>R</i> (23) <i>f</i>	1253.5912(−7)	<i>R</i> (6) <i>f</i>	1183.6528(−2) <sup>c</sup>	<i>P</i> (24) <i>e</i>	930.8638(4)	<i>P</i> (22) <i>f</i>	950.8546(9)
<i>R</i> (12) <i>e</i>	1215.2208(−1)	<i>R</i> (22) <i>f</i>	1251.2100(−28)	<i>R</i> (4) <i>f</i>	1171.6477(−2) <sup>c</sup>	<i>P</i> (25) <i>e</i>	920.8328(−38)	<i>P</i> (23) <i>f</i>	941.0026(5)
<i>R</i> (11) <i>e</i>	1210.4621(−5)	<i>R</i> (21) <i>f</i>	1248.5938(−1)	<i>R</i> (3) <i>f</i>	1165.3764(11) <sup>c</sup>	<i>P</i> (26) <i>e</i>	910.7072(3)	<i>P</i> (24) <i>f</i>	931.0589(3)
<i>R</i> (10) <i>e</i>	1205.5034(0)	<i>R</i> (20) <i>f</i>	1245.7532(−6)	<i>P</i> (1) <i>e</i>	1131.4824(−8)	<i>P</i> (27) <i>e</i>	900.5023(−4)	<i>P</i> (25) <i>f</i>	921.0253(11)
<i>R</i> (9) <i>e</i>	1200.3492(−2)	<i>R</i> (19) <i>f</i>	1242.6862(5)	<i>P</i> (2) <i>e</i>	1124.2169(−10)	<i>P</i> (5) <i>e</i>	1101.5038(4) <sup>c</sup>	<i>P</i> (26) <i>f</i>	910.9089(−20)
<i>R</i> (8) <i>e</i>	1195.0016(0)	<i>R</i> (18) <i>f</i>	1239.3989(−3)	<i>P</i> (3) <i>e</i>	1116.7954(2)	<i>P</i> (9) <i>e</i>	1069.2085(2) <sup>c</sup>	<i>P</i> (27) <i>f</i>	900.7029(5)
<i>R</i> (7) <i>e</i>	1189.4644(−1)	<i>R</i> (17) <i>f</i>	1235.8908(3)	<i>P</i> (4) <i>e</i>	1109.2236(4)	<i>P</i> (2) <i>f</i>	1124.3420(−2)	<i>P</i> (5) <i>f</i>	1101.6411(6) <sup>c</sup>
<i>R</i> (6) <i>e</i>	1183.7406(−1)	<i>R</i> (16) <i>f</i>	1232.1670(0)	<i>P</i> (5) <i>e</i>	1101.5041(1)	<i>P</i> (3) <i>f</i>	1116.9254(0)	<i>P</i> (9) <i>f</i>	1069.3603(2) <sup>c</sup>
<i>R</i> (5) <i>e</i>	1177.8322(1)	<i>R</i> (15) <i>f</i>	1228.2289(2)	<i>P</i> (6) <i>e</i>	1093.6393(2)	<i>P</i> (4) <i>f</i>	1109.3577(−1)		
<i>R</i> (4) <i>e</i>	1171.7442(−2)	<i>R</i> (14) <i>f</i>	1224.0803(0)	<i>P</i> (7) <i>e</i>	1085.6333(0)	<i>P</i> (5) <i>f</i>	1101.6412(5)		
<sup>88</sup> SrH $v = 3 - 2$									
<i>R</i> (24) <i>e</i>	1217.0663(−10)	<i>R</i> (10) <i>e</i>	1169.4315(4)	<i>R</i> (10) <i>e</i>	1169.4316(3) <sup>c</sup>	<i>R</i> (10) <i>f</i>	1169.3667(1)	<i>R</i> (6) <i>f</i>	1148.2676(34) <sup>c</sup>
<i>R</i> (23) <i>e</i>	1215.1206(−4)	<i>R</i> (9) <i>e</i>	1164.4508(1)	<i>R</i> (6) <i>e</i>	1148.3535(11) <sup>c</sup>	<i>R</i> (9) <i>f</i>	1164.3811(−1)	<i>R</i> (5) <i>f</i>	1142.5285(−13) <sup>c</sup>
<i>R</i> (22) <i>e</i>	1212.9382(13)	<i>R</i> (8) <i>e</i>	1159.2760(−5)	<i>R</i> (5) <i>e</i>	1142.6168(−14) <sup>e</sup>	<i>R</i> (8) <i>f</i>	1159.2016(−5)	<i>P</i> (2) <i>e</i>	1090.3144(−15)
<i>R</i> (21) <i>e</i>	1210.5245(15)	<i>R</i> (7) <i>e</i>	1153.9090(1)	<i>R</i> (22) <i>f</i>	1212.9382(−28)	<i>R</i> (7) <i>f</i>	1153.8298(2)	<i>P</i> (3) <i>e</i>	1083.0517(0)
<i>R</i> (20) <i>e</i>	1207.8814(10)	<i>R</i> (6) <i>e</i>	1148.3547(−1)	<i>R</i> (20) <i>f</i>	1207.8686(−9)	<i>R</i> (6) <i>f</i>	1148.2703(7)	<i>P</i> (4) <i>e</i>	1075.6371(9)
<i>R</i> (19) <i>e</i>	1205.0114(3)	<i>R</i> (5) <i>e</i>	1142.6151(3)	<i>R</i> (19) <i>f</i>	1204.9920(−3)	<i>R</i> (5) <i>f</i>	1142.5267(5)	<i>P</i> (5) <i>e</i>	1068.0764(−12)
<i>R</i> (18) <i>e</i>	1201.9168(−2)	<i>R</i> (4) <i>e</i>	1136.6946(−1)	<i>R</i> (18) <i>f</i>	1201.8915(−2)	<i>R</i> (4) <i>f</i>	1136.6018(2)	<i>P</i> (6) <i>e</i>	1060.3661(3)
<i>R</i> (17) <i>e</i>	1198.6000(1)	<i>R</i> (3) <i>e</i>	1130.5954(−1)	<i>R</i> (17) <i>f</i>	1198.5704(−8)	<i>R</i> (3) <i>f</i>	1130.4980(3)	<i>P</i> (7) <i>e</i>	1052.5149(−1)
<i>R</i> (16) <i>e</i>	1195.0646(5)	<i>R</i> (2) <i>e</i>	1124.3202(7)	<i>R</i> (16) <i>f</i>	1195.0292(3)	<i>R</i> (2) <i>f</i>	1124.2169(28)	<i>P</i> (8) <i>e</i>	1044.5233(3)
<i>R</i> (15) <i>e</i>	1191.3143(1)	<i>R</i> (1) <i>e</i>	1117.8743(2)	<i>R</i> (15) <i>f</i>	1191.2731(7)	<i>R</i> (1) <i>f</i>	1117.7653(38)	<i>P</i> (9) <i>e</i>	1036.3963(−3)
<i>R</i> (14) <i>e</i>	1187.3512(−1)	<i>R</i> (0) <i>e</i>	1111.2611(−16)	<i>R</i> (14) <i>f</i>	1187.3056(−1)	<i>R</i> (15) <i>f</i>	1191.2736(2) <sup>c</sup>	<i>P</i> (10) <i>e</i>	1028.1359(−8)
<i>R</i> (13) <i>e</i>	1183.1778(4)	<i>R</i> (15) <i>e</i>	1191.3140(4) <sup>c</sup>	<i>R</i> (13) <i>f</i>	1183.1281(−5)	<i>R</i> (13) <i>f</i>	1183.1274(2) <sup>c</sup>	<i>P</i> (11) <i>e</i>	1019.7448(−8)
<i>R</i> (12) <i>e</i>	1178.7987(0)	<i>R</i> (13) <i>e</i>	1183.1778(4) <sup>c</sup>	<i>R</i> (12) <i>f</i>	1178.7423(9)	<i>R</i> (11) <i>f</i>	1174.1552(0) <sup>c</sup>	<i>P</i> (12) <i>e</i>	1011.2261(−2)
<i>R</i> (11) <i>e</i>	1174.2157(−3)	<i>R</i> (11) <i>e</i>	1174.2153(2) <sup>c</sup>	<i>R</i> (11) <i>f</i>	1174.1550(2)	<i>R</i> (10) <i>f</i>	1169.3673(−5) <sup>c</sup>	<i>P</i> (13) <i>e</i>	1002.5837(0)
<i>P</i> (14) <i>e</i>	993.8210(−6)	<i>P</i> (21) <i>e</i>	929.3364(−56)	<i>P</i> (5) <i>f</i>	1068.2084(0)	<i>P</i> (12) <i>f</i>	1011.3835(1)	<i>P</i> (19) <i>f</i>	948.4693(−8)
<i>P</i> (15) <i>e</i>	984.9393(−3)	<i>P</i> (22) <i>e</i>	919.7014(2)	<i>P</i> (6) <i>f</i>	1060.5035(−2)	<i>P</i> (13) <i>f</i>	1002.7444(2)	<i>P</i> (21) <i>f</i>	929.5145(−2)
<i>P</i> (16) <i>e</i>	975.9429(−5)	<i>P</i> (5) <i>e</i>	1068.0748(4) <sup>c</sup>	<i>P</i> (7) <i>f</i>	1052.6551(3)	<i>P</i> (14) <i>f</i>	993.9841(2)	<i>P</i> (22) <i>f</i>	919.8887(−10)
<i>P</i> (17) <i>e</i>	966.8333(3)	<i>P</i> (6) <i>e</i>	1060.3634(30) <sup>c</sup>	<i>P</i> (8) <i>f</i>	1044.6669(9)	<i>P</i> (15) <i>f</i>	985.1060(0)	<i>P</i> (5) <i>f</i>	1068.2080(5) <sup>c</sup>
<i>P</i> (18) <i>e</i>	957.6155(−3)	<i>P</i> (2) <i>f</i>	1090.4373(−26)	<i>P</i> (9) <i>f</i>	1036.5439(−2)	<i>P</i> (16) <i>f</i>	976.1119(5)	<i>P</i> (6) <i>f</i>	1060.5004(29) <sup>c</sup>
<i>P</i> (19) <i>e</i>	948.2890(12)	<i>P</i> (3) <i>f</i>	1083.1780(−6)	<i>P</i> (10) <i>f</i>	1028.2867(−5)	<i>P</i> (17) <i>f</i>	967.0058(6)		
<i>P</i> (20) <i>e</i>	938.8612(0)	<i>P</i> (4) <i>f</i>	1075.7676(−1)	<i>P</i> (11) <i>f</i>	1019.8986(−1)	<i>P</i> (18) <i>f</i>	957.7911(−2)		



