

# Emission spectroscopy of a new ${}^2\Delta$ – $1^2\Delta$ system of VO

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## Abstract

High-resolution spectra of VO have been reinvestigated in the 12000–31000  $\text{cm}^{-1}$  region. VO was produced in a vanadium hollow cathode lamp by discharging 1.5 Torr of Ar and the spectra were recorded using a Fourier transform spectrometer. The oxygen needed to produce VO was present in the system as an impurity. Three new bands observed in the 21000–22100  $\text{cm}^{-1}$  region have been attributed to a new  ${}^2\Delta$ – $1^2\Delta$  electronic transition of VO. Two bands, with origins near 21044 and 22038  $\text{cm}^{-1}$ , have been assigned as the 0–1 and 0–0 bands of the  ${}^2\Delta_{3/2}$ – $1^2\Delta_{3/2}$  sub-band while a weak band with an origin near 21975  $\text{cm}^{-1}$  has been assigned as the 0–0 band of the corresponding  ${}^2\Delta_{5/2}$ – $1^2\Delta_{5/2}$  sub-band. A rotational analysis of these sub-bands has been obtained and spectroscopic constants have been extracted. The  $1^2\Delta$  state is known from the previous analyses of the doublet transitions of VO in the near infrared. The present observation has allowed the determination of the vibrational interval  $\Delta G_{1/2}$  and the equilibrium rotational constants for the  $1^2\Delta_{3/2}$  state.

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## 1. Introduction

VO is a molecule of astrophysical importance [1–5]. The electronic spectra of the VO radical appear from the near infrared to the visible in absorption spectra of many cool stars, and provide the basis for the spectral classification of late M-type stars [5]. These spectra have been utilized as a sensitive probe of the circumstellar environment and are of significant importance in modeling of the stellar atmospheres. VO and other oxides of vanadium are also of chemical and industrial importance because of their use in optical devices, semiconductors, catalysts, and coatings [6–11].

VO is the most extensively studied molecule in the group 5 oxide family. The ground state of VO is well established as a  ${}^4\Sigma^-$  state from numerous theoretical [12,13] and experimental [14–21] studies. Three strong

transitions of VO have been identified in the near infrared and visible regions which have been assigned as the  $A^4\Pi$ – $X^4\Sigma^-$  [14],  $B^4\Pi$ – $X^4\Sigma^-$  [15–17], and  $C^4\Sigma^-$ – $X^4\Sigma^-$  [18,19] transitions, all involving the ground state as the lower state. Two more quartet–quartet transitions of VO have been identified in the near infrared that originate from the  $D^4\Delta$  state and terminate on the  $A^4\Pi$  state and another low-lying  $A'^4\Phi$  state [20]. The near infrared region also consists of several doublet–doublet transitions [20]. Among the doublet transitions of VO, there are two  ${}^2\Pi$ – ${}^2\Delta$  transitions near 7200 and 8126  $\text{cm}^{-1}$  having a common  ${}^2\Delta$  lower state which will be referred in this paper as the  $1^2\Delta$  state. Recently another near infrared transition,  ${}^2\Phi$ – $1^2\Delta$ , has been identified near 5500  $\text{cm}^{-1}$  having its lower state in common with the two doublet–doublet transitions mentioned above [21]. There is a fourth doublet transition, which has been assigned as  ${}^2\Delta$ – $1^2\Phi$ , that does not have any state in common with the other doublet transitions [20]. The location of these doublet states is not known with any

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precision relative to the ground state since the quartet and doublet transitions do not have any state in common.

In the current work we have identified a new  ${}^2\Delta-1^2\Delta$  transition of VO in the 21000–22100  $\text{cm}^{-1}$  region having its lower state in common with the lower  $1^2\Delta$  state of three of the four known doublet transitions. In this paper we report the rotational analysis of the 0–1 and 0–0 bands of the  ${}^2\Delta_{3/2}-1^2\Delta_{3/2}$  sub-band and the 0–0 band of the  ${}^2\Delta_{5/2}-1^2\Delta_{5/2}$  sub-band. From this analysis we have determined the fundamental vibrational interval and equilibrium rotational constants for the  $1^2\Delta_{3/2}$  state.

