Spectrum of hot water in the 4750–13 000 cm^{-1} wavenumber range (0.769–2.1 μm)

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ABSTRACT

The high resolution laboratory spectrum of hot water vapour has been recorded in the 500–13 000 cm^{-1} wavenumber range and we report on the analysis of the 4750–13 000 cm^{-1} (0.769–2.1 μm) portion. The emission spectrum was recorded using an oxy-acetylene welding torch and a Fourier transform spectrometer. Line assignments in the laboratory spectrum as well as in an absorption spectrum of a sunspot umbra were made with the help of the BT2 line-list. Our torch spectrum is the first laboratory observation of the 9300 Å 'steam bands' seen in M-stars and brown dwarfs.

Key words: line: identification – molecular data – sunspots – infrared: stars.

1 INTRODUCTION

After H_2 and CO, H_2O is arguably the most important astronomical molecule. Water vapour is found in comets (Dello Russo et al. 2005, 2006), cool stars (Cushing, Rayner & Vacca 2005), brown dwarfs (Kirkpatrick 2005; Reiners et al. 2007), extrasolar planets (Tinetti et al. 2007), star-forming regions (Ashby et al. 2000) and planetary atmospheres (Lellouch et al. 2002), although detection is often difficult because of telluric absorption. Water has been detected by pure rotational and vibration–rotation transitions (but not yet by electronic transitions) based on an extensive amount of laboratory data (Bernath 2002). In general, for cool sources there are matching laboratory observations, although more work (e.g. for H_2 pressure broadening coefficients) are certainly needed. Much of the existing data is collected in the HITRAN data base (Rothman et al. 2005) or the JPL catalog (Pickett et al. 1998).

The situation for hot water vapour is much less satisfactory, particularly to shorter wavelengths. This is a serious deficiency because water vapour is a major source of opacity for cool stellar and substellar sources, and the spectroscopy of steam is an important probe of combustion processes (Teichert, Fernholz & Ebert 2003). Absorption due to 'steam bands' (Spinrad et al. 1966) can clearly be seen at wavelengths as short as 9300 Å in many sources such as M-stars and brown dwarfs (Cushing et al. 2005; Reiners et al. 2007). Sur-

prisingly, these 9300-Å steam bands have never been seen at high resolution in laboratory spectra prior to the work reported here.

For the water overtone region above 5000 cm^{-1} (or wavelengths below 2 μm) there have been numerous laboratory observations of room temperature spectra, for example recent work by Tolchenov et al. (2005), Jenouvrier et al. (2007) or Mikhailenko et al. (2007). The number of observations of spectra of hot water vapour in this short wavelength region are far fewer. They begin some 40 yr ago with the classic work of J.-P. Maillard at the Meudon Observatory using an oxy-hydrogen torch. Camy-Peyret et al. (1977) reported vibration–rotation energy levels based on 6200–9100 cm^{-1} region of this torch spectrum. More recently, Tereszchuk et al. (2002) reported on emission spectra in the 4800–7500 cm^{-1} region from water vapour at 1800 K and in sunspot absorption spectra. There are a few diode laser measurements of heated water vapour (300–1000 K) near 1.4 μm (Liu et al. 2007), hotter laser measurements (1500–1800 K) near 9400 Å (Cattaneo, Laurila & Hernberg 2004) and an intracavity Nd-glass laser experiment near 9400 cm^{-1}. The intracavity experiment used both a heated cell filled with water vapour at up to 1000 K and a plasma torch to reach 2200 K, but covered only the 9390–9450 cm^{-1} region (Petrova et al. 2006).

A few years ago we repeated the early measurements of Maillard using a oxy-acetylene welding torch and covered the 500–13 000 cm^{-1} region in emission with a Fourier transform spectrometer. So far we have published on the 500–2000 cm^{-1} (Coheur et al. 2005) and 2000–4750 cm^{-1} regions (Zobov et al. 2006). We have also reported on 'Monodromy in the water molecule', that is, on

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the highly excited bending levels (up to $9\nu_2$) that sample the linear geometry (Zobov et al. 2005). In this fourth paper on the our 3000 K torch spectrum we present the data for the remaining 4750–13 000 cm^{-1} region.

