VANADIUM OXIDE IN THE SPECTRA OF MIRA VARIABLES

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ABSTRACT

As a preliminary step in deducing $T_{\rm eff}$ and log (g) of Mira variables as a function of phase, a comparison is made between spectra synthesized from LTE stellar atmosphere models and observed spectra. The observed spectra show obvious vanadium oxide (VO) absorption bands. However, the molecular line list used to produce the synthetic spectra does not include the bound-bound VO opacities. The wavenumbers, line oscillator strengths, and lowest energy levels are needed to calculate these opacities. The equations, constants, and experimentally determined factors required to calculate the line oscillator strengths and lowest energy levels from experimentally determined wavenumbers are presented. The effect of including the wavenumbers, line oscillator strengths, and lowest energy levels of the VO B–X (0, 0) band are calculated and show the expected absorption features observed in the spectra of Mira variables. In the VO B–X (0, 0) band the line oscillator strengths range from about 0.05 to 3.

Subject headings: line: identification — molecular data — stars: late-type — stars: variables: other

1. INTRODUCTION

Over the last 4 years, we have made spectroscopic measurements of 20 Mira variable stars as a function of phase, probing their stellar atmospheres and underlying pulsation mechanisms (Castelaz et al. 2000; Castelaz & Luttermoser 1997). Figure 1 shows the phase-dependent spectra of R Leo as an example (Castelaz et al. 2000). In order to determine effective temperatures $(T_{\rm eff})$ and surface gravities [log (g)] of three Mira variables (R Leo, V CVn, and R CVn) as a function of phase, Piontek & Luttermoser (1999) compared synthetic and observed spectra. As a first approximation of $T_{\rm eff}$ and log (g), they use the LTE stellar atmosphere model ATLAS (Kurucz 1970; Johnson, Luttermoser, & Faulkner 1988; Brown et al. 1989) to synthesize spectra in the wavelength range of the observed spectra, 6000–9200 Å. Stellar atmospheric models were chosen from 7615 Kurucz models (Kurucz 1979) and 162 Indiana University (IU) models (Brown et al. 1989) that had been previously converged. Models were generally available in 200 or 250 K increments, with log (g) ranging by 0.5 from 0.0 to 2.0 and occasionally 2.5. The spectra synthesized with LTE stellar atmosphere models use the 6.6 million IU atomic and molecular line data set. Piontek & Luttermoser (1999) point out that the IU data set does not include vanadium oxide (VO). Thus, there is a noticeable difference between the synthetic and observed spectra corresponding to the B–X bands of VO (Mahanti 1935; Keenan & Schroeder 1952) in the wavelength regions 7300–7600 Å, 7800–8150 Å, and 8450–8900 Å. Figure 2 compares the synthetic with the

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observed spectrum of R Leo at phase 0.4, which clearly shows the difference. The observed spectrum shows strong VO absorption bands, whereas the synthetic spectrum does not. Hence, the addition of a VO line list to the IU data set would result in much more accurately produced spectra for Mira variables. Brett (1989) uses the just-overlapping line approximation (Tsuji 1966) to incorporate opacities for VO band heads, but not lines, in late M stars. The effects that VO had on Brett's synthetic spectra were very similar to the differences between Piontek & Luttermoser's synthetic and our observed spectra.

This paper reports on our initial work to include the bound-bound opacities of VO to our line list of atomic and molecular opacities. For this preliminary work, we will assume the atmosphere of these stars is a static, plane-parallel geometry and is in LTE. Section 2 presents the physics of the line oscillator strengths, § 3 discusses the results, and § 4 summarizes our results.

2. THE VANADIUM OXIDE LINE OSCILLATOR STRENGTH CALCULATIONS

In order to incorporate the VO line absorption in the synthetic spectra, we need to determine tables of wavenumbers, *line* oscillator strengths, and lowest energy levels, which are not readily available. The line oscillator strength, $f = f_{v'J'v''J''}$, is given by

$$f = \frac{8\pi^2 mc}{3he^2} [(\omega)(q_{v'v''})R_e^2]\left(\frac{S_{\Lambda''J''}^{\Lambda'J'}}{2J''+1}\right), \qquad (1)$$

