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Measurements of line positions and strengths of $HD^{18}O$ and $D_2^{18}O$ in the 2500–4280 cm^{-1} region

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Abstract

Measurements of line positions and strengths of $D_2^{18}O$ and $HD^{18}O$ were obtained with a Fourier transform spectrometer. The data were analyzed to obtain energy levels of the (100), (020), and (001) vibrational states of $HD^{18}O$ and the (001) and (011) states of $D_2^{18}O$ and the vibrational bands of these states connected to the ground state covered the spectral region from 2500 to 4278 cm^{-1}. 456 absorption lines of $D_2^{18}O$ and 856 lines of $HD^{18}O$ were assigned from the spectra. The measurements were of oxygen-18 enriched samples of deuterated water vapor and the spectra also contained features of $HD^{16}O$, $D_2^{16}O$, $H_2^{16}O$, $H_2^{17}O$ and $H_2^{18}O$ of which several were used as frequency calibration standards.

Keywords: HDO and D_2O infrared spectroscopy

1. Introduction

This study involves high-resolution measurements of the line center positions and absolute line strengths of the (100)-(000), (020)-(000), and (001)-(000) bands of $HD^{18}O$ and the (001)-(000) and (011)-(000) bands of $D_2^{18}O$ covering the spectral region from 2500 to 4278 cm^{-1}. The spectra were of oxygen enriched O-18 samples created from a mixture of $H_2^{18}O$ and $D_2^{16}O$. The line positions were analyzed to determine the upper state rotational energy levels.

Previous laboratory measurements of HDO and D_2O in this spectral region were analyzed for the oxygen-O-16 species and none reported observations of the O-18 derivative. Measurements of HDO include the studies of Toth et al. [1,2] and Papineau et al. [3] and for D_2O, the reports include the investigations by Papineau et al. [4], Bykov et al. [5] and He et al. [6].

2. Experimental

The spectra were obtained with a Fourier transform spectrometer (FTS) located in the McMath solar telescope facility at the Kitt peak National Observatory. The experimental conditions of the measurements are given in Table 1. The data were obtained with an absorption cell with an optical path length of 2.39 m and the sample temperatures of all the runs were at or near room temperature. The first entry in the table represents a spectral run used in two previous studies [7,8] which involved measurements in the ν_2 regions of HDO, D_2O, and H_2O and the spectra were obtained at an unapodized spectral resolution of 0.0056 cm^{-1}. This run contained useful spectra only up to about 2700 cm^{-1} however the relative amounts of the various isotopic species were determined accurately and was used here to calibrate the relative amounts of the species observed in the other spectra given in the table. The unapodized spectral resolution of the remainder of the runs were at 0.011 cm^{-1} of which the gas samples of two contained enriched oxygen O-18 and the samples of the other two were of a mixture of $HD^{16}O$ and $D_2^{16}O$.

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Table 1
Experimental conditions of deuterated water vapor samples

Path length (m)	Unapodized spectral res. (cm^{-1})	Total sample pressure (Torr)	% Abundance of isotopic species			
			$HD^{16}O$	$HD^{18}O$	$D_2^{16}O$	$D_2^{18}O$
2.39	0.0056	0.58	31.7	13.3	23.9	10.2
2.39	0.011	0.51	38.0	9.45	19.0	5.53
2.39	0.011	1.49	34.9	10.5	23.5	7.90
2.39	0.011	1.73	36.1	0.07	59.3	0.12
2.39	0.011	1.48	46.5	0.09	40.8	0.08
2.39	0.011	5.14	44.7	0.09	14.6	0.03

Note. All samples at or near room temperature (296 K)

The oxygen O-18 enriched samples were created from a mixture of $HD^{16}O$ and $H_2^{18}O$ and a discussion concerning the method used to derive the relative isotopic amounts in the sample for the first entry was given in ref. [7]. The relative amounts of the other spectra were derived from comparisons of the measured line strength values of HDO and D_2O with those obtained from the spectrum of the first entry in the 2500–2700 cm^{-1} region. Also observed in the spectra were absorptions of $H_2^{16}O$, $H_2^{18}O$, and $H_2^{17}O$ however the relative abundance of these variants in the spectra were not determined for this study.

The spectra representing all but the first entry in Table 1 were obtained with the instrument conditions as follows. The source was a 650-W quartz-iodine projection lamp and radiation at wavelengths greater than 5.7 μm was not recorded due to the cutoff properties of the N_2-cooled InSb IR detector and CaF_2 beamsplitter. The total sample pressures were measured with a Baratron gauge with a 10 Torr head. The sample temperatures were inferred from readings of one or more thermistor probes in thermal contact with the absorption cell. The estimated uncertainties in the measured pressures and temperatures were 0.5% and 0.5 K, respectively. Each spectral run consisted of eight or more co-added interferograms with each run taking 50-min or longer. The composite interferograms were transformed into spectra data at the Kitt peak facility and the spectra were transmitted to JPL. The signal-noise ratio of all the spectra in this region was about 150-to-1.

Two computer programs were used to measure the spectra. One program labeled LINEFINDER (LNF) determines line center positions and relative absorption peaks and the other used the technique of non-linear least-squares (NLLS) in which absorption positions, line strengths, linewidths, and continuum parameters are fitted simultaneously in an interactive mode on the computer. For each run, the LNF results were used as the input list to the NLLS program from which the experimental values of line positions and strengths were obtained. The measured line positions were calibrated and corrected by reference to known H_2O and HDO frequencies used as calibration standards. These line position values were computed from the vibration-rotation energy levels of the (020), (100), and (001) vibrational states of $H_2^{16}O$ given by Toth [9] and the (000) levels by Toth [10] and the (100), (020), (001) and (000) states of $HD^{16}O$ given by Toth [11].

3. Assignments and energy levels

The locations of all of the observed absorptions due to $H_2^{16}O$, $H_2^{17}O$, $H_2^{18}O$, $D_2^{16}O$, and $HD^{16}O$ were known by comparing the measured line positions with those computed using reported values of vibration-rotation energy levels [1,2,5,6,9–14]. Several of these reports [1,2,9,12,13] list measured values of the absolute line strengths of $HD^{16}O$, $H_2^{16}O$, $H_2^{17}O$, and $H_2^{18}O$ and these results were used with spectra of the non enriched oxygen samples, represented in Table 1 as the last three entries, as an additional aid in the identification of $H_2^{16}O$, $H_2^{17}O$, $H_2^{18}O$, $D_2^{16}O$, and $HD^{16}O$ features in the oxygen O-18 spectra. A given transition of $HD^{18}O$ is located a few cm^{-1} below the O-16 counter-part and the line strength (normalized to 100% of the species) should be comparable for the two. This is also true for D_2O transitions. This feature was an aid in the identification of the oxygen enriched O-18 transitions in the spectra.

The rotational energy levels of the (100), (020), and (001) vibrational states of $HD^{18}O$ were determined from the (100)-(000), and (020)-(000), and (001)-(000) band measurements by the addition to each measured transition frequency, the appropriate lower state energy level [7]. These results were weighted and averaged for each level. The same procedure was followed for deriving rotational energy level values of the (001) and (011) states of $D_2^{18}O$ using the ground state levels given by Toth [8]. The weight for each measured position was based upon the intensity of the transition and the amount (if any) of blending with other absorptions with the greatest weight given for unblended features with a moderate to strong transition strength.

Table 2 lists values of the rotational energy levels for the (100), (020), (001) states of $HD^{18}O$ and the (001) and (011) states of $D_2^{18}O$. The energy levels are listed along with associated estimated uncertainties, un, and the number, *N*, of measured transition frequencies used to derive the energy. In a few cases, only one transition could be used to

Table 2
Rotational energy levels (cm^{-1}) of the $D_2^{18}O$ vibrational states, (001) and (011), and the $HD^{18}O$ states, (001), (020), and (100)

J	K_a	K_c	$D_2^{18}O$						$HD^{18}O$								
			(001)			(011)			(001)			(020)			(100)		
			Energy	un	N	Energy	un	N	Energy	un	N	Energy	un	N	Energy	un	N
0	0	0	2767.49941	10.	1.	3927.65925	20.	1.	3696.33049	4.	2.	2767.20936	40.	1.	2709.28466	40.	1.
1	0	1	2779.50287	3.	3.	3939.67701	40.	1.	3711.66184	4.	4.	2782.72628	50.	3.	2724.42956	6.	1.
1	1	1	2786.81720	3.	2.	3947.99847	40.	1.	3724.69134	7.	5.	2801.01750	25.	2.	2738.54080	50.	2.
1	1	0	2789.30070	3.	2.	3950.60468	40.	1.	3727.44905	9.	3.	2804.09643	30.	2.	2741.17653	5.	1.
2	0	2	2802.96987	3.	2.	3963.18307	20.	2.	3741.92433	3.	6.	2813.38861	45.	2.	2754.37682	10.	2.
2	1	2	2808.34490	3.	2.	3969.43510	30.	3.	3752.58655	6.	6.	2828.95916	30.	5.	2766.18129	5.	3.
2	1	1	2815.78906	6.	3.	3977.24605	40.	3.	3760.85276	3.	6.	2838.19123	20.	4.	2774.08105	10.	3.
2	2	1	2837.65495	15.	3.	4002.09388	20.	2.	3799.80272	5.	6.	2892.72819	15.	2.	2816.10393	6.	2.
2	2	0	2838.18735	11.	2.	4002.61627	40.	2.	3800.19420	6.	4.	2893.08313	25.	2.	2816.43948	15.	1.
3	0	3	2836.97479	10.	3.	3997.25311	6.	2.	3786.37088	6.	7.	2858.50440	10.	2.	2798.47684	15.	4.
3	1	3	2840.32095	80.	1.	4001.27763	40.	1.	3794.18867	7.	5.	2870.65076	25.	4.	2807.43429	15.	3.
3	1	2	2855.11685	5.	3.	4016.81069	20.	3.	3810.66844	4.	6.	2889.06828	55.	3.	2823.18791	10.	3.
3	2	2	2873.68849	10.	1.	4038.18040	30.	3.	3845.73541	9.	9.	2939.22185	10.	3.	2861.45764	7.	3.
3	2	1	2876.19654	5.	3.	4046.65445	60.	1.	3847.63933	9.	8.	2940.96040	40.	4.	2863.09516	7.	3.
3	3	1	2916.35343	40.	1.	4085.97560	30.	2.	3917.31654	17.	4.	3036.75254	40.	3.	2937.50519	7.	2.
3	3	0	2916.42737	8.	2.	4086.03389	300.	1.	3917.35172	15.	3.	3036.77790	90.	4.	2937.53189	5.	2.
4	0	4	2880.66777	10.	1.	4041.00690	20.	2.	3844.11270	9.	5.	2917.18864	29.	4.	2855.92420	30.	4.
4	1	4	2882.46596	5.	3.	4043.24515	30.	3.	3849.25643	18.	7.	2925.86260	95.	3.	2862.08745	5.	3.
4	1	3	2906.70324	10.	3.	4068.73939	20.	2.	3876.50001	5.	4.	2956.37590	60.	2.	2888.16142	40.	1.
4	2	3	2921.27730	9.	3.	4085.84722	10.	3.	3906.64378	5.	9.	3000.56900	60.	0.	2921.64157	10.	4.
4	2	2	2928.02505	18.	3.	4092.56718	40.	2.	3912.04139	15.	8.	3005.91195	40.	3.	2926.32033	10.	3.
4	3	2	2965.33888	8.	3.	4135.05103	30.	3.	3979.15175	15.	7.	3099.28198	60.	3.	2998.45480	20.	4.
4	3	1	2965.83556	15.	3.	4135.50587	20.	3.	3979.39384	23.	5.	3099.46020	90.	1.	2998.63978	10.	4.
4	4	1	3023.27633	10.	1.	4199.88956	8.	2.	4077.54344	20.	4.	3232.28424	50.	3.	3102.92955	25.	3.
4	4	0	3023.28485	40.	1.	4199.89817	40.	1.	4077.54610	35.	5.	3232.28930	50.	3.	3102.93122	15.	3.
5	0	5	2933.68410	10.	3.	4094.42636	10.	2.	3914.45433	5.	7.	2988.63070	40.	4.	2926.02612	6.	3.
5	1	5	2934.52516	10.	3.	4095.07735	10.	2.	3917.53632	6.	7.	2994.34153	15.	2.	2929.91065	15.	4.
5	1	4	2969.66022	16.	3.	4132.18072	40.	1.	3957.74955	5.	7.	3039.58875	15.	3.	2968.49892	5.	2.
5	2	4	2980.05866	12.	3.	4145.15233	40.	1.	3982.24865	10.	9.	3077.32160	80.	0.	2996.41482	15.	4.
5	2	3	2993.61466	10.	3.	4158.37295	30.	4.	3993.76684	7.	7.	3088.44506	50.	1.	3006.52018	15.	4.
5	3	3	3026.58261	5.	3.	4196.42142	60.	2.	4056.54777	15.	6.	3177.55645	40.	2.	3074.74305	20.	4.
5	3	2	3028.43613	8.	3.	4198.12705	10.	2.	4057.48908	5.	7.	3178.25301	15.	3.	3075.46559	15.	2.
5	4	2	3084.76730	20.	3.	4261.65080	100.	3.	4154.68262	5.	7.	3310.46841	50.	1.	3178.92835	20.	4.
5	4	1	3084.84071	6.	2.	4261.71170	40.	3.	4154.70569	15.	7.	3310.48200	300.	0.	3178.94235	35.	4.
5	5	1	3158.06760	45.	2.	4343.25260	120.	2.	4279.73500	40.	4.				3311.59960	50.	2.
5	5	0	3158.06760	45.	2.	4343.25200	90.	2.	4279.73560	40.	4.				3311.59960	50.	2.
6	0	6	2996.08530	15.	2.	4155.84851	60.	2.	3997.07714	8.	5.	3072.32380	50.	2.	3008.40320	30.	3.
6	1	6	2996.31803	11.	2.	4156.58745	15.	2.	3998.79680	7.	6.	3075.84434	40.	3.	3010.68643	15.	3.
6	1	5	3042.90091	5.	2.	4206.06225	60.	2.	4053.59311	10.	6.	3137.98790	50.	2.	3063.50552	10.	3.
6	2	5	3049.63538	6.	4.	4214.45248	10.	3.	4072.21917	10.	10.	3168.76595	25.	3.	3085.48942	6.	3.
6	2	4	3072.39018	10.	2.	4237.55480	70.	2.	4092.70893	30.	6.	3188.68600	300.	0.	3103.70948	18.	3.
6	3	4	3099.88674	6.	3.	4269.90085	30.	3.	4149.43832	6.	7.	3271.55325	50.	1.	3166.32869	20.	2.

