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High-resolution spectrum of the $\nu_1 + \nu_4(E)$, $\nu_3 + \nu_4(E)$, $\nu_3 + \nu_4(A_1)$, and $\nu_3 + \nu_4(A_2)$ bands of the PH_3 molecule: assignments and preliminary analysis

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Abstract

The high-resolution ($0.005\ cm^{-1}$) Fourier transform infrared spectrum of PH_3 is recorded in the region between 3280 and $3580\ cm^{-1}$ where the following bands are located: $\nu_1 + \nu_4(E)$, $\nu_3 + \nu_4(E)$, $\nu_3 + \nu_4(A_1)$, forbidden on symmetry band $\nu_3 + \nu_4(A_2)$, and very weak bands $\nu_1 + \nu_2(A_1)$, $\nu_2 + \nu_3(E)$. Transitions are assigned to the first four ones. Vibrational analysis of known experimental data is made.

Keywords: Vibrational–rotational spectra; PH_3 molecule

1. Introduction

The high-resolution infrared spectra of phosphine can be used as an important source of information for several purposes, such as atmospheric studies of Earth and giant planets, investigation of industrial pollution, and for studies on the fundamental properties of pyramid type molecules. As a consequence, phosphine has been the subject of numerous studies of high resolution both pure

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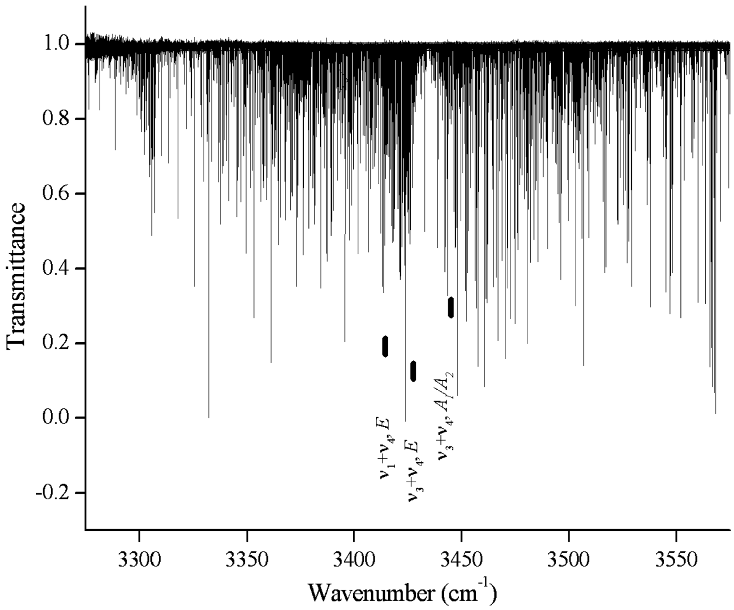

Fig. 1. An overview of the infrared spectrum from 3280 to 3580 cm^{-1} of PH_3 is shown. The vibrational band centers are approximately indicated. Experimental conditions: absorption path length 15 m, pressure 40 Pa, instrumental resolution 0.005 cm^{-1}, room temperature.

rotational and vibration–rotational spectra. However, most of the earlier studies have been devoted to the ground vibrational state, the deformational fundamentals ν_2 and ν_4 and their overtones, ν_1 and ν_3 stretching fundamentals, see, e.g., Ref. [1], references therein, and also Ref. [2]. To date, there were no high-resolution analysis of combination bands which correspond simultaneous excitations of the stretching and deformational vibrations. At the same time, high-resolution studies of such type bands can give information about the strength of connections between stretching and deformational motions in a molecule. In its turn, the last circumstance is important to understand the mechanisms of formation and/or destruction of the local mode behavior of the PH_3 molecule.

In this study, we present the assignment and preliminary analysis of the strongest of such type combination bands, $\nu_1 + \nu_4$ and $\nu_3 + \nu_4$, which are located in the region of 3280–3580 cm^{-1} and which were recorded for the first time with a high resolution (an overview of the spectrum is shown in Fig. 1). Besides the above-mentioned pure fundamental interest, the study of the $\nu_1 + \nu_4$ and $\nu_3 + \nu_4$ bands has an additional importance from an applied point of view. Since these bands are strong enough and located in a region of practically total absence of water absorption (water lines are presented in the shortwave part of the region only), they can be used to monitor the PH_3. As a consequence, the results of the present contribution can be considered as an important addition to the modern data bases.

Since the $\nu_3 + \nu_4$ band consists of three subbands, $\nu_3 + \nu_4(E)$, $\nu_3 + \nu_4(A_1)$, and $\nu_3 + \nu_4(A_2)$, experimentally recorded high-resolution spectrum is a very complicated mixture of four totally overlapped and strongly interacting bands, which show very unusual dependence of the wave numbers of transitions on quantum numbers J and K. As a consequence, a correct and unambiguous mathematical description of the spectrum is needed in additional correct information on the fundamental parameters of the PH_3 molecule. Namely, correct numerical estimations of the values of band centers and of the main resonance interaction parameters are needed. That can be made, for example, on the basis of knowledge of an intramolecular potential function. Unfortunately, as the analysis shows, such information known in the modern spectroscopic literature (see, e.g., [3]), is not completely correct. For this reason, we limit our present consideration to preliminary analysis of the spectrum and assignments of transitions.

2. Experimental details

The PH_3 sample was purchased from Nanjing Special Gas Company with the stated purity of 99.9%. The spectrum was recorded at room temperature with a Bruker IFS 120HR Fourier-transform interferometer (Hefei, China), which is equipped with a path length adjustable multi-pass gas cell. The spectrum was recorded at room temperature with a sample pressure of 40 Pa and absorption path length of 15 m. A tungsten source, a CaF2 beamsplitter, two optical band pass filters whose cutoff frequencies were 3150–4350 and 3310–2500 cm^{-1} and a liquid-nitrogen cooled InSb detector were used. The unapodized resolution was 0.005 cm^{-1}. The lines of H_2O were used to calibrate the position of the PH_3 lines by comparison with those listed in the GEISA 97 database. The accuracy of the not-very-weak unblended and nonsaturated lines was estimated to be no worse than 0.0004 –0.0005 cm^{-1}. The overview spectrum and two small parts of the recorded high resolution spectrum are presented in Figs. 2 and 3, for illustration.

3. Description of the spectrum and assignments of transition

As is seen from Fig. 1, all four bands, $\nu_1 + \nu_4(E)$, $\nu_3 + \nu_4(E)$, $\nu_3 + \nu_4(A_1)$, and $\nu_3 + \nu_4(A_2)$, are located very closely and overlap each other. Because of strong resonance interactions, all the allowed interactions on symmetry bands, $\nu_1 + \nu_4(E)$, $\nu_3 + \nu_4(E)$, and $\nu_3 + \nu_4(A_1)$ have comparable strengths. Moreover, the presence of resonance interactions leads to appearance of sets of transitions belonging to the forbidden interaction on symmetry $\nu_3 + \nu_4(A_2)$ band (some such transitions, marked by open circles, can be seen in Figs. 2 and 3). At the high frequency region, lines belonging to the water vapor can be seen. However, an overlapping of the PH_3 and H_2O bands is weak. In the long wave part of the analyzed spectrum, the bands $\nu_1 + \nu_2$ and $\nu_2 + \nu_3$ are located. However, these two bands are considerably weaker than the ones considered in the present study, and only a few of the transitions belonging to the $\nu_1 + \nu_2$ and $\nu_2 + \nu_3$ bands can be seen in the recorded spectrum.

The assignment of transitions was fulfilled on the basis of the Ground State Combination Differences method, and the ground state energies were calculated with the parameters from Ref. [1]. As a result of assignment, sets of transitions of the type $(J'\ K'\ \Gamma') \leftarrow (J\ K\ \Gamma)$ (with fixed values of the quantum numbers K, K', symmetries Γ, Γ', and different values of quantum numbers J, $J' = J, J \pm 1$) were found in the spectrum up to $K^{max} = 13$ and $J^{max} = 14$. At the same time, at that step of analysis, it was not possible to answer the question: to which concrete band does one or another concrete set of transitions $(J'\ K'\ \Gamma') \leftarrow (J\ K\ \Gamma)$ belong? Fortunately, two sets of the

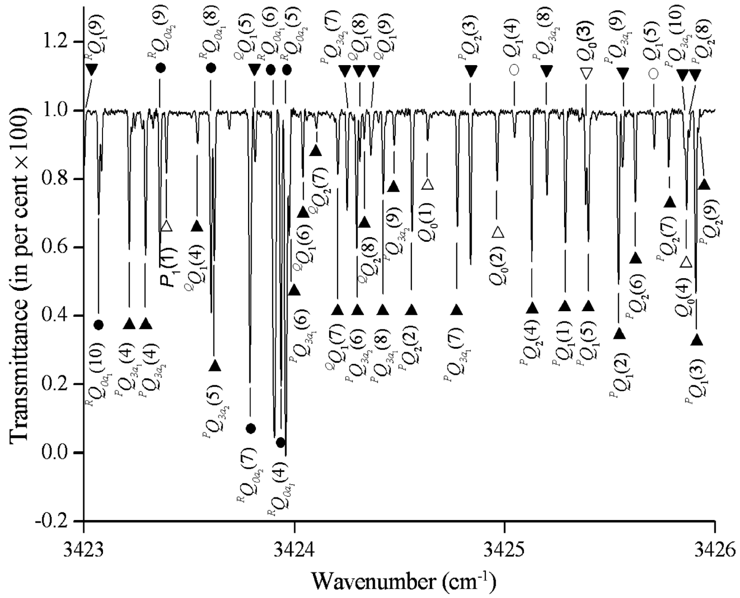

Fig. 2. A small portion of the spectrum in the region of the Q-branch of $\nu_1+\nu_4$ band is illustrated. Transitions assigned to the $\nu_1+\nu_4(E)$, $\nu_3+\nu_4(E)$, $\nu_3+\nu_4(A_1)$, and $\nu_3+\nu_4(A_2)$ bands are marked by dark triangles, dark circles, open triangles, and open circles, respectively. Set of the ${}^RQ_{K=0}(J)$ transitions of the $\nu_1+\nu_4(E)$ band is seen on the left-hand side of the figure. Some transitions which belong to the "forbidden" band $\nu_3+\nu_4(A_2)$ can also be seen.

${}^RQ_{K=0}(J)$ transitions, which undoubtedly indicate two doubly degenerated E-type bands ($\nu_1+\nu_4(E)$ and $\nu_3+\nu_4(E)$ in our case), can be found in the spectrum by way of simple visible inspection (one of them can be seen in Fig. 2). In its turn, the last circumstance allows one to make a conclusion that two E-type vibrational bands, $\nu_1+\nu_4$(E) and $\nu_3+\nu_4(E)$, are located in a longer wave region, and the $\nu_3+\nu_4(A_1)$ and $\nu_3+\nu_4(A_2)$ bands are located in a shorter wave part (see Fig. 4). Finally, more than 90 per cent of experimentally recorded lines were assigned to the four studied bands, $\nu_1+\nu_4$(E), $\nu_3+\nu_4$(E), $\nu_3+\nu_4(A_1)$, and $\nu_3+\nu_4(A_2)$. The list of transitions is presented in Table 1. In this case, Columns 4 and 5 of that table give the experimental wave numbers of transitions and their transmittances, in cm^{-1} and per cent, respectively. The quantum numbers J', K' and J, K of the upper and lower ro–vibrational states and their symmetries Γ' and Γ are presented in Columns 1 and 2, respectively. Column 3 shows the band to which the transition belongs.

Two interesting points should be specially mentioned here as the results of the assignments:

(1) the presence of experimentally recorded numerous a_1/a_2 splittings for the states ($J\ Ka_1, a_2$) with the value of quantum number $K=1$–10, and
(2) the appearance of numerous and strong enough transitions belonging to the band $\nu_3+\nu_4(A_2)$ which is forbidden on symmetry.

Both of these effects are caused by the presence of strong resonance interactions between all the four studied bands.

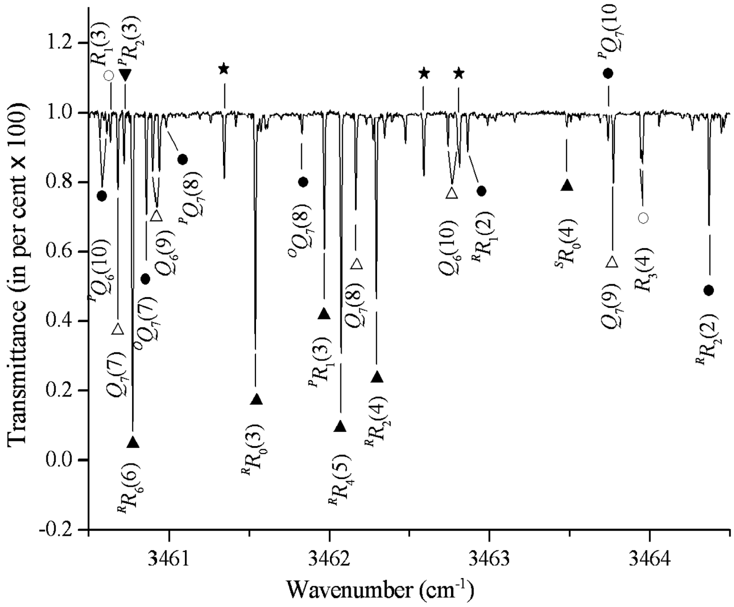

Fig. 3. A portion of the recorded spectrum in the region of the R-branch of the bands $\nu_1 + \nu_4$ and $\nu_3 + \nu_4$. Transitions assigned to the $\nu_1 + \nu_4(E)$, $\nu_3 + \nu_4(E)$, $\nu_3 + \nu_4(A_1)$, and $\nu_3 + \nu_4(A_2)$ bands are marked by dark triangles, dark circles, open triangles, and open circles, respectively. Three water vapor lines are marked by star. Some high K-value a_1/a_2 splittings can be seen.

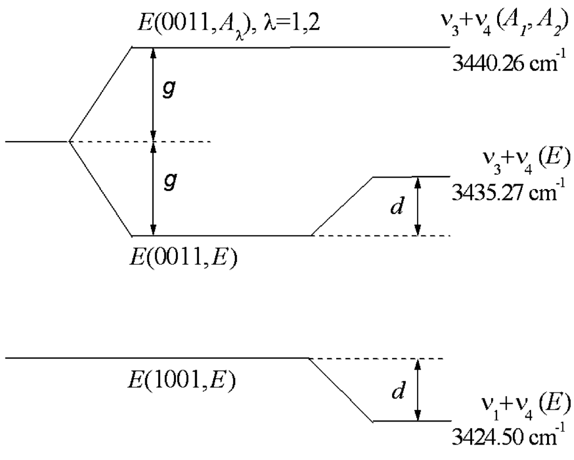

Fig. 4. Diagram of locations of some vibrational energy levels and interactions in the PH_3 molecule: g denotes splitting of the (0011) term into the E and A_1/A_2 components; d caused by the Fermi type resonance interaction between the $(1001, E)$ and $(0011, E)$ states.