where ω is the wavenumber of the line in a transition from a lower electronic state with vibrational and rotational quantum numbers v'' and J'' to upper electronic state v'' and J'. Both ω and J'' for the A–X, B–X, and C–X bands of VO are experimentally determined and given by the references in Table 1. The $q_{v'v''}$ are the Franck-Condon factors, R_e^2 is
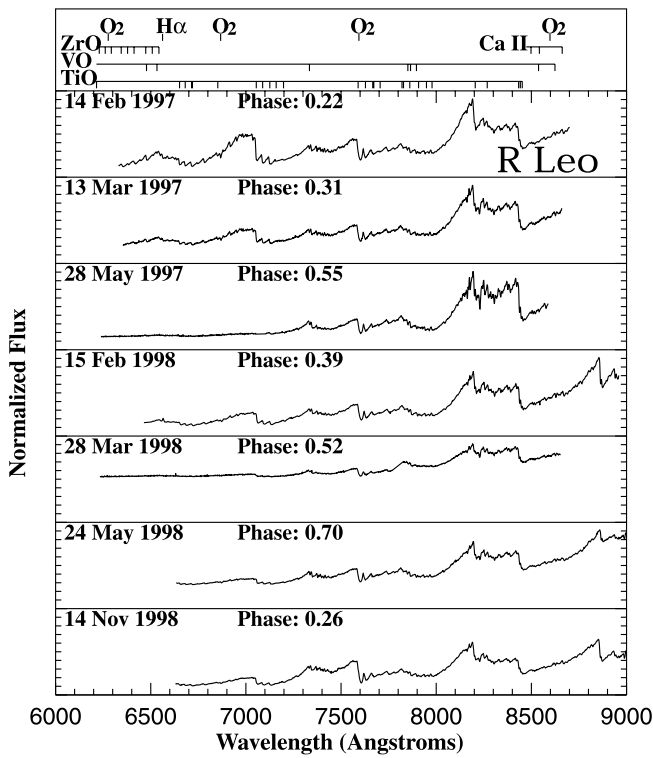
FIG. 1.—Phase-dependent spectra of R Leo. The name of the star, date, and phase are given on each spectrum. The flux is normalized to 1. Above each set of spectra are markers for the major spectral features and terrestrial oxygen. Hα is weak or not seen in most of the spectra. Note the strong VO absorption features at ∼7400 and ∼7900 Å.

the sum of the components of the electronic transition moment, and $S_{\Lambda''J''}^{\Lambda'J'}$ are the Hönl-London factors. The equations, constants, and experimentally determined factors required to calculate the line oscillator strengths given by equation (1) are found in a number of different chemistry and astrophysical publications (e.g., Huber & Herzberg 1979; Nicholls 1981; Larsson 1983; Brett 1989).
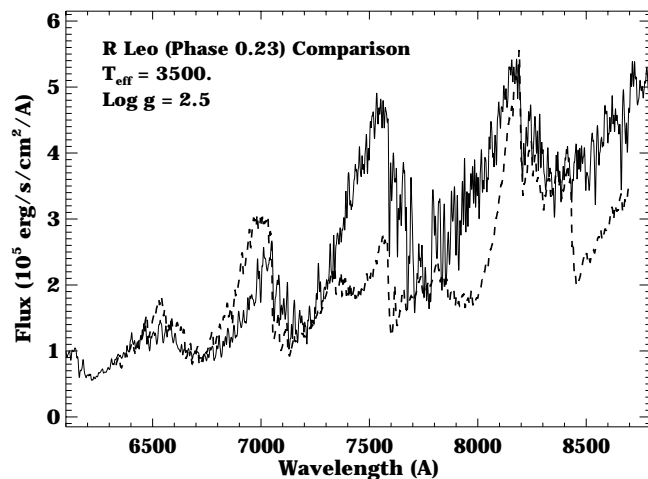

FIG. 2.—Synthetic spectrum (solid line) and observed spectrum (dashed line) of R Leo. The synthetic spectrum represents a star with $T_{eff} = 3400$ K and log $g = 2.5$ that best fits this observed spectrum of R Leo at phase 0.23. The synthetic and observed spectra have the greatest difference over the B–X VO bands (e.g., ∼7400 and ∼7900 Å). The synthetic spectrum has been convolved with a 2.0 Å Gaussian to represent the instrument profile and does not include VO molecule line opacities.