<sup>88</sup>SrH v = 4 - 3

R(24)e	1177.8902(-55)	R(9)e	1128.2788(-1)	R(16)f	1157.5371(12)	P(4)e	1041.8301(-43)	P(16)e	943.8728(-19)
R(21)e	1172.0059(-16)	R(8)e	1123.2831(4)	R(15)f	1153.9778(12)	P(5)e	1034.4175(9)	P(5)f	1034.5464(12)
R(19)e	1166.9112(-8)	R(7)e	1118.0963(-12)	R(14)f	1150.2067(-23)	P(6)e	1026.8626(6)	P(7)f	1019.2977(24)
R(18)e	1164.0180(25)	R(6)e	1112.7162(5)	R(13)f	1146.2172(5)	P(7)e	1019.1634(2)	P(8)f	1011.4612(13)
R(17)e	1160.9063(-2)	R(5)e	1107.1519(-1)	R(12)f	1142.0232(-11)	P(8)e	1011.3219(6)	P(9)f	1003.4871(-5)
R(16)e	1157.5700(2)	R(4)e	1101.4051(-16)	R(11)f	1137.6222(-16)	P(9)e	1003.3405(26)	P(10)f	995.3764(-9)
R(15)e	1154.0154(5)	R(24)f	1177.8902(47)	R(10)f	1133.0159(5)	P(10)e	995.2297(-11)	P(11)f	987.1326(-4)
R(14)e	1150.2468(-5)	R(22)f	1174.1989(26)	R(9)f	1128.2128(-1)	P(11)e	986.9819(1)	P(12)f	978.7597(-1)
R(13)e	1146.2652(-7)	R(21)f	1171.9956(27)	R(8)f	1123.2141(-13)	P(12)e	978.6061(2)	P(13)f	970.2620(-10)
R(12)e	1142.0733(4)	R(19)f	1166.8947(-8)	R(7)f	1118.0204(-5)	P(13)e	970.1061(-17)	P(14)f	961.6404(-14)
R(11)e	1137.6753(17)	R(18)f	1163.9992(-3)	R(6)f	1112.6384(-13)	P(14)e	961.4837(-45)	P(15)f	952.8963(3)
R(10)e	1133.0775(2)	R(17)f	1160.8823(-30)	R(4)f	1101.3140(9)	P(15)e	952.7341(-3)	P(16)f	944.0355(12)

