

1 Temperature-dependent absorption cross-sections of
2 HCFC-142b

3 Karine Le Bris^{*,a}, Kimberly Strong^b

4 ^a*Department of Physics, Saint Francis Xavier University, P.O. Box 5000, Antigonish,*
5 *NS, B2G 2W5, Canada*

6 ^b*Department of Physics, University of Toronto, 60 St. George Street, Toronto, Ontario,*
7 *M5S 1A7, Canada*

8 **Abstract**

9 Following the recent detection of HCFC-142b (1-chloro-1,1-difluoroethane)
10 from space, laboratory infrared absorption cross-section spectra of this molecule
11 in a pure vapour phase have been recorded in the 650-3500 cm⁻¹ spectral re-
12 gion using Fourier transform spectroscopy. The spectra have been recorded
13 at a resolution of 0.02 cm⁻¹ and a range of temperatures from 223 to 283
14 K. The resulting data show good agreement with the harmonic frequencies
15 and intensities calculated using density functional theory as well as with the
16 integrated absorption intensities of the spectral bands available in the litera-
17 ture. The new cross-sections will allow more accurate retrieval of atmospheric
18 HCFC-142b concentrations using infrared spectroscopic techniques.

19 *Key words:*

20 Hydrochlorofluorocarbons, R-142b, cross-sections, mid-infrared, FTIR,
21 gas phase, density functional theory, vibrational wavenumber, band
22 strength

*Corresponding author Tel: +1 902-867-3631 Fax: +1 902-867-2414
Email address: klebris@stfx.ca (Karine Le Bris)

23 1. Introduction

24 Hydrochlorofluorocarbons (HCFCs) are temporary substitutes for chlo-
25 rofluorocarbons (CFCs). They were introduced after the phase-out of the
26 latter by the Montreal Protocol and its subsequent amendments. Unlike
27 CFCs, which are mainly destroyed by solar ultraviolet radiation in the strato-
28 sphere, the HCFCs, which contain one or more hydrogen atoms, can react
29 with OH radicals in the troposphere to create HF and CO₂. Therefore, as
30 less chlorine and fluorine are transported to the stratosphere, the ozone de-
31 pletion potentials of HCFCs are substantially weaker than those of CFCs.
32 However, because of their C-Cl and C-F bonds, these molecules still have
33 large absorption cross-sections in the atmospheric window region (8-12 μm),
34 which give them strong global warming potentials.

35 HCFC-142b (1-chloro-1,1-difluoroethane) is a colorless gas at ambient
36 pressure. It is mainly used as a chemical intermediate to produce fluoropoly-
37 mers, as a blowing agent for expanded polystyrene and as a component of
38 refrigerant fluids. Because of its high vapour pressure and low vapour solu-
39 bility, HCFC-142b partitions mostly in the atmosphere. Today, this is the
40 third most abundant hydrochlorofluorocarbon after HCFC-22 and HCFC141-
41 b. The atmospheric lifetime of HCFC-142b is 17.9 years ±24% [1]. Its ozone
42 depletion potential has been estimated at 0.07 while its global warming po-
43 tential is evaluated to be 2310 ±810 for a horizon of 100 years [1].

44 The volume mixing ratio of HCFC-142b has been rising steadily in the
45 atmosphere since the beginning of the 1990's, exceeding 20 ppt in 2008 at
46 13-16 km with an average positive trend of more than 5% per year [2]. The
47 atmospheric concentration of HCFC-142b is now high enough to allow its

48 detection from space [2, 3]. However, the accuracy of the retrieval is limited
49 by the lack of spectroscopic knowledge of this molecule. Only three cross-
50 section spectra corresponding to the temperatures 253 K, 270 K and 287
51 K are currently available in the HITRAN 2008 database [4]. Measurements
52 of temperature-dependent infrared cross-sections of HCFC-142b vapour at
53 low temperature were reported in the 1990's [5, 6, 7] but discrepancies exist
54 between these studies. No new laboratory data at low temperature have been
55 published on this molecule since 1995.