TABLE 1
SOURCES OF J'' AND ω

VO Transition	Band (v', v'')	Approximate Wavenumber Range (cm^{-1})	Reference
$A\,^4\Pi–X\,^4\Sigma^-$	(0, 0)	9550–9250	1
$A\,^4\Pi–X\,^4\Sigma^-$	(0, 1)	8550–8350	1
$B\,^4\Pi–X\,^4\Sigma^-$	(0, 0)	12,710–12,400	2
$B\,^4\Pi–X\,^4\Sigma^-$	(1, 0)	13,630–13,350	3
$C\,^4\Pi–X\,^4\Sigma^-$	(0, 0)	17,430–17,350	1

REFERENCES.—(1) Cheung et al. 1982; (2) Adam et al. 1995; (3) Cheung et al. 1994.

We have collected the factors together here into a concise paper with the aim to report the methods for determining $q_{v'v''}$, R_e^2, and $S_{\Lambda''J''}^{\Lambda'J'}$ for VO. The same methods can be applied to other diatomic molecules but must be modified to reflect different constants of the molecules. Also, since we require the lowest energy levels of VO in the IU data set, we include those calculations.

2.1. Franck-Condon Factors

The Franck-Condon factors $(q_{v'v''})$ are calculated using the closed form, approximate, analytic equations given by Nicholls (1981). For the VO $A\,^4\Pi–X\,^4\Sigma^-$, $B\,^4\Pi–X\,^4\Sigma^-$, and $C\,^4\Pi–X\,^4\Sigma^-$ vibrational states $(v', v'') = (0, 0)$ and $(1, 0)$. Note that $(v', v'') = (1, 0) = (0, 1)$. We can write

$$q(0, 0) = \exp(-S^2/2), \qquad (2)$$

$$q(1, 0) = (S^2/2) \exp(-S^2/2), \qquad (3)$$

where $S = (\mu_A \tilde{\omega}_e)^{1/2} \Delta r_e / 5.807$.

The equations require the molecular constants Δr_e, $\tilde{\omega}_e$, and the reduced mass μ_A (12.176 amu for VO). Table 2 lists Δr_e, the difference between radii, $\tilde{\omega}_e$ (cm^{-1}) which is the mean ω_e, and the results of our calculations of the Franck-Condon factors of the (0, 0) and (1, 0) bands. The molecular constants are from Huber & Herzberg (1979) and Cheung et al. (1982).

2.2. The Sum of the Components of the Electronic Transition Moment, R_e^2

In the calculation of R_e^2, we made use of the fact that all $A–X$ $(0-v'')$ bands have a constant value and all $B–X$ $(0-v'')$ bands have a constant value (Davis, Littleton, & Phillips 1986). From the band oscillator strength equation given by

$$f_{v'v''} = \frac{8\pi^2 mc}{3he^2} [(\omega)(q_{v'v''})R_e^2], \qquad (4)$$

with the band oscillator strengths determined empirically by Brett (1990) and the Franck-Condon factors given in Table 2, we calculate R_e^2. The first two rows in Table 3 give Brett's (1990) values of $f_{v'v''}$, the wavenumber of the band head (ω), $q_{v'v''}$, and resulting R_e^2 in units of $a_0^2 e^2$, where a_0 is the Bohr

TABLE 2
THE FRANCK-CONDON FACTORS

VO Transition	Δr_e ($\times 10^{-2}$ Å)	$\tilde{\omega}_e$ (cm^{-1})	q_{00}	q_{10}
$A\,^4\Pi–X\,^4\Sigma^-$	4.74	937.4	0.684	0.260
$B\,^4\Pi–X\,^4\Sigma^-$	5.16	960.0	0.630	0.291
$C\,^4\Pi–X\,^4\Sigma^-$	8.26	937.4	0.315	0.364

TABLE 3

VALUES OF R_e^2

Band	v', v''	$f_{v'v''}$	$\omega_{v'v''}$ (cm^{-1})	$q_{v'v''}$	$A_{v'v''}$ ($\times 10^6$ s^{-1})	R_e^2 ($a_0^2 e^2$)
A–X ...	0, 0	0.005	9500	0.684	...	0.253
B–X ...	1, 0	0.08	13,420	0.291	...	6.744
A–X ...	0, 0	...	9500	0.684	0.167	0.141
B–X ...	0, 0	...	12,550	0.630	2.703	0.878
B–X ...	1, 0	...	13,420	0.291	2.500	1.755
C–X ...	0, 0	...	17,390	0.315	13.70	4.082

radius and e is the charge of an electron. Brett (1990) gives the $f_{v'v''}$ for only the A–X (0, 0) and B–X (1, 0) transitions.