## 2. Experimental details

The new VO bands were identified in an archival spectrum of vanadium recorded in 1979 at the National Solar Observatory at Kitt Peak by W. Whaling and J.W. Brault. The molecules were excited in a hollow cathode lamp and the spectra were observed using the Fourier transform spectrometer associated with the McMath–Pierce telescope of the National Solar Observatory at Kitt Peak. The vanadium cathode lamp was operated at a current of 300 mA with a flow Ar at a pressure of 1.5 Torr. The spectrometer was equipped with a UV beam splitter, midrange silicon photodiode detectors, and TC497 and WG345 filters. The spectra were recorded at 0.042  $\text{cm}^{-1}$  resolution by coadding 10 scans in about 70 min of integration.

The spectral line positions were extracted using a data reduction program called PC-DECOMP developed by J. Brault. The peak positions were determined by fitting a

Voigt line shape function to each feature. In addition to VO, the V and Ar atomic lines were also present in this spectrum. The spectra were calibrated using the measurements of the Ar atomic lines [22]. The absolute accuracy of the wavenumber scale is expected to be of the order of  $\pm 0.005 \text{ cm}^{-1}$ . The new bands are very weak in intensity compared with other known transitions of VO. The strong rotational lines of the new transition appear with a typical signal-to-noise ratio of 4:1 and have an approximate line width of 0.032  $\text{cm}^{-1}$ . The precision of measurements of strong and unblended lines of VO is expected to be better than  $\pm 0.005 \text{ cm}^{-1}$ .

## 3. Results and discussion

This spectrum consists of a number of VO bands belonging to the  $C^4\Sigma^- - X^4\Sigma^-$  transition, although no oxygen was added to the discharge. The oxygen atoms required to produce VO were probably present in the system as an impurity. We were able to identify the 0–1, 0–0, 1–0, 2–0, and 3–0 bands of the  $C^4\Sigma^- - X^4\Sigma^-$  transition along with several sequence bands involving higher vibrational levels of the upper and lower states. After a careful examination of this spectrum we noted the presence of three additional weaker bands with R heads near 21050, 21979, and 22042  $\text{cm}^{-1}$ . These bands consist of two branches and do not belong to any known transitions of VO. A rotational analysis of these bands indicated that the bands at 21050 and 22042  $\text{cm}^{-1}$  had a common upper state but the lower state constants for these two bands matched with the rotational constants of the  $v'' = 1$  and  $v'' = 0$  vibrational levels of the  $1^2\Delta_{3/2}$  state, while the band at 21979  $\text{cm}^{-1}$  had a lower