Table 1
The assigned Ro–Vibrational transitions of the $\nu_1+\nu_4(E)$, $\nu_3+\nu_4(E)$, $\nu_3+\nu_4(A_1)$, and $\nu_3+\nu_4(A_2)$ bands of the PH_3 molecule

Upper state J' K' Γ'	Lower state J K Γ	Band	Line position, exp., in cm^{-1}	Trsm., in %	Upper state J' K' Γ'	Lower state J K Γ	Band	Line position, exp., in cm^{-1}	Trsm., in %
1	2	3	4	5	1	2	3	4	5
8 4 a_2	10 6 a_1	$\nu_1+\nu_4,E$	3260.3771	96.3	5 5 e	6 5 e	$\nu_3+\nu_4,A_2$	3357.7162	83.0
12 11 a	13 12 a	$\nu_1+\nu_4,E$	3281.7052	82.3	6 3 a_2	7 3 a_1	$\nu_3+\nu_4,A_2$	3357.8609	87.9
10 10 a_2	11 9 a_1	$\nu_1+\nu_4,E$	3286.6453	95.1	6 3 a_1	7 3 a_2	$\nu_3+\nu_4,A_2$	3357.8916	84.8
11 11 a	12 12 a	$\nu_1+\nu_4,E$	3288.7901	71.6	10 3 a_2	11 3 a_1	$\nu_3+\nu_4,A_1$	3358.0777	94.5
11 10 e	12 11 e	$\nu_1+\nu_4,E$	3293.7502	86.6	8 2 e	9 2 e	$\nu_3+\nu_4,E$	3358.8324	94.8
10 10 e	11 11 e	$\nu_1+\nu_4,E$	3301.1372	76.5	11 6 a_2	12 6 a_1	$\nu_3+\nu_4,A_1$	3358.9082	97.2
10 7 a	11 6 a	$\nu_1+\nu_4,E$	3304.1230	96.2	11 6 a_1	12 6 a_2	$\nu_3+\nu_4,A_1$	3359.0154	97.5
11 7 e	12 8 e	$\nu_1+\nu_4,E$	3306.0861	92.2	6 3 e	7 4 e	$\nu_1+\nu_4,E$	3359.4767	64.3
10 5 e	11 2 e	$\nu_1+\nu_4,E$	3307.5870	98.6	5 4 a_1	6 3 a_2	$\nu_1+\nu_4,E$	3359.8107	92.6
10 8 a	11 9 a	$\nu_1+\nu_4,E$	3310.1416	69.9	6 2 e	7 1 e	$\nu_1+\nu_4,E$	3360.0523	93.2
9 7 a_1	10 6 a_2	$\nu_1+\nu_4,E$	3311.8755	98.1	10 4 e	11 5 e	$\nu_3+\nu_4,E$	3360.2295	95.7
9 9 e	10 10 e	$\nu_1+\nu_4,E$	3313.3507	68.0	6 2 e	7 2 e	$\nu_3+\nu_4,A_2$	3360.8338	81.5
10 7 e	11 8 e	$\nu_1+\nu_4,E$	3313.9553	85.4	5 5 a	6 6 a	$\nu_1+\nu_4,E$	3361.2988	14.4
9 8 a	10 9 a	$\nu_1+\nu_4,E$	3317.8489	98.7	9 3 a_2	10 0 a_1	$\nu_3+\nu_4,A_1$	3361.5110	92.0
10 4 a_1	11 3 a_2	$\nu_1+\nu_4,E$	3318.0601	98.3	9 1 e	10 1 e	$\nu_3+\nu_4,A_1$	3361.8693	92.0
11 3 e	12 4 e	$\nu_1+\nu_4,E$	3318.8477	98.8	6 1 e	7 1 e	$\nu_1+\nu_4,E$	3361.8828	97.1
8 7 a	9 6 a	$\nu_1+\nu_4,E$	3319.7176	97.8	8 4 e	9 1 e	$\nu_3+\nu_4,E$	3362.0864	95.2
10 5 a_2	11 6 a_1	$\nu_1+\nu_4,E$	3320.6694	89.1	6 2 a_1	7 3 a_2	$\nu_1+\nu_4,E$	3362.1210	67.6
10 5 a_1	11 6 a_2	$\nu_1+\nu_4,E$	3320.8681	91.7	5 4 e	6 4 e	$\nu_3+\nu_4,A_2$	3362.2615	88.5
10 3 e	11 2 e	$\nu_1+\nu_4,E$	3321.5491	97.7	8 3 e	9 2 e	$\nu_3+\nu_4,E$	3362.9033	92.2
9 5 e	10 4 e	$\nu_1+\nu_4,E$	3321.8314	97.4	9 2 e	10 2 e	$\nu_3+\nu_4,A_1$	3362.9452	67.3
9 7 e	10 8 e	$\nu_1+\nu_4,E$	3321.8656	77.3	6 1 a_1	7 0 a_2	$\nu_1+\nu_4,E$	3363.1745	93.1
11 1 a_2	12 0 a_1	$\nu_3+\nu_4,E$	3323.2514	94.9	10 5 a_2	11 6 a_1	$\nu_3+\nu_4,E$	3363.1745	93.1
8 6 e	9 5 e	$\nu_1+\nu_4,E$	3325.1346	97.9	10 5 a_1	11 6 a_2	$\nu_3+\nu_4,E$	3363.2188	94.5
9 6 e	10 7 e	$\nu_1+\nu_4,E$	3325.4871	35.3	8 2 a_1	9 3 a_2	$\nu_3+\nu_4,E$	3363.4111	94.4
8 8 a	9 9 a	$\nu_1+\nu_4,E$	3325.4871	35.3	6 1 e	7 2 e	$\nu_1+\nu_4,E$	3363.4569	76.9
9 4 a_2	10 3 a_1	$\nu_1+\nu_4,E$	3326.4961	98.0	8 4 a_2	9 3 a_1	$\nu_3+\nu_4,E$	3364.0100	94.3
10 2 a_1	11 3 a_2	$\nu_1+\nu_4,E$	3328.5605	94.9	8 4 a_1	9 3 a_2	$\nu_3+\nu_4,E$	3364.1507	96.0
9 5 a_1	10 6 a_2	$\nu_1+\nu_4,E$	3328.6043	83.8	6 1 e	7 1 e	$\nu_3+\nu_4,A_2$	3364.1899	96.7
10 1 e	11 2 e	$\nu_1+\nu_4,E$	3328.6380	97.2	5 3 e	6 2 e	$\nu_1+\nu_4,E$	3364.5054	93.1
9 5 a_2	10 6 a_1	$\nu_1+\nu_4,E$	3328.6947	75.3	8 5 e	9 4 e	$\nu_3+\nu_4,E$	3364.5206	92.6
8 7 e	9 8 e	$\nu_1+\nu_4,E$	3329.7223	63.1	11 8 a_1	12 9 a_2	$\nu_3+\nu_4,E$	3364.7106	93.3
9 4 e	10 4 e	$\nu_3+\nu_4,A_2$	3329.8306	90.7	5 4 e	6 5 e	$\nu_1+\nu_4,E$	3364.7458	46.4
9 3 e	10 2 e	$\nu_1+\nu_4,E$	3330.3028	97.4	9 3 a_1	10 3 a_2	$\nu_3+\nu_4,A_1$	3364.8870	87.0
8 5 e	9 4 e	$\nu_1+\nu_4,E$	3330.3438	97.8	6 1 a_1	7 0 a_2	$\nu_3+\nu_4,E$	3365.3909	53.6
10 1 e	11 1 e	$\nu_3+\nu_4,A_2$	3330.5180	97.7	6 1 a_1	7 0 a_2	$\nu_3+\nu_4,E$	3365.4140	64.4
10 0 e	11 1 e	$\nu_1+\nu_4,E$	3331.7679	93.7	5 2 a_2	6 0 a_1	$\nu_1+\nu_4,E$	3365.7111	86.0
10 1 a_1	11 0 a_2	$\nu_3+\nu_4,E$	3331.8834	90.4	6 1 e	7 2 e	$\nu_3+\nu_4,A_2$	3365.7625	91.9
10 1 e	11 2 e	$\nu_3+\nu_4,A_2$	3332.0544	98.8	6 4 a_1	7 6 a_2	$\nu_1+\nu_4,E$	3365.8496	97.7
9 3 a_1	10 3 a_2	$\nu_3+\nu_4,A_2$	3332.3916	91.9	8 7 a	9 6 a	$\nu_3+\nu_4,E$	3365.9404	96.6
9 3 a_2	10 3 a_1	$\nu_3+\nu_4,A_2$	3332.6843	93.2	5 3 a_1	6 3 a_2	$\nu_3+\nu_4,A_2$	3366.1362	88.6
9 4 e	10 5 e	$\nu_1+\nu_4,E$	3332.8600	98.3	5 3 a_2	6 3 a_1	$\nu_3+\nu_4,A_2$	3366.1469	88.6
8 6 e	9 7 e	$\nu_1+\nu_4,E$	3333.5051	68.6	7 2 e	8 1 e	$\nu_3+\nu_4,E$	3366.1888	93.3
9 3 e	10 4 e	$\nu_1+\nu_4,E$	3334.3874	90.4	10 6 e	11 7 e	$\nu_3+\nu_4,E$	3366.2988	90.4

Table 1 (*continued*)

Upper state J'	K'	Γ'	Lower state J	K	Γ	Band	Line position, exp., in cm^{-1}	Trsm., in %	Upper state J'	K'	Γ'	Lower state J	K	Γ	Band	Line position, exp., in cm^{-1}	Trsm., in %
8	4	a_2	9	3	a_1	$\nu_1+\nu_4,E$	3334.8661	96.3	6	1	a_2	7	3	a_1	$\nu_1+\nu_4,E$	3366.4754	98.1
8	4	a_1	9	3	a_2	$\nu_1+\nu_4,E$	3334.8868	97.3	9	3	e	10	5	e	$\nu_3+\nu_4,E$	3366.7156	97.1
9	1	e	10	1	e	$\nu_1+\nu_4,E$	3335.8308	97.4	9	4	e	10	4	e	$\nu_3+\nu_4,A_1$	3366.9394	90.3
9	2	a_1	10	3	a_2	$\nu_1+\nu_4,E$	3335.9122	92.5	9	4	e	10	5	e	$\nu_3+\nu_4,E$	3367.3085	94.4
10	1	a_1	11	3	a_2	$\nu_3+\nu_4,E$	3336.5010	96.1	7	2	e	8	2	e	$\nu_3+\nu_4,E$	3367.7547	89.9
8	5	a_1	9	6	a_2	$\nu_1+\nu_4,E$	3336.8844	73.7	5	3	e	6	4	e	$\nu_1+\nu_4,E$	3367.7861	52.6
9	2	a_2	10	3	a_1	$\nu_1+\nu_4,E$	3337.0030	91.8	7	2	a_2	8	0	a_1	$\nu_3+\nu_4,E$	3367.9185	92.4
9	1	e	10	2	e	$\nu_1+\nu_4,E$	3337.3775	94.3	4	4	a_1	5	3	a_2	$\nu_1+\nu_4,E$	3368.0985	94.6
7	7	e	8	8	e	$\nu_1+\nu_4,E$	3337.5319	51.3	10	7	e	11	7	e	$\nu_3+\nu_4,A_1$	3368.2792	97.1
8	4	e	9	4	e	$\nu_3+\nu_4,A_2$	3337.8463	89.1	8	3	a_1	9	0	a_2	$\nu_3+\nu_4,A_1$	3368.3563	89.5
7	5	e	8	4	e	$\nu_1+\nu_4,E$	3338.4169	97.4	5	2	e	6	1	e	$\nu_1+\nu_4,E$	3368.5616	91.5
9	1	e	10	1	e	$\nu_3+\nu_4,A_2$	3339.0833	98.1	8	1	e	9	1	e	$\nu_3+\nu_4,A_1$	3368.7345	88.4
8	4	e	9	5	e	$\nu_1+\nu_4,E$	3340.1640	81.0	5	2	e	6	2	e	$\nu_3+\nu_4,A_2$	3369.3815	90.4
9	0	e	10	1	e	$\nu_1+\nu_4,E$	3340.3448	90.0	9	5	e	10	5	e	$\nu_3+\nu_4,A_1$	3369.5553	94.6
9	1	a_2	10	0	a_1	$\nu_3+\nu_4,E$	3340.5178	85.1	8	2	e	9	2	e	$\nu_3+\nu_4,A_1$	3369.8891	76.8
8	3	a_2	9	3	a_1	$\nu_3+\nu_4,A_2$	3341.0224	89.3	7	4	e	8	1	e	$\nu_3+\nu_4,E$	3370.1905	96.7
8	3	a_1	9	3	a_2	$\nu_3+\nu_4,A_2$	3341.1791	89.7	9	5	a_2	10	6	a_1	$\nu_3+\nu_4,E$	3370.2698	90.2
7	6	e	8	7	e	$\nu_1+\nu_4,E$	3341.4920	58.1	5	2	a_1	6	3	a_2	$\nu_1+\nu_4,E$	3370.2840	56.9
7	5	e	8	5	e	$\nu_3+\nu_4,A_2$	3342.5094	87.6	7	3	e	8	2	e	$\nu_3+\nu_4,E$	3370.3326	96.3
8	3	e	9	4	e	$\nu_1+\nu_4,E$	3342.7885	84.4	5	1	a_2	6	0	a_1	$\nu_1+\nu_4,E$	3370.3984	92.1
7	4	a_1	8	3	a_2	$\nu_1+\nu_4,E$	3343.2361	94.9	4	4	e	5	4	e	$\nu_3+\nu_4,A_2$	3370.3984	92.1
11	7	a_2	12	6	a_1	$\nu_3+\nu_4,E$	3344.5550	95.7	5	2	a_2	6	3	a_1	$\nu_1+\nu_4,E$	3370.4570	55.7
8	2	a_2	9	3	a_1	$\nu_1+\nu_4,E$	3344.6293	85.8	9	5	a_1	10	6	a_2	$\nu_3+\nu_4,E$	3370.5541	90.3
7	5	a_1	8	6	a_2	$\nu_1+\nu_4,E$	3345.3183	63.0	9	4	a_1	10	6	a_2	$\nu_3+\nu_4,E$	3370.7345	95.5
7	5	a_2	8	6	a_1	$\nu_1+\nu_4,E$	3345.3348	53.4	9	4	a_2	10	6	a_1	$\nu_3+\nu_4,E$	3370.8330	95.2
8	2	a_1	9	3	a_2	$\nu_1+\nu_4,E$	3345.4125	85.4	7	4	a_1	8	3	a_2	$\nu_3+\nu_4,E$	3370.8962	93.3
7	4	e	8	4	e	$\nu_3+\nu_4,A_2$	3346.0161	87.5	8	0	a_1	9	3	a_2	$\nu_3+\nu_4,A_1$	3371.5682	86.9
8	1	e	9	2	e	$\nu_1+\nu_4,E$	3346.1007	90.3	8	3	a_2	9	3	a_1	$\nu_3+\nu_4,A_1$	3371.9286	91.6
6	5	e	7	4	e	$\nu_1+\nu_4,E$	3346.5322	97.5	10	8	a_1	11	9	a_2	$\nu_3+\nu_4,E$	3372.0352	88.0
11	2	e	12	1	e	$\nu_3+\nu_4,A_1$	3346.5570	98.6	10	8	a_2	11	9	a_1	$\nu_3+\nu_4,E$	3372.0487	87.6
8	1	e	9	1	e	$\nu_3+\nu_4,A_2$	3347.5562	97.0	5	1	e	6	2	e	$\nu_1+\nu_4,E$	3372.0761	68.9
7	3	e	8	2	e	$\nu_1+\nu_4,E$	3347.5767	95.8	9	6	a_2	10	6	a_1	$\nu_3+\nu_4,A_1$	3372.2504	96.2
11	3	a_2	12	0	a_1	$\nu_3+\nu_4,A_1$	3348.3211	96.1	7	5	e	8	4	e	$\nu_3+\nu_4,E$	3372.2614	95.9
7	4	e	8	5	e	$\nu_1+\nu_4,E$	3348.3459	70.1	5	1	e	6	1	e	$\nu_3+\nu_4,A_2$	3372.3914	89.2
8	0	e	9	1	e	$\nu_1+\nu_4,E$	3348.8010	84.0	7	2	a_2	8	3	a_1	$\nu_3+\nu_4,E$	3372.6213	91.3
8	1	a_1	9	0	a_2	$\nu_3+\nu_4,E$	3348.9710	75.3	4	3	e	5	2	e	$\nu_1+\nu_4,E$	3372.9187	93.5
10	3	e	11	2	e	$\nu_3+\nu_4,E$	3349.0107	85.3	4	4	e	5	5	e	$\nu_1+\nu_4,E$	3372.9856	35.2
8	1	e	9	2	e	$\nu_3+\nu_4,A_2$	3349.1130	96.0	5	1	a_2	6	0	a_1	$\nu_3+\nu_4,E$	3373.4452	53.7
6	6	e	7	7	e	$\nu_1+\nu_4,E$	3349.4735	44.1	5	0	e	6	1	e	$\nu_1+\nu_4,E$	3373.6254	61.8
7	3	a_1	8	3	a_2	$\nu_3+\nu_4,A_2$	3349.5810	82.2	9	6	e	10	7	e	$\nu_3+\nu_4,E$	3373.6513	86.5
6	5	e	7	5	e	$\nu_3+\nu_4,A_2$	3350.1816	88.3	7	7	a	8	6	a	$\nu_3+\nu_4,E$	3373.6815	96.7
11	0	a_2	12	3	a_1	$\nu_3+\nu_4,A_1$	3351.1281	94.1	8	3	e	9	5	e	$\nu_3+\nu_4,E$	3373.8708	95.7
7	3	e	8	4	e	$\nu_1+\nu_4,E$	3351.1518	73.3	5	1	e	6	2	e	$\nu_3+\nu_4,A_2$	3373.9735	91.2
11	3	a_1	12	3	a_2	$\nu_3+\nu_4,A_1$	3351.5155	95.8	8	4	e	9	4	e	$\nu_3+\nu_4,A_1$	3374.1266	91.5
6	4	a_1	7	3	a_2	$\nu_1+\nu_4,E$	3351.5366	92.0	6	2	e	7	1	e	$\nu_3+\nu_4,E$	3374.1785	93.7
7	2	e	8	1	e	$\nu_1+\nu_4,E$	3351.5556	95.7	4	3	a	5	3	a	$\nu_3+\nu_4,A_2$	3374.3929	81.7
6	3	e	7	1	e	$\nu_1+\nu_4,E$	3351.5828	61.7	8	4	e	9	5	e	$\nu_3+\nu_4,E$	3374.6095	91.2
7	2	e	8	2	e	$\nu_1+\nu_4,E$	3353.1203	96.2	6	3	e	7	1	e	$\nu_3+\nu_4,E$	3375.0127	93.2