The sum of the components of the electronic transition moment can also be calculated from the band transition probability $A_{v'v''}$ (Larsson 1983),

$$R_e^2 = 4.936 \times 10^5 \omega^3 A_{v'v''}/q_{v'v''} \ . \tag{5}$$

Karlsson et al. (1997) report lifetime measurements of 6 ± 1 μs, 0.37 ± 0.05 μs, and 73 ± 2 ns of the $A\,^4\Pi$, $B\,^4\Pi$, and $C\,^4\Sigma^-$ states of VO for the $v = 0$ levels and 0.4 μs for the $B\,^4\Pi$ state of VO for the $v = 1$ level. The last four rows of Table 3 give the band transition probabilities based on these lifetimes ($A_{v'v''} = 1$ per lifetime) for the A–X (0, 0), B–X (0, 0), B–X (1, 0), and C–X (0, 0) transitions.

2.3. The Hönl-London Factors $S^{\Lambda'J'}_{\Lambda''J''}$

The Hönl-London factors for the R, Q, and P branches of the VO A–X, B–X, and C–X bands are given by Herzberg's (1950) equations (IV-81)–(IV-83). In Herzberg's equations, we need $\Delta\Lambda = \Lambda'' - \Lambda'$. For the VO transitions we are interested in, $\Lambda'' = \Pi$ and $\Lambda' = \Sigma$. The Π and Σ states refer to the components of the electronic angular momenta. The Π states are ± 1, and the Σ state is 0. So, $\Delta\Lambda = \pm 1$, and the equations of the Hönl-London factors become for each branch and J''

$$S^R_{J''} = \frac{(J'' + 3)(J'' + 2)}{4(J'' + 1)} \ , \tag{6}$$

$$S^Q_{J''} = \frac{(J'' + 2)(J'' - 1)(2J'' + 1)}{4J''(J'' + 1)} \ , \tag{7}$$

$$S^P_{J''} = \frac{J''(J'' - 1)}{4J''} \ . \tag{8}$$

2.4. The Vanadium Oxide Lowest Energy Level, $E_{J''}$ Calculations

From Herzberg (1950), $E_{J''} \cong B_v J''(J'' + 1)$, where $B_v \cong B_e - \alpha_e(v + \frac{1}{2})$ and B_e and α_e are given by Huber & Herzberg (1979). For the VO $B\,^4\Pi$–$X\,^4\Sigma^-$ (0, 0) band, $B_e = 0.5246$ cm^{-1} and $\alpha_e = 0.004$. So, $B_v = 0.5226$ cm^{-1}, and the lowest energy level equation for the B–X (0, 0) band becomes

$$E_{J''} = 0.5226 J''(J'' + 1) \ . \tag{9}$$

3. RESULTS AND DISCUSSION

The sum of the components of the electronic transition moment is the most uncertain term used in the calculation of the line oscillator strengths. The R_e^2 depend on laboratory measurements of either the band oscillator strength or lifetime measurements. Brett (1990) calibrated opacity strengths to match observations of M giants by fitting band oscillator strengths; these relative strengths were then combined with known laboratory values of some TiO systems in their code to estimate the absolute band oscillator strength for the VO A–X and B–X systems. However, Brett (1990) warns that the absolute band oscillator strengths are lower than laboratory values for TiO by about one-half. No comparison is made with VO since VO laboratory values were not available. We use Brett's absolute band oscillator strengths for the VO A–X (0, 0) and B–X (1, 0) calculations of R_e^2, implying an uncertainty proportional to the uncertainty in the absolute band oscillator strength.

The lifetime measurements are more direct. The uncertainty in our calculation of R_e^2 for the VO A–X (0, 0), B–X (0, 0), and C–X (0, 0) systems depends primarily on the uncertainty of the lifetime measurements which are 17%, 14%, and 3%, respectively.

We can compare our calculations of R_e^2 with those of Alvarez & Plez (1998), who also use both the band oscillator strengths and lifetime measurements to calculate the sum of the components of the electronic transition moments of the VO A–X (0, 0) and B–X (0, 0) systems. For the VO A–X (0, 0) system, Alvarez & Plez (1998) calculate $R_e^2 = 0.207$ and $R_e^2 = 0.106$ using the Brett (1990) band oscillator strength and the Karlsson et al. (1997) lifetime measurements, respectively. We calculate $R_e^2 = 0.253$ for the VO A–X (0, 0) system, based on Brett's band oscillator strength and consistent with Alvarez & Plez (1998). The difference, 0.207 versus 0.253, lies in the difference in the selection of the average wavenumber. When comparing to $R_e^2 = 0.106$ determined from lifetime measurements; however, we find our value of R_e^2 is different by about a factor of 2. This is consistent with our expected uncertainty.