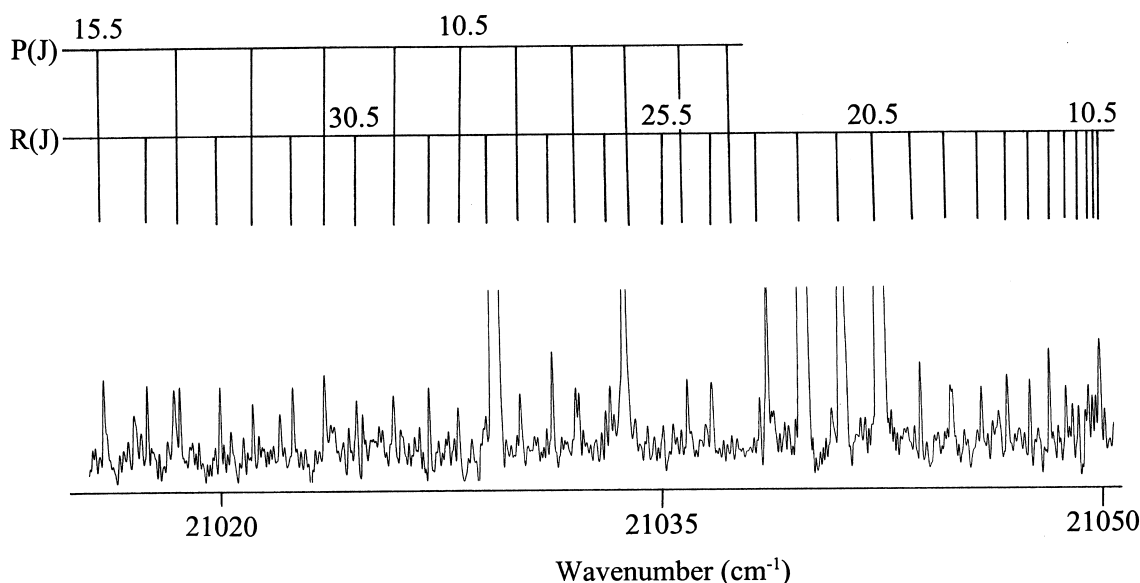


Fig. 1. An expanded portion of the 0–1 band of the new  ${}^2\Delta_{3/2}-1^2\Delta_{3/2}$  system of VO near the R head.

Table 1  
Observed line positions (in  $\text{cm}^{-1}$ ) for the new transition of VO

$J$	$R(J)$	O – C ${}^2\Delta_{3/2}-1^2\Delta_{3/2}$	$P(J)$ 0–1	O – C	$R(J)$	O – C ${}^2\Delta_{3/2}-1^2\Delta_{3/2}$	$P(J)$ 0–0	O – C	$R(J)$	O – C ${}^2\Delta_{5/2}-1^2\Delta_{5/2}$	$P(J)$ 0–0	O – C
5.5			21037.572	–1								
6.5			21035.897	3					21979.487	17		
7.5			21034.117	10					21979.608	12	21963.755	–9
8.5			21032.217	3			22024.780	5	21979.608	5	21961.802	1
9.5	21049.949	1	21030.210	–5	22042.422	–9	22022.697	–1	21979.487	–3	21959.722	3
10.5	21049.806	–8	21028.102	–7	22042.209	–2	22020.516	10	21979.245	–9	21957.559	39
11.5	21049.560	–14	21025.908	11	22041.864	–12	22018.205	6	21978.896	0	21955.202	2
12.5	21049.225	–3	21023.577	–2	22041.430	3	22015.784	6	21978.394	–17	21952.760	2
13.5	21048.789	15	21021.140	–15	22040.872	10	22013.223	–18	21977.786	–13	21950.190	–3
14.5	21048.217	3	21018.626	1	22040.192	11	22010.586	–6	b		21947.460	–43
15.5	21047.543	–5	21016.002	14	22039.390	4	22007.841	15	21976.173	–12	21944.702	16
16.5	21046.770	–6	21013.227	–19	22038.469	–8	22004.950	3	21975.192	14	21941.743	3
17.5	21045.896	–1	21010.394	–5	22037.438	–14	22001.951	–2	21974.011	–24	21938.677	13
18.5	21044.915	2	21007.441	–5	22036.320	8	21998.837	–8	21972.742	–11	21935.457	2
19.5	21043.819	–3	21004.374	–13	22035.055	–2	b	0			21932.114	3
20.5	b		21001.238	16	22033.684	–4	21992.298	13				
21.5	b		20997.964	11	22032.192	–11	21988.830	–4				
22.5	b		20994.578	–1	22030.544	–60	21985.266	–3				
23.5	21038.364	–35	20991.089	–10	22028.847	–42	21981.561	–28				
24.5	21036.729	–50	20987.470	–46	22026.972	–87	b					
25.5												
26.5	21033.275	51	20979.983	–51	22023.128	72	21969.797	–69				
27.5	21031.314	26			22020.903	21						
28.5	21029.267	19	20972.181	44	22018.596	3	21961.528	47				
29.5	21027.108	4	20968.055	22	22016.190	1	b					
30.5	21024.855	1	20963.813	–11	22013.668	–2	21952.640	–0				
31.5	21022.499	–2	20959.517	3	22011.029	–7	21948.046	–3				
32.5	21020.014	–30	20955.106	5	22008.246	–42	21943.348	4				
33.5	21017.499	16	20950.582	–3	22005.434	9	21938.523	–3				
34.5	b		20945.936	–31	22002.458	12	21933.548	–46				
35.5	21012.061	8	20941.265	17	21999.349	–5	21928.567	19				
36.5	21009.186	2	20936.448	21	b		21923.407	19				
37.5	21006.165	–47	20931.528	23	21992.794	–28	21918.115	–1				
38.5	21003.131	–7	20926.474	–9	21989.382	–2	21912.725	–4				
39.5	20999.958	–5	20921.330	–32	21985.832	1	21907.200	–30				
40.5	20996.672	–15	20916.126	–14	21982.163	–1	21901.599	–18				
41.5	20993.292	–19	20910.818	–1	21978.394	13	21895.896	6				
42.5	20989.836	3	20905.392	–8	21974.501	17	21890.053	2				
43.5	20986.258	1	20899.873	–10	21970.485	14	21884.101	3				
44.5	20982.570	–12	20894.276	7	21966.335	–9	21878.035	4				
45.5	20978.814	6	20888.558	–1			21871.849	–3				
46.5			20882.777	25			21865.545	–15				
47.5			20876.860	10								