<sup>87</sup>SrH v = 1 - 0

R(25)e	1296.3254(-36)	R(11)e	1246.6762(5)	R(1)f	1186.8699(12)	P(13)e	1066.9786(-6)	P(10)f	1093.5935(37)
R(24)e	1294.2283(-2)	R(10)e	1241.5506(-9)	P(3)e	1150.5393(14)	P(17)e	1030.0497(-3)	P(11)f	1084.9040(7)
R(20)e	1283.5401(9)	R(8)e	1230.7127(-1)	P(5)e	1134.9314(-9)	P(19)e	1010.9312(17)	P(12)f	1076.0865(5)
R(19)e	1280.3062(-25)	R(6)e	1219.1198(-15)	P(6)e	1126.9094(-19)	P(22)e	981.5080(1)	P(13)f	1067.1461(14)
R(18)e	1276.8441(11)	R(25)f	1296.3254(20)	P(7)e	1118.7440(-5)	P(25)e	951.2517(-18)	P(16)f	1039.6291(-14)
R(16)e	1269.2771(-12)	R(24)f	1294.2283(-2)	P(9)e	1102.0056(-3)	P(5)f	1135.0766(-44)	P(17)f	1030.2263(47)
R(14)e	1260.8546(4)	R(18)f	1276.8125(3)	P(10)e	1093.4394(-18)	P(7)f	1118.8973(-47)	P(21)f	991.6041(7)
R(13)e	1256.3306(16)	R(14)f	1260.8008(11)	P(11)e	1084.7417(1)	P(8)f	1110.5927(16)	P(22)f	981.7028(0)
R(12)e	1251.6056(-4)	R(13)f	1256.2751(-9)	P(12)e	1075.9220(-12)	P(9)f	1102.1652(-38)	P(23)f	971.7088(-6)

<sup>86</sup>SrH v = 1 - 0

R(24)e	1294.3147(9)	R(11)e	1246.7605(9)	R(22)f	1289.4189(-2)	R(10)f	1241.5603(9)	P(9)e	1102.0724(-8)
R(23)e	1291.9856(28)	R(10)e	1241.6342(-3)	R(21)f	1286.6265(-7)	R(9)f	1236.2311(24)	P(10)e	1093.5031(-5)
R(22)e	1289.4311(-14)	R(9)e	1236.3113(-3)	R(20)f	1283.6060(7)	R(8)f	1230.7127(7)	P(11)e	1084.8059(-4)
R(21)e	1286.6412(11)	R(8)e	1230.7954(3)	R(19)f	1280.3654(-15)	R(7)f	1225.0058(-18)	P(12)e	1075.9834(0)
R(19)e	1280.3919(-8)	R(7)e	1225.0908(2)	R(18)f	1276.8995(5)	R(6)f	1219.1086(-1)	P(13)e	1067.0399(-7)
R(18)e	1276.9319(6)	R(6)e	1219.1989(12)	R(17)f	1273.2169(7)	R(5)f	1213.0311(-11)	P(14)e	1057.9769(-5)
R(17)e	1273.2574(-21)	R(5)e	1213.1259(1)	R(16)f	1269.3199(-2)	R(4)f	1206.7717(-2)	P(15)e	1048.7991(-14)
R(16)e	1269.3612(14)	R(4)e	1206.8728(-7)	R(15)f	1265.2101(-12)	R(3)f	1200.3350(14)	P(16)e	1039.5070(-6)
R(15)e	1265.2577(-8)	R(3)e	1200.4396(17)	R(14)f	1260.8884(-4)	R(2)f	1193.7286(-8)	P(17)e	1030.1072(-19)
R(14)e	1260.9396(15)	R(2)e	1193.8392(-21)	R(13)f	1256.3602(-3)	P(1)e	1165.6240(-12)	P(18)e	1020.5982(-6)
R(13)e	1256.4184(-4)	R(24)f	1294.3147(9)	R(12)f	1251.6268(6)	P(7)e	1118.8139(-18)	P(19)e	1010.9853(7)
R(12)e	1251.6910(-6)	R(23)f	1291.9856(-28)	R(11)f	1246.6951(-16)	P(8)e	1110.5108(-17)	P(20)e	1001.2741(-6)
P(21)e	991.4622(6)	P(8)f	1110.6621(-4)	P(13)f	1067.2093(-6)	P(18)f	1020.7800(18)	P(23)f	971.7547(8)
P(4)f	1143.0173(19)	P(9)f	1102.2290(-14)	P(14)f	1058.1489(0)	P(19)f	1011.1733(-3)		
P(5)f	1135.1431(-1)	P(10)f	1093.6631(-9)	P(15)f	1048.9744(-11)	P(20)f	1001.4644(-12)		
P(6)f	1127.1205(21)	P(11)f	1084.9691(-6)	P(16)f	1039.6849(0)	P(21)f	991.6576(-25)		
P(7)f	1118.9622(-11)	P(12)f	1076.1488(8)	P(17)f	1030.2876(-8)	P(22)f	981.7505(12)		