For the VO B–X (0, 0) system, Alvarez & Plez (1998) calculate $R_e^2 = 2.590$ and $R_e^2 = 0.735$ using the Brett (1990) band oscillator strength and the Karlsson et al. (1997) lifetime measurements, respectively. Our calculation of the VO B–X (0, 0) R_e^2 is 0.878 and is consistent with the Alvarez & Plez value determined by the lifetime measurements. The difference between our value of 0.878 and the Alvarez & Plez value of 0.735 can again be attributed to the difference in selected average wavenumbers. As in the case of the VO A–X (0, 0) system, our value of R_e^2 is about a factor of 3 lower than the value Alvarez & Plez derive using the absolute band oscillator strengths given by Brett (1990). This is also consistent with our uncertainty in R_e^2.

Alvarez & Plez (1998) do not report the sum of the components of the electronic transition moments for the VO B–X (1, 0) and C–X (0, 0) systems, which we have calculated and give in Table 3. So, we cannot make a comparison. However, based on the other system comparisons, we expect the VO B–X (1, 0) and C–X (0, 0) R_e^2 to have similar uncertainties.

3.1. Line Oscillator Strengths

Line oscillator strengths for about 500 wavenumbers of the VO B–X (0, 0) band are calculated using equation (1) and are shown graphically in Figure 3. We use the values of R_e^2 calculated from the lifetimes measured by Karlsson et al. (1997). As an example of the calculation, the Franck-Condon factor is 0.630 (Table 2) and R_e^2 of B–X (0, 0) is
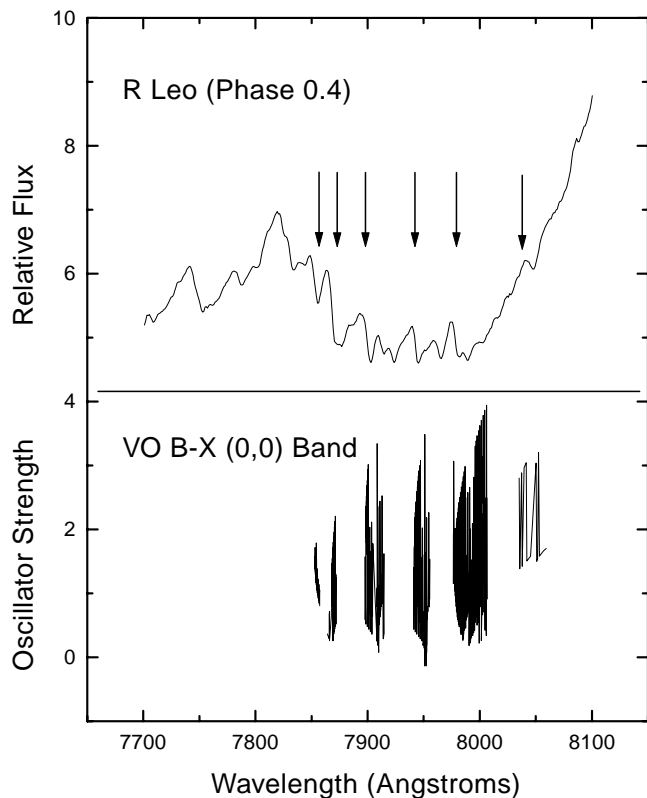
FIG. 3.—Our calculated oscillator strengths of VO $B-X$ (0, 0) are shown in the lower plot. The upper plot shows the observed spectrum of R Leo. The arrows mark the locations of the VO lines. Note that inclusion of the VO oscillator strengths in the calculation of synthetic spectra can now account for these absorption features.

0.878 $a_0^2 e^2$ (Table 3). We choose in this calculation example the R-branch, $J'' = 1.5$, $\omega = 12{,}712.7150$ cm^{-1} from the list of wavenumbers, and J'' given by Adam et al. (1995). Using these values, the Hönl-London factor is 1.575. Substituting the Franck-Condon factor, R_e^2, the Hönl-London factor, and $\omega = 12{,}712.7150$ cm^{-1} into equation (1), we find the line oscillator strength to be 0.2583. The oscillator strengths of line in the VO $B-X$ (0, 0) band range from about 0.05 to about 3. These line oscillator strengths are similar with oscillator strengths of TiO, which range from 0.1 to 10.