56 As a result, uncertainties on the spectroscopic parameters of HCFC-142b
57 are seen as one of the main sources of error for atmospheric retrievals [3].
58 New laboratory measurements are therefore crucial to enable accurate obser-
59 vations of the spatial and temporal variation of this hydrochlorofluorocarbon
60 in the atmosphere.

61 The purpose of this study is to provide new infrared (IR) cross-sections
62 of HCFC-142b at relatively high resolution (0.02 cm^{-1}) and at a range of
63 relevant atmospheric temperatures (from 223 to 283 K). The resulting ex-
64 perimental data are compared to theoretical calculations performed using
65 density functional theory and to previously published values.

66 **2. Experimental setup**

67 Experimental data are obtained using Fourier transform infrared (FTIR)
68 absorption spectroscopy. The Fourier transform spectrometer (FTS) is a
69 Bomem DA8.002 equipped with a KBr beamsplitter and operating with a
70 Globar source.

71 The gas sample (SynQuest Labs, purity $> 98\%$) is contained in a stainless

72 steel cell positioned between the FTS and a liquid nitrogen-cooled mercury
73 cadmium telluride (MCT) detector. A vacuum system equipped with a Var-
74 ian Turbo-V V250 turbo molecular pump allows the cell to be evacuated to
75 about 1.10^{-6} torr. The cell pressure is measured using 10 Torr and 1000 Torr
76 MKS baratron pressure gauges simultaneously.

77 HCFC-142b presents very intense lines in the atmospheric window region.
78 In order to avoid saturation effects while working at relevant pressures, a
79 stainless steel cell with an optical path of 3.17 cm was constructed. ZnSe
80 windows were sealed to the cell with indium O-rings to prevent leakage at
81 low temperature. The windows are maintained in place by stainless steel
82 flanges supporting teflon rings.

83 The cooling is achieved by a Neslab ULT-80 chiller sending the coolant
84 (Syltherm XLT) to a copper tube surrounding the cell. The copper tube is
85 soldered to the cell and covered by thermally conductive epoxy to provide
86 temperature homogeneity. The cell temperature is measured by a thermo-
87 couple directly inserted inside the cell. The temperature readout accuracy
88 during experiments is typically $\pm 0.1^{\circ}\text{C}$.

89 Many sources of errors and artefacts can affect an FTIR spectrum, such
90 as spectral aliasing, dynamic alignment error, blackbody emission from the
91 source aperture, non-linearity of the MCT detector in the mid-infrared, etc.
92 The spectral aliasing is reduced by the acquisition of a recursive interferogram
93 signal produced by a monochromatic reference source (He-Ne laser) and a
94 digitization resolution of 16 binary bits. The dynamic alignment is corrected
95 in the Bomem DA8 spectrometer by a patented electronic tilt correction. The
96 r.m.s. angular deviation from optimum alignment is less than 10^{-6} radians

97 in normal laboratory conditions (data provided by the manufacturer).

98 The blackbody emission from the source aperture comes from the warm-
99 ing of the iris by the light source. The warm annulus around the aperture
100 acts as a second infrared source emitting off-axis thermal radiation. This
101 leads to distortion of the signal shape and intensities as the aperture size
102 decreases. To reduce this warm aperture artefact, a second iris is inserted
103 between the DA8 spectrometer and the MCT detector at the focal point of
104 the beam [8]. After this installation, no variation of the cross-section signal
105 with the aperture size has been observed.

106 The non-linearity of the MCT detector, corresponding to the non-linearity
107 between the measured signal and the photon flux, essentially affects the cen-
108 tral fringe of the interferogram, which leads to a zero-level offset in the ab-
109 sorption spectrum. Correction of non-linearity is applied on the raw inter-
110 ferograms before the phase correction and the Fourier transformation. We
111 adjusted the response of the detector to the light intensity by a curve whose
112 only unknown parameter is an empirically chosen DC output value [9]. This
113 parameter is adjusted by a minimization of the transmission in the spectral
114 region below the cut-off wavenumber. The residual baseline offset is sub-
115 tracted from the spectra after phase correction and Fourier transformation.