<sup>88</sup>SrH

v'	N'	p'	v''	N''	p''	v'	N'	p'	v''	N''	p''
0	1	e	0	0	e	1	2	e	1	1	e
0	2	e	0	1	e	1	2	f	1	1	f
0	1	f	0	0	e	1	1	f	0	0	e
											14.268285(-1) <sup>f</sup>
											14.148543(1) <sup>f</sup>
											1179.7891(0)

(continued on next page)

Table 1 (continued)

Line	Wavenumber		Line	Wavenumber		Line	Wavenumber		Line	Wavenumber			
0	2	<i>f</i>	0	1	<i>f</i>		1	0	<i>e</i>	0	1	<i>f</i>	1165.6634(–27)
<sup>86</sup> SrH													
<i>v'</i>	<i>N'</i>	<i>p'</i>	<i>v''</i>	<i>N''</i>	<i>P''</i>								
0	2	<i>e</i>	0	1	<i>e</i>								14.595189(–1) <sup>f</sup>
<sup>86</sup> SrD													
<i>v'</i>	<i>N'</i>	<i>p'</i>	<i>v''</i>	<i>N''</i>	<i>P''</i>	<i>v'</i>	<i>N'</i>	<i>p'</i>	<i>v''</i>	<i>N''</i>	<i>P''</i>		
0	3	<i>e</i>	0	2	<i>e</i>	0	4	<i>e</i>	0	3	<i>e</i>		14.800171(3) <sup>f</sup>
<sup>88</sup> SrD													
<i>v'</i>	<i>N'</i>	<i>p'</i>	<i>v''</i>	<i>N''</i>	<i>P''</i>	<i>v'</i>	<i>N'</i>	<i>p'</i>	<i>v''</i>	<i>N''</i>	<i>P''</i>		
0	3	<i>e</i>	0	2	<i>e</i>	0	4	<i>f</i>	0	3	<i>f</i>		14.729609(–4) <sup>f</sup>
0	4	<i>e</i>	0	3	<i>e</i>	1	4	<i>e</i>	1	3	<i>e</i>		14.560702(8) <sup>f</sup>
<sup>88</sup> SrD <i>v</i> = 1 – 0													
<i>R</i> (1) <i>e</i>	848.8145(12) <sup>g</sup>		<i>R</i> (10) <i>e</i>	878.2188(–4) <sup>g</sup>		<i>R</i> (8) <i>f</i>	872.0829(2) <sup>g</sup>		<i>P</i> (4) <i>e</i>	826.4335(3) <sup>g</sup>		<i>P</i> (15) <i>f</i>	780.6339(1) <sup>g</sup>
<i>R</i> (3) <i>e</i>	855.7882(–12) <sup>g</sup>		<i>R</i> (1) <i>f</i>	848.7563(1) <sup>g</sup>		<i>R</i> (10) <i>f</i>	878.1738(–4) <sup>g</sup>		<i>P</i> (3) <i>e</i>	830.2964(–13) <sup>g</sup>		<i>P</i> (4) <i>f</i>	826.5010(9) <sup>g</sup>
<i>R</i> (4) <i>e</i>	859.1799(15) <sup>g</sup>		<i>R</i> (3) <i>f</i>	855.7312(–5) <sup>g</sup>		<i>P</i> (16) <i>e</i>	776.0922(–1) <sup>g</sup>		<i>P</i> (2) <i>e</i>	834.1002(10) <sup>g</sup>		<i>P</i> (3) <i>f</i>	830.3630(–12) <sup>g</sup>
<i>R</i> (8) <i>e</i>	872.1316(–2) <sup>g</sup>		<i>R</i> (4) <i>f</i>	859.1261(6) <sup>g</sup>		<i>P</i> (15) <i>e</i>	780.5517(–3) <sup>g</sup>		<i>P</i> (16) <i>f</i>	776.1762(–4) <sup>g</sup>		<i>P</i> (2) <i>f</i>	834.1660(4) <sup>g</sup>
<sup>88</sup> SrD <i>v</i> = 2 – 1													
<i>R</i> (4) <i>e</i>	841.6044(11) <sup>g</sup>		<i>R</i> (17) <i>e</i>	879.0299(1) <sup>g</sup>		<i>R</i> (8) <i>f</i>	854.2738(2) <sup>g</sup>		<i>P</i> (17) <i>e</i>	755.2681(3) <sup>g</sup>			
<i>R</i> (5) <i>e</i>	844.8788(7) <sup>g</sup>		<i>R</i> (21) <i>e</i>	888.1630(–9) <sup>g</sup>		<i>R</i> (10) <i>f</i>	860.2468(–6) <sup>g</sup>		<i>P</i> (15) <i>e</i>	764.1206(–2) <sup>g</sup>			
<i>R</i> (8) <i>e</i>	854.3218(–10) <sup>g</sup>		<i>R</i> (4) <i>f</i>	841.5509(14) <sup>g</sup>		<i>R</i> (17) <i>f</i>	878.9986(–1) <sup>g</sup>		<i>P</i> (17) <i>f</i>	755.3524(–7) <sup>g</sup>			
<i>R</i> (10) <i>e</i>	860.2911(–14) <sup>g</sup>		<i>R</i> (5) <i>f</i>	844.8264(15) <sup>g</sup>		<i>R</i> (21) <i>f</i>	888.1382(–5) <sup>g</sup>		<i>P</i> (15) <i>f</i>	764.2016(–2) <sup>g</sup>			
<sup>88</sup> SrD <i>v</i> = 3 – 2													
<i>R</i> (6) <i>e</i>	830.3966(–9) <sup>g</sup>		<i>R</i> (15) <i>e</i>	855.7882(23) <sup>g</sup>		<i>R</i> (8) <i>f</i>	836.4617(0) <sup>g</sup>		<i>R</i> (17) <i>f</i>	860.6415(1) <sup>g</sup>		<i>P</i> (7) <i>f</i>	780.8316(5) <sup>g</sup>
<i>R</i> (8) <i>e</i>	836.5066(5) <sup>g</sup>		<i>R</i> (17) <i>e</i>	860.6714(3) <sup>g</sup>		<i>R</i> (11) <i>f</i>	845.1414(–12) <sup>g</sup>		<i>R</i> (26) <i>f</i>	878.9378(4) <sup>g</sup>		<i>P</i> (5) <i>f</i>	788.5928(1) <sup>g</sup>
<i>R</i> (11) <i>e</i>	845.1819(–12) <sup>g</sup>		<i>R</i> (26) <i>e</i>	878.9519(1) <sup>g</sup>		<i>R</i> (14) <i>f</i>	853.2071(3) <sup>g</sup>		<i>P</i> (7) <i>e</i>	780.7621(8) <sup>g</sup>			
<i>R</i> (14) <i>e</i>	853.2432(–4) <sup>g</sup>		<i>R</i> (6) <i>f</i>	830.3474(–3) <sup>g</sup>		<i>R</i> (15) <i>f</i>	855.7564(4) <sup>g</sup>		<i>P</i> (5) <i>e</i>	788.5269(–5) <sup>g</sup>			