(*continued on next page*)

Table 2 (*continued*)

J	K_a	K_c	$D_2^{18}O$						$HD^{18}O$								
			(001)			(011)			(001)			(020)			(100)		
			Energy	un	N	Energy	un	N	Energy	un	N	Energy	un	N	Energy	un	N
6	3	3	3104.85273	8.	3.	4274.52680	100.	3.	4152.13394	10.	7.	3273.56557	130.	0.	3168.41497	45.	2.
6	4	3	3158.71444	10.	3.	4335.86418	60.	2.	4247.42960	16.	7.				3270.27580	30.	3.
6	4	2	3159.05946	6.	3.	4336.15035	40.	3.	4247.54263	10.	6.				3270.35282	15.	3.
6	5	2	3232.62409	50.	3.				4372.00213	25.	4.				3402.45990		
6	5	1	3232.63279	50.	3.				4372.00440	35.	4.				3402.46220	40.	2.
6	6	1	3321.53715	50.	1.	4515.20315	80.	1.	4522.87150	60.	3.				3562.49320	20.	2.
6	6	0	3321.53715	50.	1.	4515.20315	80.	1.	4522.87150	60.	3.				3562.49320	20.	2.
7	0	7	3067.29120	20.	2.	4227.17911	20.	2.	4091.93777	10.	6.	3168.09267	60.	2.	3102.95394	15.	2.
7	1	7	3067.79433	6.	3.	4227.92620	30.	2.	4092.84985	15.	6.	3170.15800	40.	3.	3104.22930	15.	2.
7	1	6	3125.55486	5.	3.	4289.41305	40.	2.	4163.05044	5.	6.	3250.66850	50.	2.	3172.32250	8.	2.
7	2	6	3129.62485	15.	3.	4294.61192	40.	1.	4176.19152	21.	8.	3274.28302	40.	1.	3188.54295	10.	4.
7	2	5	3163.47359	24.	3.	4329.27320	60.	3.	4208.36444	15.	6.	3306.28002	50.	1.	3217.52514	5.	3.
7	3	5	3184.93465	10.	3.	4355.19760	120.	0.	4257.65862	10.	8.	3381.13442	40.	1.	3273.08923	15.	3.
7	3	4	3195.46277	10.	3.	4365.15880	15.	3.	4263.91537	25.	6.	3385.92378	40.	1.	3278.01088	15.	3.
7	4	4	3245.09611	35.	3.	4422.51398	40.	1.	4355.83857	6.	7.				3377.03160	30.	4.
7	4	3	3246.26215	10.	3.	4423.47639	30.	3.	4356.24188	15.	5.				3377.30815	15.	3.
7	5	3	3319.41035	20.	3.				4479.78634	18.	3.				3508.59320	45.	3.
7	5	2	3319.45597	17.	3.				4479.79737	12.	4.				3508.59959	50.	3.
7	6	2	3404.32408	80.	3.	4600.52360	50.	1.	4630.12080	50.	3.				3668.07266	50.	3.
7	6	1	3404.32408	80.	3.	4600.52360	50.	1.	4630.12080	50.	3.				3668.07266	50.	3.
7	7	1	3508.72914	50.	2.	4714.77854	60.	1.	4805.81902	25.	2.				3854.27382	50.	0.
7	7	0	3508.72914	50.	2.	4714.77854	60.	1.	4805.81902	25.	2.				3854.27382	50.	0.
8	0	8	3148.35307	10.	3.	4307.75812	40.	2.	4199.08880	6.	5.	3275.94150	50.	3.	3209.70825	10.	3.
8	1	8	3148.24458	2.	3.	4307.77793	40.	2.	4199.55602	9.	5.	3277.11191	40.	2.	3210.39562	10.	3.
8	1	7	3217.26524	8.	3.	4381.71260	40.	2.	4285.19844	14.	5.	3376.64425	25.	2.	3294.06360	30.	2.
8	2	7	3219.72964	3.	3.	4384.94516	30.	2.	4293.79586	8.	4.	3393.71895	20.	1.	3305.23755	30.	2.
8	2	6	3265.77225	8.	3.	4431.94285	40.	1.	4339.98275	8.	4.	3440.57208	300.	0.	3347.35378	15.	2.
8	3	6	3281.32828	30.	4.	4451.93454	60.	3.	4380.94633	29.	4.				3394.81815	30.	3.
8	3	5	3300.07303	29.	3.				4393.29536	40.	6.				3404.72586	30.	3.
8	4	5	3343.79640	10.	3.	4521.51072	80.	2.	4479.92172	28.	7.				3499.21686	15.	3.
8	4	4	3346.92489	15.	3.	4524.04318	80.	1.	4481.08400	12.	6.				3500.02095	30.	3.
8	5	4	3418.50668	27.	3.				4603.14226	30.	5.				3630.02750	55.	3.
8	5	3	3418.68659	30.	3.				4603.18928	29.	4.				3630.05360	60.	3.
8	6	3	3500.98637	45.	3.				4752.78200	40.	3.				3788.80987	50.	3.
8	6	2	3500.99921	40.	3.				4752.78200	40.	3.				3788.80987	50.	3.
8	7	2	3606.01000	10.	3.				4811.68778	100.	1.				4927.87870	15.	2.
8	7	1	3606.01000	10.	3.				4811.68778	100.	1.				4927.87870	15.	2.
8	8	1	3718.91289	35.	1.				5127.39110	300.	0.						
8	8	0	3718.91289	35.	1.				5127.39110	300.	0.						
9	0	9	3238.78850	10.	2.	4397.64207	40.	2.	4318.58237	30.	3.	3395.93143	50.	1.	3328.71667	15.	3.
9	1	9	3238.79300	15.	2.	4397.66924	40.	2.	4318.81500	20.	5.	3396.58122	50.	1.	3329.07682	20.	2.
9	1	8	3318.02300	13.	4.	4482.89810	50.	1.	4419.42460	30.	3.	3515.06208	300.	1.	3428.03283	40.	1.
9	2	8	3320.02446	10.	3.				4424.68308	20.	6.	3526.78411	300.	2.	3435.25113	30.	2.

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9	2	7	3378.11785	10.	3.	4545.98126	60.	1.	4486.63268	20.	4.				3492.41512	30.	1.
9	3	7	3388.65659	17.	3.	4559.72964	80.	1.	4518.95842	15.	2.				3531.23097	25.	2.
9	3	6	3417.96020	20.	3.	4588.34905	25.	2.	4540.34850	35.	4.				3548.79307	25.	2.
9	4	6	3454.59033	37.	3.				4619.62323	50.	2.				3636.80708	15.	2.
9	4	5	3461.58000	10.	1.				4622.47576	60.	2.				3638.80487	50.	1.
9	5	5	3529.94478	50.	2.				4742.12222	300.	1.				3766.80403	70.	2.
9	5	4	3530.51721	10.	3.				4742.28248	15.	2.				3766.90309	50.	2.
9	6	4	3610.06649	50.	2.				4890.88400	200.	1.						
9	6	3	3610.09290	48.	3.				4890.88700	200.	1.						
9	7	3	3715.53060	90.	3.				5065.24626	80.	2.						
9	7	2	3715.53060	90.	3.				5065.24626	80.	2.						
9	8	2	3832.35033	150.	1.				5264.06863	300.	1.						
9	8	1	3832.35033	150.	1.				5264.06863	300.	1.						
10	0	10	3338.64703	10.	1.	4496.84327	60.	2.	4450.44258	15.	3.	3528.11600	300.	0.	3460.01012	5.	2.
10	1	10	3338.64703	10.	1.	4496.85688	40.	2.	4450.55715	15.	3.	3528.46811	50.	0.	3460.19593	15.	2.
10	1	9	3427.93216	50.	2.	4593.07130	40.	2.	4565.50415	10.	5.				3574.24940	15.	1.
10	2	9	3432.03890	300.	1.	4593.32313	25.	2.	4568.55209	15.	4.				3578.28154	40.	1.
10	2	8	3499.59142	30.	1.	4668.76295	60.	1.	4647.24589	15.	2.				3651.79004	15.	1.
10	3	8	3506.59839	25.	2.	4678.37634	80.	2.	4671.28800	60.	1.				3681.98546	40.	1.
10	3	7	3548.08682	20.	1.				4704.66655	35.	3.				3710.03650	30.	1.
10	4	7	3577.15964	15.	2.				4774.79803	40.	2.				3791.06063	50.	1.
10	4	6	3590.51852	50.	2.				4780.92896	50.	1.				3794.07406	50.	1.
10	5	6	3653.69965	55.	3.				4896.76088	50.	1.						
10	5	5	3655.24666	40.	2.				4897.21906	50.	1.						
10	6	5	3731.55416	30.	3.												
10	6	4	3731.64549	300.	1.												
10	7	4	3837.30020	100.	2.												
10	7	3	3837.30200	100.	2.												
11	0	11	3447.90990	40.	2.	4605.35900	200.	1.	4594.67237	25.	4.				3603.59612	10.	2.
11	1	11	3447.91256	40.	2.	4605.36200	300.	1.	4594.72784	45.	3.				3603.69115	20.	2.
11	1	10	3547.08147	12.	2.	4712.35177	60.	1.	4723.46099	15.	2.				3731.49273	50.	1.
11	2	10	3547.14030	40.	1.	4711.82530	60.	1.	4725.15720	50.	3.				3734.07725	40.	1.
11	2	9	3629.79297	40.	2.	4800.22158	60.	1.	4820.73799	50.	1.						
11	3	9	3635.44138	12.	2.				4837.52855	50.	2.						
11	3	8	3689.24270	15.	3.				4885.47486	50.	1.						
11	4	8	3711.15271	50.	2.												
11	4	7	3733.50035	140.	1.												
11	5	7	3789.96075	50.	1.												
11	5	6	3793.31415	55.	2.												
12	0	12	3566.58300	200.	2.	4723.18848	300.	1.	4751.25688	50.	3.				3759.46655	50.	1.
12	1	12	3566.58520	200.	2.	4723.18848	300.	1.	4751.28350	50.	4.				3759.51460	50.	1.
12	1	11	3675.52643	10.	2.	4841.83796	300.	0.	4893.43740	50.	0.						
12	2	11	3675.56920	64.	2.				4894.31414	50.	1.						
12	2	10	3768.73912	25.	2.												
12	3	10	3776.55200	300.	0.												
12	3	9	3839.90950	10.	2.												
12	4	9	3855.77216	50.	1.												
12	4	8	3888.63827	90.	1.												
13	0	13	3694.64767	90.	2.	4850.29812	100.	1.	4920.16705	50.	1.				3927.45855	300.	0.

(*continued on next page*)

Table 2 (*continued*)

J	K_a	K_c	$D_2^{18}O$				$HD^{18}O$									
			(001)			(011)			(001)			(020)			(100)		
			Energy	un	*N*	Energy	un	*N*	Energy	un	*N*	Energy	un	*N*	Energy	un	*N*
13	1	13	3694.64767	90.	2.	4850.29812	100.	1.	4920.18796	50.	1.				3927.45855	300.	0.
13	1	12	3813.28488	50.	1.				5075.54074	300.	0.						
13	2	12	3813.30715	20.	1.				5075.88863	50.	1.						
13	2	11	3916.58426	55.	2.												
14	0	14	3832.08295	40.	2.				5101.38118	50.	1.						
14	1	14	3832.08295	40.	2.				5101.38753	300.	1.						
14	1	13	3959.09070	50.	0.												
14	2	13	3959.11565	50.	1.												
15	0	15	3978.85202	100.	1.				5294.88155	300.	0.						
15	1	15	3978.85202	100.	1.				5294.88155	300.	0.						

un is the estimated uncertainty of the energy level value in $cm^{-1} \times 10^5$; *N* are the number of observed transition frequencies used to derive the energy.

determine the upper state level and the estimated uncertainty of these values was based upon the quality of the measured transition. In a few other cases, $N=0$ and for these, the upper state level value was derived from calculations and given large uncertainties. In fact all levels given with uncertainties of $\pm 0.003\ cm^{-1}$ may be in error by as much as $\pm 0.03\ cm^{-1}$ and were included here mainly to aid in future studies of these molecules in this spectral region.

4. Results

Table 3 is a listing of measurements of $HD^{18}O$ and $D_2^{18}O$ covering the region from 2517 to 3020 cm^{-1}. Another comparable listing was made for the upper spectral region but not included here due to space limitations. A complete listing of the measurements can be obtained from the author. Each entry in Table 3 gives the molecule, mo, observed position, observed minus computed position, o−c, the estimated uncertainty in the computed position, un, rotational quantum assignment, observed strength in cm^{-2}/atm at 296 K, estimated uncertainty in percent for the strength, *%s,* the lower level energy level, and the vibrational band. The notation for molecule is mol=49 for $HD^{18}O$ and mol=80 for $D_2^{18}O$. The values of o−c were determined from the measured and computed positions derived from the energy levels given in Table 2 and the ground state levels given in ref. [7] for $HD^{18}O$ and ref. [8] for $D_2^{18}O$ and the uncertainties, un, were derived from the expression:

$$\text{un} = \{\text{un(upper)}^2 + \text{un(lower)}^2\}^{1/2}. \quad (1)$$

The measured line strengths, *S*, for each run was normalized to 100% of the sample by the relation:

$$S(100\%) = S(\text{measured})/\text{RA}, \quad (2)$$

where RA is the relative abundance of the species and listed in Table 1.

A few of the entries given in Table 3 contain an asterisk located in front of the observed position. These lines contain doubled transitions and the strength is the sum of the strengths of the two comparable transitions and the rotational quantum assignment pertains to the stronger of the transitions for $D_2^{18}O$.

Figs. 1−4 display short scans of the oxygen O-18 enriched spectrum with a total pressure of 1.49 Torr. The isotopic species are labeled in the figures with rotational quantum assignments followed by the upper state notation given for the $HD^{18}O$ and $D_2^{18}O$ transitions. The observed spectrum in each figure is overlaid with a synthetic spectrum created from the NLLS program. The upper portion of each figure shows a residual plot giving the percent differences between the observed and computed spectra.