116 **3. Data analysis**

117 For each temperature, a series of spectra were recorded at a minimum of
118 six different pressures between 2 and 12 torr. Each Pressure-Temperature
119 (P-T) spectrum is composed of at least 200 unapodised scans. The resulting
120 spectrum, for each temperature, is a composite spectrum from the P-T spec-

121 trum sets extrapolated to the zero-torr limit. A 200-scan primary baseline
122 spectrum with an empty cell was recorded at each temperature. Secondary
123 control baselines of at least 20 scans were also taken before and after each
124 sample measurement to account for the small intensity variations that can
125 occur during the long periods (typically several hours) of acquisitions. If
126 necessary, the primary baseline is adjusted to the secondary baselines by a
127 polynomial regression prior to the division of each sample spectrum by the
128 adjusted baseline spectrum.

129 The cross-section, $\sigma(\nu)$, in $\text{cm}^2/\text{molecule}$ is calculated for each P-T set
130 using the well-known Beer-Lambert law:

$$I(\nu) = I_0(\nu)e^{-\chi(\nu)} \quad (1)$$

131 with optical depth:

$$\chi(\nu) = \sigma(\nu) \frac{PT_0}{TP_0} N_L L \quad (2)$$

132 where ν is the wavenumber (cm^{-1}); $I_0(\nu)$, the light intensity passing through
133 the empty cell (baseline); $I(\nu)$, the light intensity passing through the sample
134 gas cell; N_L is the Loschmidt's constant (2.6868×10^{19} molecules/ cm^3); L , the
135 length of the cell (cm); and P_0 and T_0 , the standard conditions for pressure
136 and temperature.

137 To prevent saturation effects in an optically thick medium while keeping
138 a good signal-to-noise ratio at every wavenumber, the points corresponding
139 to optically thick ($\chi(\nu) > 1.1$) or optically thin ($\chi(\nu) < 0.1$) conditions are
140 eliminated. This way, a linear behaviour is obtained for strong absorption
141 bands from the low-pressure measurements while the weak absorption fea-
142 tures are represented by the high-pressure measurements.

143 The shapes of the ro-vibrational transition lines, as well as the peaks of the
144 *Q*-branches, are pressure-dependent due to collisional broadening. The cross-
145 section for each wavenumber is obtained at the zero-torr limit by the linear
146 least-square fit of the experimental apparent cross-section of the remaining
147 values ($0.1 < \chi(\nu) < 1.1$) versus the pressure.

148 The errors on optical path length, temperature readout, pressure, baseline
149 drift, and sample purity have been evaluated to account for less than $\pm 3\%$.
150 The other sources of error in spectral measurements come from the residual
151 MCT non-linearity, a possible residual baseline drift and the errors induced
152 by the data reduction. For each wavenumber, we calculated the standard
153 deviation Δ between the linear fit and the apparent cross-section values as
154 a function of pressure. The error for each wavenumber is chosen at the 95%
155 confidence limit (2Δ).

156 4. Results

157 HCFC-142b is a near-prolate asymmetric top molecule belonging to the
158 *Cs* symmetry group (Figure 1). As a consequence, it has 18 fundamental
159 vibration modes (11 with *A'* symmetry and 7 with *A''* symmetry). Twelve
160 of those fundamental modes have active absorption bands in the spectral
161 window region between 650 and 3500 cm^{-1} .

162 All the bands present a sharp *Q*-branch surrounded by less intense *P*-
163 and *R*-branch structures (Figure 2). No significant variation of the integrated
164 band strength with temperature has been observed from 223 to 283 K for any
165 of the bands (Figure 3). Therefore, we can confirm that the superimposed
166 hot bands and combination bands of HCFC-142b do not play a significant

167 role in our range of temperatures.