2 LABORATORY SPECTRA

2.1 Experimental background

The laboratory spectra reported by Coheur et al. (2005) were obtained by recording emission from an oxy-acetylene torch using a Bruker IFS 120 M Fourier transform spectrometer between 500 and 13 000 cm^{-1}. In the region considered here (4750–13 000 cm^{-1}), InSb, InGaAs and Si detectors were used with a CaF$_2$ window and beamsplitter. Either a 1.4 or a 2 mm aperture was chosen and the spectral resolution was set to 0.05 cm^{-1} (18 cm maximum optical path difference) or 0.1 cm^{-1}(9 cm maximum optical path difference).

Spectra were recorded with the torch at atmospheric pressure which, combined with a temperature of about 3000 K, leads to broadened lines with many blends and an uncertainty of about 0.02 cm^{-1} in the determination of line positions. A few lines have fitting errors larger than this value; information on this is given in the archived version of the spectrum.

As is obvious from Fig. 1, the spectra are very dense, showing, in addition to water lines, emission features of CO, CO$_2$ and OH. In the region considered here, we identified 1939 OH emission lines using data taken from Mélen et al. (1995) and Colin et al. (2002). Indeed at wavenumbers above 12 365 cm^{-1} the only lines we could assign are due to OH. 159 CO lines were identified by using the HITEMP data base (Rothman et al. 1998) as a reference. Many of the possible OH and CO lines identified in the spectrum and marked in the line-list are likely due to water. These transitions match CO or OH line positions but only for transitions with higher vibrational or rotational quantum numbers than expected for a 3000 K source.

Including multiple assignment 37 628 lines were measured in the 4750–13 150 cm^{-1} interval, although the spectrum becomes quite sparse at higher wavenumbers. Two absorption spectra of sunspots (Wallace et al. 1996, 2001) were analysed at the same time as the laboratory emission spectra. These sunspot spectra have an estimated water vapor temperature of 3200 K. The first covered the *K*-band (4251–4962 cm^{-1}) contains 3134 lines. Previous analysis (Polyansky et al. 1997c; Zobov et al. 2000) had led to the assignment of 717 absorption features due to water vapour. Use of the
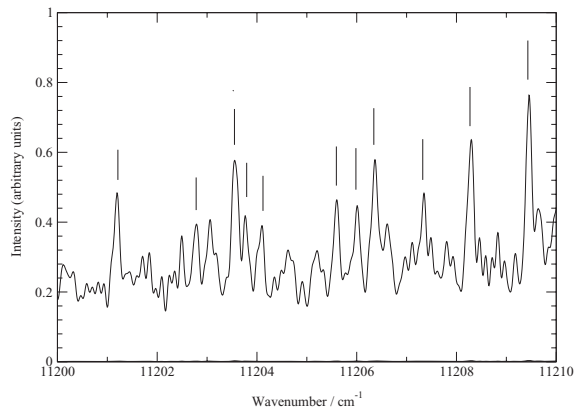
torch spectrum allows us to more than double the number of water features identified. The second sunspot spectrum covered the 5540–7000 cm^{-1} region (*H* band). In this region only a minority of the features are due to water. However, again the use of the flame spectrum allows us to more than double the number of water assignments.

Figs 1–3 present small portions of the laboratory emission spectra. Two of these portions are chosen to overlap the sunspot absorption spectra of Wallace et al. (1996), which are given for comparison. Tables 1–3, respectively, present the corresponding emission spectrum line-list for these small portions of the spectrum only. The full line-list as well as new versions of the sunspot spectra with updated assignments can be found in the electronic archive.
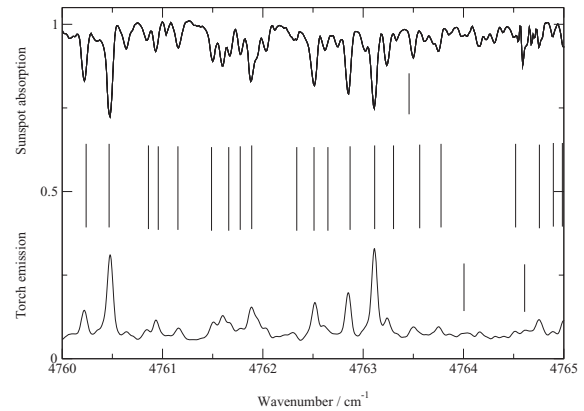
Figure 2. Sunspot spectrum of Wallace et al. (1996) and laboratory emission spectrum in a small region of the *K* band. Lines assigned in both spectra are indicated by the vertical lines in the centre of the figure. The vertical lines close to one spectrum indicate assignments to that spectrum only. Table 2 tabulates the laboratory lines in this region. Note that the intensity scale refers to the sunspot absorption; the absolute intensity of the laboratory emission spectrum was not determined.