Table 3
Measured and computed line positions (cm^{-1}) and observed strengths (cm^{-2}/atm at 296 K) for the (001)-(000) band of $D_2^{18}O$ and the (100)-(000) and (020)-(000) bands of $HD^{18}O$

Mol	Observed position	o−c	un	upper			Lower			Observed strength	%s	Lower level	Band
				J	K_a	K_c	J	K_a	K_c				
49	2517.19620	−4.	16.	10	2	8	11	2	9	1.91×10^{-2}	10.	1134.59380	100 000
49	2520.33800	193.	50.	12	1	12	13	1	13	1.72×10^{-2}	10.	1239.17853	100 000
49	2530.81800	-21.	27.	9	3	6	10	3	7	3.86×10^{-2}	10.	1017.97486	100 000
49	2533.47400	24.	30.	9	2	7	10	2	8	4.42×10^{-2}	10.	958.94136	100 000
49	2535.47170	0.	12.	11	0	11	12	0	12	3.11×10^{-2}	3.	1068.12442	100 000
49	2535.52400	23.	26.	11	1	11	12	1	12	3.01×10^{-2}	4.	1068.16738	100 000
49	2536.51440	0.	41.	10	2	9	11	2	10	3.55×10^{-2}	10.	1041.76714	100 000
49	2538.86830	49.	51.	9	5	4	10	5	5	1.18×10^{-2}	10.	1228.03528	100 000
49	2539.08550	69.	72.	9	5	5	10	5	6	1.17×10^{-2}	10.	1227.71922	100 000
49	2539.39030	15.	17.	9	4	6	10	4	7	2.33×10^{-2}	10.	1097.41693	100 000
49	2542.68820	20.	25.	9	3	7	10	3	8	4.03×10^{-2}	5.	988.54297	100 000
49	2548.93330	0.	40.	9	1	8	10	1	9	7.29×10^{-2}	5.	879.09953	100 000
49	2550.44080	3.	9.	10	0	10	11	0	11	6.55×10^{-2}	4.	909.56935	100 000
49	2550.54050	-3.	17.	10	1	10	11	1	11	7.09×10^{-2}	10.	909.65540	100 000
49	2550.60390	0.	16.	8	2	6	9	2	7	9.80×10^{-2}	5.	796.74988	100 000
49	2551.17900	−27.	31.	8	3	5	9	3	6	7.19×10^{-2}	3.	853.54659	100 000
49	2551.94000	−28.	31.	9	2	8	10	2	9	7.44×10^{-2}	3.	883.31085	100 000
49	2556.26120	−29.	30.	8	4	4	9	4	5	3.78×10^{-2}	5.	943.75946	100 000
49	*2557.17800	−143.	50.	8	6	3	9	6	4	1.45×10^{-2}	10.	1231.63044	100 000
49	2557.36520	16.	60.	8	5	3	9	5	4	2.08×10^{-2}	15.	1072.68856	100 000
49	2557.44600	−182.	55.	8	5	4	9	5	5	1.68×10^{-2}	10.	1072.57968	100 000
49	2557.62240	−13.	16.	8	4	5	9	4	6	4.19×10^{-2}	10.	941.59433	100 000
49	2559.77000	−13.	31.	8	3	6	9	3	7	6.60×10^{-2}	10.	835.04802	100 000
49	2563.18720	−22.	30.	8	1	7	9	1	8	1.26×10^{-1}	5.	730.87618	100 000
49	2565.20270	25.	19.	9	0	9	10	0	10	1.20×10^{-1}	5.	763.51422	100 000
49	2568.47530	4.	6.	7	2	5	8	2	6	1.67×10^{-1}	4.	649.04988	100 000
49	2571.41180	−30.	15.	7	3	4	8	3	5	1.10×10^{-1}	10.	706.59878	100 000
49	*2575.04600	50.	50.	7	6	2	8	6	3	1.63×10^{-2}	10.	1093.02716	100 000
49	2575.07500	−4.	15.	7	4	3	8	4	4	6.45×10^{-2}	4.	802.23311	100 000
49	2575.44370	−50.	50.	7	5	2	8	5	3	2.64×10^{-2}	3.	933.15539	100 000
49	2575.46950	−36.	45.	7	5	3	8	5	4	2.59×10^{-2}	3.	933.12334	100 000
49	2575.67240	3.	30.	7	4	4	8	4	5	6.35×10^{-2}	10.	801.35923	100 000
49	2576.96550	−7.	15.	7	3	5	8	3	6	1.23×10^{-1}	3.	696.12366	100 000
49	2577.61550	8.	9.	7	1	6	8	1	7	2.14×10^{-1}	4.	594.70708	100 000
49	2578.49700	−48.	15.	3	0	3	4	2	2	8.82×10^{-3}	10.	219.97936	100 000
49	2579.73841	−3.	16.	8	0	8	9	0	9	2.11×10^{-1}	4.	629.96981	100 000
49	2580.09000	−16.	11.	8	1	8	9	1	9	2.06×10^{-1}	5.	630.30546	100 000
49	2582.99287	3.	10.	7	2	6	8	2	7	1.90×10^{-1}	5.	605.55011	100 000
49	2586.91045	5.	18.	6	2	4	7	2	5	2.63×10^{-1}	2.	516.79908	100 000
49	2591.06770	55.	45.	6	3	3	7	3	4	1.79×10^{-1}	3.	577.34782	100 000
49	2592.56732	−4.	10.	6	1	5	7	1	6	3.43×10^{-1}	3.	470.93816	100 000
49	*2592.59240	−12.	25.	6	6	1	7	6	2	1.46×10^{-2}	10.	969.90068	100 000
49	*2593.14220	−53.	100.	6	5	2	7	5	3	6.55×10^{-2}	4.	809.31717	100 000
49	2593.45840	41.	30.	6	4	3	7	4	4	8.62×10^{-2}	10.	676.81781	100 000
49	2594.02410	8.	16.	7	0	7	8	0	8	3.14×10^{-1}	2.	508.92992	100 000
49	2594.20060	17.	21.	6	3	4	7	3	5	1.94×10^{-1}	5.	572.12826	100 000
80	2594.45860	0.	120.	12	3	9	13	3	10	1.67×10^{-2}	10.	1245.45090	001 000
49	2594.65390	23.	15.	7	1	7	8	1	8	3.21×10^{-1}	3.	509.57563	100 000
80	2594.84220	−40.	63.	13	2	11	14	2	12	2.16×10^{-2}	10.	1321.74166	001 000
80	*2596.09030	0.	141.	15	0	15	16	0	16	2.81×10^{-2}	10.	1382.76172	001 000
49	2598.68545	5.	7.	6	2	5	7	2	6	2.88×10^{-1}	7.	486.80402	100 000
80	2601.14130	101.	146.	11	4	7	12	4	8	5.13×10^{-2}	10.	1132.36006	001 000
80	2603.16360	−38.	56.	11	5	6	12	5	7	2.74×10^{-2}	10.	1190.15017	001 000
49	2604.15800	−14.	10.	8	0	8	8	2	7	8.57×10^{-3}	10.	605.55011	100 000
80	2605.48700	26.	34.	10	6	5	11	6	6	2.63×10^{-2}	15.	1126.06742	001 000
49	2605.70475	19.	16.	5	2	3	6	2	4	4.04×10^{-1}	10.	400.81562	100 000
80	2605.88290	18.	47.	12	2	10	13	2	11	2.39×10^{-2}	15.	1162.85640	001 000
80	2606.05390	52.	18.	11	3	8	12	3	9	6.03×10^{-2}	2.	1083.18932	001 000
80	*2606.22910	−289.	51.	13	1	12	14	1	13	4.78×10^{-2}	8.	1207.05289	001 000

(*continued on next page*)

Table 3 (*continued*)

Mol	Observed position	o−c	un	upper			Lower			Observed strength	%s	Lower level	Band
				J	K_a	K_c	J	K_a	K_c				
80	*2607.14330	0.	108.	14	1	14	15	1	15	5.50×10^{-2}	7.	1224.93965	001 000
80	2607.42400	0.	51.	11	5	7	12	5	8	1.45×10^{-2}	10.	1182.53675	001 000
49	2608.03940	−40.	30.	6	0	6	7	0	7	4.59×10^{-1}	3.	400.36340	100 000
49	2608.23480	−2.	6.	5	1	4	6	1	5	4.66×10^{-1}	4.	360.26410	100 000
49	2609.11252	0.	15.	6	1	6	7	1	7	4.48×10^{-1}	2.	401.57391	100 000
49	2609.88240	3.	15.	5	3	2	6	3	3	2.25×10^{-1}	3.	465.58322	100 000
49	*2610.48330	108.	50.	5	5	0	6	5	1	5.12×10^{-2}	10.	701.11738	100 000
49	2610.85670	25.	35.	5	4	1	6	4	2	1.04×10^{-1}	3.	568.08590	100 000
49	2610.92630	−21.	20.	5	4	2	6	4	3	1.04×10^{-1}	3.	568.00184	100 000
80	2611.11810	130.	64.	11	4	8	12	4	9	2.38×10^{-2}	10.	1100.03591	001 000
49	2611.38140	−3.	20.	5	3	3	6	3	4	2.31×10^{-1}	6.	463.36162	100 000
49	2614.49590	−20.	15.	5	2	4	6	2	5	3.92×10^{-1}	3.	381.91872	100 000
80	2615.23860	−29.	51.	10	4	6	11	4	7	4.86×10^{-2}	10.	975.27963	001 000
80	2616.77120	29.	47.	11	2	9	12	2	10	7.79×10^{-2}	8.	1013.02206	001 000
80	2617.22180	−45.	66.	12	2	11	13	2	12	7.03×10^{-2}	10.	1058.34695	001 000
80	2617.24800	7.	21.	12	1	11	13	1	12	3.44×10^{-2}	3.	1058.27850	001 000
80	*2617.54400	70.	105.	9	7	2	10	7	3	2.92×10^{-2}	10.	1097.98730	001 000
80	2617.56000	9.	53.	10	5	5	11	5	6	2.61×10^{-2}	10.	1037.68675	001 000
80	2617.86180	18.	40.	10	3	7	11	3	8	5.75×10^{-2}	10.	930.22520	001 000
80	*2618.11610	65.	93.	13	0	13	14	0	14	1.04×10^{-1}	8.	1076.53222	001 000
80	2619.67420	48.	57.	10	5	6	11	5	7	5.13×10^{-2}	2.	1034.02593	001 000
80	2620.00620	−23.	49.	9	6	3	10	6	4	3.37×10^{-2}	10.	990.08647	001 000
80	2620.03310	9.	16.	11	3	9	12	3	10	3.45×10^{-2}	4.	1015.40837	001 000
49	2621.80663	1.	6.	5	0	5	6	0	6	6.11×10^{-1}	3.	304.21950	100 000
80	2622.89640	12.	17.	10	4	7	11	4	8	8.96×10^{-2}	10.	954.26336	001 000
49	2623.50300	9.	15.	5	1	5	6	1	6	6.01×10^{-1}	3.	306.40774	100 000
49	*2623.81600	−42.	50.	4	4	0	5	5	1	9.26×10^{-3}	10.	608.47288	020 000
80	2625.86520	83.	11.	5	0	5	6	2	4	1.30×10^{-2}	10.	307.81973	001 000
80	2627.50610	32.	33.	10	2	8	11	2	9	7.32×10^{-2}	5.	872.08564	001 000
49	2627.82530	4.	10.	4	3	1	5	3	2	2.34×10^{-1}	2.	370.81452	100 000
49	2628.02470	11.	16.	4	4	0	5	4	1	8.03×10^{-2}	5.	474.90663	100 000
49	2628.03980	−16.	25.	4	4	1	5	4	2	7.83×10^{-2}	5.	474.88959	100 000
80	2628.16670	11.	16.	11	1	10	12	1	11	1.29×10^{-1}	5.	918.91488	001 000
49	2628.41005	−10.	20.	4	3	2	5	3	3	2.61×10^{-1}	10.	370.04465	100 000
80	*2629.00580	−25.	206.	12	1	12	13	1	13	1.94×10^{-1}	4.	937.57915	001 000
80	2629.73785	0.	12.	9	4	5	10	4	6	1.53×10^{-1}	5.	831.84215	001 000
80	2630.18880	−26.	26.	10	3	8	11	3	9	1.34×10^{-1}	4.	876.40933	001 000
80	2630.36500	−27.	28.	9	3	6	10	3	7	2.15×10^{-1}	5.	787.59493	001 000
49	2630.39925	0.	10.	4	2	3	5	2	4	4.57×10^{-1}	3.	291.24232	100 000
80	2631.29210	−8.	13.	9	5	4	10	5	5	8.03×10^{-2}	10.	899.22503	001 000
80	*2631.40920	1.	18.	8	7	2	9	7	3	2.69×10^{-2}	10.	974.60081	001 000
80	2632.26760	34.	64.	9	5	5	10	5	6	3.70×10^{-2}	10.	897.67752	001 000
80	2634.58000	−272.	47.	8	6	2	9	6	3	2.17×10^{-2}	10.	866.41649	001 000
80	2634.59540	−32.	51.	8	6	3	9	6	4	4.47×10^{-2}	4.	866.39065	001 000
49	2634.78330	−50.	6.	5	0	5	5	2	4	1.76×10^{-2}	10.	291.24232	100 000
80	2635.01420	−42.	38.	9	4	6	10	4	7	7.03×10^{-2}	10.	819.57571	001 000
49	2635.45987	−26.	30.	4	0	4	5	0	5	7.49×10^{-1}	2.	220.46407	100 000
49	2637.86429	−2.	6.	4	1	4	5	1	5	7.39×10^{-1}	2.	224.22314	100 000
80	2638.18533	6.	11.	9	2	7	10	2	8	2.48×10^{-1}	5.	739.93258	001 000
80	2638.97390	0.	51.	10	1	9	11	1	10	1.07×10^{-1}	4.	788.95826	001 000
49	2639.32000	−254.	40.	3	3	1	4	4	0	9.46×10^{-3}	10.	397.43000	020 000
49	2639.34900	−78.	90.	3	3	0	4	4	1	8.67×10^{-3}	10.	397.42812	020 000
80	*2639.81080	−38.	43.	11	0	11	12	0	12	3.32×10^{-1}	4.	808.09872	001 000
49	2640.81470	32.	30.	4	0	4	4	2	3	1.62×10^{-2}	10.	215.10982	100 000
80	2641.29130	19.	23.	9	3	7	10	3	8	1.12×10^{-1}	4.	747.36548	001 000
49	2641.36982	0.	10.	3	1	2	4	1	3	6.75×10^{-1}	3.	181.81809	100 000
49	2643.11574	−6.	8.	3	2	1	4	2	2	4.85×10^{-1}	3.	219.97936	100 000
80	2643.59308	−21.	30.	8	3	5	9	3	6	1.82×10^{-1}	6.	656.47974	001 000
80	2644.23780	14.	19.	8	4	4	9	4	5	1.23×10^{-1}	3.	702.68723	001 000
80	2644.40660	−33.	32.	8	5	3	9	5	4	6.15×10^{-2}	4.	774.27966	001 000
80	2644.79310	31.	28.	8	5	4	9	5	5	1.23×10^{-1}	4.	773.71389	001 000
49	2645.02565	−3.	6.	3	3	0	4	3	1	1.94×10^{-1}	5.	292.50621	100 000

(*continued on next page*)

Table 3 (*continued*)