168 The shape of the bands is strongly dependent on the temperature. The
169 Q -branches become sharper as the temperature decreases due to the change
170 of relative populations of the rotational states of the vibrational bands. This
171 leads to a significant increase in the cross-sections at the band centers with
172 decreasing temperature (Figure 4).

173 The uncertainty on the integrated band strength is stable with tempera-
174 ture for all bands with the exception of the ν_8 band. The increased uncer-
175 tainty on the integrated strength of the ν_8 band as the temperature decreases
176 is likely due to the intense sharpening of the ν_8 Q -branch which worsens the
177 data reduction error on the main peak.

178 Weak features of magnitude lower than 10^{-20} $\text{cm}^2/\text{molecule}$, which can be
179 attributed either to overtones and combination band or sample impurity, are
180 present at all temperatures in the spectral region between $1500\text{-}2800$ cm^{-1} .

181 5. Data Validation

182 5.1. Comparison with theoretical calculation of vibrational modes and inten- 183 sities

184 The unconstrained geometric optimizations and harmonic vibrational fre-
185 quencies of HCFC-142b are calculated using density functional theory (DFT)
186 with Gaussian 03 [10].

187 Previous ab-initio calculations for HCFC-142b have been carried out at
188 the RHF/6-31* [11] and MP2/6-31G** [12] levels . The present DFT calcu-
189 lations are performed using the Becke's three-parameter functionals for the
190 exchange and the Lee-Yang-Parr and Perdew-Wang non-local functionals for

191 correlation (respectively B3LYP and B3PW91). For each functional set, two
192 basis sets are used: the Pople's type valence triple-zeta basis supplemented by
193 multiple polarization and diffuse functions (6-311++(3df,3pd)) and the aug-
194 mented correlation-consistent polarized quadruple-zeta (aug-cc-pVQZ) basis.

195 We observe a very good agreement between the geometries from the four
196 levels of theory. The choice of the correlation functionals and the size of
197 the basis sets have only a weak influence on the geometry. The harmonic
198 wavenumber positions present little sensitivity to basis sets, with an average
199 difference below 0.2%, and to the correlation functionals, with an average
200 difference around 0.7%. The variations of intensity with basis sets are also
201 weak in both cases, with the exception of the ν_{10} band, corresponding to
202 C-Cl stretching. It may be noted that the inclusion of diffuse functions
203 on hydrogen atoms has almost no influence on the geometry and harmonic
204 frequencies of HCFC-142b. However, the choice of correlation functionals
205 does have a strong influence on the intensities, with an average difference
206 between LYP and PW91 above 12% and a maximum difference between
207 25-30% for the ν_4 and ν_{15} bands. Comparison with experimental data is
208 therefore essential to test the validity of the methods.

209 Table 1 presents the assignment, the calculated harmonic wavenumber
210 and the integrated strength of the fundamentals modes. The strongest bands
211 correspond to C-C, C-Cl and C-F stretching vibrations. All of them fall in the
212 800-1250 cm^{-1} atmospheric window region, which explains the high global
213 warming potential of this molecule.

214 The weak fundamental C-H stretching vibrations fall in the 3000 cm^{-1}
215 spectral region. The superimposed CH_3 deformation vibrations lie in the

216 1400 cm^{-1} region. Only the ν_4 mode presents a medium intensity in this
217 window.

218 The theoretical values of the harmonic frequencies have been compared
219 to the experimental data (Figure 5). The experimental line center is chosen
220 at the barycentre of the Q -band. All four levels of theory give excellent re-
221 sults after an average linear scaling: $\nu_{exp} = (1.06 \pm 0.01)\nu_{theo} - (59.3 \pm 7.7)$,
222 with ν_{exp} and ν_{theo} , the respective experimental and theoretical harmonic
223 wavenumber values in cm^{-1} . The theoretical values for line intensity in the
224 mid-IR spectral windows also fit relatively well the data after linear scal-
225 ing with the experimental integrated absorption strength. We obtained an
226 average $I_{exp} = (1.01 \pm 0.05)I_{theo} + (0.22 \pm 0.14) \times 10^{-17}$ for B3LYP and
227 $I_{exp} = (1.10 \pm 0.02)I_{theo} + (0.08 \pm 0.05) \times 10^{-17}$ for B3PW91, with I_{exp} and
228 I_{theo} the respective experimental and theoretical integrated band strengths
229 in $\text{cm}/\text{molecule}$. However, B3PW91 gives the best correlation with an R^2 of
230 0.999 for both basic sets.