Figure 1. A small region of the near-infrared laboratory emission spectrum. The assigned lines are indicated by the vertical lines; see Table 1 for details.

Figure 3. Sunspot spectrum of Wallace et al. (1996) and laboratory emission spectrum in a small region of the *H* band. Lines assigned in both spectra are indicated by the vertical lines in the centre of the figure. The vertical lines close to one spectrum indicate assignments to that spectrum only. Table 3 tabulates the laboratory lines in this region. Note that the intensity scale refers to the sunspot absorption; the absolute intensity of the laboratory emission spectrum was not determined.
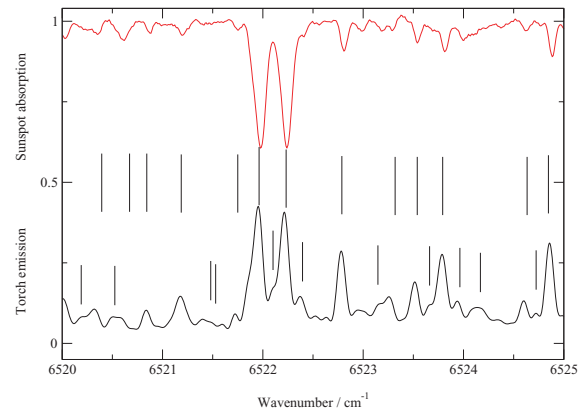
Table 1. Lines identified in the laboratory emission spectrum corresponding to Fig. 1. The intensity, I, is in arbitrary units and the width w is in millicm^{-1}. Lines with two assignments are given twice except for the lines due to quasi-degenerate doublets for which the ortho-transition is given and labelled d. The notes on the assignments are: t trivial assignment, n transition to new energy level, and c new energy level confirmed by combination differences. The full line-list is available as Supplementary Material in the online version of this article.

$\tilde{\nu}/$cm^{-1}	I	w	J'	K'_a	K'_c	$J'_{\prime}$	K''_a	K''_c	$(v'_1, v'_2, v'_3)-(v''_1, v''_2, v''_3)$	Notes
11201.2570	.014	119	14	0	14	13	0	13	003-000	t
11202.5605	.014	32								
11202.8456	.009	103	22	1	21	21	1	20	003-000	dnc
11203.1360	.010	148								
11203.6293	.020	140	14	1	13	13	1	12	003-000	dt
11203.8410	.012	96	12	2	10	11	2	9	003-000	t
11204.1488	.010	128	13	3	11	12	3	10	003-000	t
11204.6964	.006	207								
11205.2649	.006	157								
11205.6637	.013	110	11	4	8	10	4	7	003-000	t
11206.0738	.011	122	21	2	20	20	2	19	003-000	dnc
11206.4345	.017	149	15	1	15	14	1	14	003-000	dt
11206.6778	.008	134								
11207.4153	.012	87	16	1	15	15	1	14	003-000	nc
11208.3553	.020	124	14	2	12	13	2	11	003-000	t
11208.3553	.020	124	20	1	19	19	1	18	003-000	nc
11209.5187	.028	119	15	3	13	14	3	12	003-000	nc
11209.5187	.028	119	19	5	15	18	5	14	003-000	nc
11209.7156	.010	134								

Table 2. Lines identified in the laboratory emission spectrum corresponding to Fig. 2. The intensity, I, is in arbitrary units and the width w is in 10^{-3} cm^{-1}. Lines with two assignments are given twice except for lines due to quasi-degenerate doublets for which the ortho-transition is given and labelled d. The notes on the assignments are: t trivial assignment, n transition to new energy level, and c new energy level confirmed by combination differences. The full line-list is available as Supplementary Material in the online version of this article.