Table 1 (*continued*)

Upper state J' K' Γ'	Lower state J K Γ	Band	Line position, exp., in cm^{-1}	Trsm., in %	Upper state J' K' Γ'	Lower state J K Γ	Band	Line position, exp., in cm^{-1}	Trsm., in %
6 5 a	7 6 a	$\nu_1+\nu_4, E$	3353.2270	27.2	7 3 a_2	8 0 a_1	$\nu_3+\nu_4, A_1$	3375.3826	84.4
7 2 a_1	8 3 a_2	$\nu_1+\nu_4, E$	3353.2542	79.0	7 2 a_1	8 3 a_2	$\nu_3+\nu_4, E$	3375.6008	90.2
7 2 a_2	8 3 a_1	$\nu_1+\nu_4, E$	3353.7807	78.2	7 1 e	8 1 e	$\nu_3+\nu_4, A_1$	3375.7918	85.6
6 4 e	7 4 e	$\nu_3+\nu_4, A_2$	3354.1497	86.9	4 3 e	5 4 e	$\nu_1+\nu_4, E$	3376.1131	43.6
7 1 e	8 2 e	$\nu_1+\nu_4, E$	3354.7976	84.1	6 3 e	7 2 e	$\nu_3+\nu_4, E$	3376.5868	84.7
9 4 e	10 1 e	$\nu_3+\nu_4, E$	3354.8647	96.8	8 5 e	9 5 e	$\nu_3+\nu_4, A_1$	3376.7927	94.9
10 2 e	11 1 e	$\nu_3+\nu_4, A_1$	3355.1796	93.6	7 2 e	8 2 e	$\nu_3+\nu_4, A_1$	3377.0378	85.8
9 3 e	10 2 e	$\nu_3+\nu_4, E$	3355.8180	93.2	4 2 e	5 1 e	$\nu_1+\nu_4, E$	3377.1008	89.5
7 1 e	8 1 e	$\nu_3+\nu_4, A_2$	3355.9218	96.8	4 1 a_1	5 0 a_2	$\nu_1+\nu_4, E$	3377.4350	95.5
6 3 e	7 2 e	$\nu_1+\nu_4, E$	3356.0706	94.2	5 1 a_1	6 3 a_2	$\nu_3+\nu_4, E$	3377.7863	90.0
10 1 e	11 2 e	$\nu_3+\nu_4, A_1$	3356.2197	93.9	6 4 e	7 1 e	$\nu_3+\nu_4, E$	3377.7863	90.0
9 6 e	10 4 e	$\nu_3+\nu_4, E$	3356.3657	96.6	8 5 a_2	9 6 a_1	$\nu_3+\nu_4, E$	3378.1703	89.0
6 4 e	7 5 e	$\nu_1+\nu_4, E$	3356.5421	58.0	8 5 a_1	9 6 a_2	$\nu_3+\nu_4, E$	3378.3083	92.3
9 4 a_1	10 3 a_2	$\nu_3+\nu_4, E$	3356.6632	93.3	7 3 e	8 4 e	$\nu_3+\nu_4, E$	3378.4934	77.2
9 4 a_2	10 3 a_1	$\nu_3+\nu_4, E$	3356.7648	87.0	6 4 a_1	7 3 a_2	$\nu_3+\nu_4, E$	3378.6900	92.4
7 0 e	8 1 e	$\nu_1+\nu_4, E$	3357.1351	77.2	4 2 a_2	5 3 a_1	$\nu_1+\nu_4, E$	3378.7423	50.9
9 5 e	10 4 e	$\nu_3+\nu_4, E$	3357.1778	95.6	4 2 a_1	5 3 a_2	$\nu_1+\nu_4, E$	3378.8201	51.0
7 1 a_2	8 0 a_1	$\nu_3+\nu_4, E$	3357.2552	67.9	7 0 a_2	8 3 a_1	$\nu_3+\nu_4, A_1$	3378.8893	83.0
8 2 e	9 1 e	$\nu_3+\nu_4, E$	3357.2767	94.9	7 3 a_1	8 3 a_2	$\nu_3+\nu_4, A_1$	3379.2139	88.9
7 1 e	8 2 e	$\nu_3+\nu_4, A_2$	3357.4851	94.1	6 5 a_1	7 3 a_2	$\nu_3+\nu_4, E$	3379.3632	95.2
10 0 a_1	11 3 a_2	$\nu_3+\nu_4, A_1$	3357.6586	92.5	6 5 a_2	7 3 a_1	$\nu_3+\nu_4, E$	3379.4123	96.7
8 6 a_1	9 6 a_2	$\nu_3+\nu_4, A_1$	3379.4975	96.8	9 5 a_2	9 3 a_1	$\nu_1+\nu_4, E$	3403.1848	97.2
8 6 a_2	9 6 a_1	$\nu_3+\nu_4, A_1$	3379.5206	96.7	8 5 e	8 2 e	$\nu_1+\nu_4, E$	3403.8708	96.2
9 8 a	10 9 a	$\nu_3+\nu_4, E$	3379.5646	64.9	7 6 e	7 5 e	$\nu_1+\nu_4, E$	3404.1355	75.6
11 11 e	11 10 e	$\nu_1+\nu_4, E$	3379.6444	96.8	8 6 e	8 5 e	$\nu_1+\nu_4, E$	3404.9757	75.4
6 5 e	7 4 e	$\nu_3+\nu_4, E$	3379.9775	93.9	4 4 e	5 4 e	$\nu_3+\nu_4, A_1$	3405.2807	92.4
4 1 e	5 1 e	$\nu_3+\nu_4, A_2$	3380.5875	98.3	3 0 a_2	4 0 a_1	$\nu_3+\nu_4, A_1$	3405.5964	66.2
4 1 e	5 2 e	$\nu_1+\nu_4, E$	3380.6652	61.2	9 6 e	9 5 e	$\nu_1+\nu_4, E$	3405.7322	78.3
8 6 e	9 7 e	$\nu_3+\nu_4, E$	3381.0689	75.8	1 1 a_2	2 0 a_1	$\nu_3+\nu_4, E$	3406.3369	73.4
4 1 a_1	5 0 a_2	$\nu_3+\nu_4, E$	3381.4943	52.0	3 1 e	4 1 e	$\nu_3+\nu_4, A_1$	3406.3724	73.6
7 4 e	8 4 e	$\nu_3+\nu_4, A_1$	3381.5622	83.8	10 6 e	10 5 e	$\nu_1+\nu_4, E$	3406.4004	83.1
6 0 a_1	7 0 a_2	$\nu_3+\nu_4, A_1$	3381.7253	96.2	4 4 e	5 5 e	$\nu_3+\nu_4, E$	3406.4694	82.3
4 0 e	5 1 e	$\nu_1+\nu_4, E$	3381.9221	56.7	1 1 e	2 2 e	$\nu_1+\nu_4, E$	3406.5274	43.9
4 1 e	5 2 e	$\nu_3+\nu_4, A_2$	3382.1762	90.5	9 8 a	9 9 a	$\nu_1+\nu_4, E$	3406.6517	88.8
6 3 a_1	7 0 a_2	$\nu_3+\nu_4, A_1$	3382.6184	83.0	5 4 e	5 2 e	$\nu_1+\nu_4, E$	3406.9332	97.8
3 3 a	4 3 a	$\nu_3+\nu_4, A_2$	3382.6908	86.1	11 6 e	11 5 e	$\nu_1+\nu_4, E$	3407.0769	87.3
7 4 e	8 5 e	$\nu_3+\nu_4, E$	3382.7868	92.1	3 2 a_2	4 3 a_1	$\nu_3+\nu_4, E$	3407.3175	77.7
6 1 e	7 1 e	$\nu_3+\nu_4, A_1$	3382.8408	94.9	1 0 e	2 1 e	$\nu_1+\nu_4, E$	3407.4850	61.3
5 2 e	6 1 e	$\nu_3+\nu_4, E$	3383.0063	91.6	3 2 a_1	4 3 a_2	$\nu_3+\nu_4, E$	3407.6002	74.1
6 2 a_2	7 3 a_1	$\nu_3+\nu_4, E$	3383.2361	86.0	10 8 a	10 9 a	$\nu_1+\nu_4, E$	3407.7041	87.3
5 3 e	6 1 e	$\nu_3+\nu_4, E$	3383.6020	95.6	5 5 e	5 4 e	$\nu_1+\nu_4, E$	3408.0012	74.1
10 10 a_2	10 9 a_1	$\nu_1+\nu_4, E$	3384.2088	90.4	7 4 e	7 2 e	$\nu_1+\nu_4, E$	3408.2996	96.7
7 5 e	8 5 e	$\nu_3+\nu_4, A_1$	3384.2842	94.6	3 2 e	4 2 e	$\nu_3+\nu_4, A_1$	3408.3316	80.3
8 7 e	9 8 e	$\nu_3+\nu_4, E$	3384.3880	84.9	6 5 e	6 4 e	$\nu_1+\nu_4, E$	3408.7256	66.5
6 1 e	7 2 e	$\nu_3+\nu_4, A_1$	3384.4142	84.3	2 2 e	3 1 e	$\nu_3+\nu_4, E$	3409.3240	94.9
3 3 e	4 4 e	$\nu_1+\nu_4, E$	3384.4958	34.5	7 5 e	7 4 e	$\nu_1+\nu_4, E$	3409.4319	67.4
6 2 e	7 2 e	$\nu_3+\nu_4, A_1$	3384.6484	96.0	8 7 e	8 8 e	$\nu_1+\nu_4, E$	3409.6817	92.3

Table 1 (*continued*)

Upper state J'	K'	Γ'	Lower state J	K	Γ	Band	Line position, exp., in cm^{-1}	Trsm., in %	J'	K'	Γ'	Lower state J	K	Γ	Band	Line position, exp., in cm^{-1}	Trsm., in %
7	4	a_1	8	6	a_2	$\nu_3+\nu_4, E$	3385.1371	87.9	8	5	e	8	4	e	$\nu_1+\nu_4, E$	3410.1577	71.0
3	1	a_2	4	0	a_1	$\nu_1+\nu_4, E$	3385.1826	83.3	9	4	a_1	9	0	a_2	$\nu_1+\nu_4, E$	3410.3227	97.8
5	3	e	6	2	e	$\nu_3+\nu_4, E$	3385.1826	83.3	3	0	a_2	4	3	a_1	$\nu_3+\nu_4, A_1$	3410.3779	94.3
3	2	e	4	1	e	$\nu_1+\nu_4, E$	3385.6521	90.2	9	5	e	9	4	e	$\nu_1+\nu_4, E$	3410.4140	77.7
7	5	a_2	8	6	a_1	$\nu_3+\nu_4, E$	3385.8363	81.3	9	7	e	9	8	e	$\nu_1+\nu_4, E$	3410.6097	89.9
7	5	a_1	8	6	a_2	$\nu_3+\nu_4, E$	3386.0423	89.8	3	3	a_1	4	3	a_2	$\nu_3+\nu_4, A_1$	3410.8594	89.0
4	1	a_2	5	3	a_1	$\nu_3+\nu_4, E$	3386.1665	66.6	3	3	a_2	4	3	a_1	$\nu_3+\nu_4, A_1$	3410.8724	90.8
11	10	a_2	11	9	a_1	$\nu_1+\nu_4, E$	3386.2694	89.3	10	5	e	10	4	e	$\nu_1+\nu_4, E$	3411.0806	83.8
6	0	a_1	7	3	a_2	$\nu_3+\nu_4, A_1$	3386.4523	80.0	3	3	e	4	4	e	$\nu_3+\nu_4, E$	3411.2754	62.5
6	3	e	7	4	e	$\nu_3+\nu_4, E$	3386.6677	78.2	10	7	e	10	8	e	$\nu_1+\nu_4, E$	3411.4548	91.0
6	3	a_2	7	3	a_1	$\nu_3+\nu_4, A_1$	3386.7517	86.8	11	7	e	11	8	e	$\nu_1+\nu_4, E$	3412.3063	92.6
3	2	a_1	4	3	a_2	$\nu_1+\nu_4, E$	3387.2136	43.8	6	5	e	6	5	e	$\nu_3+\nu_4, A_2$	3412.3962	94.5
3	2	a_2	4	3	a_1	$\nu_1+\nu_4, E$	3387.2403	41.5	4	4	a_1	4	3	a_2	$\nu_1+\nu_4, E$	3412.5719	49.5
8	8	a	9	9	a	$\nu_3+\nu_4, E$	3387.3027	48.2	7	6	e	7	7	e	$\nu_1+\nu_4, E$	3412.5969	88.3
5	5	a	6	3	a	$\nu_3+\nu_4, E$	3387.4683	97.0	5	4	a_1	5	3	a_2	$\nu_1+\nu_4, E$	3413.1458	35.3
5	5	e	6	4	e	$\nu_3+\nu_4, E$	3387.9626	96.2	5	3	e	5	1	e	$\nu_1+\nu_4, E$	3413.1761	97.0
5	3	e	6	2	e	$\nu_3+\nu_4, E$	3388.2797	98.0	8	6	e	8	7	e	$\nu_1+\nu_4, E$	3413.4187	85.8
7	6	e	8	7	e	$\nu_3+\nu_4, E$	3388.8512	66.9	6	4	a_1	6	3	a_2	$\nu_1+\nu_4, E$	3413.7129	33.3
9	9	e	9	8	e	$\nu_1+\nu_4, E$	3388.9419	92.6	6	3	e	6	1	e	$\nu_1+\nu_4, E$	3413.7408	94.9
3	1	e	4	2	e	$\nu_1+\nu_4, E$	3389.2479	48.5	2	0	a_1	3	0	a_2	$\nu_3+\nu_4, A_1$	3413.9615	70.6
6	4	e	7	4	e	$\nu_3+\nu_4, A_1$	3389.2479	48.5	7	4	a_1	7	3	a_2	$\nu_1+\nu_4, E$	3414.2314	46.1
5	0	a_2	6	0	a_1	$\nu_3+\nu_4, A_1$	3389.5015	89.7	7	3	e	7	1	e	$\nu_1+\nu_4, E$	3414.2732	92.4
3	1	a_2	4	0	a_1	$\nu_3+\nu_4, E$	3389.6184	52.5	8	4	a_2	8	3	a_1	$\nu_1+\nu_4, E$	3414.6598	64.8
5	2	a_2	6	3	a_1	$\nu_3+\nu_4, E$	3390.1058	81.5	8	4	a_1	8	3	a_2	$\nu_1+\nu_4, E$	3414.6765	64.0
3	0	e	4	1	e	$\nu_1+\nu_4, E$	3390.3215	55.5	8	3	e	8	1	e	$\nu_1+\nu_4, E$	3414.7478	93.8
5	1	e	6	1	e	$\nu_3+\nu_4, A_1$	3390.4357	83.4	2	1	e	3	1	e	$\nu_3+\nu_4, A_1$	3414.7686	72.9
6	4	e	7	5	e	$\nu_3+\nu_4, E$	3390.4454	85.6	4	4	e	4	4	e	$\nu_3+\nu_4, A_2$	3414.8848	87.8
10	9	e	10	8	e	$\nu_1+\nu_4, E$	3390.5475	91.5	9	4	a_1	9	3	a_2	$\nu_1+\nu_4, E$	3414.9988	72.9
5	2	e	6	1	e	$\nu_3+\nu_4, A_1$	3390.6447	89.9	9	4	a_2	9	3	a_1	$\nu_1+\nu_4, E$	3415.0546	71.2
5	2	a_1	6	3	a_2	$\nu_3+\nu_4, E$	3391.1231	81.4	10	4	a_2	10	3	a_1	$\nu_1+\nu_4, E$	3415.1421	78.0
4	2	e	5	1	e	$\nu_3+\nu_4, E$	3391.7936	91.9	9	3	e	9	1	e	$\nu_1+\nu_4, E$	3415.1625	93.2
6	5	e	7	5	e	$\nu_3+\nu_4, A_1$	3392.0030	93.3	10	4	a_1	10	3	a_2	$\nu_1+\nu_4, E$	3415.3547	81.5
5	1	e	6	2	e	$\nu_3+\nu_4, A_1$	3392.0159	88.1	6	5	a	6	6	a	$\nu_1+\nu_4, E$	3415.4673	70.4
4	3	e	5	1	e	$\nu_3+\nu_4, E$	3392.0364	97.1	5	4	e	5	4	e	$\nu_3+\nu_4, A_2$	3415.6109	97.3
11	9	e	11	8	e	$\nu_1+\nu_4, E$	3392.0782	92.3	0	0	e	1	1	e	$\nu_1+\nu_4, E$	3416.1301	73.4
7	7	e	8	8	e	$\nu_3+\nu_4, E$	3392.1688	63.6	7	5	a_2	7	6	a_1	$\nu_1+\nu_4, E$	3416.4040	60.2
5	2	e	6	2	e	$\nu_3+\nu_4, A_1$	3392.2257	89.0	8	5	a_2	8	6	a_1	$\nu_1+\nu_4, E$	3416.7176	82.4
6	4	a_2	7	6	a_1	$\nu_3+\nu_4, E$	3392.8954	90.3	9	4	e	9	4	e	$\nu_1+\nu_4, E$	3416.7576	82.4
6	4	a_1	7	6	a_2	$\nu_3+\nu_4, E$	3393.0035	90.0	8	5	a_1	8	6	a_2	$\nu_1+\nu_4, E$	3416.7576	82.4
2	1	a_1	3	0	a_2	$\nu_1+\nu_4, E$	3393.4066	94.9	2	2	e	3	2	e	$\nu_3+\nu_4, A_1$	3416.7741	84.9
4	3	e	5	2	e	$\nu_3+\nu_4, E$	3393.6232	87.6	3	3	e	3	2	e	$\nu_1+\nu_4, E$	3416.9479	66.4
6	5	a_1	7	6	a_2	$\nu_3+\nu_4, E$	3393.6765	70.6	9	5	a_1	9	6	a_2	$\nu_1+\nu_4, E$	3417.2541	85.7
6	5	a_2	7	6	a_1	$\nu_3+\nu_4, E$	3393.7268	71.8	9	5	a_2	9	6	a_1	$\nu_1+\nu_4, E$	3417.3443	84.1
8	8	e	8	7	e	$\nu_1+\nu_4, E$	3393.7373	88.8	4	3	e	4	2	e	$\nu_1+\nu_4, E$	3417.3842	51.3
12	9	e	12	8	e	$\nu_1+\nu_4, E$	3394.1184	95.2	5	3	e	5	2	e	$\nu_1+\nu_4, E$	3417.8296	46.6
2	2	e	3	1	e	$\nu_1+\nu_4, E$	3394.2365	92.6	10	5	a_2	10	6	a_1	$\nu_1+\nu_4, E$	3418.0657	86.5
5	0	a_2	6	3	a_1	$\nu_3+\nu_4, A_1$	3394.2486	79.0	5	4	e	5	5	e	$\nu_1+\nu_4, E$	3418.1129	79.2
5	3	a_1	6	3	a_2	$\nu_3+\nu_4, A_1$	3394.5466	85.2	6	3	e	6	2	e	$\nu_1+\nu_4, E$	3418.2356	47.3