231 5.2. Comparison with published values

232 The integrated band intensities of the HCFC-142b cross-section spec-
233 tra are compared with data available in the literature (Table 2). The inte-
234 grated intensities of the four absorption bands ν_8 , (ν_7, ν_{15}) , (ν_6, ν_5, ν_{14}) , and
235 (ν_4, ν_3, ν_{13}) between 650 and 1500 cm^{-1} are reported. No previous values
236 for the ν_1, ν_2, ν_{12} bands around 3000 cm^{-1} have been found in literature.
237 At most temperatures, our integrated absorption band strengths show good
238 agreement with earlier measurements for a pure vapour [5, 6], as well as for
239 N_2 -broadened vapour [7, 13]. No constant relative difference is observed with
240 any of the data sets, which indicates that there were no significant systematic

241 errors in the measurements.

242 The largest discrepancies between authors appears at 233 K. A disparity
243 close to 20% for the ν_6 , ν_5 , ν_{14} absorption bands exists between Newnham
244 and Ballard [5] and Cappellani and Restelli [7]. As previously mentioned,
245 our integrated band strengths do not exhibit trends and our values at 233 K,
246 midway between the values of these two studies, remain consistent with our
247 results at other temperatures.

248 **6. Conclusions**

249 Absorption cross-sections of HCFC-142b at a spectral resolution of 0.02
250 cm^{-1} have been recorded in the mid-infrared between 650 and 3500 cm^{-1}
251 at seven different temperatures (223, 233, 243, 253, 263 , 273, and 283 K).
252 The main sources of errors in the measurements have been investigated and
253 accounted for in the final results. The integrated intensities of the harmonic
254 wavenumber bands show good agreement with the data available in the liter-
255 ature and with theoretical calculations using DTF. The availability of cross-
256 section spectra at 10-K steps between 223 and 283 K should, therefore, allow
257 the reduction of uncertainties on HCFC-142b volume mixing ratio retrieval
258 from space missions. The cross-sections are provided online in supplementary
259 data files and are also available from the corresponding author.

260 **7. Acknowledgments**

261 This work was supported by the Canadian Space Agency (CSA) and the
262 Natural Sciences and Engineering Research Council of Canada (NSERC).
263 We thank Paul Chen for technical support, and Prof. James R. Drummond

264 and the NSERC Industrial Research Chair in Atmospheric Remote Sounding
265 from Space (sponsored by COMDEV, Bomem, Environment Canada, CSA,
266 and NSERC) for the use of the Bomem DA8 Fourier transform spectrometer.
267 We also thank Dr. Stella M.L. Melo from the CSA for helpful discussions.

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Figure 1: Geometrical structure of HCFC-142b.

Figure 2: Survey spectrum of HCFC-142b in the mid-infrared at 263 K.

Figure 3: Variation of the integrated strength of the five main absorption bands of HCFC-142b in the mid-infrared.

Figure 4: Cross-section of the P - and Q -branches of the ν_{15} band of HCFC-142b at seven different temperatures.

Figure 5: Comparison between experimental and theoretical harmonic frequencies of HCFC-142b for the four levels of theory.

Figure 6: Comparison between experimental and theoretical band strengths of HCFC-142b for the four levels of theory.