<sup>a</sup> Calculated minus observed values of the line positions computed with the Dunham constants of Tables 5 and 6.

<sup>b</sup> From Ref. [81].

<sup>c</sup> From Ref. [84], see text.

<sup>d</sup> From Ref. [83], see text.

<sup>e</sup> From Ref. [85].

<sup>f</sup> From Ref. [87], see text.

<sup>g</sup> From Ref. [86].

Table 2  
Spectroscopic constants (in  $\text{cm}^{-1}$ ) for the  $X^2\Sigma^+$  ground state of  $^{40}\text{CaH}$  (all uncertainties are  $2\sigma$ )

$v$	$T_v$	$B_v$	$10^4 D_v$	$10^9 H_v$	$10^{13} L_v$	$10^2 \gamma_v$	$10^6 \gamma_{D,v}$
0	0.0	4.2286902(7)	1.851405(150)	6.835(31)	−4.11(18)	4.3566(2)	−5.04(12)
1	1260.12775(22)	4.1317220(39)	1.84939(19)	6.819(32)	−4.3(2)	4.211(2)	−5.02(13)
2	2481.99888(30)	4.0342454(60)	1.84957(31)	6.774(55)	−4.7(3)	4.065(4)	−5.02(14)
3	3665.4141(4)	3.935887(9)	1.85277(56)	6.61(13)	−4.9(9)	3.920(5)	−5.1(2)
4	4809.9464(6)	3.836122(12)	1.86000(64)	5.94(9)	–	3.777(9)	−5.5(3)

Table 3  
Spectroscopic constants (in  $\text{cm}^{-1}$ ) for the  $X^2\Sigma^+$  ground state of  $^{88}\text{SrH}$  (all uncertainties are  $2\sigma$ )

$v$	$T_v$	$B_v$	$10^4 D_v$	$10^9 H_v$	$10^{13} L_v$	$10^2 \gamma_v$	$10^6 \gamma_{D,v}$
0	0.0	3.6334432(16)	1.35664(21)	3.959(47)	−1.52(29)	12.3991(8)	−11.37(13)
1	1172.80311(17)	3.5531837(17)	1.35436(18)	3.946(38)	−1.7(2)	11.9871(13)	−11.23(12)
2	2311.45036(29)	3.4726241(50)	1.35330(27)	3.951(50)	−2.2(3)	11.580(3)	−11.14(12)
3	3415.8717(4)	3.391531(6)	1.35282(26)	3.61(3)	–	11.179(5)	−11.3(2)
4	4485.8394(11)	3.309615(17)	1.3558(7)	3.46(8)	–	10.762(10)	−10.7(3)

determined for these vibrational levels. The spectral lines corresponding to  $e$  and  $f$  parity components of the same rotational transition were fully resolved in the SrH spectrum. However, in the CaH spectrum, the splitting was not resolved in about one third of the R branch lines, and the DPARFIT program was modified so that the spin-rotation interaction constants ( $\gamma$  and  $\gamma_D$ ) were not fitted for the unresolved lines of CaH and CaD. In order to minimize the number of digits, the constants of Tables 2 and 3 have been sequentially rounded and refitted [91] starting from the highest order parameter of the highest observed vibrational level. The new constants of the  $v=0$  level and the fundamental band origin ( $\nu_{1\rightarrow 0}$ ) of  $^{40}\text{CaH}$  and  $^{88}\text{SrH}$  are compared with previous studies in Table 4. The new  $B_0$  and  $\gamma_0$  constants are very precise because we included all the pure rotational data [83,84,87] in our fits, and in addition to that, we obtained a more complete set of band constants for the  $v=0$  to 4 levels.

The next step was to combine all the data of CaH with CaD, and SrH with SrD in Dunham fits. The energy expression for a  $^2\Sigma^+$  state is different from the ordinary Dunham expansion because of the spin-rotation interaction term in the Hamiltonian operator. The energy expressions,

$$E_{v,N} = \sum_{l,m} Y_{l,m} \left( v + \frac{1}{2} \right)^l [N(N+1)]^m + \frac{1}{2} (N) \sum_{l,m} \gamma_{l,m} \left( v + \frac{1}{2} \right)^l [N(N+1)]^{m-1} \quad (2)$$

$$E_{v,N} = \sum_{l,m} Y_{l,m} \left( v + \frac{1}{2} \right)^l [N(N+1)]^m - \frac{1}{2} (N+1) \times \sum_{l,m} \gamma_{l,m} \left( v + \frac{1}{2} \right)^l [N(N+1)]^{m-1} \quad (3)$$

were used for  $e$  ( $J = N + 1/2$ ) and  $f$  ( $J = N - 1/2$ ) parities, respectively. As formulated by Le Roy [92], the Dunham

Table 4  
A comparison of some  $^{40}\text{CaH}$  and  $^{88}\text{SrH}$  constants (all values are in  $\text{cm}^{-1}$ , and all uncertainties are  $2\sigma$ )