Mol	Observed position	o−c	un	upper			Lower			Observed strength	%s	Lower level	Band
				J	K_a	K_c	J	K_a	K_c				
80	*2645.16250	−16.	54.	7	7	0	8	7	1	3.82×10^{-2}	10.	863.56648	001 000
49	2645.19580	−5.	8.	3	3	1	4	3	2	1.93×10^{-1}	3.	292.30934	100 000
49	2645.76780	−27.	25.	8	1	7	9	1	8	6.90×10^{-3}	10.	730.87618	020 000
49	2645.97080	−89.	52.	8	0	8	9	0	9	1.12×10^{-2}	10.	629.96981	020 000
49	2646.34780	−2.	8.	3	2	2	4	2	3	4.80×10^{-1}	3.	215.10982	100 000
80	2647.38440	−8.	11.	8	4	5	9	4	6	2.33×10^{-1}	2.	696.41192	001 000
49	2648.65120	14.	40.	3	2	1	4	3	2	1.31×10^{-2}	10.	292.30934	020 000
80	*2649.06100	80.	81.	7	6	1	8	6	2	1.01×10^{-1}	5.	755.26388	001 000
80	2649.08980	0.	9.	8	2	6	9	2	7	2.15×10^{-1}	10.	616.68245	001 000
49	2649.28860	−18.	15.	3	0	3	4	0	4	7.88×10^{-1}	3.	149.18806	100 000
80	2649.64750	−13.	16.	9	1	8	10	1	9	3.40×10^{-1}	4.	668.37537	001 000
49	2650.42190	−43.	15.	6	1	6	6	1	5	2.04×10^{-2}	5.	360.26410	100 000
80	*2650.52625	0.	14.	10	1	10	11	1	11	5.47×10^{-1}	3.	688.12078	001 000
80	2651.01570	24.	18.	9	2	8	10	2	9	1.70×10^{-1}	3.	669.00900	001 000
49	2652.22586	0.	15.	3	1	3	4	1	4	7.39×10^{-1}	3.	155.20843	100 000
80	2652.73980	−14.	32.	8	3	6	9	3	7	3.66×10^{-1}	3.	628.58834	001 000
49	2655.96190	48.	50.	7	1	6	8	1	7	1.25×10^{-2}	10.	594.70708	020 000
49	2656.18800	33.	30.	8	2	7	8	2	6	1.38×10^{-2}	10.	649.04988	100 000
80	2657.02700	−12.	18.	7	5	2	8	5	3	1.62×10^{-1}	3.	662.42885	001 000
80	2657.15480	−21.	22.	7	5	3	8	5	4	7.85×10^{-2}	3.	662.25534	001 000
80	2657.46660	−15.	13.	7	3	4	8	3	5	4.93×10^{-1}	3.	537.99602	001 000
80	2658.34670	5.	19.	7	4	3	8	4	4	3.39×10^{-1}	5.	587.91550	001 000
49	2658.41590	−3.	10.	2	1	1	3	1	2	6.50×10^{-1}	4.	115.66512	100 000
80	2659.93110	33.	36.	7	4	4	8	4	5	1.61×10^{-1}	4.	585.16534	001 000
80	2660.16690	3.	9.	8	1	7	9	1	8	2.67×10^{-1}	4.	557.09837	001 000
80	2660.57108	25.	26.	7	2	5	8	2	6	6.39×10^{-1}	4.	502.90276	001 000
80	2661.13830	−4.	18.	9	1	9	10	1	10	2.69×10^{-1}	5.	577.65466	001 000
80	2661.15270	27.	14.	9	0	9	10	0	10	5.46×10^{-1}	4.	577.63607	001 000
49	2661.22800	−8.	40.	7	1	7	8	0	8	1.11×10^{-2}	10.	508.92992	020 000
80	2661.35460	−3.	9.	8	2	7	9	2	8	5.17×10^{-1}	3.	558.37501	001 000
49	2662.28180	1.	6.	2	2	1	3	2	2	3.47×10^{-1}	10.	153.82214	100 000
49	2663.61148	10.	10.	2	0	2	3	0	3	8.72×10^{-1}	3.	90.76544	100 000
80	2664.47220	−11.	12.	7	3	5	8	3	6	2.62×10^{-1}	6.	520.46234	001 000
49	2666.31720	−29.	15.	5	1	5	5	1	4	3.89×10^{-2}	7.	263.59316	100 000
49	2666.59402	0.	6.	2	1	2	3	1	3	6.70×10^{-1}	3.	99.58727	100 000
49	2667.04930	−44.	50.	6	1	5	7	1	6	1.76×10^{-2}	10.	470.93816	020 000
80	2669.28460	0.	51.	6	5	2	7	5	3	1.84×10^{-1}	5.	563.33949	001 000
80	2670.54029	5.	11.	7	1	6	8	1	7	7.32×10^{-1}	3.	455.01462	001 000
80	2671.52120	0.	8.	8	1	8	9	1	9	7.79×10^{-1}	3.	476.72338	001 000
80	2671.67250	−10.	22.	8	0	8	9	0	9	3.99×10^{-1}	3.	476.68047	001 000
80	2671.77080	0.	11.	6	3	3	7	3	4	3.27×10^{-1}	3.	433.08193	001 000
80	2671.91013	5.	12.	6	4	2	7	4	3	1.98×10^{-1}	4.	487.14938	001 000
49	2671.96090	50.	50.	6	0	6	7	0	7	3.11×10^{-2}	5.	400.36340	020 000
80	2672.13420	16.	17.	7	2	6	8	2	7	2.48×10^{-1}	3.	457.49081	001 000
80	2672.57006	−10.	14.	6	4	3	7	4	4	3.66×10^{-1}	4.	486.14428	001 000
80	2672.81345	9.	14.	6	2	4	7	2	5	4.31×10^{-1}	3.	399.57682	001 000
80	2674.15620	41.	11.	3	0	3	4	2	2	4.30×10^{-2}	10.	162.81900	001 000
49	2674.27140	97.	40.	6	1	6	7	1	7	3.29×10^{-2}	10.	401.57391	020 000
49	2675.51738	−3.	5.	1	1	0	2	1	1	4.42×10^{-1}	3.	65.65913	100 000
80	2676.47655	4.	8.	6	3	4	7	3	5	6.74×10^{-1}	2.	423.41023	001 000
49	2678.53100	6.	6.	1	0	1	2	0	2	6.40×10^{-1}	3.	45.89862	100 000
49	2679.32460	−5.	15.	5	1	4	6	1	5	3.11×10^{-2}	10.	360.26410	020 000
49	2680.26940	4.	5.	4	1	4	4	1	3	7.00×10^{-2}	4.	181.81809	100 000
80	2680.87990	−1.	13.	6	1	5	7	1	6	5.14×10^{-1}	5.	362.02100	001 000
49	2680.94250	−77.	50.	1	1	1	2	1	2	5.12×10^{-1}	6.	57.59753	100 000
80	*2681.11460	248.	45.	5	5	0	6	5	1	2.11×10^{-1}	6.	476.95548	001 000
49	2681.96170	−23.	25.	6	2	5	7	2	6	1.81×10^{-2}	10.	486.80402	020 000
80	2682.04028	−5.	22.	7	0	7	8	0	8	1.04×10^{0}	2.	385.25087	001 000
80	2682.44429	0.	8.	7	1	7	8	1	8	5.24×10^{-1}	2.	385.35004	001 000
80	2683.08510	3.	8.	6	2	5	7	2	6	9.61×10^{-1}	3.	366.55031	001 000
49	2684.36920	11.	20.	2	1	1	3	2	2	1.72×10^{-2}	10.	153.82214	020 000

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Table 3 (*continued*)

Mol	Observed position	o−c	un	upper			Lower			Observed strength	%s	Lower level	Band
				J	K_a	K_c	J	K_a	K_c				
49	2684.41180	60.	40.	5	0	5	6	0	6	4.12×10^{-2}	10.	304.21950	020 000
80	2685.00147	4.	11.	5	4	1	6	4	2	4.05×10^{-1}	3.	399.83928	001 000
80	2685.22050	38.	22.	5	4	2	6	4	3	2.23×10^{-1}	4.	399.54718	001 000
80	2685.79460	−33.	11.	5	2	3	6	2	4	1.08×10^{0}	4.	307.81973	001 000
80	2686.09833	−1.	11.	5	3	2	6	3	3	7.62×10^{-1}	2.	342.33779	001 000
49	2687.93380	1.	15.	5	1	5	6	1	6	3.84×10^{-2}	5.	306.40774	020 000
49	2688.21910	−27.	30.	8	3	6	8	3	5	2.12×10^{-2}	10.	706.59878	100 000
80	2688.72630	20.	9.	5	3	3	6	3	4	3.85×10^{-1}	4.	337.85651	001 000
80	2689.43550	84.	16.	9	1	8	9	3	7	3.16×10^{-2}	10.	628.58834	001 000
80	2690.86280	54.	13.	8	0	8	8	2	7	2.19×10^{-2}	10.	457.49081	001 000
80	2691.46408	16.	19.	5	1	4	6	1	5	1.25×10^{0}	3.	278.19630	001 000
49	2691.76880	−37.	15.	3	1	3	3	1	2	1.15×10^{-1}	8.	115.66512	100 000
80	2692.10628	−4.	300.	10	2	9	10	2	8	1.97×10^{-2}	10.	739.93258	001 000
80	2692.74420	−28.	19.	6	0	6	7	0	7	6.09×10^{-1}	10.	303.34082	001 000
49	2692.96580	30.	29.	4	0	4	5	1	5	2.41×10^{-2}	10.	224.22314	020 000
80	2693.22996	0.	10.	8	1	8	8	1	7	3.47×10^{-2}	10.	455.01462	001 000
49	2693.86600	0.	40.	0	0	0	1	0	1	3.53×10^{-1}	3.	15.41866	100 000
80	2694.23385	11.	14.	5	2	4	6	2	5	5.75×10^{-1}	4.	285.82492	001 000
49	2694.67000	13.	15.	5	2	4	5	2	3	1.06×10^{-1}	3.	301.74495	100 000
49	2695.74160	19.	16.	7	3	5	7	3	4	5.02×10^{-2}	5.	577.34782	100 000
49	*2695.78310	39.	50.	8	6	2	8	6	3	3.32×10^{-2}	5.	1093.02716	100 000
49	2696.72420	−37.	29.	4	0	4	5	0	5	6.80×10^{-2}	10.	220.46407	020 000
80	2696.80330	40.	11.	8	1	7	8	3	6	2.24×10^{-2}	10.	520.46234	001 000
49	2696.87260	49.	55.	8	5	4	8	5	3	2.43×10^{-2}	10.	933.15539	100 000
49	2696.92970	−56.	60.	8	5	3	8	5	4	2.41×10^{-2}	6.	933.12334	100 000
80	2697.76480	0.	40.	4	4	0	5	4	1	1.60×10^{-1}	5.	325.52005	001 000
80	2697.81728	0.	11.	4	4	1	5	4	2	3.30×10^{-1}	3.	325.45905	001 000
49	*2698.17300	110.	51.	7	6	2	7	6	1	5.22×10^{-2}	10.	969.90076	100 000
49	2698.66200	28.	30.	8	4	4	8	4	5	2.73×10^{-2}	10.	801.35923	100 000
49	2699.26890	39.	45.	7	5	3	7	5	2	4.82×10^{-2}	10.	809.32469	100 000
49	2699.28290	48.	50.	7	5	2	7	5	3	4.82×10^{-2}	10.	809.31717	100 000
80	2699.39049	−13.	18.	4	2	2	5	2	3	6.15×10^{-1}	4.	228.63443	001 000
49	2699.91210	−43.	30.	7	4	4	7	4	3	5.86×10^{-2}	4.	677.11907	100 000
80	2700.00940	16.	16.	4	3	1	5	3	2	3.92×10^{-1}	4.	265.82632	001 000
49	*2700.26650	6.	25.	6	6	1	6	6	0	1.26×10^{-1}	6.	862.22676	100 000
49	2700.52220	3.	5.	2	1	2	2	1	1	2.27×10^{-1}	2.	65.65913	100 000
49	2700.74530	−17.	20.	6	3	4	6	3	3	1.19×10^{-1}	8.	465.58322	100 000
80	2701.16060	4.	9.	4	3	2	5	3	3	8.03×10^{-1}	4.	264.17832	001 000
49	*2701.34610	0.	40.	6	5	1	6	5	2	1.86×10^{-1}	4.	701.11610	100 000
49	2701.64050	104.	95.	4	1	4	5	1	5	5.62×10^{-2}	10.	224.22314	020 000
49	2701.66140	−81.	10.	4	2	3	4	2	2	2.39×10^{-1}	3.	219.97936	100 000
49	2702.18800	−190.	30.	6	4	3	6	4	2	1.21×10^{-1}	10.	568.08590	100 000
49	2702.35110	12.	15.	6	4	2	6	4	3	1.24×10^{-1}	3.	568.00184	100 000
80	2702.66180	19.	12.	4	1	3	5	1	4	7.85×10^{-1}	3.	204.04163	001 000
80	2702.76315	9.	12.	5	0	5	6	0	6	1.63×10^{0}	3.	230.92104	001 000
80	2703.10910	−16.	12.	5	1	5	6	1	6	7.85×10^{-1}	3.	231.41590	001 000
49	*2703.12670	−2.	50.	5	5	0	5	5	1	3.62×10^{-1}	8.	608.47288	100 000
49	2703.92865	12.	20.	5	3	3	5	3	2	1.98×10^{-1}	3.	370.81452	100 000
49	2704.02180	8.	20.	5	4	2	5	4	1	2.32×10^{-1}	4.	474.90663	100 000
49	2704.05280	4.	35.	5	4	1	5	4	2	2.24×10^{-1}	3.	474.88959	100 000
49	2705.05300	−35.	45.	6	3	3	6	3	4	1.21×10^{-1}	3.	463.36162	100 000
49	2705.39760	−93.	95.	4	1	4	5	0	5	1.91×10^{-2}	10.	220.46407	020 000
49	2705.42090	−4.	15.	5	3	2	5	3	3	1.87×10^{-1}	5.	370.04465	100 000
49	*2705.50080	−230.	16.	4	4	0	4	4	1	8.47×10^{-1}	8.	397.42812	100 000
80	2705.77340	7.	13.	7	1	7	7	1	6	3.59×10^{-2}	15.	362.02100	001 000
49	2705.93138	−5.	7.	3	2	2	3	2	1	3.96×10^{-1}	3.	155.52621	100 000
49	2705.94880	21.	20.	4	3	2	4	3	1	3.65×10^{-1}	3.	292.50621	100 000
49	2706.33044	0.	10.	4	3	1	4	3	2	3.67×10^{-1}	4.	292.30934	100 000
49	2706.39192	23.	50.	1	1	1	1	1	0	4.75×10^{-1}	3.	32.14911	100 000
80	2706.74400	−154.	3.	1	0	1	2	2	0	1.61×10^{-2}	10.	72.75733	001 000
49	2707.24960	−59.	55.	3	1	2	4	1	3	5.42×10^{-2}	10.	181.81809	020 000
49	2707.27450	5.	8.	3	3	1	3	3	0	6.40×10^{-1}	3.	230.23074	100 000

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Table 3 (*continued*)