Table 1: Theoretical harmonic wavenumbers and intensities of the fundamental modes of HCFC-142b. Wavenumbers are in cm^{-1} , bands strengths are in 10^{-17} $\text{cm}^2/\text{molecule}$. (a):6-311++ , (b):Aug-cc-pvqz. st:stretch, def: deformation.

Label	Assignment	Wavenumber						Band strength	
		B3LYP		B3PW91		B3LYP		B3LYP	B3PW91
		(a)	(b)	(a)	(b)	(a)	(b)	(a)	(b)
A'									
ν_1	CH ₃ sym st.	3141.36	3136.41	3157.78	3152.34	0.06	0.06	0.05	0.05
ν_2	CH ₃ sym st.	3063.13	3059.54	3071.15	3066.82	0.03	0.03	0.03	0.03
ν_3	CH ₃ sym def.	1483.52	1483.83	1474.41	1474.57	0.01	0.01	0.01	0.01
ν_4	CH ₃ sym def.	1421.65	1422.37	1412.26	1412.58	0.46	0.47	0.62	0.63
ν_5	CF ₂ sym st., C-C st.	1217.65	1216.27	1231.51	1229.66	2.00	1.99	1.93	1.94
ν_6	C-Cl st., CF ₂ sym. def.	1129.57	1129.39	1128.24	1127.67	2.72	2.67	3.01	2.95
ν_7	CF ₂ sym. st.	892.16	889.67	903.03	900.49	2.10	2.14	1.83	1.88
ν_8	C-C-Cl def.	669.26	668.25	678.87	677.57	0.98	0.98	0.94	0.94

Table 1 – continued from previous page

Label	Assignment	Wavenumber				Band strength			
		B3LYP		B3PW91		B3LYP		B3PW91	
		(a)	(b)	(a)	(b)	(a)	(b)	(a)	(b)
ν_9	CF ₂ scissor	538.74	538.32	543.53	543.01	0.22	0.22	0.21	0.21
ν_{10}	C-Cl st.	424.24	421.51	431.71	428.52	0.05	0.05	0.04	0.04
ν_{11}	CClF ₂ -CH ₃ rock	301.07	299.86	301.40	299.99	0.02	0.02	0.02	0.02
A'									
ν_{12}	CH ₂ asym. st.	3157.99	3153.42	3173.96	3169.17	0.03	0.03	0.02	0.02
ν_{13}	CH ₃ asym. def	1480.50	1480.27	1471.51	1470.95	0.06	0.06	0.06	0.06
ν_{14}	CF ₂ asym. st.	1185.37	1183.27	1194.77	1192.94	2.36	2.33	2.64	2.61
ν_{15}	CF ₂ asym. st.	963.01	961.31	968.74	967.87	1.20	1.2	0.93	0.97
ν_{16}	CF ₂ rock	430.36	429.96	431.12	430.89	0.00	0.00	0.00	0.00
ν_{17}	CClF ₂ -CH ₃ twist	330.49	329.79	332.15	331.29	0.01	0.01	0.01	0.01
ν_{18}	torsion	236.96	235.49	239.07	238.32	0.00	0.00	0.00	0.00

Table 2: Comparison of the experimental infrared integrated band strengths ($\times 10^{-17}$ cm/molecule) with published values when available. (a) The first two temperature sets for Ref. [13] are at 297 and 277 K. (b) The first temperature set for Ref. [5] is at 296 K. (c) The first two temperature sets for Ref. [6] are at 287 and 270 K.