Table 1 (*continued*)

Upper state J' K' Γ'	Lower state J K Γ	Band	Line position, exp., in cm^{-1}	Trsm., in %	Upper state J' K' Γ'	Lower state J K Γ	Band	Line position, exp., in cm^{-1}	Trsm., in %
5 3 e	6 4 e	$\nu_3+\nu_4, E$	3394.6273	74.8	3 3 a	3 3 a	$\nu_3+\nu_4, A_2$	3418.2892	80.4
5 3 a_2	6 3 a_1	$\nu_3+\nu_4, A_1$	3394.8511	97.4	9 4 e	9 4 e	$\nu_3+\nu_4, A_2$	3418.4142	94.0
9 8 e	9 7 e	$\nu_1+\nu_4, E$	3395.0143	81.2	4 2 a_2	4 0 a_1	$\nu_1+\nu_4, E$	3418.4354	95.3
4 4 e	5 2 e	$\nu_3+\nu_4, E$	3395.2903	95.9	7 3 e	7 2 e	$\nu_1+\nu_4, E$	3418.5594	50.7
2 2 a	3 3 a	$\nu_1+\nu_4, E$	3395.7466	20.2	11 3 e	11 2 e	$\nu_1+\nu_4, E$	3418.7099	84.5
8 6 e	8 4 e	$\nu_1+\nu_4, E$	3395.9233	98.3	6 4 e	6 5 e	$\nu_1+\nu_4, E$	3418.7565	71.5
2 1 e	3 1 e	$\nu_1+\nu_4, E$	3396.2573	85.7	8 3 e	8 2 e	$\nu_1+\nu_4, E$	3418.7691	56.0
10 8 e	10 7 e	$\nu_1+\nu_4, E$	3396.2573	85.7	10 3 e	10 2 e	$\nu_1+\nu_4, E$	3418.8294	71.0
5 3 e	6 5 e	$\nu_3+\nu_4, E$	3396.3194	97.4	9 3 e	9 2 e	$\nu_1+\nu_4, E$	3418.8471	63.8
6 6 e	7 7 e	$\nu_3+\nu_4, E$	3396.9390	60.8	6 2 a_2	6 0 a_1	$\nu_1+\nu_4, E$	3419.2277	88.2
12 11 a	12 12 a	$\nu_1+\nu_4, E$	3396.9619	96.4	7 4 e	7 5 e	$\nu_1+\nu_4, E$	3419.3858	71.8
5 4 e	6 4 e	$\nu_3+\nu_4, A_1$	3397.1573	89.8	9 2 a_1	9 0 a_2	$\nu_1+\nu_4, E$	3419.7990	79.7
4 0 a_1	5 0 a_2	$\nu_3+\nu_4, A_1$	3397.4673	79.2	8 4 e	8 5 e	$\nu_1+\nu_4, E$	3420.0042	75.3
6 5 e	7 7 e	$\nu_3+\nu_4, E$	3397.5643	95.9	6 3 a_2	6 3 a_1	$\nu_3+\nu_4, A_2$	3420.0376	95.4
11 8 e	11 7 e	$\nu_1+\nu_4, E$	3397.6066	90.5	6 3 a_1	6 3 a_2	$\nu_3+\nu_4, A_2$	3420.0685	94.9
2 1 e	3 2 e	$\nu_1+\nu_4, E$	3397.8567	47.0	7 3 a_1	7 3 a_2	$\nu_3+\nu_4, A_2$	3420.5768	91.4
2 1 a_1	3 0 a_2	$\nu_3+\nu_4, E$	3397.8833	58.4	4 3 e	4 4 e	$\nu_1+\nu_4, E$	3420.5993	75.3
4 3 a_1	5 0 a_2	$\nu_3+\nu_4, A_1$	3397.9171	91.0	4 2 e	4 1 e	$\nu_3+\nu_4, A_2$	3420.6601	96.3
4 1 e	5 1 e	$\nu_3+\nu_4, A_1$	3398.2619	76.2	8 3 a_2	8 3 a_1	$\nu_3+\nu_4, A_2$	3420.8132	80.8
5 4 e	6 5 e	$\nu_3+\nu_4, E$	3398.3743	76.3	2 2 e	2 1 e	$\nu_1+\nu_4, E$	3420.9384	59.6
7 7 a	7 6 a	$\nu_1+\nu_4, E$	3398.5345	73.1	9 3 a_1	9 3 a_2	$\nu_3+\nu_4, A_2$	3420.9546	87.2
4 2 a_1	5 3 a_2	$\nu_3+\nu_4, E$	3398.5800	84.8	8 3 a_1	8 3 a_2	$\nu_3+\nu_4, A_2$	3420.9684	80.7
2 0 e	3 1 e	$\nu_1+\nu_4, E$	3398.8407	56.8	5 2 e	5 2 e	$\nu_3+\nu_4, A_2$	3421.1191	89.0
4 2 a_2	5 3 a_1	$\nu_3+\nu_4, E$	3399.2532	77.2	5 3 e	5 4 e	$\nu_1+\nu_4, E$	3421.1349	65.5
8 7 a	8 6 a	$\nu_1+\nu_4, E$	3399.5898	66.6	3 2 e	3 1 e	$\nu_1+\nu_4, E$	3421.2396	38.8
4 1 e	5 2 e	$\nu_3+\nu_4, A_1$	3399.8486	94.8	9 4 e	9 5 e	$\nu_1+\nu_4, E$	3421.4747	91.6
5 5 e	6 5 e	$\nu_3+\nu_4, A_1$	3399.9277	96.1	4 2 e	4 1 e	$\nu_1+\nu_4, E$	3421.5610	36.7
4 2 e	5 2 e	$\nu_3+\nu_4, A_1$	3400.1311	81.7	6 3 e	6 4 e	$\nu_1+\nu_4, E$	3421.6695	65.9
11 10 e	11 11 e	$\nu_1+\nu_4, E$	3400.2023	97.3	5 2 e	5 1 e	$\nu_1+\nu_4, E$	3421.8799	37.5
9 7 a_1	9 6 a_2	$\nu_1+\nu_4, E$	3400.5246	85.9	7 3 e	7 4 e	$\nu_1+\nu_4, E$	3422.1671	68.4
3 2 e	4 1 e	$\nu_3+\nu_4, E$	3400.5768	92.1	6 2 e	6 1 e	$\nu_1+\nu_4, E$	3422.2095	45.7
9 7 a_2	9 6 a_1	$\nu_1+\nu_4, E$	3400.6238	84.8	7 2 e	7 1 e	$\nu_1+\nu_4, E$	3422.5310	57.7
10 7 a	10 6 a	$\nu_1+\nu_4, E$	3401.5194	73.4	1 0 a_2	2 0 a_1	$\nu_3+\nu_4, A_1$	3422.5700	75.7
1 1 a_2	2 0 a_1	$\nu_1+\nu_4, E$	3401.8212	95.2	8 3 e	8 4 e	$\nu_1+\nu_4, E$	3422.6017	74.4
5 5 a	6 6 a	$\nu_3+\nu_4, E$	3401.8468	43.8	5 2 e	5 2 e	$\nu_3+\nu_4, A_2$	3422.7055	78.3
3 3 e	4 2 e	$\nu_3+\nu_4, E$	3402.0752	93.4	1 1 e	1 1 e	$\nu_1+\nu_4, E$	3422.7348	97.6
4 0 a_1	5 3 a_2	$\nu_3+\nu_4, A_1$	3402.2328	85.7	8 2 e	8 1 e	$\nu_1+\nu_4, E$	3422.7670	66.5
8 5 a_2	8 3 a_1	$\nu_1+\nu_4, E$	3402.4777	97.0	11 1 a_1	11 0 a_2	$\nu_1+\nu_4, E$	3422.7760	80.3
11 7 a	11 6 a	$\nu_1+\nu_4, E$	3402.5037	88.6	3 2 a_1	3 3 a_2	$\nu_1+\nu_4, E$	3422.8131	60.6
4 3 a_2	5 3 a_1	$\nu_3+\nu_4, A_1$	3402.5891	85.8	3 2 a_2	3 3 a_1	$\nu_1+\nu_4, E$	3422.8382	69.2
4 3 a_1	5 3 a_2	$\nu_3+\nu_4, A_1$	3402.6818	91.8	9 3 e	9 4 e	$\nu_1+\nu_4, E$	3422.9718	71.7
4 3 e	5 4 e	$\nu_3+\nu_4, E$	3402.8411	67.8	9 2 e	9 1 e	$\nu_1+\nu_4, E$	3423.0032	84.1
9 5 a_1	9 3 a_2	$\nu_1+\nu_4, E$	3403.0969	96.8	6 2 e	6 2 e	$\nu_3+\nu_4, A_2$	3423.0032	84.1
6 6 e	6 5 e	$\nu_1+\nu_4, E$	3403.1566	83.8	10 1 a_2	10 0 a_1	$\nu_1+\nu_4, E$	3423.0717	69.6
4 2 a_2	4 3 a_1	$\nu_1+\nu_4, E$	3423.2162	59.4	5 4 e	5 2 e	$\nu_3+\nu_4, E$	3440.5628	92.5
4 2 a_1	4 3 a_2	$\nu_1+\nu_4, E$	3423.2938	58.1	6 4 a_2	6 3 a_1	$\nu_3+\nu_4, E$	3440.7579	92.4
9 1 a_1	9 0 a_2	$\nu_1+\nu_4, E$	3423.3596	54.2	5 5 a	5 3 a	$\nu_3+\nu_4, E$	3440.8040	96.5

Table 1 (*continued*)