$\tilde{\nu}/$cm^{-1}	I	w	J'	K'_a	K'_c	J''	K''_a	K''_c	$(v'_1, v'_2, v'_3) - (v'_1, v'_2, v'_3)$	Notes
4760.2262	.007	49	18	3	15	19	3	16	041-030	t
4760.4842	.028	60	20	0	20	21	0	21	031-020	dt
4760.6564	.002	62								
4760.8446	.003	51	17	4	14	18	4	15	111-100	t
4760.9434	.006	69	17	2	16	18	2	17	111-100	dt
4761.1651	.004	77	10	0	10	11	0	11	141-130	nc
4761.5038	.004	58	17	3	14	18	3	15	111-100	nc
4761.6160	.007	135								
4761.6921	.003	17	12	2	10	13	2	11	131-120	nc
4761.7798	.003	81	8	5	4	9	5	5	230-021	t
4761.8937	.008	80	14	0	14	15	0	15	061-050	t
4761.9824	.004	152								
4762.2806	.002	95	25	6	20	24	4	21	001-000	t
4762.5243	.012	59	20	1	20	21	1	21	012-001	dt
4762.6275	.003	92	23	8	16	24	8	17	021-010	t
4762.8575	.015	56	21	2	20	22	2	21	031-020	t
4763.1192	.030	55	23	1	23	24	1	24	011-000	dt
4763.2512	.005	59	22	3	19	21	1	20	001-000	dt
4763.5142	.003	75	24	5	19	25	5	20	101-010	nc
4763.7563	.003	75	17	3	15	18	3	16	111-100	t
4764.0340	.001	98	15	10	6	16	9	7	211-021	dnc
4764.1723	.002	49								
4764.5185	.002	47	25	3	22	24	2	23	100-000	dt
4764.6299	.002	117								OH
4764.7617	.006	76	8	1	8	9	1	9	220-011	t
4764.7617	.006	76	13	7	6	14	8	7	110-000	t
4764.9013	.002	59	22	5	18	23	5	19	021-010	nc

Table 3. Lines identified in the laboratory emission spectrum corresponding to Fig. 3. The intensity, I, is in arbitrary units and the width w is in millicm^{-1}. Lines with two assignments are given twice except for lines due to quasi-degenerate doublets for which the ortho-transition is given and labelled d. The notes on the assignments are: t trivial assignment, n transition to new energy level, and c new energy level confirmed by combination differences. The full line-list is available as Supplementary Material in the online version of this article.

$\tilde{v}$/cm^{-1}	I	w	J'	K'_a	K'_c	J''	K''_a	K''_c	$(v'_1, v'_2, v'_3) - (v''_1, v''_2, v''_3)$	Notes
6520.0548	.373	101								
6520.2503	.159	40	18	10	8	19	10	9	101-000	nc
6520.3611	.269	86	14	6	8	15	6	9	041-020	t
6520.3611	.269	86	17	13	5	18	13	6	101-000	dnc
6520.5601	.182	54	4	4	1	4	4	0	410-111	t
6520.6425	.135	62	15	2	13	16	2	14	201-100	n
6520.7565	.003	34								
6520.8869	.253	66	11	4	8	12	4	9	041-020	t
6520.9746	.044	31								
6521.2254	.385	130	12	4	8	13	4	9	031-010	t
6521.2254	.385	130	10	4	7	11	5	6	022-100	t
6521.4557	.112	73								
6521.5410	.055	45	2	2	0	2	2	1	321-220	t
6521.5410	.055	45	9	5	5	10	5	6	310-011	t
6521.6396	.030	11	10	5	6	11	4	7	230-110	t
6521.7713	.216	25	4	0	4	5	0	5	203-102	t
6521.7713	.216	25	7	5	2	7	5	3	410-111	t
6521.9056	.437	51								
6521.9997	1.540	96								OH
6522.1511	.286	43	12	3	9	13	3	10	031-010	t
6522.1511	.286	43	7	1	6	8	1	7	104-003	t
6522.2608	1.320	105								OH
6522.4238	.333	45	17	10	8	18	10	9	111-010	nc
6522.4565	.075	335								
6522.8291	.877	80	25	2	24	26	2	25	101-000	dt
6522.8291	.877	80	8	7	2	8	7	1	301-200	t
6523.0144	.123	412								OH
6523.0144	.123	412								
6523.0203	.089	20								
6523.2069	.199	40	11	4	8	12	3	9	201-001	t
6523.3008	.280	92	7	0	7	8	0	8	041-020	t
6523.5611	.473	85	15	3	13	16	3	14	201-100	nc
6523.7037	.162	30	16	1	15	17	1	16	021-000	t
6523.8326	.839	107	17	1	17	18	1	18	201-100	dnc
6523.8326	.839	107	10	4	7	11	4	8	300-001	t
6523.9945	.237	43	15	7	9	16	7	10	041-020	nc
6524.1867	.151	149	17	6	11	18	6	12	021-000	nc
6524.1867	.151	149	8	7	1	9	8	2	023-101	t
6524.6475	.275	74	18	3	15	19	3	16	021-000	t
6524.6475	.275	74	11	4	7	12	2	10	220-001	t
6524.7905	.042	210	14	10	4	15	10	5	121-020	nc
6524.7905	.042	210	8	2	6	9	4	5	141-040	nc
6524.9061	1.060	81	1	1	0	2	1	1	400-101	t
6524.9061	1.060	81	26	0	26	27	0	27	101-000	dt
6524.9061	1.060	81	5	5	0	5	5	1	410-111	dt
6524.9061	1.060	81	10	6	4	11	6	5	103-002	t