Temperature	Label	Integrated band strength				
		This work	Ref. [13] ^a	Ref. [5]	Ref. [6] ^b	Ref. [7]
293 K	ν_8		0.74	0.71 ± 0.01		0.74
	ν_7, ν_{15}		2.53	2.49 ± 0.07		2.38
	ν_6, ν_5, ν_{14}		7.06	7.34 ± 0.10		6.94
	ν_4, ν_3, ν_{13}		0.64	0.58 ± 0.04		0.60
283 K	ν_8	0.69 ± 0.02			0.75 ± 0.05	
	ν_7, ν_{15}	2.41 ± 0.07			2.58 ± 0.14	
	ν_6, ν_5, ν_{14}	6.99 ± 0.19			7.19 ± 0.20	
	ν_4, ν_3, ν_{13}	0.57 ± 0.02			0.61 ± 0.09	
	ν_2, ν_1, ν_{12}	0.13 ± 0.01				
273 K	ν_8	0.70 ± 0.03	0.74	0.70 ± 0.04	0.69 ± 0.05	0.75
	ν_7, ν_{15}	2.42 ± 0.07	2.50	2.56 ± 0.07	2.51 ± 0.14	2.45
	ν_6, ν_5, ν_{14}	6.91 ± 0.19	7.05	7.06 ± 0.13	7.11 ± 0.20	7.12
	ν_4, ν_3, ν_{13}	0.64 ± 0.02	0.63	0.61 ± 0.03	0.64 ± 0.09	0.62
	ν_2, ν_1, ν_{12}	0.15 ± 0.01				
263 K	ν_8	0.68 ± 0.06				
	ν_7, ν_{15}	2.35 ± 0.06				
	ν_6, ν_5, ν_{14}	6.74 ± 0.18				

Table 2 – continued from previous page

Temperature	Label	Integrated band strength				
		This work	Ref. [13] ^a	Ref. [5] ^b	Ref. [6] ^c	Ref. [7] ^c
	ν_4, ν_3, ν_{13}	0.59 ± 0.02				
	ν_2, ν_1, ν_{12}	0.14 ± 0.01				
253 K	ν_8	0.68 ± 0.07		0.69 ± 0.03	0.68 ± 0.05	
	ν_7, ν_{15}	2.36 ± 0.07		2.41 ± 0.08	2.40 ± 0.14	
	ν_6, ν_5, ν_{14}	6.76 ± 0.19		6.16 ± 0.43	6.96 ± 0.20	
	ν_4, ν_3, ν_{13}	0.65 ± 0.02		0.65 ± 0.05	0.78 ± 0.09	
	ν_2, ν_1, ν_{12}	0.13 ± 0.02				
243 K	ν_8	0.67 ± 0.11				
	ν_7, ν_{15}	2.29 ± 0.07				
	ν_6, ν_5, ν_{14}	6.58 ± 0.18				
	ν_4, ν_3, ν_{13}	0.64 ± 0.02				
	ν_2, ν_1, ν_{12}	0.13 ± 0.02				
233 K	ν_8	0.67 ± 0.15		0.71 ± 0.01		0.75
	ν_7, ν_{15}	2.35 ± 0.07		2.30 ± 0.04		2.51
	ν_6, ν_5, ν_{14}	6.92 ± 0.21		6.19 ± 0.02		7.38
	ν_4, ν_3, ν_{13}	0.61 ± 0.02		0.62 ± 0.05		0.64
	ν_2, ν_1, ν_{12}	0.13 ± 0.01				
223 K	ν_8	0.64 ± 0.15				
	ν_7, ν_{15}	2.30 ± 0.08				
	ν_6, ν_5, ν_{14}	6.67 ± 0.19				
	ν_4, ν_3, ν_{13}	0.58 ± 0.02				
	ν_2, ν_1, ν_{12}	0.12 ± 0.01				

Table 2 – continued from previous page

Temperature	Label	Integrated band strength				
		This work	Ref. [13] ^a	Ref. [5] ^b	Ref. [6] ^c	Ref. [7] ^c
213 K	ν_8			0.70 ± 0.07		
	ν_7, ν_{15}			2.46 ± 0.05		
	ν_6, ν_5, ν_{14}			6.80 ± 0.28		
	ν_4, ν_3, ν_{13}			0.60 ± 0.04		
203 K	ν_8			0.79 ± 0.09		
	ν_7, ν_{15}			2.34 ± 0.26		
	ν_6, ν_5, ν_{14}			6.90 ± 0.10		
	ν_4, ν_3, ν_{13}			0.58 ± 0.03		