Upper state J' K' Γ'	Lower state J K Γ	Band	Line position, exp., in cm^{-1}	Trsm., in %	Upper state J' K' Γ'	Lower state J K Γ	Band	Line position, exp., in cm^{-1}	Trsm., in %
1 1 e	2 1 e	$\nu_3+\nu_4, A_1$	3423.3906	81.7	6 4 a_1	6 3 a_2	$\nu_3+\nu_4, E$	3440.8663	90.2
4 1 e	4 1 e	$\nu_1+\nu_4, E$	3423.5389	90.4	6 3 e	6 1 e	$\nu_3+\nu_4, E$	3440.9320	97.7
3 1 a_1	3 0 a_2	$\nu_1+\nu_4, E$	3423.6036	40.3	7 4 e	7 1 e	$\nu_3+\nu_4, E$	3441.1663	97.7
8 1 a_2	8 0 a_1	$\nu_1+\nu_4, E$	3423.6036	40.3	1 1 e	1 1 e	$\nu_3+\nu_4, A_1$	3441.1969	79.6
5 2 a_1	5 3 a_2	$\nu_1+\nu_4, E$	3423.6190	56.1	5 5 e	5 4 e	$\nu_3+\nu_4, E$	3441.3119	84.4
4 1 a_2	4 0 a_1	$\nu_1+\nu_4, E$	3423.7884	20.2	2 1 e	2 1 e	$\nu_3+\nu_4, A_1$	3441.4699	88.8
7 1 a_1	7 0 a_2	$\nu_1+\nu_4, E$	3423.7884	20.2	6 4 e	6 2 e	$\nu_3+\nu_4, E$	3441.5245	91.6
5 1 e	5 1 e	$\nu_1+\nu_4, E$	3423.8132	85.0	7 4 a_2	7 3 a_1	$\nu_3+\nu_4, E$	3441.8933	93.7
6 1 a_2	6 0 a_1	$\nu_1+\nu_4, E$	3423.9048	43.0	3 1 e	3 1 e	$\nu_3+\nu_4, A_1$	3441.9588	90.3
5 1 a_1	5 0 a_2	$\nu_1+\nu_4, E$	3423.9597	0.90	6 5 e	6 4 e	$\nu_3+\nu_4, E$	3442.1720	80.3
6 2 a_2	6 3 a_1	$\nu_1+\nu_4, E$	3423.9757	63.6	2 1 a_1	1 0 a_2	$\nu_3+\nu_4, E$	3442.3892	39.0
6 1 e	6 1 e	$\nu_1+\nu_4, E$	3424.0407	80.6	7 5 a_2	7 3 a_1	$\nu_3+\nu_4, E$	3442.5930	95.6
7 2 e	7 2 e	$\nu_1+\nu_4, E$	3424.1054	94.8	8 3 e	8 2 e	$\nu_3+\nu_4, E$	3442.6810	97.3
7 1 e	7 1 e	$\nu_1+\nu_4, E$	3424.2071	81.4	4 1 e	4 1 e	$\nu_3+\nu_4, A_1$	3442.7221	95.1
7 2 a_1	7 3 a_2	$\nu_1+\nu_4, E$	3424.2511	70.8	7 4 e	7 2 e	$\nu_3+\nu_4, E$	3442.7402	95.0
6 2 a_1	6 3 a_2	$\nu_1+\nu_4, E$	3424.2973	59.8	7 5 a_1	7 3 a_2	$\nu_3+\nu_4, E$	3442.7983	87.9
8 1 e	8 1 e	$\nu_1+\nu_4, E$	3424.3121	85.1	3 2 a_2	3 3 a_1	$\nu_3+\nu_4, E$	3442.9153	92.5
8 2 e	8 2 e	$\nu_1+\nu_4, E$	3424.3324	91.8	4 2 a_1	4 3 a_2	$\nu_3+\nu_4, E$	3443.0544	88.9
9 1 e	9 1 e	$\nu_1+\nu_4, E$	3424.3640	87.1	6 6 e	6 5 e	$\nu_3+\nu_4, E$	3443.0763	87.1
8 2 a_2	8 3 a_1	$\nu_1+\nu_4, E$	3424.4231	75.6	8 8 a	8 6 a	$\nu_3+\nu_4, E$	3443.1307	85.8
9 2 a_1	9 3 a_2	$\nu_1+\nu_4, E$	3424.4752	89.8	3 2 a_1	3 3 a_2	$\nu_3+\nu_4, E$	3443.1990	88.6
2 1 e	2 2 e	$\nu_1+\nu_4, E$	3424.5607	64.6	7 5 e	7 4 e	$\nu_3+\nu_4, E$	3443.2753	92.5
1 1 a_1	1 0 a_2	$\nu_3+\nu_4, E$	3424.6349	91.2	2 0 e	1 1 e	$\nu_1+\nu_4, E$	3443.3478	83.0
7 2 a_2	7 3 a_1	$\nu_1+\nu_4, E$	3424.7764	65.9	5 2 a_2	5 3 a_1	$\nu_3+\nu_4, E$	3443.4429	90.3
3 1 e	3 2 e	$\nu_1+\nu_4, E$	3424.8395	55.0	2 2 e	2 2 e	$\nu_3+\nu_4, A_1$	3443.4781	63.9
2 1 a_2	2 0 a_1	$\nu_3+\nu_4, E$	3424.9661	79.3	3 3 e	2 2 e	$\nu_1+\nu_4, E$	3443.6526	32.6
4 1 e	4 1 e	$\nu_3+\nu_4, A_2$	3425.0497	92.1	4 2 a_2	4 3 a_1	$\nu_3+\nu_4, E$	3443.7275	88.1
4 1 e	4 2 e	$\nu_1+\nu_4, E$	3425.1307	55.8	5 1 e	5 1 e	$\nu_3+\nu_4, A_1$	3443.7531	94.8
8 2 a_1	8 3 a_2	$\nu_1+\nu_4, E$	3425.2035	75.3	7 6 a_1	7 3 a_2	$\nu_3+\nu_4, A_1$	3443.7742	94.2
1 0 e	1 1 e	$\nu_1+\nu_4, E$	3425.2912	61.3	8 4 a_2	8 3 a_1	$\nu_3+\nu_4, E$	3443.8039	96.4
3 1 a_1	3 0 a_2	$\nu_3+\nu_4, E$	3425.3879	72.4	3 2 e	3 2 e	$\nu_3+\nu_4, A_1$	3443.9227	75.9
5 1 e	5 2 e	$\nu_1+\nu_4, E$	3425.4001	61.6	8 4 a_1	8 3 a_2	$\nu_3+\nu_4, E$	3443.9401	92.2
2 0 e	2 1 e	$\nu_1+\nu_4, E$	3425.5418	49.2	7 6 e	7 5 e	$\nu_3+\nu_4, E$	3444.0213	84.5
9 2 a_2	9 3 a_1	$\nu_1+\nu_4, E$	3425.5605	83.6	8 5 e	8 4 e	$\nu_3+\nu_4, E$	3444.3355	90.5
6 1 e	6 2 e	$\nu_1+\nu_4, E$	3425.6212	73.1	9 3 e	9 2 e	$\nu_3+\nu_4, E$	3444.3630	98.5
5 1 e	5 1 e	$\nu_3+\nu_4, A_2$	3425.7109	88.8	5 2 a_1	5 3 a_2	$\nu_3+\nu_4, E$	3444.4576	84.2
7 1 e	7 2 e	$\nu_1+\nu_4, E$	3425.7805	83.3	4 2 e	4 2 e	$\nu_3+\nu_4, A_1$	3444.5965	81.2
10 2 a_1	10 3 a_2	$\nu_1+\nu_4, E$	3425.8549	84.8	8 7 e	8 4 e	$\nu_3+\nu_4, A_1$	3444.6704	98.4
4 1 a_2	4 0 a_1	$\nu_3+\nu_4, E$	3425.8653	71.1	7 7 a	7 6 a	$\nu_3+\nu_4, E$	3444.7510	80.2
8 1 e	8 2 e	$\nu_1+\nu_4, E$	3425.8779	92.1	8 2 e	8 4 e	$\nu_3+\nu_4, E$	3444.8979	94.3
3 0 e	3 1 e	$\nu_1+\nu_4, E$	3425.9086	46.2	6 1 e	6 1 e	$\nu_3+\nu_4, A_1$	3444.9982	94.9
9 1 e	9 2 e	$\nu_1+\nu_4, E$	3425.9219	93.7	8 6 e	8 5 e	$\nu_3+\nu_4, E$	3445.1561	78.4
5 1 a_1	5 0 a_2	$\nu_3+\nu_4, E$	3426.3538	74.2	9 4 a_1	9 3 a_2	$\nu_3+\nu_4, E$	3445.2238	95.3
4 0 e	4 1 e	$\nu_1+\nu_4, E$	3426.3824	50.3	9 4 a_2	9 3 a_1	$\nu_3+\nu_4, E$	3445.3236	94.4
4 1 e	4 2 e	$\nu_3+\nu_4, A_2$	3426.6417	89.2	6 2 a_2	6 3 a_1	$\nu_3+\nu_4, E$	3445.4121	83.5
6 1 a_2	6 0 a_1	$\nu_3+\nu_4, E$	3426.8116	78.5	7 3 a_1	7 0 a_2	$\nu_3+\nu_4, A_1$	3445.4834	95.6
7 1 e	7 1 e	$\nu_3+\nu_4, A_2$	3426.8963	89.3	5 2 e	5 2 e	$\nu_3+\nu_4, A_1$	3445.5498	86.7
5 0 e	5 1 e	$\nu_1+\nu_4, E$	3426.9433	61.3	9 5 e	9 4 e	$\nu_3+\nu_4, E$	3445.7615	93.2

Table 1 (*continued*)

Upper state J' K' Γ'	Lower state J K Γ	Band	Line position, exp., in cm^{-1}	Trsm., in %	Upper state J' K' Γ'	Lower state J K Γ	Band	Line position, exp., in cm^{-1}	Trsm., in %
7 1 a_1	7 0 a_2	$\nu_3+\nu_4, E$	3427.1925	83.8	8 7 a	8 6 a	$\nu_3+\nu_4, E$	3445.8152	82.5
5 1 e	5 2 e	$\nu_3+\nu_4, A_2$	3427.2975	84.3	8 8 e	8 7 e	$\nu_3+\nu_4, E$	3446.3180	92.0
8 1 e	8 1 e	$\nu_3+\nu_4, A_2$	3427.3256	92.7	9 7 e	9 4 e	$\nu_3+\nu_4, A_1$	3446.3790	97.7
11 1 a_1	11 3 a_2	$\nu_1+\nu_4, E$	3427.3933	95.4	3 3 a_1	3 3 a_2	$\nu_3+\nu_4, A_1$	3446.4575	55.9
8 1 a_2	8 0 a_1	$\nu_3+\nu_4, E$	3427.4742	88.3	3 3 a_2	3 3 a_1	$\nu_3+\nu_4, A_1$	3446.4707	55.2
6 0 e	6 1 e	$\nu_1+\nu_4, E$	3427.5439	73.5	9 6 e	9 5 e	$\nu_3+\nu_4, E$	3446.5030	89.6
9 1 e	9 1 e	$\nu_3+\nu_4, A_2$	3427.6181	94.9	7 2 a_1	7 3 a_2	$\nu_3+\nu_4, E$	3446.5980	82.3
10 1 a_2	10 3 a_1	$\nu_1+\nu_4, E$	3427.7189	92.8	6 2 e	6 2 e	$\nu_3+\nu_4, A_1$	3446.8136	89.4
10 1 e	10 1 e	$\nu_3+\nu_4, A_2$	3427.7879	97.2	8 3 a_2	8 0 a_1	$\nu_3+\nu_4, A_1$	3447.0196	94.8
6 1 e	6 2 e	$\nu_3+\nu_4, A_2$	3427.9268	83.4	4 3 a_2	4 3 a_1	$\nu_3+\nu_4, A_1$	3447.0641	61.2
4 0 e	4 2 e	$\nu_1+\nu_4, E$	3427.9747	83.4	9 7 a_1	9 6 a_2	$\nu_3+\nu_4, E$	3447.1039	89.7
9 1 a_1	9 3 a_2	$\nu_1+\nu_4, E$	3428.0361	92.0	4 3 a_1	4 3 a_2	$\nu_3+\nu_4, A_1$	3447.1565	67.4
6 4 a_1	6 6 a_2	$\nu_1+\nu_4, E$	3428.0897	97.6	4 3 e	4 4 e	$\nu_3+\nu_4, E$	3447.3266	92.9
7 0 e	7 1 e	$\nu_1+\nu_4, E$	3428.1102	84.4	6 6 e	5 4 e	$\nu_1+\nu_4, E$	3447.4298	97.9
8 1 a_2	8 3 a_1	$\nu_1+\nu_4, E$	3428.3061	90.6	3 1 a_2	2 0 a_1	$\nu_1+\nu_4, E$	3447.4677	92.2
3 1 a_1	3 3 a_2	$\nu_1+\nu_4, E$	3428.3986	97.3	9 8 e	9 7 e	$\nu_3+\nu_4, E$	3447.5107	90.5
7 1 e	7 2 e	$\nu_3+\nu_4, A_2$	3428.4706	82.1	5 0 a_2	5 3 a_1	$\nu_3+\nu_4, A_1$	3447.5831	95.9
7 1 a_1	7 3 a_2	$\nu_1+\nu_4, E$	3428.5132	92.0	9 9 e	9 8 e	$\nu_3+\nu_4, E$	3447.7664	93.7
1 1 a_2	0 0 a_1	$\nu_1+\nu_4, E$	3428.5299	93.0	5 3 a_1	5 3 a_2	$\nu_3+\nu_4, A_1$	3447.8811	75.5
8 0 e	8 1 e	$\nu_1+\nu_4, E$	3428.5689	91.6	3 2 e	2 1 e	$\nu_1+\nu_4, E$	3447.9405	50.5
6 1 a_2	6 3 a_1	$\nu_1+\nu_4, E$	3428.6521	93.0	5 3 e	5 4 e	$\nu_3+\nu_4, E$	3447.9759	89.8
5 1 a_1	5 3 a_2	$\nu_1+\nu_4, E$	3428.7236	94.7	4 4 a_1	3 3 a_2	$\nu_1+\nu_4, E$	3448.1701	5.50
9 0 e	9 1 e	$\nu_1+\nu_4, E$	3428.8779	95.0	5 3 a_2	5 3 a_1	$\nu_3+\nu_4, A_1$	3448.1866	72.6
8 1 e	8 2 e	$\nu_3+\nu_4, A_2$	3428.8903	86.1	7 1 e	7 2 e	$\nu_3+\nu_4, A_1$	3448.3405	92.1
8 4 a_1	8 6 a_2	$\nu_1+\nu_4, E$	3428.9170	95.2	10 7 a_2	10 6 a_1	$\nu_3+\nu_4, E$	3448.5651	92.2
5 3 e	5 5 e	$\nu_1+\nu_4, E$	3429.0071	97.7	10 7 a_1	10 6 a_2	$\nu_3+\nu_4, E$	3448.5844	92.1
10 0 e	10 1 e	$\nu_1+\nu_4, E$	3429.0395	97.3	6 0 a_1	6 3 a_2	$\nu_3+\nu_4, A_1$	3448.6288	96.2
9 4 a_1	9 6 a_2	$\nu_1+\nu_4, E$	3429.1560	95.9	9 3 a_1	9 0 a_2	$\nu_3+\nu_4, A_1$	3448.7731	94.8
9 1 e	9 2 e	$\nu_3+\nu_4, A_2$	3429.1749	90.2	6 3 e	6 4 e	$\nu_3+\nu_4, E$	3448.8600	89.6
10 4 a_2	10 6 a_1	$\nu_1+\nu_4, E$	3429.2100	90.6	10 8 e	10 7 e	$\nu_3+\nu_4, E$	3448.8874	92.1
10 1 e	10 2 e	$\nu_3+\nu_4, A_2$	3429.3350	93.7	6 3 a_2	6 3 a_1	$\nu_3+\nu_4, A_1$	3448.9280	82.8
6 3 e	6 5 e	$\nu_1+\nu_4, E$	3429.3699	96.8	10 10 a	10 9 a	$\nu_3+\nu_4, E$	3449.0887	84.9
10 4 a_1	10 6 a_2	$\nu_1+\nu_4, E$	3429.4260	95.1	1 0 a_2	0 0 a_1	$\nu_3+\nu_4, A_1$	3449.2793	83.4
11 3 e	11 5 e	$\nu_1+\nu_4, E$	3429.5328	96.2	6 3 a_1	6 3 a_2	$\nu_3+\nu_4, A_1$	3449.5206	81.6
7 3 e	7 5 e	$\nu_1+\nu_4, E$	3429.6456	94.8	4 4 e	4 4 e	$\nu_3+\nu_4, A_1$	3449.7668	52.8
7 0 e	7 2 e	$\nu_1+\nu_4, E$	3429.6834	97.6	9 2 e	9 1 e	$\nu_3+\nu_4, A_1$	3449.9410	95.7
10 3 e	10 5 e	$\nu_1+\nu_4, E$	3429.7262	94.9	7 7 e	6 5 e	$\nu_1+\nu_4, E$	3449.9780	88.7
8 3 e	8 5 e	$\nu_1+\nu_4, E$	3429.7983	94.2	8 1 e	8 2 e	$\nu_3+\nu_4, A_1$	3450.0684	93.0
9 3 e	9 5 e	$\nu_1+\nu_4, E$	3429.8129	94.0	7 3 a_1	7 3 a_2	$\nu_3+\nu_4, A_1$	3450.2106	88.6
5 2 e	5 4 e	$\nu_1+\nu_4, E$	3429.8390	96.9	5 4 e	5 4 e	$\nu_3+\nu_4, A_1$	3450.5058	65.6
6 2 e	6 4 e	$\nu_1+\nu_4, E$	3430.1384	94.6	11 10 a	11 9 a	$\nu_3+\nu_4, E$	3450.5454	87.0
7 2 e	7 4 e	$\nu_1+\nu_4, E$	3430.4247	95.3	11 8 e	11 7 e	$\nu_3+\nu_4, E$	3450.5631	94.2
8 2 e	8 4 e	$\nu_1+\nu_4, E$	3430.6204	95.3	11 7 a_2	11 6 a_1	$\nu_3+\nu_4, E$	3450.6647	97.3
4 1 a_2	4 3 a_1	$\nu_3+\nu_4, E$	3430.6454	98.4	11 7 a_1	11 6 a_2	$\nu_3+\nu_4, E$	3450.6900	96.6
4 1 a_1	4 3 a_2	$\nu_3+\nu_4, E$	3430.7342	96.6	10 3 a_2	10 0 a_1	$\nu_3+\nu_4, A_1$	3450.7332	94.8
5 1 a_1	5 3 a_2	$\nu_3+\nu_4, E$	3431.1204	97.5	7 3 a_2	7 3 a_1	$\nu_3+\nu_4, A_1$	3451.0814	84.4
0 0 a_1	1 0 a_2	$\nu_3+\nu_4, A_1$	3431.3543	85.1	12 12 e	12 11 e	$\nu_3+\nu_4, E$	3451.3320	97.6

Table 1 (*continued*)