Mol	Observed position	o−c	un	upper			Lower			Observed strength	%s	Lower level	Band
				J	K_a	K_c	J	K_a	K_c				
49	2707.32962	3.	5.	3	3	0	3	3	1	6.55×10^{-1}	3.	230.20230	100 000
49	2708.12458	−2.	6.	2	2	1	2	2	0	7.14×10^{-1}	2.	107.97933	100 000
49	2708.60000	−220.	30.	8	3	5	8	3	6	2.34×10^{-2}	10.	696.12366	100 000
49	2708.80899	0.	15.	2	2	0	2	2	1	7.19×10^{-1}	2.	107.63049	100 000
49	2709.27310	8.	7.	3	2	1	3	2	2	4.07×10^{-1}	4.	153.82214	100 000
49	2711.71653	3.	5.	1	1	0	1	1	1	4.79×10^{-1}	5.	29.46003	100 000
80	2713.32750	11.	13.	3	3	0	4	3	1	5.44×10^{-1}	2.	203.09998	001 000
80	2713.37758	4.	6.	3	2	1	4	2	2	1.17×10^{0}	2.	162.81900	001 000
80	2713.48368	2.	11.	4	1	4	5	1	5	1.83×10^{0}	4.	168.98230	001 000
80	2713.69020	0.	40.	3	3	1	4	3	2	2.71×10^{-1}	3.	202.66323	001 000
49	2713.80140	6.	45.	2	0	2	3	1	3	2.71×10^{-2}	10.	99.58727	020 000
80	2714.63906	3.	8.	3	1	2	4	1	3	1.60×10^{0}	2.	140.47782	001 000
49	2715.27780	−6.	15.	5	2	3	5	2	4	1.15×10^{-1}	8.	291.24232	100 000
49	2715.44230	−3.	25.	3	1	3	4	1	4	5.22×10^{-2}	4.	155.20843	020 000
49	2716.48370	18.	10.	2	1	1	2	1	2	2.31×10^{-1}	5.	57.59753	100 000
80	2717.26396	0.	11.	3	2	2	4	2	3	6.15×10^{-1}	4.	156.42453	001 000
80	2718.02810	−34.	11.	5	0	5	5	2	4	1.16×10^{-1}	8.	215.65566	001 000
80	2718.12162	−11.	15.	6	1	6	6	1	5	1.02×10^{-1}	4.	278.19630	001 000
49	2720.98120	16.	40.	3	2	1	4	2	2	3.03×10^{-2}	10.	219.97936	020 000
49	2721.46280	10.	25.	3	1	3	4	0	4	2.47×10^{-2}	10.	149.18806	020 000
49	2721.79050	−26.	18.	6	2	4	6	2	5	6.01×10^{-2}	10.	381.91872	100 000
49	2722.52590	−21.	20.	2	1	1	3	1	2	5.17×10^{-2}	10.	115.66512	020 000
49	2722.62270	−47.	45.	2	0	2	3	0	3	6.75×10^{-2}	10.	90.76544	020 000
49	2723.60050	−14.	10.	3	1	2	3	1	3	1.34×10^{-1}	3.	99.58727	100 000
80	2723.92768	83.	80.	3	1	3	4	1	4	9.14×10^{-1}	10.	116.39410	001 000
49	2724.11200	−3.	11.	3	2	2	4	2	3	2.26×10^{-2}	3.	215.10982	020 000
49	2724.42951	−5.	6.	1	0	1	0	0	0	3.47×10^{-1}	3.	0.00000	100 000
49	2725.03720	−34.	40.	5	0	5	5	1	4	1.74×10^{-2}	10.	263.59316	020 000
49	2725.12930	55.	50.	1	0	1	2	1	2	2.07×10^{-2}	10.	57.59753	020 000
80	2727.27352	−2.	7.	2	1	1	3	1	2	7.32×10^{-1}	3.	88.51552	001 000
80	2727.32108	11.	11.	2	2	0	3	2	1	4.12×10^{-1}	3.	110.86638	001 000
80	2728.46080	−96.	10.	3	0	3	3	2	2	7.21×10^{-2}	4.	108.51303	001 000
80	2729.14207	15.	15.	2	2	1	3	2	2	8.32×10^{-1}	5.	108.51303	001 000
49	2729.23680	−53.	60.	4	3	2	5	3	3	1.29×10^{-2}	10.	370.04465	020 000
49	2729.37150	−39.	30.	2	1	2	3	1	3	5.02×10^{-2}	4.	99.58727	020 000
80	2730.04800	−3.	18.	7	2	6	7	2	5	5.47×10^{-2}	10.	399.57682	001 000
80	2730.48400	47.	12.	5	1	5	5	1	4	6.74×10^{-2}	10.	204.04163	001 000
80	2732.17670	−15.	18.	9	3	7	9	3	6	2.36×10^{-2}	10.	656.47974	001 000
80	2732.86796	−1.	4.	2	0	2	3	0	3	8.61×10^{-1}	4.	70.10190	001 000
80	*2732.95320	−4.	87.	8	8	1	8	8	0	1.08×10^{-1}	7.	985.95965	001 000
80	2734.50082	1.	4.	2	1	2	3	1	3	1.49×10^{0}	2.	73.84409	001 000
49	2735.37050	−5.	29.	4	0	4	4	1	3	2.10×10^{-2}	3.	181.81809	020 000
49	2736.72130	4.	5.	2	1	2	1	1	1	4.39×10^{-1}	3.	29.46003	100 000
49	2736.82750	−16.	50.	1	0	1	2	0	2	6.11×10^{-2}	10.	45.89862	020 000
49	2737.17270	42.	50.	6	1	5	6	2	4	1.12×10^{-2}	10.	400.81562	020 000
49	2737.84300	−80.	15.	5	1	4	5	2	3	2.08×10^{-2}	10.	301.74495	020 000
49	2738.19300	−72.	30.	2	1	2	3	0	3	2.01×10^{-2}	10.	90.76544	020 000
49	2738.43760	30.	30.	1	1	0	2	1	1	3.76×10^{-2}	10.	65.65913	020 000
49	2738.95806	−10.	10.	2	0	2	1	0	1	6.21×10^{-1}	4.	15.41866	100 000
80	*2739.31420	130.	114.	10	7	4	10	7	3	4.17×10^{-2}	10.	1097.98730	001 000
80	2740.34168	−1.	3.	1	1	0	2	1	1	9.72×10^{-1}	3.	48.95901	001 000
49	2740.88010	79.	15.	3	0	3	2	1	2	7.34×10^{-3}	10.	57.59753	100 000
80	*2740.93040	61.	91.	9	7	2	9	7	3	9.67×10^{-2}	3.	974.60081	001 000
80	2741.46790	21.	31.	10	6	5	10	6	4	2.16×10^{-2}	10.	990.08647	001 000
80	2741.81600	35.	8.	6	2	5	6	2	4	1.37×10^{-1}	8.	307.81973	001 000
49	2741.93193	−1.	10.	2	1	1	1	1	0	4.33×10^{-1}	3.	32.14911	100 000
80	2741.98840	26.	8.	4	1	4	4	1	3	2.07×10^{-1}	5.	140.47782	001 000
80	*2742.44357	5.	22.	8	7	2	8	7	1	1.79×10^{-1}	10.	863.56648	001 000
49	2742.83920	−8.	10.	3	0	3	3	1	2	3.12×10^{-2}	10.	115.66512	020 000
80	2743.33220	−6.	31.	8	3	6	8	3	5	1.04×10^{-1}	5.	537.99602	001 000
80	2743.65000	0.	56.	9	6	4	9	6	3	3.07×10^{-2}	10.	866.41649	001 000

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Table 3 (*continued*)

Mol	Observed position	o−c	un	upper			Lower			Observed strength	%s	Lower level	Band
				J	K_a	K_c	J	K_a	K_c				
80	2743.70280	55.	54.	9	6	3	9	6	4	5.37×10^{-2}	5.	866.39065	001 000
80	2743.76044	−2.	3.	1	0	1	2	0	2	1.34×10^{0}	2.	35.74241	001 000
80	*2743.84870	0.	52.	7	7	0	7	7	1	3.45×10^{-1}	4.	764.88044	001 000
80	2745.23500	3.	3.	1	1	1	2	1	2	5.14×10^{-1}	3.	41.58223	001 000
80	2745.72280	31.	47.	8	6	3	8	6	2	1.34×10^{-1}	4.	755.26388	001 000
80	2745.74060	0.	41.	8	6	2	8	6	3	7.03×10^{-2}	4.	755.25861	001 000
49	2746.58800	102.	5.	7	2	5	7	1	6	7.64×10^{-3}	10.	470.93816	100 000
80	*2747.75460	−58.	81.	7	6	1	7	6	2	3.45×10^{-1}	7.	656.56890	001 000
49	2750.57680	−37.	50.	1	0	1	1	1	0	2.70×10^{-2}	10.	32.14911	020 000
80	*2751.24430	0.	51.	6	6	1	6	6	0	2.15×10^{-1}	4.	570.29285	001 000
49	2751.79070	0.	40.	0	0	0	1	0	1	2.37×10^{-2}	10.	15.41866	020 000
80	2751.85210	−62.	13.	7	3	5	7	3	4	9.67×10^{-2}	5.	433.08193	001 000
80	2751.90340	30.	39.	9	4	6	9	4	5	3.19×10^{-2}	10.	702.68723	001 000
49	2752.57822	0.	15.	3	0	3	2	0	2	7.83×10^{-1}	3.	45.89862	100 000
49	2753.82723	8.	8.	3	2	2	2	2	1	3.19×10^{-1}	3.	107.63049	100 000
80	2754.47400	−62.	56.	10	5	6	10	5	5	3.92×10^{-2}	10.	899.22503	001 000
80	*2755.03385	−13.	46.	5	5	0	5	5	1	1.42×10^{0}	2.	403.03362	001 000
49	2755.11587	4.	7.	3	2	1	2	2	0	3.33×10^{-1}	3.	107.97933	100 000
80	2755.41738	0.	10.	0	0	0	1	0	1	3.82×10^{-1}	3.	12.08203	001 000
80	*2755.66860	−1.	50.	6	5	2	6	5	1	5.98×10^{-1}	5.	476.95548	001 000
80	2755.68460	0.	51.	6	5	1	6	5	2	2.54×10^{-1}	4.	476.94819	001 000
80	2755.88130	40.	19.	8	4	5	8	4	4	1.56×10^{-1}	3.	587.91550	001 000
80	2756.02870	21.	21.	7	5	3	7	5	2	1.42×10^{-1}	10.	563.38186	001 000
80	2756.07770	−13.	28.	8	5	4	8	5	3	1.53×10^{-1}	4.	662.42885	001 000
80	2756.11660	12.	19.	7	5	2	7	5	3	3.00×10^{-1}	4.	563.33949	001 000
49	2756.33900	207.	30.	4	0	4	3	1	3	1.17×10^{-3}	10.	99.58727	100 000
80	2756.43130	5.	32.	8	5	3	8	5	4	8.49×10^{-2}	6.	662.25534	001 000
80	2756.80350	18.	12.	9	5	4	9	5	5	8.90×10^{-2}	4.	773.71389	001 000
49	2757.09790	12.	10.	6	1	5	6	1	6	2.10×10^{-2}	10.	306.40774	100 000
49	2757.52882	3.	10.	3	1	2	2	1	1	6.55×10^{-1}	4.	65.65913	100 000
80	2757.54888	−7.	9.	6	3	4	6	3	3	3.85×10^{-1}	3.	342.33779	001 000
80	2757.94700	27.	36.	7	4	4	7	4	3	1.48×10^{-1}	3.	487.14938	001 000
80	2758.45836	6.	10.	4	2	3	4	2	2	5.68×10^{-1}	3.	162.81900	001 000
80	2758.87524	8.	13.	6	4	3	6	4	2	5.41×10^{-1}	2.	399.83928	001 000
80	2759.24701	−24.	21.	5	4	2	5	4	1	3.43×10^{-1}	3.	325.52005	001 000
80	2759.51300	72.	10.	6	4	2	6	4	3	2.81×10^{-1}	5.	399.54718	001 000
80	2760.11760	−27.	14.	7	4	3	7	4	4	2.92×10^{-1}	3.	486.14428	001 000
80	2760.75626	−3.	7.	5	3	3	5	3	2	3.30×10^{-1}	3.	265.82632	001 000
49	2761.53630	63.	15.	3	1	3	2	0	2	1.23×10^{-2}	10.	45.89862	100 000
80	2761.75950	−5.	17.	8	4	4	8	4	5	7.15×10^{-2}	10.	585.16534	001 000
80	2762.23910	20.	13.	4	3	2	4	3	1	1.11×10^{0}	3.	203.09998	001 000
80	2762.94778	0.	13.	3	3	0	3	3	1	1.84×10^{0}	4.	153.47959	001 000
80	2763.17220	−13.	16.	4	3	1	4	3	2	5.86×10^{-1}	3.	202.66323	001 000
49	2763.30000	−3.	30.	2	1	2	2	1	1	2.48×10^{-2}	10.	65.65913	020 000
80	2764.25790	9.	9.	5	3	2	5	3	3	6.50×10^{-1}	2.	264.17832	001 000
80	2764.47871	−2.	3.	1	1	1	1	1	0	5.25×10^{-1}	2.	22.33847	001 000
80	2764.89760	−2.	15.	2	2	1	2	2	0	1.70×10^{0}	4.	72.75733	001 000
49	2765.15950	74.	30.	4	0	4	3	0	3	7.83×10^{-1}	4.	90.76544	100 000
80	2765.92618	−10.	11.	2	2	0	2	2	1	9.14×10^{-1}	3.	72.26107	001 000
80	2766.99622	0.	11.	6	3	3	6	3	4	1.91×10^{-1}	4.	337.85651	001 000
80	2767.68346	−5.	6.	3	2	1	3	2	2	1.00×10^{0}	4.	108.51303	001 000
49	2767.81925	−18.	10.	4	2	3	3	2	2	4.53×10^{-1}	3.	153.82214	100 000
49	2768.25290	40.	20.	4	3	2	3	3	1	1.83×10^{-1}	4.	230.20230	100 000
49	2768.40870	−34.	11.	4	3	1	3	3	0	1.81×10^{-1}	2.	230.23074	100 000
49	2768.86820	−19.	25.	1	1	1	1	1	0	4.68×10^{-2}	10.	32.14911	020 000
80	2769.42313	1.	3.	1	1	0	1	1	1	1.07×10^{0}	3.	19.87758	001 000
49	2770.79412	0.	10.	4	2	2	3	2	1	4.21×10^{-1}	2.	155.52621	100 000
49	2771.32000	−201.	5.	4	1	4	3	0	3	1.54×10^{-2}	15.	90.76544	100 000
80	2771.60070	18.	18.	4	2	2	4	2	3	3.07×10^{-1}	10.	156.42453	001 000
80	2772.05290	36.	12.	7	3	4	7	3	5	1.87×10^{-1}	4.	423.41023	001 000
49	2772.49630	0.	40.	4	1	3	3	1	2	6.40×10^{-1}	2.	115.66512	100 000
80	2774.20690	7.	6.	2	1	1	2	1	2	2.67×10^{-1}	3.	41.58223	001 000

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Table 3 (*continued*)