2.2 Analysis

Line assignments were performed using the BT2 line-list (Barber et al. 2006). This line-list was computed in order to model the spectrum of water vapour in cool stars and is thus suitable for the temperatures considered here. BT2 contains all transitions between levels of water with $J \leqslant 50$ and energy less than 30 000 cm^{-1} above the $J = 0$ ground state. Transition wavenumbers and wavefunctions were calculated using the spectroscopically determined potential energy surface of Shirin et al. (2003); transition intensities were obtained using the dipole moment surface of Schwenke & Partridge (2000).

The first step in analysing the torch spectrum was to mark transitions belonging to other species: OH and CO as discussed above.

The second step was to make trivial assignments – that is assignments that can be made using previously determined experimental energy levels (Tennyson et al. 2001). Simple checks were made using the theoretical intensities to ensure that the intensity of each assigned transition was consistent with observation. It was possible to assign a high proportion of lines in this fashion, a total of 21 605.

Two different methods were used to assign new lines. For transitions involving states with high J but low K_a, the method of branches

(Polyansky et al. 1997a; Polyansky, Tennyson & Bernath 1997b) was used to follow a series of transitions with quantum numbers which simply differ by one in J. This method was used for 28 bands starting with transitions to (011) with energy 5330 cm^{-1} up to the vibrational state (203) with energy 17 495 cm^{-1} and yielded about 700 new energy levels.

For transitions with J in the range of 15–25 and intermediate values of K_a, the error (O$-$C) obtained using the BT2 predictions varies smoothly with K_a and K_c. This means that the positions of experimentally determined energy levels could be predicted with sufficient accuracy for new assignments to be made. This method yielded about 1000 new energy levels.

A full copy of the assigned lines from the laboratory spectrum for the 4750–13 150 cm^{-1} region has been placed in the electronic archive. Tables 1–3 give portions of it and Table 4 summarizes the information obtained as a function of vibrational states analysed. It can be seen that our analysis has extended the range of rotational excitation for a significant number of vibrational states. A set of newly determined H$_2$^{16}O energy levels have been placed in the electronic archive. We estimate the error for each of these levels to be about 0.02 cm^{-1}, similar to the error in determining the line positions in the laboratory emission spectrum.

In the paper of Petrova et al. (2006), the line positions and the assignments of about 50 strong lines at $T = 2200$ K in the range 9392–9456 cm^{-1} are reported. The assignments of 18 lines coincide with ours. For the other lines, we either have a different assignment or have no assignment at all. The line positions of their assigned lines, as calculated using the previously determined experimental energy levels (Tennyson et al. 2001), are correct within experimental error. However, their assigned lines that we do not see are too weak to appear in our spectra according to the BT2 line-list (Barber et al. 2006) at a temperature of 3000 K. We find that using line intensity information as given by the BT2 line-list is crucial in our assignments of the torch spectra.

3 SUNSPOT SPECTRA

Following the assignment of high-temperature laboratory water lines, we reconsidered the assignment of the sunspot spectra (Wallace et al. 1995) in the two regions overlapped by the laboratory spectrum assigned above. No determination of the new rovibrational levels was attempted using the sunspot spectra. The sunspot absorption spectra are recorded only in limited frequency ranges mostly due to telluric absorption and this prevents the use of combination differences to confirm the assignments. Instead trivial assignments have been made using BT2 theoretical line-list and known energy levels including, in particular, those determined in our previous studies of the torch spectrum in lower frequency regions (Coheur et al. 2005; Zobov et al. 2006). The transitions in sunspot spectra are assigned by simply matching sunspot and laboratory spectra.