	$\nu_{1\rightarrow 0}$	$B_0$	$10^4 D_0$	$10^9 H_0$	$10^{13} L_0$	$10^2 \gamma_0$	$10^6 \gamma_{D,0}$
$^{40}\text{CaH}$							
This work	1260.12775(22)	4.2286902(7)	1.851405(150)	6.835(31)	−4.11(18)	4.3566(2)	−5.04(12)
Ref. [84]	–	4.22868994(24)	1.850 <sup>a</sup>	–	–	4.355530(62)	–
Ref. [83]	–	4.2286893(13)	1.84985(100)	6.30(24)	–	4.35668(80)	−4.84(80)
Ref. [82]	1260.12859(110)	4.228689(44)	1.8498(26)	6.27(46)	–	4.3569(174)	4.50(96)
Ref. [81]	1260.1277(70)	4.22865(100)	1.850(26)	5.9 <sup>b</sup>	–	4.670(116)	–
$^{88}\text{SrH}$							
This work	1172.80311(17)	3.6334432(16)	1.35664(21)	3.959(47)	−1.52(29)	12.3991(8)	−11.37(13)
Ref. [87]	1172.80608(31)	3.63344198(99)	1.35450(89)	3.536(180) <sup>c</sup>	–	12.39878(63)	−11.22(66) <sup>c</sup>

<sup>a</sup> Fixed to the value taken from Ref. [81].

<sup>b</sup> Fixed to  $Y_{0,3}$  value.

<sup>c</sup> Common for  $v=0$  and 1.

constants of two isotopomers of the A–B molecule are related via the following equation:

$$Y_{l,m}^\alpha = \left\{ Y_{l,m}^1 + \frac{\Delta M_A^\alpha}{M_A^\alpha} \delta_{l,m}^A + \frac{\Delta M_B^\alpha}{M_B^\alpha} \delta_{l,m}^B \right\} \left( \frac{\mu_1}{\mu_\alpha} \right)^{m+l/2}. \quad (4)$$

The  $\delta_{l,m}$ 's are the Born–Oppenheimer breakdown parameters for the atoms A and B with masses  $M_A$  and  $M_B$ , and  $\mu$ 's are reduced masses. The index 1 is for the main (reference) isotopomer and  $\alpha$  is the index for the other isotopomer(s). The  $\gamma_{l,m}$  constants of two isotopomers are related by a reduced mass relationship

$$\gamma_{l,m}^\alpha = \gamma_{l,m}^1 \left( \frac{\mu_1}{\mu_\alpha} \right)^{m+l/2}. \quad (5)$$

For the CaH and CaD molecules, only one isotope of calcium ( $^{40}\text{Ca}$ ) has been observed, and Eq. (4) becomes simpler

$$Y_{l,m}^{\text{CaD}} = \left\{ Y_{l,m}^{\text{CaH}} + \frac{M_D - M_H}{M_D} \delta_{l,m}^{\text{H}} \right\} \left( \frac{\mu_{\text{CaH}}}{\mu_{\text{CaD}}} \right)^{m+l/2}. \quad (6)$$

The Dunham constants of  $^{40}\text{CaH}$  and  $^{40}\text{CaD}$ , and the Born–Oppenheimer breakdown constants ( $\delta_{l,m}^{\text{H}}$ ) have been

determined in a combined fit using the DPARFIT program [90], and are compared with the constants of Petitprez et al. [81] in Table 5. For the SrH and SrD molecules, we combined the data of five isotopomers, and performed a similar fit. The Dunham constants of  $^{88}\text{SrH}$  and  $^{88}\text{SrD}$ , and the Born–Oppenheimer breakdown constants are presented in Table 6, and compared with the previously determined constants [85,86]. Only the constants of  $^{40}\text{CaH}$  and  $^{88}\text{SrH}$  and the Born–Oppenheimer breakdown parameters in Tables 5 and 6 were fitted to experimental data, and the constants of  $^{40}\text{CaD}$  and  $^{88}\text{SrD}$  are derived using Eqs. (4)–(6) and the constants of the corresponding hydrides. By using the sequential rounding and refitting technique [91], starting from the parameter with largest relative uncertainty, we minimized the number of digits required for  $^{40}\text{CaH}$  and  $^{88}\text{SrH}$  constants in Tables 5 and 6. Of course, the derived Dunham constants for  $^{40}\text{CaD}$  and  $^{88}\text{SrD}$  require more digits as determined by the parameter sensitivities [91]. No Born–Oppenheimer breakdown correction for strontium isotopic species was required ( $\delta_{l,m}^{\text{Sr}} = 0$ ), and, therefore, the Dunham constants of  $^{87}\text{SrH}$  and  $^{86}\text{SrH}$  are related to those of  $^{88}\text{SrH}$  by simple reduced mass ratios, and are not shown in Table 6.

Table 5

Dunham and Born–Oppenheimer breakdown constants (in  $\text{cm}^{-1}$ ) for the  $X^2\Sigma^+$  ground state of  $^{40}\text{CaH}$  and  $^{40}\text{CaD}$  (all uncertainties are  $2\sigma$ )