Mol	Observed position	o−c	un	upper			Lower			Observed strength	%s	Lower level	Band
				J	K_a	K_c	J	K_a	K_c				
49	2774.63610	−30.	30.	1	1	0	1	1	1	4.04×10^{-2}	10.	29.46003	020 000
49	2774.70227	5.	15.	5	1	5	4	1	4	6.26×10^{-1}	4.	155.20843	100 000
49	2775.95000	−75.	15.	5	2	4	5	0	5	1.84×10^{-2}	10.	220.46407	100 000
49	2776.83805	−1.	7.	5	0	5	4	0	4	7.00×10^{-1}	2.	149.18806	100 000
80	2777.95900	0.	11.	5	2	3	5	2	4	3.15×10^{-1}	3.	215.65566	001 000
80	2779.50290	3.	3.	1	0	1	0	0	0	7.85×10^{-1}	3.	0.00000	001 000
80	2779.61040	−29.	30.	8	3	5	8	3	6	3.46×10^{-2}	10.	520.46234	001 000
49	2780.72200	−59.	15.	5	1	5	4	0	4	1.72×10^{-2}	10.	149.18806	100 000
80	2781.27270	−6.	6.	3	1	2	3	1	3	3.16×10^{-1}	3.	73.84409	001 000
49	2781.30500	0.	16.	5	2	4	4	2	3	4.41×10^{-1}	2.	215.10982	100 000
49	2781.50030	7.	21.	5	4	2	4	4	1	8.37×10^{-2}	3.	397.42812	100 000
49	2781.51200	−35.	35.	5	4	1	4	4	0	8.37×10^{-2}	3.	397.43000	100 000
49	2782.43370	−1.	20.	5	3	3	4	3	2	2.27×10^{-1}	3.	292.30934	100 000
49	2784.18000	−6.	30.	6	0	6	5	1	5	2.09×10^{-2}	10.	224.22314	100 000
49	2784.74880	−6.	15.	2	2	1	2	2	0	4.62×10^{-2}	10.	107.97933	020 000
49	2785.45290	26.	25.	2	2	0	2	2	1	4.72×10^{-2}	10.	107.63049	020 000
49	2786.46330	1.	15.	6	1	6	5	1	5	5.42×10^{-1}	2.	224.22314	100 000
49	2786.54075	−7.	15.	5	2	3	4	2	2	4.21×10^{-1}	2.	219.97936	100 000
49	2786.68085	2.	5.	5	1	4	4	1	3	5.71×10^{-1}	3.	181.81809	100 000
49	2787.13780	−46.	40.	3	2	1	3	2	2	2.45×10^{-2}	10.	153.82214	020 000
49	2787.93945	32.	30.	6	0	6	5	0	5	6.55×10^{-1}	15.	220.46407	100 000
49	2788.18010	55.	10.	7	2	6	7	0	7	1.40×10^{-2}	10.	400.36340	100 000
80	2788.46730	−2.	3.	2	1	2	1	1	1	1.01×10^{0}	4.	19.87758	001 000
80	2789.37200	14.	22.	9	3	6	9	3	7	4.23×10^{-2}	10.	628.58834	001 000
80	2790.30890	−24.	11.	4	1	3	4	1	4	1.04×10^{-1}	6.	116.39410	001 000
49	2790.80200	−13.	40.	4	2	2	4	2	3	1.64×10^{-2}	10.	215.10982	020 000
80	2790.88786	2.	3.	2	0	2	1	0	1	6.91×10^{-1}	2.	12.08203	001 000
49	2792.29270	9.	20.	2	1	1	2	0	2	3.18×10^{-2}	10.	45.89862	020 000
80	2793.45063	4.	6.	2	1	1	1	1	0	5.00×10^{-1}	4.	22.33847	001 000
49	*2793.98970	268.	100.	6	5	2	5	5	1	5.37×10^{-2}	4.	608.47288	100 000
49	2794.24706	−4.	6.	6	2	5	5	2	4	3.59×10^{-1}	4.	291.24232	100 000
49	2795.38610	−11.	30.	6	4	3	5	4	2	9.26×10^{-2}	3.	474.88959	100 000
49	2795.44610	−9.	16.	6	4	2	5	4	1	1.19×10^{-1}	3.	474.90663	100 000
49	2796.54610	−10.	15.	7	0	7	6	1	6	1.76×10^{-2}	10.	306.40774	100 000
80	2796.92320	−8.	25.	7	2	5	7	2	6	9.61×10^{-2}	3.	366.55031	001 000
49	2797.82156	0.	15.	7	1	7	6	1	6	4.14×10^{-1}	2.	306.40774	100 000
49	2798.30340	56.	55.	3	1	2	3	0	3	3.45×10^{-2}	10.	90.76544	020 000
49	2799.49940	27.	30.	2	1	2	1	1	1	4.59×10^{-2}	10.	29.46003	020 000
49	2799.91233	−3.	10.	6	1	5	5	1	4	4.50×10^{-1}	2.	263.59316	100 000
80	2800.67770	−22.	19.	5	1	4	5	1	5	1.35×10^{-1}	10.	168.98230	001 000
49	2801.01770	20.	25.	1	1	1	0	0	0	2.10×10^{-2}	10.	0.00000	020 000
80	2801.23238	0.	10.	3	0	3	2	0	2	1.77×10^{0}	4.	35.74241	001 000
80	2801.91220	−34.	15.	2	2	1	2	0	2	2.59×10^{-2}	10.	35.74241	001 000
49	2801.96470	17.	18.	6	2	4	5	2	3	3.55×10^{-1}	5.	301.74495	100 000
80	2803.43924	3.	5.	3	2	1	2	2	0	8.20×10^{-1}	2.	72.75733	001 000
49	*2805.84590	0.	52.	7	6	2	6	6	1	1.71×10^{-2}	10.	862.22676	100 000
49	2805.97650	5.	10.	4	2	3	3	1	2	1.05×10^{-2}	10.	115.66512	100 000
49	2806.04300	88.	20.	2	1	1	1	1	0	4.32×10^{-2}	10.	32.14911	020 000
80	2806.15789	5.	5.	3	1	2	2	1	1	1.48×10^{0}	2.	48.95901	001 000
49	2806.52180	0.	40.	3	3	1	3	3	0	3.16×10^{-2}	4.	230.23074	020 000
49	2806.57490	−70.	90.	3	3	0	3	3	1	2.94×10^{-2}	10.	230.20230	020 000
49	2806.62420	−3.	10.	7	2	6	6	2	5	2.65×10^{-1}	4.	381.91872	100 000
49	2806.74200	7.	40.	5	3	3	5	3	2	1.22×10^{-2}	10.	370.81452	020 000
49	2806.77560	−17.	60.	4	3	2	4	3	1	1.44×10^{-2}	10.	292.50621	020 000
80	2806.96930	8.	10.	4	2	3	4	0	4	8.73×10^{-2}	3.	114.30808	001 000
49	2807.15010	−76.	90.	4	3	1	4	3	2	1.31×10^{-2}	10.	292.30934	020 000
49	2807.18740	−44.	60.	4	1	3	4	0	4	2.63×10^{-2}	10.	149.18806	020 000
49	*2807.47830	120.	45.	7	5	3	6	5	2	6.75×10^{-2}	6.	701.11610	100 000
49	2808.20900	64.	15.	5	3	2	5	3	3	9.90×10^{-3}	10.	370.04465	020 000
80	2808.28090	−54.	12.	8	2	6	8	2	7	3.10×10^{-2}	10.	457.49081	001 000
80	2808.62183	−4.	6.	4	1	4	3	1	3	1.84×10^{0}	4.	73.84409	001 000

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Table 3 (*continued*)

Mol	Observed position	o−c	un	upper			Lower			Observed strength	%s	Lower level	Band
				J	K_a	K_c	J	K_a	K_c				
49	2808.82175	4.	10.	8	1	8	7	1	7	2.76×10^{-1}	4.	401.57391	100 000
49	2809.03020	44.	30.	7	4	4	6	4	3	9.46×10^{-2}	15.	568.00184	100 000
49	2809.22225	0.	15.	7	4	3	6	4	2	8.13×10^{-2}	3.	568.08590	100 000
49	2809.34489	4.	10.	8	0	8	7	0	7	2.94×10^{-1}	3.	400.36340	100 000
49	2809.72750	−11.	15.	7	3	5	6	3	4	1.70×10^{-1}	2.	463.36162	100 000
49	2810.03220	−2.	10.	8	1	8	7	0	7	2.04×10^{-2}	10.	400.36340	100 000
80	2810.56587	0.	10.	4	0	4	3	0	3	9.84×10^{-1}	2.	70.10190	001 000
80	2811.85927	−2.	13.	4	3	2	3	3	1	5.70×10^{-1}	2.	153.47959	001 000
49	2812.05835	−5.	9.	7	1	6	6	1	5	3.13×10^{-1}	3.	360.26410	100 000
80	2812.12630	24.	14.	5	2	4	5	0	5	4.82×10^{-2}	10.	167.93260	001 000
80	2812.29150	−4.	18.	4	3	1	3	3	0	2.90×10^{-1}	2.	153.54402	001 000
49	2812.42766	0.	15.	7	3	4	6	3	3	1.64×10^{-1}	3.	465.58322	100 000
49	2812.60580	2.	10.	3	0	3	2	0	2	8.82×10^{-2}	3.	45.89862	020 000
80	2812.76419	−8.	9.	4	2	3	3	2	2	1.25×10^{0}	4.	108.51303	001 000
49	2813.05290	−33.	25.	3	1	3	2	1	2	7.24×10^{-2}	3.	57.59753	020 000
49	2813.54060	10.	30.	2	1	2	1	0	1	2.62×10^{-2}	10.	15.41866	020 000
49	2816.70951	−1.	7.	7	2	5	6	2	4	2.51×10^{-1}	2.	400.81562	100 000
80	2817.15879	12.	18.	4	2	2	3	2	1	6.03×10^{-1}	2.	110.86638	001 000
49	2817.60150	13.	29.	4	0	4	3	1	3	2.53×10^{-2}	3.	99.58727	020 000
80	2818.13106	0.	11.	5	1	5	4	1	4	9.43×10^{-1}	2.	116.39410	001 000
80	2818.18772	0.	10.	4	1	3	3	1	2	8.38×10^{-1}	3.	88.51552	001 000
80	2818.71520	86.	9.	6	2	5	6	0	6	7.38×10^{-2}	10.	230.92104	001 000
49	*2818.90880	−39.	52.	8	6	3	7	6	2	1.50×10^{-2}	10.	969.90068	100 000
49	2819.14090	−14.	15.	9	0	9	8	1	8	9.66×10^{-3}	10.	509.57563	100 000
80	2819.37593	−9.	11.	5	0	5	4	0	4	1.86×10^{0}	4.	114.30808	001 000
49	2819.50130	11.	20.	9	1	9	8	1	8	1.80×10^{-1}	3.	509.57563	100 000
80	2819.74200	−84.	13.	9	2	7	9	2	8	3.29×10^{-2}	6.	558.37501	001 000
49	2819.78672	−3.	16.	9	0	9	8	0	8	1.83×10^{-1}	3.	508.92992	100 000
49	2820.14700	10.	20.	9	1	9	8	0	8	1.27×10^{-2}	10.	508.92992	100 000
49	2820.70970	−63.	55.	8	5	4	7	5	3	2.99×10^{-2}	10.	809.31717	100 000
49	2820.72940	49.	60.	8	5	3	7	5	2	2.67×10^{-2}	10.	809.32469	100 000
80	2820.89298	15.	21.	5	4	2	4	4	1	1.63×10^{-1}	3.	263.87447	001 000
80	2820.95920	−4.	8.	5	4	1	4	4	0	3.23×10^{-1}	2.	263.88147	001 000
49	2821.89900	274.	6.	6	2	5	5	1	4	1.56×10^{-2}	10.	263.59316	100 000
80	2821.98940	−57.	9.	7	1	6	7	1	7	6.85×10^{-2}	6.	303.56489	001 000
49	2822.39900	−5.	15.	8	4	5	7	4	4	6.01×10^{-2}	10.	676.81781	100 000
49	2822.69020	31.	30.	8	3	6	7	3	5	1.00×10^{-1}	10.	572.12826	100 000
49	2822.90300	112.	30.	8	4	4	7	4	3	6.40×10^{-2}	10.	677.11907	100 000
49	2823.12566	22.	30.	8	1	7	7	1	6	2.08×10^{-1}	4.	470.93816	100 000
49	2823.40920	5.	55.	3	1	2	2	1	1	5.81×10^{-2}	5.	65.65913	020 000
80	2823.63401	−12.	13.	5	2	4	4	2	3	6.56×10^{-1}	3.	156.42453	001 000
80	2823.91941	3.	7.	5	3	3	4	3	2	3.99×10^{-1}	2.	202.66323	001 000
49	2824.09470	84.	40.	4	2	2	4	1	3	2.40×10^{-2}	10.	181.81809	020 000
49	2824.75240	26.	25.	3	1	3	2	0	2	3.32×10^{-2}	10.	45.89862	020 000
49	2825.29600	72.	40.	3	2	1	3	1	2	2.24×10^{-2}	10.	115.66512	020 000
80	2825.33606	−9.	13.	5	3	2	4	3	1	7.79×10^{-1}	2.	203.09998	001 000
49	2826.27600	67.	95.	4	1	4	3	1	3	8.52×10^{-2}	10.	99.58727	020 000
80	2826.31300	−66.	32.	8	3	6	8	1	7	3.45×10^{-2}	7.	455.01462	001 000
49	2826.73280	−26.	10.	4	2	2	3	1	3	5.27×10^{-3}	10.	99.58727	100 000
80	2827.33583	10.	15.	6	1	6	5	1	5	1.77×10^{0}	3.	168.98230	001 000
49	2827.37830	26.	30.	8	3	5	7	3	4	1.14×10^{-1}	3.	577.34782	100 000
80	2828.15288	18.	17.	6	0	6	5	0	5	3.44×10^{-1}	5.	167.93260	001 000
49	2828.27870	−15.	10.	7	2	6	6	1	5	1.72×10^{-2}	10.	360.26410	100 000
80	2829.18225	−15.	17.	5	1	4	4	1	3	1.59×10^{0}	3.	140.47782	001 000
80	*2829.59290	243.	50.	6	5	2	5	5	1	2.02×10^{-1}	10.	403.03362	001 000
49	2829.70130	28.	30.	9	2	8	8	2	7	1.21×10^{-1}	15.	605.55011	100 000
49	2829.89050	3.	16.	10	1	10	9	1	9	1.08×10^{-1}	10.	630.30546	100 000
49	2830.04031	0.	14.	10	0	10	9	0	9	1.02×10^{-1}	4.	629.96981	100 000
49	2830.55470	0.	15.	8	2	6	7	2	5	1.52×10^{-1}	4.	516.79908	100 000
80	2830.58210	−32.	34.	10	2	8	10	2	9	1.05×10^{-2}	10.	669.00900	001 000
80	2830.79570	4.	11.	5	2	3	4	2	2	1.25×10^{0}	4.	162.81900	001 000
49	2831.59140	4.	10.	3	2	2	2	2	1	2.45×10^{-2}	10.	107.63049	020 000

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Table 3 (*continued*)