For the K-band region, we used data published by Wallace & Livingston (1992). The 4251–4962 cm^{-1} region was re-analysed. This region contains 3134 lines of which 717 had been previously assigned to water (Polyansky et al. 1997c; Zobov et al. 2000). A further 116 lines had been assigned to CO and 17 to OH in the later sunspot atlas (Wallace et al. 1996). A comparison with laboratory flame spectra allowed a further 948 lines to be definitely assigned to water. A list of K-band sunspot transitions is given in the electronic archive with these assignments. 57 per cent of the lines are assigned in this spectrum so there remains work to be done in this region.

Table 4. Summary of newly determined energy levels of H$_2$^{16}O by vibrational state (v_1', v_2', v_3').

(v_1', v_2', v_3')	N	J_{max}(old)	J_{max}(new)
011	56	35	35
021	57	30	33
200	86	29	29
101	151	29	33
111	145	26	31
041	27	25	21
121	73	20	22
022	29	24	17
300	145	15	25
201	136	16	32
102	118	13	27
003	93	15	26
131	33	17	17
032	30	12	19
310	30	13	22
211	102	14	27
112	25	12	16
141	38	11	14
042	34	9	16
320	7	10	14
221	5	12	14
400	29	11	20
301	30	14	24
023	6	11	14
202	8	12	14
103	32	14	23
004	61	11	22
151	17	8	11
330	5	8	9
311	15	12	15
203	12	11	18
002	4	32	15
031	10	29	18
210	7	14	14
012	15	27	16
013	1	13	10
122	3	11	11
071	1	11	1
231	1	10	10
500	1	9	10
510	2	11	11

Notes. N is the number of newly determined energy levels; J_{max}(old) is the highest rotational level determined previously; J_{max}(new) is the highest rotational level determined in this work.

The newer umbral spectral atlas of Wallace, Hinkle & Livingston (2001) covers the region 4000–8640 cm^{-1}. This atlas lists 3554 lines in the 5540–7000 cm^{-1} region and associates 546 of them with water. Our previous paper on the laboratory spectrum of hot water (1800 K) recorded in the 4878–7552 cm^{-1} region at the University of Waterloo also looked at the sunspot spectrum in this region (Tereszchuk et al. 2002). Besides the water lines there are many lines due to other species: CO (480 lines), OH (363 lines), FeH and Fe I (154 lines), CN (202 lines), Mg I (2 lines), Ti I (13 lines), K I (3 lines) and Ca I (6 lines) (Wallace et al. 2001). Use of the laboratory flame spectrum allowed us to assign a further 872 lines in the spectrum to water bring the total number of assigned lines to 2641 or 74 per cent of the total. A copy of the line-list with these assignments has been placed in the electronic archive.

4 CONCLUSION

We have extended the analysis of the hot water spectrum below 1 μm to cover the steam bands seen at 9300 Å in cool stars and brown dwarfs.

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SUPPLEMENTARY MATERIAL

The following supplementary material is available for this article.

Table 1. Lines identified in the sunspot absorption spectrum in the range 4251–4962 cm^{-1}. See Fig. 2 for sample. Lines with two assignments are given twice except for lines due to quasi-degenerate doublets for which the ortho-transition is given and labelled d. The notes on the assignments are: t trivial assignment, and o assigned previously.

Table 2. Lines identified in the laboratory emission spectrum. The intensity, I, is in arbitrary units and the width w is in 10^{-3} cm^{-1}. Lines with two assignments are given twice except for lines due to quasi-degenerate doublets for which the ortho-transition is given and labelled d. The notes on the assignments are: t trivial assignment, n transition to new energy level, and c new energy level confirmed by combination differences.

Table 3. Lines identified in the sunspot absorption spectrum in the range 5540–7000 cm^{-1}. See Fig. 3 for a sample. Lines with two assignments are given twice except for lines due to quasi-degenerate doublets for which the ortho-transition is given and labelled d. The notes on the assignments are: t trivial assignment, and o assigned previously.

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