Note. O – C are observed minus calculated wavenumbers in the units of  $10^3 \text{ cm}^{-1}$  and “b” marks lines overlapped by strong atomic lines.

state rotational constant similar to the  $v'' = 0$  vibrational level of the  $1^2\Delta_{5/2}$  state [20,21]. This observation led us to conclude that the 21 050 and 22 042  $\text{cm}^{-1}$  bands were in fact the 0–1 and 0–0 bands of the  $^2\Delta_{3/2}$ – $1^2\Delta_{3/2}$  sub-band of a new electronic transition, and the 21 979  $\text{cm}^{-1}$  band was the 0–0 band of the corresponding  $^2\Delta_{5/2}$ – $1^2\Delta_{5/2}$  sub-band. An attempt to locate the 0–1 band of the  $^2\Delta_{5/2}$ – $1^2\Delta_{5/2}$  sub-band was unsuccessful, probably because of its very weak intensity. The bands with  $1^2\Delta_{5/2}$  lower state are generally weaker in intensity as compared to those with  $^2\Delta_{3/2}$  as the lower state.

A part of the spectrum of the 0–1 band has been provided in Fig. 1 where lines belonging to the head-forming  $R$  branch and a few low  $J$   $P$  lines have been marked. Lines up to  $R(45.5)$ ,  $P(47.5)$ , and  $R(45.5)$ ,  $P(46.5)$  have been observed in the 0–1 and 0–0 bands of the  $^2\Delta_{3/2}$ – $1^2\Delta_{3/2}$  sub-band while only low  $J$  lines up to  $R(18.5)$ ,  $P(19.5)$  were identified in the 0–0 band of the  $^2\Delta_{5/2}$ – $1^2\Delta_{5/2}$  sub-band. The rotational constants for the upper and lower states were determined by fitting the lines of both sub-bands separately using a simple energy expression:

$$F_v(J) = T_v + B_v J(J+1) - D_v [J(J+1)]^2 + H_v [J(J+1)]^3, \quad (1)$$

although the observed electronic states most likely obey Hund's case (a) coupling.

The rotational lines were given weights based on their relative intensity and extent of blending. The inclusion of the higher order constant  $H_v$  for the lower  $1^2\Delta_{3/2}$  spin components is likely a reflection of interactions of this state with other close-lying electronic states. In the final fit lines belonging to the 0–0, 1–0, 2–1, and 3–1 bands of the  $1^2\Pi_{1/2}$ – $1^2\Delta_{3/2}$  transition of Merer et al. [20] were also included with the line positions of the 0–1 and 0–0 bands of the new  $^2\Delta_{3/2}$ – $1^2\Delta_{3/2}$  sub-band. Similarly the lines of the 0–0 and 1–0 bands of Merer et al.'s  $1^2\Pi_{3/2}$ – $1^2\Delta_{5/2}$  sub-band were combined with the 0–0 band of the new  $^2\Delta_{5/2}$ – $1^2\Delta_{5/2}$  sub-band. The  $1^2\Pi_{1/2}$  and  $1^2\Pi_{3/2}$  states were represented by the following simple energy level formula:

$$F_v(J) = T_v + B_v J(J+1) - D_v [J(J+1)]^2 + H_v [J(J+1)]^3 \pm 1/2 [p_v (J+1/2) + p_{D_v} (J+1/2)^3 + p_{H_v} (J+1/2)^5], \quad (2)$$

where  $p_v$ ,  $p_{D_v}$ , and  $p_{H_v}$  are  $\Omega$ -doubling constants in the  $1^2\Pi$  state.

The observed line positions of the new transition are provided in Table 1 and the molecular constants for the new state are provided in Table 2. In this table we have also provided the revised rotational constants for the  $v = 0, 1, 2$ , and 3 vibrational levels of the  $1^2\Pi_{1/2}$  spin component and the  $v = 0$  and 1 vibrational levels of the  $1^2\Pi_{3/2}$  spin component for completeness. These con-

Table 2  
Spectroscopic constants (in  $\text{cm}^{-1}$ ) for  $1^2\Delta$ ,  $1^2\Pi$ , and the new  $^2\Delta$  states of VO

State	Constant <sup>a</sup>	$v = 0$	$v = 1$	$v = 2$	$v = 3$
$^2\Delta_{5/2}$	$T_v$	$b + 21974.8220(50)$	—	—	—
	$B_v$	0.495643(57)	—	—	—
	$10^6 \times D_v$	6.71(12)	—	—	—
$^2\Delta_{3/2}$	$T_v$	$a + 22037.8008(35)$	—	—	—
	$B_v$	0.493460(21)	—	—	—
	$10^7 \times D_v$	6.38(18)	—	—	—
	$10^{11} \times H_v$	–2.02(50)	—	—	—
$1^2\Pi_{3/2}$	$T_v$	$b + 7147.7256(16)$	$b + 8074.7007(22)$	—	—
	$B_v$	0.521151(18)	0.518190(19)	—	—
	$10^7 \times D_v$	6.85(11)	7.57(13)	—	—
$1^2\Pi_{1/2}$	$T_v$	$a + 7256.4286(17)$	$a + 8183.7202(15)$	$a + 9101.8076(41)$	$a + 10010.1195(45)$
	$B_v$	0.518588(16)	0.515322(16)	0.512010(18)	0.508509(21)
	$10^7 \times D_v$	6.288(65)	6.422(68)	7.183(91)	6.91(12)
	$10^2 \times p_v$	2.9003(90)	3.0400(89)	3.1515(51)	3.3291(71)
	$10^7 \times p_{D_v}$	–3.87(68)	–3.60(66)	—	—
$1^2\Delta_{5/2}$	$T_v$	$b^b$	—	—	—
	$B_v$	0.552272(21)	—	—	—
	$10^7 \times D_v$	6.81(22)	—	—	—
	$10^{10} \times H_v$	–3.064(84)	—	—	—
$1^2\Delta_{3/2}$	$T_v$	$a^b$	$a + 992.8929(42)$	—	—
	$B_v$	0.550903(17)	0.546809(22)	—	—
	$10^7 \times D_v$	7.016(92)	8.14(18)	—	—
	$10^{11} \times H_v$	–1.42(18)	–6.03(51)	—	—

<sup>a</sup> Values in parentheses are one standard deviation in the last digits quoted.

<sup>b</sup> Unknown values, fixed to zero in the fit.