Upper state J' K' Γ'	Lower state J K Γ	Band	Line position, exp., in cm^{-1}	Trsm., in %	Upper state J' K' Γ'	Lower state J K Γ	Band	Line position, exp., in cm^{-1}	Trsm., in %
5 1 a_2	5 3 a_1	v_3+v_4,E	3431.5270	94.1	5 4 e	4 2 e	v_1+v_4,E	3451.3994	98.2
6 1 a_2	6 3 a_1	v_3+v_4,E	3431.5591	97.2	6 4 e	6 4 e	v_3+v_4,A_1	3451.4363	73.4
7 1 a_1	7 3 a_2	v_3+v_4,E	3431.9183	97.2	3 1 e	2 2 e	v_1+v_4,E	3451.5436	89.1
8 1 a_2	8 3 a_1	v_3+v_4,E	3432.1767	96.6	8 3 a_2	8 3 a_1	v_3+v_4,A_1	3451.7222	92.1
7 1 a_2	7 3 a_1	v_3+v_4,E	3432.9537	92.3	5 4 e	5 5 e	v_3+v_4,E	3451.7407	97.8
1 1 a_2	0 0 a_1	v_3+v_4,E	3433.0468	49.9	12 8 e	12 7 e	v_3+v_4,E	3451.7677	96.9
8 1 a_1	8 3 a_2	v_3+v_4,E	3433.4382	92.6	12 11 e	12 10 e	v_3+v_4,E	3451.8727	96.1
9 1 a_2	9 3 a_1	v_3+v_4,E	3433.7236	93.9	3 1 a_2	2 0 a_1	v_3+v_4,E	3451.9046	34.0
10 1 a_1	10 3 a_2	v_3+v_4,E	3433.7946	95.7	12 9 e	12 8 e	v_3+v_4,E	3451.9880	95.2
11 1 a_2	11 3 a_1	v_3+v_4,E	3433.8326	97.5	12 10 a_2	12 9 a_1	v_3+v_4,E	3452.1808	95.6
2 2 e	2 1 e	v_3+v_4,E	3436.0256	94.5	12 10 a_1	12 9 a_2	v_3+v_4,E	3452.1929	93.7
3 2 e	3 1 e	v_3+v_4,E	3436.1641	96.0	13 13 a	13 12 a	v_3+v_4,E	3452.2507	96.4
11 7 a_1	11 3 a_2	v_3+v_4,E	3436.7217	97.3	8 8 a	7 6 a	v_1+v_4,E	3452.3845	97.8
5 3 e	5 1 e	v_3+v_4,E	3436.9205	97.5	7 3 e	7 5 e	v_3+v_4,E	3452.4013	97.2
7 4 a_1	7 0 a_2	v_3+v_4,E	3437.1666	96.3	5 5 e	4 4 e	v_1+v_4,E	3452.4870	25.7
3 3 e	3 2 e	v_3+v_4,E	3437.6658	88.2	11 2 e	11 1 e	v_3+v_4,A_1	3452.5316	91.8
4 2 e	4 2 e	v_3+v_4,E	3437.8454	96.0	7 4 e	7 4 e	v_3+v_4,A_1	3452.5777	83.4
2 1 a_1	1 0 a_2	v_1+v_4,E	3437.9132	94.8	3 0 e	2 1 e	v_1+v_4,E	3452.6100	70.6
2 2 e	1 1 e	v_1+v_4,E	3438.7443	45.6	6 4 e	6 5 e	v_3+v_4,E	3452.6602	96.9
4 4 e	4 2 e	v_3+v_4,E	3439.7560	92.0	8 3 a_1	8 3 a_2	v_3+v_4,A_1	3452.8231	87.1
11 3 a_1	11 0 a_2	v_3+v_4,A_1	3452.9114	95.5	6 3 a_1	5 3 a_2	v_3+v_4,A_2	3473.4033	82.9
4 3 e	3 2 e	v_1+v_4,E	3452.9755	38.8	8 5 a_2	7 3 a_1	v_1+v_4,E	3473.4735	97.3
13 12 e	13 11 e	v_3+v_4,E	3453.0656	97.5	8 5 a_1	7 3 a_2	v_1+v_4,E	3473.5154	97.5
5 5 e	5 5 e	v_3+v_4,A_1	3453.2939	49.6	4 3 e	3 2 e	v_3+v_4,E	3473.6801	69.3
9 3 a_1	9 3 a_2	v_3+v_4,A_1	3453.4489	94.9	4 4 e	3 1 e	v_3+v_4,E	3473.7515	91.0
13 10 a_1	13 9 a_2	v_3+v_4,E	3453.6996	96.1	4 2 a_1	3 0 a_2	v_3+v_4,E	3473.8591	83.6
13 10 a_2	13 9 a_1	v_3+v_4,E	3453.7215	96.5	9 8 e	8 7 e	v_1+v_4,E	3474.9297	48.0
2 2 e	1 1 e	v_3+v_4,E	3453.8321	83.8	6 2 e	5 1 e	v_1+v_4,E	3475.5281	75.2
8 4 e	8 4 e	v_3+v_4,A_1	3453.9391	89.5	7 5 e	6 5 e	v_3+v_4,A_2	3475.7635	87.6
10 2 e	10 2 e	v_3+v_4,A_1	3453.9974	95.7	8 6 e	7 5 e	v_1+v_4,E	3476.0154	49.5
4 2 a_1	3 0 a_2	v_1+v_4,E	3454.0981	96.7	6 2 e	5 2 e	v_3+v_4,A_2	3476.3283	94.5
14 13 a	14 12 a	v_3+v_4,E	3454.1239	96.9	7 4 a_1	6 3 a_2	v_1+v_4,E	3476.4076	45.0
6 5 e	6 5 e	v_3+v_4,A_1	3454.2176	61.7	7 3 e	6 1 e	v_1+v_4,E	3476.4333	96.9
6 5 a	5 3 a	v_1+v_4,E	3454.4243	95.6	6 2 e	5 2 e	v_1+v_4,E	3477.1161	96.0
8 4 e	8 5 e	v_3+v_4,E	3454.4497	93.6	11 11 e	10 10 e	v_1+v_4,E	3477.2794	62.2
4 3 a	3 3 a	v_3+v_4,A_2	3454.4653	82.0	6 2 a_2	5 3 a_1	v_1+v_4,E	3477.3101	86.7
9 3 a_2	9 3 a_1	v_3+v_4,A_1	3454.7166	90.7	4 0 a_1	3 0 a_2	v_3+v_4,A_1	3477.5120	66.9
14 12 e	14 11 e	v_3+v_4,E	3454.8268	97.6	6 2 a_1	5 3 a_2	v_1+v_4,E	3477.6319	86.6
7 5 e	7 5 e	v_3+v_4,A_1	3455.3242	70.8	4 3 a_1	3 0 a_2	v_3+v_4,A_1	3477.9612	93.2
10 3 a_2	10 3 a_1	v_3+v_4,A_1	3455.3823	93.4	4 1 e	3 1 e	v_3+v_4,A_1	3478.3097	65.0
9 4 e	9 4 e	v_3+v_4,A_1	3455.5288	93.3	6 1 e	5 2 e	v_1+v_4,E	3478.9460	80.0
9 4 e	9 5 e	v_3+v_4,E	3455.9221	93.3	7 4 e	6 4 e	v_3+v_4,A_2	3479.2247	84.3
6 6 e	5 5 e	v_1+v_4,E	3456.5242	36.3	10 9 e	9 8 e	v_1+v_4,E	3479.2922	58.5
8 5 e	8 5 e	v_3+v_4,A_1	3456.6324	81.1	10 7 e	9 5 e	v_1+v_4,E	3479.5114	98.1
10 3 a_1	10 3 a_2	v_3+v_4,A_1	3456.7421	92.3	6 1 e	5 1 e	v_3+v_4,A_2	3479.6650	96.4
7 5 a_2	7 3 a_1	v_3+v_4,E	3456.9050	96.5	4 1 e	3 2 e	v_3+v_4,A_1	3479.9053	98.5
6 6 a	6 6 a	v_3+v_4,A_1	3456.9678	29.2	8 4 e	7 2 e	v_1+v_4,E	3479.9575	96.6
4 2 e	3 1 e	v_1+v_4,E	3457.1481	56.2	4 2 e	3 2 e	v_3+v_4,A_1	3480.1879	69.9

Table 1 (*continued*)

Upper state J' K' Γ'	Lower state J K Γ	Band	Line position, exp., in cm^{-1}	Trsm., in %	Upper state J' K' Γ'	Lower state J K Γ	Band	Line position, exp., in cm^{-1}	Trsm., in %
4 1 a_1	3 0 a_2	$\nu_1+\nu_4,E$	3457.4808	98.2	9 7 a_1	8 6 a_2	$\nu_1+\nu_4,E$	3480.3988	60.0
10 4 e	10 5 e	$\nu_3+\nu_4,E$	3457.5852	93.0	9 7 a_2	8 6 a_1	$\nu_1+\nu_4,E$	3480.4972	60.0
5 4 a_1	4 3 a_2	$\nu_1+\nu_4,E$	3457.6200	13.8	7 3 e	6 2 e	$\nu_1+\nu_4,E$	3480.7241	65.7
4 2 e	3 2 e	$\nu_3+\nu_4,A_2$	3457.8428	89.6	5 2 e	4 1 e	$\nu_3+\nu_4,E$	3480.7850	91.0
8 5 a_2	8 6 a_1	$\nu_3+\nu_4,E$	3458.0439	96.5	6 1 a_1	5 0 a_2	$\nu_3+\nu_4,E$	3480.8635	19.7
7 6 a_2	7 6 a_1	$\nu_3+\nu_4,A_1$	3458.0762	61.4	8 5 e	7 4 e	$\nu_1+\nu_4,E$	3481.1733	55.8
7 6 a_1	7 6 a_2	$\nu_3+\nu_4,A_1$	3458.0872	60.6	6 1 e	5 2 e	$\nu_3+\nu_4,A_2$	3481.2523	92.2
9 5 e	9 5 e	$\nu_3+\nu_4,A_1$	3458.1690	87.7	7 4 e	6 5 e	$\nu_1+\nu_4,E$	3481.5999	96.0
2 0 a_1	1 0 a_2	$\nu_3+\nu_4,A_1$	3458.4673	72.7	6 1 a_2	5 3 a_1	$\nu_1+\nu_4,E$	3481.9867	96.3
4 2 e	3 2 e	$\nu_1+\nu_4,E$	3458.7448	95.9	7 2 a_2	6 0 a_1	$\nu_1+\nu_4,E$	3482.2059	94.6
4 2 a_2	3 3 a_1	$\nu_1+\nu_4,E$	3458.8149	95.4	4 0 a_1	3 3 a_2	$\nu_3+\nu_4,A_1$	3482.3048	97.2
4 2 a_1	3 3 a_2	$\nu_1+\nu_4,E$	3458.8927	94.4	4 3 a_2	3 3 a_1	$\nu_3+\nu_4,A_1$	3482.6617	80.9
2 1 e	1 1 e	$\nu_3+\nu_4,A_1$	3459.2764	87.6	4 3 a_1	3 3 a_2	$\nu_3+\nu_4,A_1$	3482.7544	72.7
8 6 a_1	8 6 a_2	$\nu_3+\nu_4,A_1$	3459.3713	72.7	5 3 e	4 2 e	$\nu_3+\nu_4,E$	3482.9727	74.6
8 6 a_2	8 6 a_1	$\nu_3+\nu_4,A_1$	3459.3938	72.4	5 2 a_2	4 0 a_1	$\nu_3+\nu_4,E$	3483.1354	74.8
10 5 e	10 5 e	$\nu_3+\nu_4,A_1$	3459.9805	93.6	5 4 e	4 1 e	$\nu_3+\nu_4,E$	3483.4366	93.4
5 4 e	4 4 e	$\nu_3+\nu_4,A_2$	3460.0967	89.7	11 10 a_2	10 9 a_1	$\nu_1+\nu_4,E$	3483.8318	47.3
10 5 a_2	10 6 a_1	$\nu_3+\nu_4,E$	3460.5705	92.8	7 3 e	6 4 e	$\nu_1+\nu_4,E$	3484.3600	91.9
10 5 a_1	10 6 a_2	$\nu_3+\nu_4,E$	3460.6147	94.0	5 3 e	4 1 e	$\nu_3+\nu_4,E$	3484.4761	96.7
4 1 e	3 1 e	$\nu_3+\nu_4,A_2$	3460.6369	91.6	8 6 e	7 7 e	$\nu_1+\nu_4,E$	3484.5213	60.9
7 7 e	7 7 e	$\nu_3+\nu_4,A_1$	3460.6825	77.9	7 2 e	6 1 e	$\nu_1+\nu_4,E$	3484.6887	83.4
4 1 e	3 2 e	$\nu_1+\nu_4,E$	3460.7222	85.3	10 8 e	9 7 e	$\nu_1+\nu_4,E$	3484.9510	63.5
7 7 a	6 6 a	$\nu_1+\nu_4,E$	3460.7751	8.30	5 4 e	4 2 e	$\nu_3+\nu_4,E$	3485.0290	96.0
7 5 e	7 7 e	$\nu_3+\nu_4,E$	3460.8616	70.8	5 5 a	4 3 a	$\nu_3+\nu_4,E$	3485.2777	87.3
9 6 a_2	9 6 a_1	$\nu_3+\nu_4,A_1$	3460.9011	83.0	9 6 e	8 5 e	$\nu_1+\nu_4,E$	3485.5726	61.8
9 6 a_1	9 6 a_2	$\nu_3+\nu_4,A_1$	3460.9386	83.1	8 4 a_2	7 3 a_1	$\nu_1+\nu_4,E$	3485.6553	65.3
8 6 e	8 7 e	$\nu_3+\nu_4,E$	3460.9818	95.8	8 4 a_1	7 3 a_2	$\nu_1+\nu_4,E$	3485.6739	64.2
4 1 a_1	3 0 a_2	$\nu_3+\nu_4,E$	3461.5386	31.8	8 3 e	7 1 e	$\nu_1+\nu_4,E$	3485.7245	97.2
8 5 e	8 7 e	$\nu_3+\nu_4,E$	3461.8298	93.9	5 5 e	4 4 e	$\nu_3+\nu_4,E$	3485.7973	41.7
4 0 e	3 1 e	$\nu_1+\nu_4,E$	3461.9696	60.4	7 2 e	6 2 e	$\nu_1+\nu_4,E$	3486.2695	95.4
6 5 e	5 4 e	$\nu_1+\nu_4,E$	3462.0742	30.7	7 2 a_1	6 3 a_2	$\nu_1+\nu_4,E$	3486.4270	84.7
8 7 e	8 7 e	$\nu_3+\nu_4,A_1$	3462.1661	72.0	7 2 a_2	6 3 a_1	$\nu_1+\nu_4,E$	3486.9533	83.8
4 1 e	3 2 e	$\nu_3+\nu_4,A_2$	3462.2329	96.6	5 4 e	4 1 e	$\nu_3+\nu_4,A_1$	3487.0074	96.1
4 1 a_1	3 3 a_2	$\nu_1+\nu_4,E$	3462.2738	92.2	5 0 a_2	4 0 a_1	$\nu_3+\nu_4,A_1$	3487.2763	74.8
5 3 e	4 2 e	$\nu_1+\nu_4,E$	3462.2952	46.5	8 5 a_1	7 6 a_2	$\nu_1+\nu_4,E$	3487.8299	98.3
10 6 a_1	10 6 a_2	$\nu_3+\nu_4,A_1$	3462.7423	90.4	5 3 a_2	4 0 a_1	$\nu_3+\nu_4,A_1$	3487.8802	85.4
10 6 a_2	10 6 a_1	$\nu_3+\nu_4,A_1$	3462.8038	89.8	7 1 e	6 2 e	$\nu_1+\nu_4,E$	3487.9449	80.3
3 2 e	2 1 e	$\nu_3+\nu_4,E$	3462.8656	88.7	5 1 e	4 1 e	$\nu_3+\nu_4,A_1$	3488.2138	68.9
5 2 a_2	4 0 a_1	$\nu_1+\nu_4,E$	3463.4854	96.0	5 2 e	4 1 e	$\nu_3+\nu_4,A_1$	3488.4237	94.3
4 0 e	3 2 e	$\nu_1+\nu_4,E$	3463.5657	97.9	8 4 e	7 4 e	$\nu_3+\nu_4,A_2$	3488.6748	87.7
10 6 e	10 7 e	$\nu_3+\nu_4,E$	3463.7428	92.0	7 1 e	6 1 e	$\nu_3+\nu_4,A_2$	3489.0546	97.9
9 7 e	9 7 e	$\nu_3+\nu_4,A_1$	3463.7755	79.8	11 9 e	10 8 e	$\nu_1+\nu_4,E$	3489.5776	74.1
5 3 a_1	4 3 a_2	$\nu_3+\nu_4,A_2$	3463.9446	86.9	6 2 e	5 1 e	$\nu_3+\nu_4,E$	3489.6543	93.0
5 3 a_2	4 3 a_1	$\nu_3+\nu_4,A_2$	3463.9551	85.3	8 3 e	7 2 e	$\nu_1+\nu_4,E$	3489.7522	74.1
7 5 a_2	6 3 a_1	$\nu_1+\nu_4,E$	3464.2665	95.0	5 1 e	4 2 e	$\nu_3+\nu_4,A_1$	3489.8056	94.3
8 7 e	8 8 e	$\nu_3+\nu_4,E$	3464.3472	98.1	5 2 e	4 2 e	$\nu_3+\nu_4,A_1$	3490.0158	69.6
3 3 e	2 2 e	$\nu_3+\nu_4,E$	3464.3701	67.3	10 7 a	9 6 a	$\nu_1+\nu_4,E$	3490.1696	48.4
8 8 e	7 7 e	$\nu_1+\nu_4,E$	3464.8421	34.6	9 5 e	8 4 e	$\nu_1+\nu_4,E$	3490.2276	70.8