	$^{40}\text{CaH}$		$^{40}\text{CaD}$	
	This work	Ref. [81]	This work	Ref. [81]
$Y_{1,0}$	1298.39996(130)	1298.3999(80)	929.903553	929.9312(90)
$Y_{2,0}$	−19.18099(100)	−19.1842(56)	−9.813622	−9.8342(34)
$10^2 Y_{3,0}$	4.210(31)	4.373(172)	1.03831	1.605(64)
$10^3 Y_{4,0}$	−9.426(31)	−9.635(174)	−2.01787	2.532(46)
$Y_{0,1}$	4.2770434(38)	4.277019(138)	2.19469905	2.194646(140)
$10^2 Y_{1,1}$	−9.66314(98)	−9.6894(40)	−3.548718	−3.5593(28)
$10^4 Y_{2,1}$	−1.486(58)	1.051(164)	−0.390573	0.276(44)
$10^2 Y_{3,1}$	0.00(15)	−7.665(194)	0.00	−1.442(36)
$10^6 Y_{4,1}$	−7.473(130)	−	−1.00698	−
$10^4 Y_{0,2}$	−1.85266(20)	−1.8471(112)	−0.48831	−0.48549(94)
$10^7 Y_{1,2}$	2.42(26)	4.29(38)	0.45543	0.807(70)
$10^8 Y_{2,2}$	1.30(76)	−15.15(150)	0.17517	−2.04(20)
$10^8 Y_{3,2}$	−2.429(81)	−	−0.234354	−
$10^9 Y_{0,3}$	6.814(38)	5.900(184)	0.918178	0.795(24)
$10^{11} Y_{1,3}$	7.7(31)	−	0.7429	−
$10^{11} Y_{2,3}$	−3.58(36)	−	−0.24731	−
$10^{13} Y_{0,4}$	−4.0(2)	−	−0.27633	−
$10^{14} Y_{1,4}$	−3.0(13)	−	−0.14839	−
$10^2 \gamma_{0,1}$	4.4280(9)	4.391(140)	2.270122	2.251(72)
$10^3 \gamma_{1,1}$	−1.425(18)	−1.719(146)	−0.52309	−0.631(54)
$10^6 \gamma_{2,1}$	−9.0(43)	−	−2.37	−
$10^6 \gamma_{0,2}$	−5.0(1)	84.5(26)	−1.314	2.22(72)
$\delta_{1,0}^{\text{H}}$	0.6501(53)	−	−	−
$\delta_{2,0}^{\text{H}}$	0.078(6)	−	−	−
$10^2 \delta_{3,0}^{\text{H}}$	−2.765(240)	−	−	−
$10^3 \delta_{4,0}^{\text{H}}$	3.5(3)	−	−	−
$\delta_{0,1}^{\text{H}}$	0.007686(3)	−	−	−
$10^2 \delta_{1,1}^{\text{H}}$	−0.0085(7)	−	−	−
$10^4 \delta_{0,2}^{\text{H}}$	−0.0104(7)	−	−	−

Table 6

Dunham and Born–Oppenheimer breakdown constants (in  $\text{cm}^{-1}$ ) for the  $X^2\Sigma^+$  ground state of  $^{88}\text{SrH}$  and  $^{88}\text{SrD}$  (all uncertainties are  $2\sigma$ )

	$^{88}\text{SrH}$		$^{88}\text{SrD}$	
	This work	Ref. [85]	This work	Ref. [86]
$Y_{1,0}$	1207.03454(140)	1206.8912(30)	858.896638	858.8547(28)
$Y_{2,0}$	−17.16492(110)	−17.02566(186)	−8.678401	−8.63901(168)
$10^2 Y_{3,0}$	4.030(35)	−1.162(30)	1.34104	−0.056(26)
$10^3 Y_{4,0}$	−6.505(38)	–	−1.665827	–
$Y_{0,1}$	3.6734952(35)	3.673447(44)	1.86067025	1.860651(80)
$10^2 Y_{1,1}$	−8.00602(78)	−8.0132(32)	−2.883574	−2.8822(26)
$10^4 Y_{2,1}$	−0.882(56)	0.223(182)	−0.225866	−0.304(58)
$10^5 Y_{3,1}$	0.00(15)	−4.02(30)	0.00	–
$10^6 Y_{4,1}$	−4.456(160)	–	−0.57746	–
$10^4 Y_{0,2}$	−1.35785(23)	−1.3505(28)	−0.348875	−0.3506(24)
$10^7 Y_{1,2}$	2.37(16)	0.0 <sup>a</sup>	0.43174	1.29(84)
$10^8 Y_{2,2}$	1.60(69)	–	0.20735	−3.17(138)
$10^8 Y_{3,2}$	−1.35(8)	–	−0.124452	–
$10^9 Y_{0,3}$	3.955(52)	3.03(38)	0.512531	0.91(50)
$10^{11} Y_{1,3}$	3.0(17)	–	0.27656	–
$10^{11} Y_{2,3}$	−2.01(29)	–	−0.13181	–
$10^{13} Y_{0,4}$	−1.5(3)	–	−0.09837	–
$10^{14} Y_{1,4}$	−1.8(8)	–	−0.08397	–
$10^2 \gamma_{0,1}$	12.605(2)	12.622(84)	6.37873	6.376(90)
$10^3 \gamma_{1,1}$	−4.131(19)	−4.062(76)	−1.48711	−1.476(60)
$10^6 \gamma_{2,1}$	9.0(44)	–	2.3	–
$10^6 \gamma_{0,2}$	−11.4(2)	−11.6(32)	−2.919	−2.60(146)
$10^7 \gamma_{1,2}$	1.3(2)	–	0.2368	–
$\delta_{1,0}^{\text{H}}$	0.6987(38)	–	–	–
$\delta_{2,0}^{\text{H}}$	0.0311(31)	–	–	–
$10^2 \delta_{3,0}^{\text{H}}$	−0.61(7)	–	–	–
$\delta_{0,1}^{\text{H}}$	0.006753(5)	–	–	–
$10^2 \delta_{1,1}^{\text{H}}$	−0.0084(7)	–	–	–
$10^4 \delta_{0,2}^{\text{H}}$	−0.009(1)	–	–	–

<sup>a</sup> Fixed to zero.

#### 4. Discussion

Having a more complete set of data for  $v = 0$  to 4 of  $^{40}\text{CaH}$  and  $^{88}\text{SrH}$ , we were able to determine a more reliable set of band constants for these vibrational levels compared to the previous work [81–84,87]. The new experimental data allowed us to determine higher order Dunham constants for the ground states of  $\text{CaH}$  and  $\text{SrH}$ , and by including the pure rotational data we were able to determine the equilibrium rotational constants ( $B_e \approx Y_{0,1}$ ) with high precision. Using the  $B_e$  values of  $^{40}\text{CaH}$  and  $^{88}\text{SrH}$ , we calculated the equilibrium bond distances ( $r_e$ ) to be 2.0023603(9) Å for  $\text{CaH}$  and 2.1460574(10) Å for  $\text{SrH}$ . The  $Y_{3,1}$  constants in both  $\text{CaH}$  and  $\text{SrH}$  are very small (smaller than their uncertainties), but the higher order  $Y_{4,1}$  constants are larger. In the sequential rounding and refitting process, the  $Y_{3,1}$  constants have been rounded to zero for both  $\text{CaH}$  and  $\text{SrH}$ .