Table 3  
Effective equilibrium spectroscopic constants (in  $\text{cm}^{-1}$ ) for  $1^2\Delta_{3/2}$ ,  $1^2\Pi_{1/2}$ , and  $1^2\Pi_{3/2}$  states of VO

Constant	$1^2\Delta_{3/2}$	$1^2\Pi_{1/2}$	$1^2\Pi_{3/2}$
$B_e$	0.552950(22)	0.520305(79)	0.522632(22)
$\alpha_e$	0.004094(28)	0.003346(38)	0.002961(26)
$r_e$ (Å)	1.582556(31)	1.631440(13)	1.627804(34)
$\omega_e$	[992.8929(42)] <sup>a</sup>	935.948(15)	[926.9751(27)] <sup>a</sup>
$\omega_e x_e$	—	4.1737(72)	—
$\omega_e y_e$	—	−0.0952(15)	—

<sup>a</sup> The values in square brackets are the first vibrational interval  $\Delta G_{1/2}$  rather than  $\omega_e$ .

stants have been used to evaluate effective equilibrium constants for the  $1^2\Pi_{1/2}$ ,  $1^2\Pi_{3/2}$ , and  $1^2\Delta_{3/2}$  states of VO, which are provided in Table 3. As the spin–orbit constants are unknown, no Hund’s case (a) fits were attempted.

The present observations allow the fundamental vibrational interval to be determined along with the equilibrium rotational constants for the  $1^2\Delta_{3/2}$  state. The spectroscopic constants for the  $v=0$  and 1 vibrational levels of the  $1^2\Delta_{3/2}$  state provide  $\Delta G_{1/2} = 992.8929(42) \text{ cm}^{-1}$ ,  $B_e = 0.552950(22)$ ,  $\alpha_e = 0.004094(28) \text{ cm}^{-1}$ , and  $r_e = 1.582556(31) \text{ Å}$  for this spin component. A vibrational interval of  $\Delta G_{1/2} = 1019.9 \text{ cm}^{-1}$  was estimated for the  $1^2\Delta$  state by Merer et al. [20] by assuming that a weak, unanalyzed band at  $7120.362 \text{ cm}^{-1}$  was the 0–1 band of the  $1^2\Pi_{3/2}$ – $1^2\Delta_{5/2}$  transition. This value for  $\Delta G_{1/2}$  is quite different than the value of  $992.8929(42) \text{ cm}^{-1}$  obtained in the present work, casting doubt on the tentative assignment of the  $7120 \text{ cm}^{-1}$  band. It must be noted that the experimental bond length of the  $1^2\Delta_{3/2}$  state ( $r_e = 1.582556(31) \text{ Å}$ ) is shorter than the bond length of the ground state ( $r_e = 1.58932 \text{ Å}$ ) but the vibrational interval for the  $1^2\Delta_{3/2}$  state is smaller than that for the ground state of VO. A weak perturbation has been observed in the  $2^2\Delta_{3/2}$  spin component of the upper  $2^2\Delta$  state near  $J = 25.5$ . The rotational lines near the perturbation are very weak in intensity and several lines could not be measured with certainty because of weak intensity and overlapped by strong atomic lines.

#### 4. Conclusion

The emission spectrum of VO has been observed in the  $12000$ – $31000 \text{ cm}^{-1}$  region using a Fourier transform spectrometer. Two new bands with R heads near  $21050$  and  $22042 \text{ cm}^{-1}$  have been identified as the 0–1 and 0–0 bands of the  $2^2\Delta_{3/2}$ – $1^2\Delta_{3/2}$  sub-band while a weak band with R head at  $21979 \text{ cm}^{-1}$  has been identified as the 0–0 band of the  $2^2\Delta_{5/2}$ – $1^2\Delta_{5/2}$  sub-band of a new  $2^2\Delta$ – $1^2\Delta$  electronic transition. The  $1^2\Delta$  state is known from

the analysis of other near infrared doublet–doublet transitions by Merer et al. [20] and Ram et al. [21]. A rotational analysis of the observed sub-bands provides improved spectroscopic constants. In particular, the vibrational interval for the  $1^2\Delta_{3/2}$  state as well as the equilibrium rotational constants for this state have been determined. In addition, by including the observed lines for Merer et al.’s  $1^2\Pi_{1/2}$ – $1^2\Delta_{3/2}$  transition near  $7200 \text{ cm}^{-1}$ , we have been able to determine the equilibrium vibrational and rotational constants for the  $1^2\Pi_{1/2}$  state.

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