Table 1 (*continued*)

Upper state J' K' Γ'	Lower state J K Γ	Band	Line position, exp., in cm^{-1}	Trsm., in %	Upper state J' K' Γ'	Lower state J K Γ	Band	Line position, exp., in cm^{-1}	Trsm., in %
11 6 a_2	11 6 a_1	$\nu_3+\nu_4, A_1$	3465.0183	95.4	7 0 e	6 1 e	$\nu_1+\nu_4, E$	3490.2680	57.6
11 6 a_1	11 6 a_2	$\nu_3+\nu_4, A_1$	3465.1251	95.9	7 1 a_2	6 0 a_1	$\nu_3+\nu_4, E$	3490.3828	45.2
5 2 e	4 2 e	$\nu_3+\nu_4, A_2$	3465.5794	97.1	6 3 e	5 1 e	$\nu_3+\nu_4, E$	3490.4881	96.2
5 3 e	4 4 e	$\nu_1+\nu_4, E$	3465.6216	96.7	7 1 e	6 2 e	$\nu_3+\nu_4, A_2$	3490.6349	89.4
10 7 e	10 7 e	$\nu_3+\nu_4, A_1$	3465.7230	89.0	7 1 a_1	6 3 a_2	$\nu_1+\nu_4, E$	3490.6895	95.0
6 5 e	5 5 e	$\nu_3+\nu_4, A_2$	3465.7631	88.4	8 4 e	7 5 e	$\nu_1+\nu_4, E$	3491.0437	94.6
5 2 e	4 1 e	$\nu_1+\nu_4, E$	3466.3402	66.3	8 2 a_1	7 0 a_2	$\nu_1+\nu_4, E$	3491.4753	94.9
7 6 e	6 5 e	$\nu_1+\nu_4, E$	3466.3498	37.4	8 3 a_2	7 3 a_1	$\nu_3+\nu_4, A_2$	3491.8113	90.6
8 6 e	7 4 e	$\nu_1+\nu_4, E$	3466.9366	97.2	7 0 e	6 2 e	$\nu_1+\nu_4, E$	3491.8492	96.2
6 4 a_1	5 3 a_2	$\nu_1+\nu_4, E$	3467.0476	20.7	8 3 a_1	7 3 a_2	$\nu_3+\nu_4, A_2$	3491.9670	90.5
6 3 e	5 1 e	$\nu_1+\nu_4, E$	3467.0618	92.5	6 3 e	5 2 e	$\nu_3+\nu_4, E$	3492.0759	82.7
5 2 e	4 2 e	$\nu_3+\nu_4, A_2$	3467.1716	89.2	5 3 a_1	4 3 a_2	$\nu_3+\nu_4, A_1$	3492.3552	73.3
11 7 e	11 7 e	$\nu_3+\nu_4, A_1$	3467.8493	95.5	7 2 e	6 4 e	$\nu_1+\nu_4, E$	3492.6180	98.8
3 0 a_2	2 0 a_1	$\nu_3+\nu_4, A_1$	3467.8825	66.0	5 3 a_2	4 3 a_1	$\nu_3+\nu_4, A_1$	3492.6612	82.6
5 2 e	4 2 e	$\nu_1+\nu_4, E$	3467.9333	97.8	6 4 e	5 1 e	$\nu_3+\nu_4, E$	3493.2622	90.1
5 2 a_1	4 3 a_2	$\nu_1+\nu_4, E$	3468.0931	90.5	8 3 e	7 4 e	$\nu_1+\nu_4, E$	3493.6177	85.6
5 1 a_2	4 0 a_1	$\nu_1+\nu_4, E$	3468.1733	95.0	8 2 e	7 1 e	$\nu_1+\nu_4, E$	3493.7424	88.2
5 2 a_2	4 3 a_1	$\nu_1+\nu_4, E$	3468.2664	89.3	6 4 a_2	5 3 a_1	$\nu_3+\nu_4, E$	3494.0929	68.2
9 8 a	9 9 a	$\nu_3+\nu_4, E$	3468.3677	95.0	6 4 a_1	5 3 a_2	$\nu_3+\nu_4, E$	3494.2007	67.9
3 1 e	2 1 e	$\nu_3+\nu_4, A_1$	3468.6610	68.9	9 4 a_1	8 3 a_2	$\nu_1+\nu_4, E$	3494.7897	74.9
9 9 e	8 8 e	$\nu_1+\nu_4, E$	3468.9014	41.7	9 4 a_2	8 3 a_1	$\nu_1+\nu_4, E$	3494.8485	73.5
10 8 a_1	10 9 a_2	$\nu_3+\nu_4, E$	3469.5974	86.4	6 5 a_1	5 3 a_2	$\nu_3+\nu_4, E$	3494.8711	84.3
10 8 a_2	10 9 a_1	$\nu_3+\nu_4, E$	3469.6094	86.4	6 5 a_2	5 3 a_1	$\nu_3+\nu_4, E$	3494.9246	86.0
6 4 e	5 4 e	$\nu_3+\nu_4, A_2$	3469.6914	85.2	5 4 e	4 4 e	$\nu_3+\nu_4, A_1$	3494.9922	85.2
5 1 e	4 2 e	$\nu_1+\nu_4, E$	3469.8658	81.6	10 6 e	9 5 e	$\nu_1+\nu_4, E$	3495.0160	59.7
5 1 e	4 1 e	$\nu_3+\nu_4, A_2$	3470.1718	94.2	11 8 e	10 7 e	$\nu_1+\nu_4, E$	3495.0497	78.3
7 4 e	6 2 e	$\nu_1+\nu_4, E$	3470.4651	96.2	7 1 a_2	6 3 a_1	$\nu_3+\nu_4, E$	3495.1301	96.6
3 2 e	2 2 e	$\nu_3+\nu_4, A_1$	3470.6271	78.7	8 1 e	7 1 e	$\nu_1+\nu_4, E$	3495.2879	97.7
8 7 a	7 6 a	$\nu_1+\nu_4, E$	3470.6594	15.8	8 2 e	7 2 e	$\nu_1+\nu_4, E$	3495.3161	98.6
11 8 a_1	11 9 a_2	$\nu_3+\nu_4, E$	3470.9988	93.3	8 2 a_2	7 3 a_1	$\nu_1+\nu_4, E$	3495.4189	86.0
5 1 a_2	4 0 a_1	$\nu_3+\nu_4, E$	3471.2203	34.1	6 5 e	5 4 e	$\nu_3+\nu_4, E$	3495.5192	52.1
5 0 e	4 1 e	$\nu_1+\nu_4, E$	3471.4039	55.2	8 2 a_1	7 3 a_2	$\nu_1+\nu_4, E$	3496.2005	83.6
6 3 e	5 2 e	$\nu_1+\nu_4, E$	3471.5600	55.9	6 6 e	5 5 e	$\nu_3+\nu_4, E$	3496.4438	36.9
7 5 e	6 4 e	$\nu_1+\nu_4, E$	3471.6246	45.1	8 1 e	7 2 e	$\nu_1+\nu_4, E$	3496.8616	81.0
5 1 e	4 2 e	$\nu_3+\nu_4, A_2$	3471.7626	94.1	9 5 a_1	8 6 a_2	$\nu_1+\nu_4, E$	3497.1263	97.8
4 2 e	3 1 e	$\nu_3+\nu_4, E$	3471.8411	89.9	6 0 a_1	5 0 a_2	$\nu_3+\nu_4, A_1$	3497.1973	79.7
6 4 e	5 5 e	$\nu_1+\nu_4, E$	3472.1228	98.2	9 5 a_2	8 6 a_1	$\nu_1+\nu_4, E$	3497.2216	96.0
6 2 a_1	5 0 a_2	$\nu_1+\nu_4, E$	3472.8661	95.0	6 3 a_1	5 0 a_2	$\nu_3+\nu_4, A_1$	3498.0893	82.9
5 0 e	4 2 e	$\nu_1+\nu_4, E$	3472.9958	95.9	9 4 e	8 4 e	$\nu_3+\nu_4, A_2$	3498.2273	91.9
10 10 a_2	9 9 a_1	$\nu_1+\nu_4, E$	3473.0113	26.5	6 1 e	5 1 e	$\nu_3+\nu_4, A_1$	3498.3166	78.9
5 1 a_1	4 3 a_2	$\nu_1+\nu_4, E$	3473.1972	98.2	6 2 e	5 1 e	$\nu_3+\nu_4, A_1$	3498.5509	85.7
6 3 a_2	5 3 a_1	$\nu_3+\nu_4, A_2$	3473.3724	79.7	9 3 e	8 2 e	$\nu_1+\nu_4, E$	3498.6240	82.7
6 2 a_2	5 3 a_1	$\nu_3+\nu_4, E$	3498.7471	98.5	8 1 e	7 2 e	$\nu_3+\nu_4, A_1$	3521.0515	89.3
8 1 a_2	7 3 a_1	$\nu_1+\nu_4, E$	3499.3020	93.1	8 0 a_1	7 3 a_2	$\nu_3+\nu_4, A_1$	3522.3559	82.1
7 2 e	6 1 e	$\nu_3+\nu_4, E$	3499.3219	92.0	9 3 e	8 1 e	$\nu_3+\nu_4, E$	3522.5738	97.8
8 0 e	7 1 e	$\nu_1+\nu_4, E$	3499.5443	63.7	8 3 a_2	7 3 a_1	$\nu_3+\nu_4, A_1$	3522.7177	77.8
10 5 e	9 4 e	$\nu_1+\nu_4, E$	3499.6647	81.7	9 4 e	8 1 e	$\nu_3+\nu_4, E$	3523.1677	96.8

Table 1 (*continued*)

Upper state J' K' Γ'	Lower state J K Γ	Band	Line position, exp., in cm^{-1}	Trsm., in %	Upper state J' K' Γ'	Lower state J K Γ	Band	Line position, exp., in cm^{-1}	Trsm., in %
8 1 a_1	7 0 a_2	v_3+v_4,E	3499.7087	52.8	8 3 a_1	7 3 a_2	v_3+v_4,A_1	3523.8202	86.5
8 1 e	7 2 e	v_3+v_4,A_2	3499.8740	89.7	9 3 e	8 2 e	v_3+v_4,E	3524.1395	87.2
11 7 a	10 6 a	v_1+v_4,E	3499.9014	70.3	9 8 a	8 6 a	v_3+v_4,E	3524.1978	94.8
6 2 e	5 2 e	v_3+v_4,A_1	3500.1380	78.4	9 5 a_2	8 3 a_1	v_3+v_4,E	3524.5538	92.2
12 9 e	11 8 e	v_1+v_4,E	3500.3383	86.8	11 1 a_1	10 3 a_2	v_1+v_4,E	3524.6879	92.0
9 2 a_2	8 0 a_1	v_1+v_4,E	3500.6515	95.2	9 4 e	8 2 e	v_3+v_4,E	3524.7335	95.2
9 3 a_1	8 3 a_2	v_3+v_4,A_2	3500.7463	95.2	9 5 a_1	8 3 a_2	v_3+v_4,E	3524.8364	85.5
8 3 e	7 5 e	v_1+v_4,E	3500.8383	98.4	8 4 e	7 4 e	v_3+v_4,A_1	3524.9549	79.5
7 2 e	6 2 e	v_3+v_4,E	3500.9024	90.0	9 4 a_1	8 3 a_2	v_3+v_4,E	3525.0176	85.1
9 3 a_2	8 3 a_1	v_3+v_4,A_2	3501.0354	92.9	9 4 a_2	8 3 a_1	v_3+v_4,E	3525.1170	89.2
8 0 e	7 2 e	v_1+v_4,E	3501.1181	95.5	9 5 e	8 4 e	v_3+v_4,E	3525.5743	83.0
9 4 e	8 5 e	v_1+v_4,E	3501.3142	95.0	9 7 e	8 4 e	v_3+v_4,A_1	3526.1925	91.3
8 2 e	7 4 e	v_1+v_4,E	3501.6357	98.2	9 6 e	8 5 e	v_3+v_4,E	3526.3436	60.5
7 3 e	6 1 e	v_3+v_4,E	3501.8990	95.3	11 1 a_2	10 0 a_1	v_3+v_4,E	3526.4887	87.3
6 0 a_1	5 3 a_2	v_3+v_4,A_1	3501.9629	84.6	9 6 a_2	8 3 a_1	v_3+v_4,A_1	3526.5351	95.8
6 3 a_2	5 3 a_1	v_3+v_4,A_1	3502.2624	70.9	9 6 a_1	8 3 a_2	v_3+v_4,A_1	3526.5714	95.6
9 3 e	8 4 e	v_1+v_4,E	3502.7834	91.0	9 7 a_2	8 6 a_1	v_3+v_4,E	3526.9405	63.6
6 3 a_1	5 3 a_2	v_3+v_4,A_1	3502.8549	84.1	9 7 a_1	8 6 a_2	v_3+v_4,E	3526.9779	62.3
7 4 e	6 1 e	v_3+v_4,E	3503.3242	88.2	9 8 e	8 7 e	v_3+v_4,E	3527.4240	56.1
7 3 e	6 2 e	v_3+v_4,E	3503.4805	82.9	8 5 e	7 5 e	v_3+v_4,A_1	3527.6723	82.9
10 4 a_2	9 3 a_1	v_1+v_4,E	3503.6999	84.1	9 9 e	8 8 e	v_3+v_4,E	3527.7258	46.8
10 4 a_1	9 3 a_2	v_1+v_4,E	3503.9182	86.4	9 0 a_2	8 0 a_1	v_3+v_4,A_1	3528.1366	85.9
7 4 a_2	6 3 a_1	v_3+v_4,E	3504.0687	74.4	9 2 e	8 1 e	v_3+v_4,A_1	3529.7085	92.1
9 2 a_1	8 3 a_2	v_1+v_4,E	3504.2661	87.6	9 3 a_2	8 0 a_1	v_3+v_4,A_1	3529.8068	91.2
11 6 e	10 5 e	v_1+v_4,E	3504.4338	80.8	9 1 e	8 1 e	v_3+v_4,A_1	3530.1716	89.6
7 6 e	6 4 e	v_3+v_4,E	3504.5627	96.7	8 6 a_1	7 6 a_2	v_3+v_4,A_1	3530.4406	88.2
7 5 a_2	6 3 a_1	v_3+v_4,E	3504.7685	86.2	8 6 a_2	7 6 a_1	v_3+v_4,A_1	3530.4635	88.1
6 4 e	5 4 e	v_3+v_4,A_1	3504.7854	79.5	11 1 a_2	10 3 a_1	v_3+v_4,E	3531.1355	97.4
7 5 a_1	6 3 a_2	v_3+v_4,E	3504.9740	87.9	9 2 e	8 2 e	v_3+v_4,A_1	3531.2745	89.1
7 7 e	6 4 e	v_3+v_4,A_1	3505.2893	76.9	9 1 e	8 2 e	v_3+v_4,A_1	3531.7366	90.6
9 2 a_2	8 3 a_1	v_1+v_4,E	3505.3544	85.4	9 0 a_2	8 3 a_1	v_3+v_4,A_1	3532.8393	91.9
7 5 e	6 4 e	v_3+v_4,E	3505.4686	76.0	8 5 e	7 7 e	v_3+v_4,E	3532.9347	98.6
9 1 e	8 2 e	v_1+v_4,E	3505.6990	85.4	9 3 a_1	8 3 a_2	v_3+v_4,A_1	3533.2399	82.9
7 6 e	6 5 e	v_3+v_4,E	3506.2359	48.1	8 7 e	7 7 e	v_3+v_4,A_1	3533.2713	95.2
7 5 e	6 2 e	v_3+v_4,A_1	3506.4028	96.8	9 3 a_2	8 3 a_1	v_3+v_4,A_1	3534.5097	88.0
10 5 a_2	9 6 a_1	v_1+v_4,E	3506.7150	95.2	10 3 e	9 2 e	v_3+v_4,E	3534.8365	90.1
7 4 e	6 1 e	v_3+v_4,A_1	3506.8420	94.2	10 5 a_1	9 3 a_2	v_3+v_4,E	3535.1070	94.7
7 7 a	6 6 a	v_3+v_4,E	3506.9918	13.9	10 4 e	9 2 e	v_3+v_4,E	3535.2324	97.7
7 0 a_2	6 0 a_1	v_3+v_4,A_1	3507.3139	82.3	9 4 e	8 4 e	v_3+v_4,A_1	3535.3412	85.9
10 3 e	9 2 e	v_1+v_4,E	3507.3735	89.0	9 4 e	8 5 e	v_3+v_4,E	3535.7627	97.9
6 5 e	5 5 e	v_3+v_4,A_1	3507.5848	86.9	10 7 e	9 4 e	v_3+v_4,A_1	3537.0209	93.0
9 1 a_1	8 3 a_2	v_1+v_4,E	3507.8267	92.0	10 7 a_2	9 6 a_1	v_3+v_4,E	3537.2149	73.3
8 2 e	7 1 e	v_3+v_4,E	3508.0195	91.1	10 7 a_1	9 6 a_2	v_3+v_4,E	3537.2339	69.5
7 3 a_2	6 0 a_1	v_3+v_4,A_1	3508.5104	84.6	10 8 e	9 7 e	v_3+v_4,E	3537.5816	67.8
7 2 e	6 1 e	v_3+v_4,A_1	3508.6045	85.5	10 5 e	9 2 e	v_3+v_4,A_1	3537.6277	95.1
9 0 e	8 1 e	v_1+v_4,E	3508.6482	71.8	10 9 e	9 8 e	v_3+v_4,E	3537.8346	61.3
9 1 a_2	8 0 a_1	v_3+v_4,E	3508.8145	66.1	10 10 a	9 9 a	v_3+v_4,E	3537.8914	29.7