Mol	Observed position	o−c	un	upper			Lower			Observed strength	%s	Lower level	Band
				J	K_a	K_c	J	K_a	K_c				
80	2833.25510	−29.	11.	6	4	3	5	4	2	4.22×10^{-1}	7.	325.45905	001 000
49	2833.42130	−97.	40.	5	0	5	4	1	4	2.81×10^{-2}	10.	155.20843	020 000
80	2833.53930	−11.	8.	6	4	2	5	4	1	2.15×10^{-1}	3.	325.52005	001 000
49	2833.68000	−69.	70.	9	5	5	8	5	4	2.19×10^{-2}	10.	933.12334	100 000
49	2833.74720	−50.	50.	9	5	4	8	5	3	1.79×10^{-2}	10.	933.15539	100 000
80	2833.97970	−2.	8.	6	2	5	5	2	4	1.22×10^{0}	2.	215.65566	001 000
80	*2834.03180	57.	80.	7	6	1	6	6	0	1.12×10^{-1}	5.	570.29285	001 000
49	2834.30200	261.	30.	8	2	7	7	1	6	1.11×10^{-2}	15.	470.93816	100 000
80	2834.47878	1.	10.	8	2	7	8	0	8	3.59×10^{-2}	5.	385.25087	001 000
49	*2834.85720-398.		50.	4	4	0	4	4	1	3.00×10^{-2}	10.	397.42812	020 000
49	2835.10710	−21.	25.	9	3	7	8	3	6	7.44×10^{-2}	10.	696.12366	100 000
49	2835.44770	−15.	15.	9	4	6	8	4	5	2.99×10^{-2}	10.	801.35923	100 000
49	2835.55490	1.	10.	4	2	2	3	0	3	1.14×10^{-2}	10.	90.76544	100 000
80	2835.70844	2.	8.	6	3	4	5	3	3	8.03×10^{-1}	2.	264.17832	001 000
80	2836.37050	34.	21.	7	0	7	6	0	6	1.51×10^{0}	5.	230.92104	001 000
80	2836.37840	−3.	8.	7	1	7	6	1	6	7.56×10^{-1}	5.	231.41590	001 000
49	2836.57120	−56.	50.	9	4	5	8	4	4	3.32×10^{-2}	10.	802.23311	100 000
80	2838.85930	2.	9.	6	1	5	5	1	4	6.74×10^{-1}	3.	204.04163	001 000
80	2839.02720	79.	9.	6	3	3	5	3	2	3.97×10^{-1}	7.	265.82632	001 000
49	2839.13310	0.	15.	5	1	5	4	1	4	8.18×10^{-2}	4.	155.20843	020 000
49	2839.44270	6.	40.	5	0	5	4	0	4	8.87×10^{-2}	8.	149.18806	020 000
49	2840.00570	0.	21.	11	1	11	10	1	10	6.90×10^{-2}	10.	763.68545	100 000
49	2840.08190	0.	15.	11	0	11	10	0	10	6.01×10^{-2}	10.	763.51422	100 000
49	2840.71130	52.	60.	4	1	3	3	1	2	6.55×10^{-2}	7.	115.66512	020 000
80	*2841.12950	−6.	18.	8	7	2	7	7	1	4.16×10^{-2}	3.	764.88044	001 000
80	2841.30070	108.	15.	9	1	8	9	1	9	2.72×10^{-2}	10.	476.72338	001 000
49	2842.19450	21.	25.	9	3	6	8	3	5	6.45×10^{-2}	10.	706.59878	100 000
80	2842.46220	4.	22.	7	5	3	6	5	2	8.38×10^{-2}	10.	476.94819	001 000
80	2842.50020	−29.	18.	7	5	2	6	5	1	1.70×10^{-1}	8.	476.95548	001 000
49	2842.92850	−9.	20.	4	3	2	3	2	1	1.78×10^{-2}	10.	155.52621	100 000
80	2843.34340	−59.	22.	9	2	8	9	0	9	7.97×10^{-3}	10.	476.68047	001 000
49	2843.36500	−24.	30.	9	2	7	8	2	6	9.56×10^{-2}	10.	649.04988	100 000
80	2843.75560	−15.	11.	6	2	4	5	2	3	5.92×10^{-1}	4.	228.63443	001 000
80	2843.79980	−13.	17.	7	2	6	6	2	5	5.11×10^{-1}	2.	285.82492	001 000
80	*2844.41850	103.	46.	8	6	3	7	6	2	1.15×10^{-1}	6.	656.56890	001 000
80	2844.67970	1.	7.	8	1	8	7	1	7	1.17×10^{0}	2.	303.56489	001 000
49	2844.81860	96.	10.	4	3	1	3	2	2	1.64×10^{-2}	10.	153.82214	100 000
80	2845.01225	0.	16.	8	0	8	7	0	7	6.44×10^{-1}	5.	303.34082	001 000
80	2845.54862	−31.	36.	7	4	4	6	4	3	2.43×10^{-1}	3.	399.54718	001 000
80	*2846.39100	32.	170.	9	8	1	8	8	0	1.44×10^{-2}	15.	985.95965	001 000
80	2846.42284	−3.	13.	7	4	3	6	4	2	4.16×10^{-1}	3.	399.83928	001 000
49	2846.93700	−44.	41.	10	3	8	9	3	7	4.03×10^{-2}	10.	835.04802	100 000
80	2847.07818	4.	13.	7	3	5	6	3	4	3.97×10^{-1}	3.	337.85651	001 000
80	2847.35855	−1.	11.	7	1	6	6	1	5	1.11×10^{0}	3.	278.19630	001 000
49	2849.46630	0.	50.	10	4	7	9	4	6	2.35×10^{-2}	10.	941.59433	100 000
49	2849.85920	0.	50.	12	1	12	11	1	11	3.09×10^{-2}	10.	909.65540	100 000
49	2849.89720	0.	50.	12	0	12	11	0	11	3.39×10^{-2}	10.	909.56935	100 000
49	2850.31460	0.	50.	10	4	6	9	4	5	2.36×10^{-2}	10.	943.75946	100 000
49	2850.38550	−24.	40.	4	2	2	3	2	1	3.21×10^{-2}	5.	155.52621	020 000
49	2850.76640	0.	40.	11	2	10	10	2	9	3.00×10^{-2}	3.	883.31085	100 000
49	2851.62120	0.	40.	6	1	6	5	1	5	7.64×10^{-2}	3.	224.22314	020 000
49	2851.85920	−53.	50.	6	0	6	5	0	5	7.44×10^{-2}	6.	220.46407	020 000
80	*2851.96350	−62.	92.	9	7	2	8	7	1	4.60×10^{-2}	10.	863.56648	001 000
49	2852.39320	0.	50.	11	1	10	10	1	9	3.49×10^{-2}	10.	879.09953	100 000
80	2853.12493	−5.	12.	7	3	4	6	3	3	7.09×10^{-1}	2.	342.33779	001 000
80	2853.17933	0.	6.	8	2	7	7	2	6	8.03×10^{-1}	3.	366.55031	001 000
80	2853.44300	4.	16.	9	1	9	8	1	8	4.18×10^{-1}	8.	385.35004	001 000
80	2853.53754	−9.	14.	9	0	9	8	0	8	8.96×10^{-1}	2.	385.25087	001 000
49	2854.76330	−39.	20.	5	3	3	4	2	2	1.14×10^{-2}	10.	219.97936	100 000
80	2854.80700	−88.	51.	9	6	4	8	6	3	2.88×10^{-2}	10.	755.25861	001 000
80	2854.82870	−32.	50.	9	6	3	8	6	2	5.77×10^{-2}	10.	755.26388	001 000

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Table 3 (*continued*)

Mol	Observed position	o−c	un	upper			Lower			Observed strength	%s	Lower level	Band
				J	K_a	K_c	J	K_a	K_c				
49	2855.04020	4.	16.	10	2	8	9	2	7	4.11×10^{-2}	10.	796.74988	100 000
80	2855.16700	−19.	28.	8	5	4	7	5	3	1.51×10^{-1}	6.	563.33949	001 000
80	2855.24420	−4.	14.	8	1	7	7	1	6	4.35×10^{-1}	4.	362.02100	001 000
80	2855.30500	27.	31.	8	5	3	7	5	2	7.44×10^{-2}	3.	563.38186	001 000
49	2855.38000	−27.	40.	6	1	6	5	0	5	3.06×10^{-2}	10.	220.46407	020 000
80	2855.65364	−22.	25.	7	2	5	6	2	4	9.20×10^{-1}	2.	307.81973	001 000
49	2856.48980	−11.	31.	10	3	7	9	3	6	3.57×10^{-2}	2.	853.54659	100 000
49	2857.33310	98.	15.	5	2	3	4	0	4	1.43×10^{-2}	10.	149.18806	100 000
80	2857.65220	8.	14.	8	4	5	7	4	4	3.19×10^{-1}	4.	486.14428	001 000
49	2857.77060	−6.	15.	5	1	4	4	1	3	5.22×10^{-2}	3.	181.81809	020 000
80	2857.91845	40.	31.	8	3	6	7	3	5	5.60×10^{-1}	4.	423.41023	001 000
80	2859.77550	−1.	18.	8	4	4	7	4	3	1.60×10^{-1}	3.	487.14938	001 000
49	2860.57900	−8.	15.	2	2	1	1	1	0	2.40×10^{-2}	4.	32.14911	020 000
49	2861.68450	−43.	60.	7	0	7	6	1	6	2.13×10^{-2}	4.	306.40774	020 000
80	2862.53365	0.	13.	9	2	8	8	2	7	2.71×10^{-1}	2.	457.49081	001 000
80	*2862.70030	91.	101.	10	7	4	9	7	3	4.04×10^{-2}	10.	974.60081	001 000
80	2863.00841	3.	16.	9	1	8	8	1	7	5.77×10^{-1}	2.	455.01462	001 000
49	2863.62290	−20.	25.	2	2	0	1	1	1	2.33×10^{-2}	10.	29.46003	020 000
49	2863.75000	−26.	40.	7	1	7	6	1	6	5.81×10^{-2}	10.	306.40774	020 000
49	2863.87360	43.	60.	7	0	7	6	0	6	6.06×10^{-2}	3.	304.21950	020 000
80	2865.16330	−21.	39.	10	6	5	9	6	4	3.91×10^{-2}	10.	866.39065	001 000
80	2865.22900	0.	301.	10	6	4	9	6	3	2.17×10^{-2}	10.	866.41649	001 000
49	2865.93900	50.	40.	7	1	7	6	0	6	2.11×10^{-2}	10.	304.21950	020 000
80	2866.19545	2.	13.	8	2	6	7	2	5	3.32×10^{-1}	4.	399.57682	001 000
80	2866.99130	20.	30.	8	3	5	7	3	4	2.59×10^{-1}	2.	433.08193	001 000
80	2867.68910	−34.	51.	9	5	5	8	5	4	6.03×10^{-2}	6.	662.25534	001 000
80	2868.08836	0.	12.	9	5	4	8	5	3	1.25×10^{-1}	5.	662.42885	001 000
80	2868.19420	−5.	18.	9	3	7	8	3	6	1.90×10^{-1}	2.	520.46234	001 000
49	2868.46570	0.	50.	5	2	3	4	2	2	3.40×10^{-2}	10.	219.97936	020 000
80	2869.42510	11.	38.	9	4	6	8	4	5	1.29×10^{-1}	5.	585.16534	001 000
80	2870.25790	0.	41.	11	1	11	10	1	10	2.08×10^{-1}	4.	577.65466	001 000
80	2870.27390	7.	41.	11	0	11	10	0	10	4.08×10^{-1}	3.	577.63607	001 000
80	2870.83300	−79.	50.	10	1	9	9	1	8	2.00×10^{-1}	10.	557.09837	001 000
49	2872.69910	29.	25.	4	4	1	3	3	0	2.38×10^{-2}	15.	230.23074	100 000
49	2872.72880	−12.	15.	4	4	0	3	3	1	1.64×10^{-2}	15.	230.20230	100 000
49	2873.56400	128.	10.	3	2	2	2	1	1	2.30×10^{-2}	10.	65.65913	020 000
49	2874.36770	11.	50.	8	0	8	7	1	7	1.66×10^{-2}	10.	401.57391	020 000
80	2875.21500	−9.	15.	9	2	7	8	2	6	4.43×10^{-1}	4.	502.90276	001 000
49	2875.53800	0.	40.	8	1	8	7	1	7	4.61×10^{-2}	5.	401.57391	020 000
49	2875.57840	30.	50.	8	0	8	7	0	7	4.98×10^{-2}	10.	400.36340	020 000
49	2876.74900	49.	40.	8	1	8	7	0	7	1.86×10^{-2}	10.	400.36340	020 000
49	2877.52380	17.	25.	6	2	5	5	2	4	2.24×10^{-2}	10.	291.24232	020 000
80	2878.01031	26.	27.	10	3	8	9	3	7	2.78×10^{-1}	5.	628.58834	001 000
80	2878.13130	0.	43.	11	2	10	10	2	9	1.28×10^{-1}	4.	669.00900	001 000
80	*2878.46650	208.	200.	12	1	12	11	1	11	3.97×10^{-1}	4.	688.12078	001 000
80	2878.70600	−10.	16.	11	1	10	10	1	9	2.53×10^{-1}	3.	668.37537	001 000
80	2879.96420	2.	22.	9	3	6	8	3	5	3.64×10^{-1}	2.	537.99602	001 000
80	2879.98590	14.	55.	10	5	6	9	5	5	8.32×10^{-2}	5.	773.71389	001 000
80	2880.74760	−12.	16.	10	4	7	9	4	6	1.83×10^{-1}	6.	696.41192	001 000
80	2880.96700	0.	41.	10	5	5	9	5	4	4.01×10^{-2}	5.	774.27966	001 000
49	2881.25300	131.	90.	3	3	0	3	2	1	7.88×10^{-3}	10.	155.52621	020 000
49	2883.36300	13.	40.	3	2	1	2	1	2	1.60×10^{-2}	10.	57.59753	020 000
49	2885.74680	0.	16.	5	3	2	4	3	1	1.44×10^{-2}	10.	292.50621	020 000
80	2886.30510	45.	65.	12	2	11	11	2	10	1.53×10^{-1}	4.	789.26455	001 000
49	2886.35580	0.	50.	9	0	9	8	1	8	1.12×10^{-2}	10.	509.57563	020 000
49	2886.42100	−114.	20.	5	4	2	4	3	1	1.37×10^{-2}	10.	292.50621	100 000
80	*2886.54830	−65.	91.	13	0	13	12	0	12	2.72×10^{-1}	4.	808.09872	001 000
80	2886.56810	−7.	14.	12	1	11	11	1	10	6.21×10^{-2}	10.	788.95826	001 000
49	2886.63200	−101.	35.	5	4	1	4	3	2	1.50×10^{-2}	10.	292.30934	100 000
49	2887.65130	0.	50.	9	1	9	8	0	8	1.03×10^{-2}	10.	508.92992	020 000
80	2887.83100	−29.	51.	10	4	6	9	4	5	7.85×10^{-2}	8.	702.68723	001 000
80	2888.07580	−10.	19.	11	3	9	10	3	8	6.68×10^{-2}	5.	747.36548	001 000

(*continued on next page*)

Table 3 (*continued*)