The Born–Oppenheimer breakdown constants for hydrogen atom ( $\delta_{l,m}^{\text{H}}$ ) are large, which is expected for diatomic hydrides with small reduced masses. In fact, for both  $\text{CaH}$  and  $\text{SrH}$ , the number of Born–Oppenheimer breakdown

parameters required for the vibrational energy ( $\delta_{l,0}^{\text{H}}$ ) is equal to the number of observed vibrational intervals in the  $\text{CaD}$  [81] and  $\text{SrD}$  [86] infrared spectra. Therefore, the simple reduced mass ratio is not appropriate for the Dunham constants representing the vibrational energy ( $Y_{l,0}$ ) in this range of the potential well. However, fewer correction parameters were required for the rotational and centrifugal distortion constants ( $Y_{l,1}$  and  $Y_{l,2}$ ). The reduced mass relationship in Eq. (5) for the spin-rotation interaction constants ( $\gamma_{l,m}$ ) was satisfactory, and no correction was required for those constants.

Although  $\text{BeH}_2$  and  $\text{MgH}_2$  molecules are linear [6,7,9], theoretical calculations have predicted bent structures for  $\text{SrH}_2$  and  $\text{BaH}_2$  [1–3]. In the case of  $\text{CaH}_2$ , the results from different studies are not consistent with each other. Three ab initio calculations predicted a linear structure for  $\text{CaH}_2$  [1,3,5], and in another study by Bytheway et al. [2] the H–Ca–H bond angle was calculated to be 157 degrees. The infrared spectrum of  $\text{CaH}_2$  trapped in krypton and xenon matrices at 12 K was recorded by Xiao et al. [93], and assuming a bent structure for this molecule, they assigned a very weak absorption band to the symmetric stretching mode of  $\text{CaH}_2$ .

Table 7

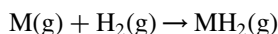
A comparison of bond lengths and atomization energies of alkaline earth hydrides ( $2\sigma$  uncertainties are reported for all experimental values)

Metal	$r_e$ (Å) M–H	Ref.	$r_e$ (Å) H–M–H	Ref.	Atomization energy of $MH_2(g)$ (kcal/mol)	Ref.	$\Delta E$ (kcal/mol) $M(g) + H_2(g) \rightarrow MH_2(g)$	$MH_2(g)$ Observed?
Be	1.342436(2)	[8]	1.326407(6)	[7]	140.9	[97]	–37.6 <sup>a</sup>	Yes
Mg	1.7297612(9)	[95]	[1.703327(6)] <sup>b</sup>	[9]	98.6	[98]	+4.7 <sup>a</sup>	Yes
Ca	2.0023603(9) <sup>c</sup>		2.03	[1]	84.2 <sup>d</sup>	[5]	+19.1 <sup>a</sup>	No
Sr	2.146057(1) <sup>c</sup>		2.18	[1]	–		–	No
Ba	2.231882(2)	[96]	2.27	[1]	–		–	No

<sup>a</sup> Calculated using the dissociation energy of  $H_2$  (103.3 kcal/mol) from Ref. [94].<sup>b</sup>  $r_0$  value from Ref. [9].<sup>c</sup> This work.<sup>d</sup> A slightly different value (81.3 kcal/mol) is reported in Ref. [4].

One of our goals in this work was to record the vibration–rotation emission spectra of gaseous  $CaH_2$ ,  $SrH_2$  and  $BaH_2$  to determine their structures. Although we observed the vibration–rotation transitions of  $CaH$ ,  $SrH$  and  $BaH$  with high signal-to-noise ratios, no metal dihydride was found in the spectra.

We have compared molecular properties of alkaline earth hydrides in Table 7 to investigate the reason why we could not observe  $CaH_2$ ,  $SrH_2$  and  $BaH_2$  in the gas phase. It can be seen in Table 7 that the M–H bond distances change very slightly from  $MH(g)$  to  $MH_2(g)$  because the unpaired electron of the metal monohydride is in a non-bonding molecular orbital. Furthermore, as the M–H bond distance increases from Be to Ca, the total atomization energy of  $MH_2(g)$  decreases (Table 7). The dissociation energy of  $H_2(g)$  is 103.3 kcal/mol [94], and therefore the overall reaction



is predicted to be exoergic for beryllium, nearly ergoneutral for magnesium, and endoergic for calcium. This means that  $CaH_2(g)$  is not stable with respect to  $Ca(g) + H_2(g)$ , and therefore is more difficult to produce compared to  $BeH_2(g)$  and  $MgH_2(g)$ . There is no calculation of the atomization energies of  $SrH_2(g)$  and  $BaH_2(g)$ , but following the pattern observed for Be, Mg and Ca, one can predict that those molecules are even less stable with respect to the metal atom and molecular hydrogen.

## 5. Conclusion

High resolution Fourier transform infrared emission spectra of  $CaH$  and  $SrH$  were recorded and the vibration–rotation transitions of these molecules were observed in their  $X^2\Sigma^+$  ground electronic states. The new data were combined with previous diode laser infrared and pure rotational data of  $CaH/D$  and  $SrH/D$ , and spectroscopic constants for  $v = 0$  to 4 levels of  $^{40}CaH$  and  $^{88}SrH$  were determined. In addition, the Dunham constants and the Born–Oppenheimer breakdown correction parameters were

obtained in combined isotopomer fits. One of the goals in this work was to obtain the vibration–rotation emission spectra of  $CaH_2(g)$ ,  $SrH_2(g)$  and  $BaH_2(g)$ , but none of these species were found.

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