Table 1 (*continued*)

Upper state J' K' Γ'	Lower state J K Γ	Band	Line position, exp., in cm^{-1}	Trsm., in %	Upper state J' K' Γ'	Lower state J K Γ	Band	Line position, exp., in cm^{-1}	Trsm., in %
7 1 e	6 1 e	$\nu_3+\nu_4, A_1$	3508.9247	84.8	9 5 e	8 5 e	$\nu_3+\nu_4, A_1$	3538.0091	86.5
9 1 e	8 2 e	$\nu_3+\nu_4, A_2$	3508.9519	91.2	10 0 a_1	9 0 a_2	$\nu_3+\nu_4, A_1$	3538.8397	87.1
9 4 a_2	8 6 a_1	$\nu_1+\nu_4, E$	3509.0890	99.0	10 1 e	9 1 e	$\nu_3+\nu_4, A_1$	3540.4885	93.5
7 1 a_2	6 6 a_1	$\nu_3+\nu_4, E$	3509.5104	97.3	10 3 a_1	9 0 a_2	$\nu_3+\nu_4, A_1$	3540.6297	94.4
8 2 e	7 2 e	$\nu_3+\nu_4, E$	3509.5932	94.9	9 6 a_2	8 6 a_1	$\nu_3+\nu_4, A_1$	3540.7749	88.8
9 3 e	8 5 e	$\nu_1+\nu_4, E$	3509.6526	98.5	9 6 a_1	8 6 a_2	$\nu_3+\nu_4, A_1$	3540.8117	88.4
10 2 a_1	9 0 a_2	$\nu_1+\nu_4, E$	3509.7419	96.6	10 2 e	9 1 e	$\nu_3+\nu_4, A_1$	3540.9844	94.2
7 2 e	6 2 e	$\nu_3+\nu_4, A_1$	3510.1855	82.1	10 1 e	9 2 e	$\nu_3+\nu_4, A_1$	3542.0453	92.7
8 4 a_1	7 0 a_2	$\nu_3+\nu_4, E$	3510.2122	89.1	10 2 e	9 2 e	$\nu_3+\nu_4, A_1$	3542.5413	92.9
7 0 a_2	6 3 a_1	$\nu_3+\nu_4, A_1$	3512.0614	85.4	10 0 a_1	9 3 a_2	$\nu_3+\nu_4, A_1$	3543.5160	94.6
7 3 a_1	6 3 a_2	$\nu_3+\nu_4, A_1$	3512.3866	73.3	9 7 e	8 7 e	$\nu_3+\nu_4, A_1$	3543.6886	93.1
8 4 e	7 1 e	$\nu_3+\nu_4, E$	3512.8291	94.3	10 3 a_2	9 3 a_1	$\nu_3+\nu_4, A_1$	3543.9392	87.4
7 3 a_2	6 3 a_1	$\nu_3+\nu_4, A_1$	3513.2581	84.5	10 3 a_1	9 3 a_2	$\nu_3+\nu_4, A_1$	3545.3056	90.4
9 1 a_2	8 3 a_1	$\nu_3+\nu_4, E$	3513.5164	94.8	10 3 e	9 5 e	$\nu_3+\nu_4, E$	3545.8033	96.8
8 3 e	7 2 e	$\nu_3+\nu_4, E$	3513.6648	83.6	10 4 e	9 5 e	$\nu_3+\nu_4, E$	3546.1987	97.7
8 2 a_1	7 3 a_2	$\nu_3+\nu_4, E$	3514.1990	86.2	11 9 e	10 8 e	$\nu_3+\nu_4, E$	3547.9144	61.0
10 2 a_1	9 3 a_2	$\nu_1+\nu_4, E$	3514.4177	87.8	11 8 e	10 7 e	$\nu_3+\nu_4, E$	3548.0070	78.9
10 1 e	9 2 e	$\nu_1+\nu_4, E$	3514.4644	89.2	11 7 a_2	10 6 a_1	$\nu_3+\nu_4, E$	3548.0608	88.1
7 4 e	6 4 e	$\nu_3+\nu_4, A_1$	3514.7707	78.7	11 7 a_1	10 6 a_2	$\nu_3+\nu_4, E$	3548.0866	87.1
8 4 a_2	7 3 a_1	$\nu_3+\nu_4, E$	3514.7999	86.4	11 10 a	10 9 a	$\nu_3+\nu_4, E$	3548.1097	38.9
8 4 a_1	7 3 a_2	$\nu_3+\nu_4, E$	3514.9384	87.6	11 6 a_2	10 3 a_1	$\nu_3+\nu_4, A_1$	3548.3478	94.7
8 5 e	7 4 e	$\nu_3+\nu_4, E$	3515.3487	76.7	11 6 a_1	10 3 a_2	$\nu_3+\nu_4, A_1$	3548.4503	94.6
8 7 e	7 4 e	$\nu_3+\nu_4, A_1$	3515.6852	90.8	10 5 e	9 5 e	$\nu_3+\nu_4, A_1$	3548.5944	90.1
8 2 e	7 4 e	$\nu_3+\nu_4, E$	3515.9128	98.4	10 5 a_1	9 6 a_2	$\nu_3+\nu_4, E$	3549.2650	95.9
11 3 e	10 2 e	$\nu_1+\nu_4, E$	3515.9915	95.8	11 0 a_2	10 0 a_1	$\nu_3+\nu_4, A_1$	3549.7808	88.1
8 6 a_1	7 3 a_2	$\nu_3+\nu_4, A_1$	3516.1280	95.1	10 6 a_1	9 6 a_2	$\nu_3+\nu_4, A_1$	3551.3921	91.0
8 6 a_2	7 3 a_1	$\nu_3+\nu_4, A_1$	3516.1495	96.1	10 6 a_2	9 6 a_1	$\nu_3+\nu_4, A_1$	3551.4537	92.3
8 6 e	7 5 e	$\nu_3+\nu_4, E$	3516.1959	57.8	11 3 a_2	10 0 a_1	$\nu_3+\nu_4, A_1$	3551.5578	96.5
10 1 a_2	9 3 a_1	$\nu_1+\nu_4, E$	3516.2771	91.1	10 7 e	9 7 e	$\nu_3+\nu_4, A_1$	3554.4169	94.3
8 5 e	7 2 e	$\nu_3+\nu_4, A_1$	3516.5863	96.1	11 3 a_1	10 3 a_2	$\nu_3+\nu_4, A_1$	3554.8230	91.8
8 7 a	7 6 a	$\nu_3+\nu_4, E$	3516.8843	38.8	11 3 a_2	10 3 a_1	$\nu_3+\nu_4, A_1$	3556.2065	91.9
8 4 e	7 1 e	$\nu_3+\nu_4, A_1$	3517.0611	93.7	12 12 e	11 11 e	$\nu_3+\nu_4, E$	3557.7851	69.5
8 8 e	7 7 e	$\nu_3+\nu_4, E$	3517.4233	40.2	12 8 e	11 7 e	$\nu_3+\nu_4, E$	3557.9278	90.5
7 5 e	6 5 e	$\nu_3+\nu_4, A_1$	3517.5380	82.8	12 9 e	11 8 e	$\nu_3+\nu_4, E$	3558.2080	91.3
10 0 e	9 1 e	$\nu_1+\nu_4, E$	3517.5728	79.4	12 11 e	11 10 e	$\nu_3+\nu_4, E$	3558.2381	74.8
8 0 a_1	7 0 a_2	$\nu_3+\nu_4, A_1$	3517.6297	84.7	12 10 a_2	11 9 a_1	$\nu_3+\nu_4, E$	3558.4687	79.5
10 1 a_1	9 0 a_2	$\nu_3+\nu_4, E$	3517.6817	75.6	12 10 a_1	11 9 a_2	$\nu_3+\nu_4, E$	3558.4772	79.1
10 1 e	9 2 e	$\nu_3+\nu_4, A_2$	3517.8793	93.2	11 6 a_2	10 6 a_1	$\nu_3+\nu_4, A_1$	3562.4148	95.1
10 4 a_1	9 6 a_2	$\nu_1+\nu_4, E$	3518.0770	98.4	11 6 a_1	10 6 a_2	$\nu_3+\nu_4, A_1$	3562.5213	94.7
8 2 e	7 1 e	$\nu_3+\nu_4, A_1$	3519.0751	89.7	13 13 a	12 12 a	$\nu_3+\nu_4, E$	3567.5067	58.5
8 3 a_1	7 0 a_2	$\nu_3+\nu_4, A_1$	3519.0940	87.7	13 12 e	12 11 e	$\nu_3+\nu_4, E$	3568.2198	80.9
10 0 e	9 2 e	$\nu_1+\nu_4, E$	3519.1293	97.1	13 10 a_1	12 9 a_2	$\nu_3+\nu_4, E$	3568.6774	87.8
8 1 e	7 1 e	$\nu_3+\nu_4, A_1$	3519.4776	87.4	13 10 a_2	12 9 a_1	$\nu_3+\nu_4, E$	3568.6991	87.6
7 6 a_2	6 6 a_1	$\nu_3+\nu_4, A_1$	3520.3165	91.7	13 11 e	12 10 e	$\nu_3+\nu_4, E$	3568.7088	90.3
7 6 a_1	6 6 a_2	$\nu_3+\nu_4, A_1$	3520.3278	91.2	14 13 a	13 12 a	$\nu_3+\nu_4, E$	3578.0483	74.0
8 2 e	7 2 e	$\nu_3+\nu_4, A_1$	3520.6493	86.4	14 12 e	13 11 e	$\nu_3+\nu_4, E$	3578.6418	89.9

4. Estimation of vibrational parameters

For an analysis of high-resolution vibrational–rotational spectra of the bands which are located in higher wavelength regions, at least, approximate information about corresponding band centers can be very important. In this respect, it is useful to have information about harmonic frequencies ω_λ and anharmonic coefficients $x_{\lambda\mu}$ of a molecule. As to the PH_3, such information, in principle, can be found in Ref. [3] where an ab initio quartic force field was derived. It should be mentioned, however, that the assumption about local mode behavior of the PH_3 molecule was additionally used in [3]. From this point, it would be interesting to compare the results of such ab initio calculations with the results of direct determination of vibrational spectroscopic parameters from experimental data.

At the moment, "experimental" values of vibrational energies are known for 12 vibrational states: the v_2 and v_4 bands were considered in [1]; the v_1, v_3, $2v_2$, $2v_4(A_1)$, $2v_4(E)$, and v_2+v_4 were analyzed in Refs. [2,4]; information about the v_1+v_4, $v_3+v_4(E)$, $v_3+v_4(A_1)$, and $v_3+v_4(A_2)$ bands is presented in the present contribution. A simple calculation which can be made on this base lead to the results presented in Column 2 of Table 2. In that table, ω_λ, $x_{\lambda\mu}$, and g_{44} correspond to the usual notations used in vibrational–rotational spectroscopy [5]; g is the value of the E/A_λ vibrational splitting of the states $(0011, E)$ and $(0011, A_\lambda)$ $(\lambda = 1,2)$; d is the absolute values of shifts of the $(0011, E)$ and $(1001, E)$ terms caused by Fermi-type resonance interaction, see Fig. 4. For comparison, Column 3 of Table 2 presents the values of corresponding parameters obtained on the basis of ab initio calculations from [3]. Good correlations between the data in both Columns 2 and 3 can be seen for the first four parameters. It is not an unexcepted result because practically the same experimental data were used for corrections of ab initio calculations in [3].

The correspondence between the data in Columns 2 and 3 of Table 2 is worse for the other parameters presented. In this case, it is interesting to analyze situation with the three last combinations of parameters in Column 2. Firstly, let us use the x_{14} and x_{34} parameters from [3] in the last two

Table 2
Some vibrational spectroscopic parameters of the PH_3 molecule[a]

Parameters	Our	From Ref. [3]
1	2	3
x_{22}	−5.85	−5.46
x_{24}	−2.29	−2.78
x_{44}	−2.87	−3.59
g_{44}	2.03	1.97
$\omega_2 + \frac{1}{2}x_{12} + x_{23}$	1006.11	1009.49
$\omega_4 + \frac{1}{2}x_{14} + x_{34}$	1126.04	1116.25
$2g - d$	5.04	—
$x_{14} - d$	−14.94	−16.07[b]
$x_{34} + d$	−7.44	−17.87[b]

[a]All the values are given in cm^{-1}.
[b]Here x_{14} and x_{34} from [3] are given.

lines of Table 2. In this case, it is possible to determine two values of the d parameter, and they are 20.85 and -1.13 cm^{-1}, respectively. Comparison of these two values with each other allows one to come to the conclusion that the ab initio values of the parameters x_{14} and x_{34} do not satisfy the real experimental data. On the other hand, if one assumes the Fermi interaction is absent between the states $(0011, E)$ and $(1001, E)$, (i.e., $d = 0$ in Column 2), then results for the x_{14} and x_{34} parameters are $x_{34} = -7.44$ cm^{-1}, and $x_{14} = -14.94$ cm^{-1}, respectively. This result strongly differs from the values of corresponding parameters of [3], see Column 3.

It is well known in molecular spectroscopy that the anharmonic coefficients $x_{\lambda\mu}$ are negative, as a rule. As a consequence, data from Column 2 of Table 2 lead to the following condition for the d parameter, $-7.44 < d < 14.94$ cm^{-1}. At the same time, it should be mentioned that many manifestations of the local mode behavior can be seen in the vibration–rotation spectra of both the PH_3 molecule, and its deuterated species [5,6]. For this reason, one can assume that real values of the x_{14} and x_{34} parameters have to be close to each other. Under this assumption, one will obtain $x_{14} = x_{34} = -9.94$ cm^{-1}, $g = 5.02$ cm^{-1}, and $d = 5.00$ cm^{-1}. As the result of the discussion, we believe that these last values of parameters are not far from reality.

5. Conclusion

The high-resolution (0.005 cm^{-1}) Fourier transform infrared spectrum of PH_3 molecule was recorded for the first time in the region between 3280 and 3580 cm^{-1}, and assignments of the recorded transitions were fulfilled. In this case, because of strong resonance interactions between all the vibrational states of the studied poliad, transitions were assigned not only to the allowed bands $v_1 + v_4(E)$, $v_3 + v_4(E)$, and $v_3 + v_4(A_1)$, but also to the band $v_3 + v_4(A_2)$ which is forbidden on symmetry. Numerous a_1/a_2 splittings for the states $(J\ Ka_1, a_2)$ with the value of quantum number $K = 1$–10 were found in the experimental spectrum. Some pure vibrational spectroscopic parameters of the PH_3 molecule are estimated on the basis of analysis of experimental data.

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