Mol	Observed position	o−c	un	upper			Lower			Observed strength	%s	Lower level	Band
				J	K_a	K_c	J	K_a	K_c				
80	2889.86010	−29.	40.	11	2	9	10	2	8	1.62×10^{-1}	10.	739.93258	001 000
49	2890.40400	−40.	50.	7	1	6	6	1	5	3.16×10^{-2}	10.	360.26410	020 000
80	2891.57700	0.	51.	11	4	8	10	4	7	4.85×10^{-2}	4.	819.57571	001 000
80	2891.60690	−18.	21.	10	3	7	9	3	6	1.14×10^{-1}	8.	656.47974	001 000
49	2892.36430	0.	40.	7	2	6	6	2	5	2.74×10^{-2}	5.	381.91872	020 000
80	2894.08950	38.	56.	11	5	6	10	5	5	5.78×10^{-2}	10.	899.22503	001 000
80	2894.24548	0.	23.	13	2	12	12	2	11	4.47×10^{-2}	10.	919.06167	001 000
80	2894.37000	0.	51.	13	1	12	12	1	11	8.73×10^{-2}	3.	918.91488	001 000
80	*2894.50380	0.	64.	14	1	14	13	1	13	1.36×10^{-1}	3.	937.57915	001 000
49	2896.09160	−56.	15.	7	3	4	6	2	5	1.00×10^{-2}	10.	381.91872	100 000
80	2896.65330	−18.	28.	12	2	10	11	2	9	4.52×10^{-2}	5.	872.08564	001 000
49	2900.30810	−7.	15.	6	4	2	5	3	3	1.07×10^{-2}	10.	370.04465	100 000
80	2900.76870	0.	52.	14	2	13	13	2	12	4.54×10^{-2}	7.	1058.34695	001 000
80	2901.50880	0.	51.	12	4	9	11	4	8	6.68×10^{-2}	10.	954.26336	001 000
80	2901.64770	−7.	25.	11	3	8	10	3	7	1.15×10^{-1}	10.	787.59493	001 000
80	2903.56260	40.	60.	13	2	11	12	2	10	4.73×10^{-2}	4.	1013.02206	001 000
49	2905.17300	21.	25.	6	2	5	5	1	4	1.56×10^{-2}	15.	263.59316	020 000
49	2905.46440	0.	50.	7	2	5	6	2	4	2.04×10^{-2}	10.	400.81562	020 000
49	2905.70630	21.	25.	8	1	7	7	1	6	1.69×10^{-2}	10.	470.93816	020 000
49	2906.91510	17.	20.	8	2	7	7	2	6	1.67×10^{-2}	10.	486.80402	020 000
80	2909.68430	0.	36.	12	3	9	11	3	8	2.59×10^{-2}	10.	930.22520	001 000
49	2911.44830	−8.	30.	7	4	4	6	3	3	6.26×10^{-3}	10.	465.58322	100 000
80	2913.35800	−64.	91.	12	4	8	11	4	7	2.55×10^{-2}	10.	975.27963	001 000
49	2913.94700	47.	15.	7	4	3	6	3	4	1.00×10^{-2}	10.	463.36162	100 000
49	*2914.17119	−29.	50.	5	5	0	4	4	1	1.98×10^{-2}	10.	397.42812	100 000
80	2917.26700	53.	14.	7	3	4	6	1	5	4.09×10^{-2}	10.	278.19630	001 000
49	2917.77300	20.	40.	7	3	5	6	3	4	1.45×10^{-2}	10.	463.36162	020 000
49	2920.34100	44.	40.	7	3	4	6	3	3	9.66×10^{-3}	10.	465.58322	020 000
49	2920.35500	0.	300.	9	1	8	8	1	7	1.41×10^{-2}	10.	594.70708	020 000
49	2921.23400	0.	300.	9	2	8	8	2	7	1.45×10^{-2}	10.	605.55011	020 000
49	2921.86920	16.	16.	8	4	5	7	3	4	8.47×10^{-3}	10.	577.34782	100 000
49	2928.77200	−121.	40.	3	3	1	2	2	0	2.45×10^{-2}	10.	107.97933	020 000
49	2929.14810	69.	90.	3	3	0	2	2	1	2.68×10^{-2}	10.	107.63049	020 000
49	2943.75640	63.	60.	4	3	2	3	2	1	2.14×10^{-2}	10.	155.52621	020 000
49	2957.57700	−9.	40.	5	3	3	4	2	2	1.59×10^{-2}	10.	219.97936	020 000
49	2963.14320	1.	16.	5	3	2	4	2	3	1.39×10^{-2}	10.	215.10982	020 000
49	2969.80830	0.	50.	6	3	4	5	2	3	1.06×10^{-2}	10.	301.74495	020 000
49	3002.05350	0.	50.	4	4	1	3	3	0	1.87×10^{-2}	10.	230.23074	020 000
49	3002.08700	0.	50.	4	4	0	3	3	1	1.83×10^{-2}	10.	230.20230	020 000
49	3017.96220	0.	50.	5	4	2	4	3	1	1.26×10^{-2}	10.	292.50621	020 000

mol is the molecule with the notation: 80 = $D_2^{18}O$ and 49 = $HD^{1*}O$. o−c is the observed minus the computed position in $cm^{-1} \times 10^5$. un is the estimated uncertainty in the computed line position in $cm^{-1} \times 10^5$. *%s* is the estimated uncertainty in the observed strength in percent. an asterisk, *, denotes a doubled absorption with the rotational quantum assignment given for the stronger transition ($D_2^{18}O$) and the value of the strength given is the sum of the strengths of the two comparable transitions. Strengths are normalized to 100% of the isotopic species. lower levels (cm^{-1}) are ground state levels of $D_2^{18}O$ and $HD^{18}O$ given in refs. 8 and 7, respectively.

5. Discussion

Several of the features in the O-18 enriched spectra were not assigned of which the majority had observed peak height absorptions of 10% or less. Transitions not assigned and have observable absorptions in the present spectra belong to the following bands and molecules: (100)-(000) and (110)-(000) bands of $D_2^{18}O$ and the (011)-(010) band of $HD^{18}O$. Other unassigned transitions that may appear in these spectra are of the (030)-(000) band of $D_2^{18}O$, the (001)-(000) bands of $HD^{17}O$ and $D_2^{17}O$ and the (100)-(000) band of $HD^{17}O$. Two very weak, unassigned lines appear in Fig. 1 and one in Fig. 4 and others may be present and dominated by the assigned absorptions in all the figures. The optical densities of the present spectra were not large enough to do an adequate analysis of the unassigned features.

Several lines in the (100)-(000) and (001)-(000) bands of $HD^{18}O$ have enough transition intensity to be included in the HITRAN [15] listing. In fact 73 transitions of the (100)-(000) band and 148 of the (001)-(000) band have strengths of at least 10^{-7} cm^{-2}/atm at 296 K or greater for un-normalized samples (normal H_2O). These transitions have been included in a listing of water vapor parameters by this author. This compilation covers the 500–8000 cm^{-1} region and is available on the website, http://mark4sun.jpl.nasa.gov, given under 'science data'.

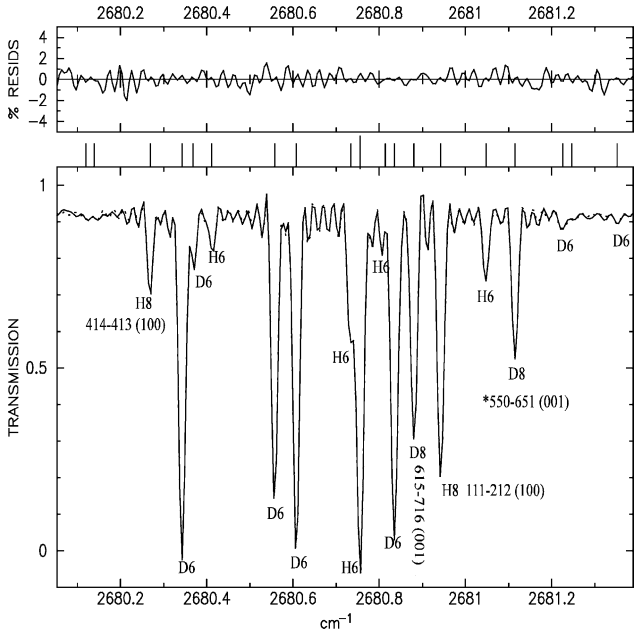

Fig. 1. Short scan spectra of oxygen enriched O-18 deuterated water vapor. The observed spectrum is overlaid with a synthetic spectrum, which is the result from a non-linear-least squares fit of the observed features. The upper portion of the figure is a residual plot showing the percent differences between the observed and computed spectra. The sample pressure was 1.48 Torr and the absorption path length was 2.39 m. The absorption features are labeled in terms of the isotopic species as follows: H6 = $HD^{16}O$, H8 = $HD^{18}O$, D6 = $D_2^{16}O$, and D8 = $D_2^{18}O$. The O-18 species also show the quantum assignments (QA) for the rotational transitions followed, in parenthesis, with the upper vibrational state of the band connecting to the ground state. One feature has an asterisk in front of the QA and this denotes that the feature is composed of two comparable transitions with the QA of the stronger transition shown.

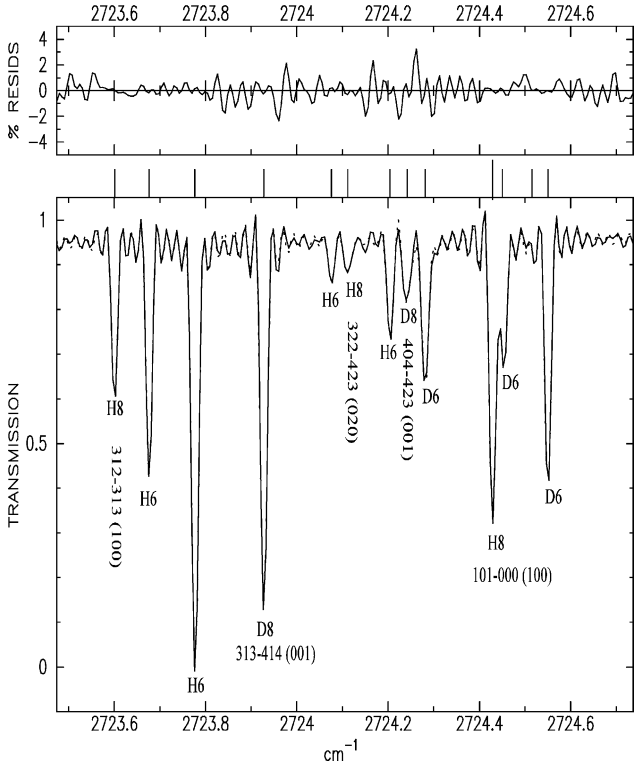

Fig. 2. Short scan spectra of oxygen enriched O-18 deuterated water vapor. The observed spectrum is overlaid with a synthetic spectrum, which is the result from a non-linear-least squares fit of the observed features. The upper portion of the figure is a residual plot showing the percent differences between the observed and computed spectra. The sample pressure was 1.48 Torr and the absorption path length was 2.39 m. The absorption features are labeled in terms of the isotopic species as follows: H6 = $HD^{16}O$, H8 = $HD^{18}O$, D6 = $D_2^{16}O$, and D8 = $D_2^{18}O$. The O-18 species also show the quantum assignments (QA) for the rotational transitions followed, in parenthesis, with the upper vibrational state of the band connecting to the ground state.

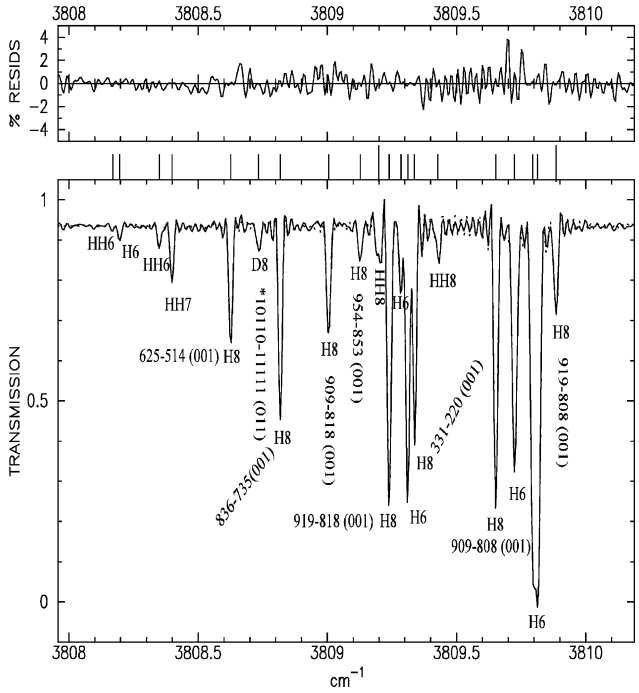

Fig. 3. Short scan spectra of oxygen enriched O-18 deuterated water vapor. The observed spectrum is overlaid with a synthetic spectrum, which is the result from a non-linear-least squares fit of the observed features. The upper portion of the figure is a residual plot showing the percent differences between the observed and computed spectra. The sample pressure was 1.48 Torr and the absorption path length was 2.39 m. The absorption features are labeled in terms of the isotopic species as follows: H6 = $HD^{16}O$, H8 = $HD^{18}O$, D6 = $D_2^{16}O$, D8 = $D_2^{18}O$, HH6 = $H_2^{16}O$, HH7 = $H_2^{17}O$, and HH8 = $H_2^{18}O$. The O-18 species also show the quantum assignments (QA) for the rotational transitions followed, in parenthesis, with the upper vibrational state of the band connecting to the ground state. One feature has an asterisk in front of the QA and this denotes that the feature is composed of two comparable transitions with the QA of the stronger transition shown.

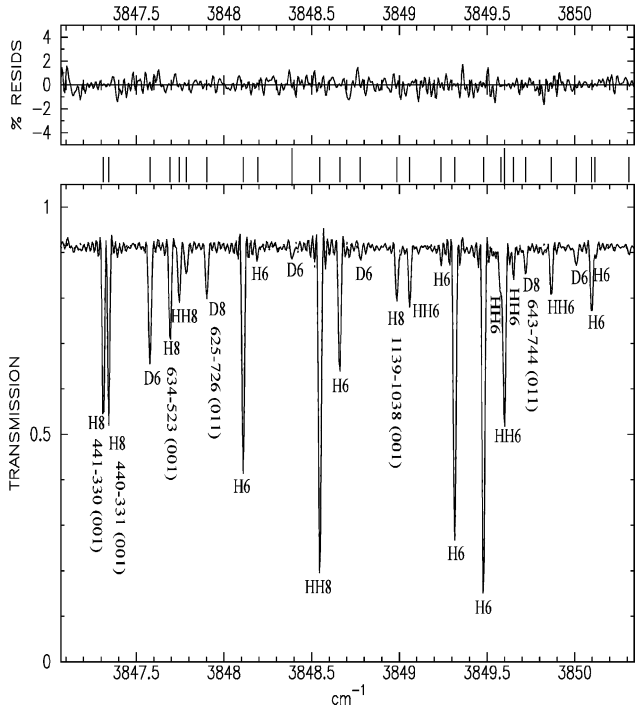

Fig. 4. Short scan spectra of oxygen enriched O-18 deuterated water vapor. The observed spectrum is overlaid with a synthetic spectrum, which is the result from a non-linear-least squares fit of the observed features. The upper portion of the figure is a residual plot showing the percent differences between the observed and computed spectra. The sample pressure was 1.48 Torr and the absorption path length was 2.39 m. The absorption features are labeled in terms of the isotopic species as follows: H6 = $HD^{16}O$, H8 = $HD^{18}O$, D6 = $D_2^{16}O$, D8 = $D_2^{18}O$, HH6 = $H_2^{16}O$, HH7 = $H_2^{17}O$, and HH8 = $H_2^{18}O$. The O-18 species also show the quantum assignments (QA) for the rotational transitions followed, in parenthesis, with the upper vibrational state of the band connecting to the ground state.

6. Conclusion

Reported in this study for the first time are measurements and assignments in the (100)-(000), (020)-(000), and (001)-(000) bands of $HD^{18}O$ and the (001) and (011) bands of $D_2^{18}O$. The data were analyzed to obtain energy levels of the (100), (020), and (001) vibrational states of $HD^{18}O$ and the (001) and (011) states of $D_2^{18}O$ and the vibrational bands of these states connected to the ground state covered the spectral region from 2500 to 4278 cm^{-1}. 456 absorption lines of $D_2^{18}O$ and 856 lines of $HD^{18}O$ were assigned from the spectra. The measurements were of oxygen-18 enriched samples of deuterated water vapor and the spectra also contained features of $HD^{16}O$, $D_2^{16}O$, $H_2^{16}O$, $H_2^{17}O$ and $H_2^{18}O$ of which several were used as frequency calibration standards. The measured line strengths were listed in compilations that contain the observed and computed transition frequencies. 73 lines in the (100)-(000) band and 148 lines in the (001)-(000) band of $HD^{18}O$ have enough transition intensity to be included in the HITRAN [15] listing. These have been included in a water vapor compilation by this author that covers the 500 to 8000 cm^{-1} region and is available on the website, http://mark4sun.jpl.nasa.gov, given under 'science data'.

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