Figure 4 shows the synthetic spectrum of a cool star [$T_{\text{eff}} = 3200$ K, log (g) = 2.0] calculated with ATLAS, with and without the VO $B-X$ (0, 0) band. The dashed line shows a synthetic spectrum without VO, whereas the thin solid line shows one with VO at solar abundance. Finally, the thick solid line shows a synthetic spectrum with VO calculated with an enhancement of the vanadium 10 times solar abundance.

3.2. Lowest Energy Levels

Table 4 shows our calculations of $E_{J''}$ of the $J'' = 0.5$, 1.5, 2.5, and 3.5 levels of the $B\,^4\Pi$ and $X\,^4\Sigma^-$ $v = 0$ states compared with those given by Adam et al. (1995) for the same J'' levels. Adam et al. analyzed the $B-X$ (0, 0) band from Doppler-limited Fourier transform emission spectra, along with wavelength-resolved laser-induced fluorescence and sub-Doppler intermodulated fluorescence spectra. A least-squares fit of the sub-Doppler data with more than 3000 hyperfine transition frequencies to 38 parameters gives the energy levels. Adam et al. (1995) show a plot of the energy
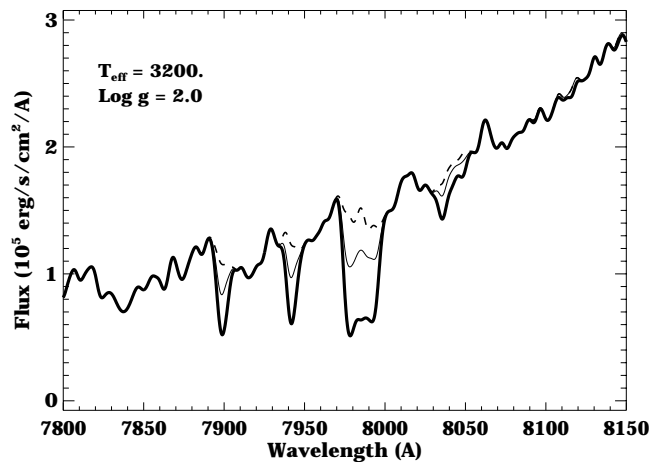

FIG. 4.—Effects of VO shown in synthetic spectra of a 3200 K model with log g = 2.0. The thin solid line has the VO $B-X$ (0, 0) lines included with vanadium set at the solar abundance, whereas the dashed line shows spectra from the same model with the VO lines turned off. The thick solid line repeats the VO calculations, but with the vanadium abundance set to 10 times the solar value. All of the synthetic spectra are convolved with a 3.0 Å FWHM Gaussian. The synthetic spectra with VO only include the $B-X$ (0, 0) bands so that all of the observed VO features are not modeled at this time.

levels for $(J + \frac{1}{2})^2$ from 0 to 6000 and lists the energies for $J = 0.5$, 1.5, 2.5, and 3.5. Our calculations of $E_{J''}$ are within $\sim 10\%$ of the values given by Adam et al. (1995). Also, as a result of the fit, Adam et al. (1995) give the rotation constant $B_v = 0.512652$ cm^{-1}. If we use this value, rather than $B_v = 0.5246$ cm^{-1} calculated from molecular constants, then the energy levels for $J = 0.5$, 1.5, 2.5, and 3.5 are 0.385, 1.922, 4.485, and 8.074 cm^{-1}. These are consistent with our calculations of the energy levels, but still within 10% of those given by Adam et al.

For further comparison, we also calculated $E_{J''}$ using (Herzberg 1950, eq. [III-147])

$$E_{J''} = BJ''(J'' + 1) + (A - B)\Lambda^2 , \qquad (10)$$

where

$$B = \frac{h}{8\pi^2 c \mu_A r_e^2} ,$$

$$A = \frac{h}{8\pi^2 c R_e^2} .$$

For the $B-X$ band, $\Lambda = 0$ and $r_e = 1.589$ Å, so $B = 0.548$ cm^{-1} and $A = 1.40$ cm^{-1}. With these values, we calculate $E_{J''}$ from equation (9) and find the same lowest energy levels that we calculated using equation (8) and shown in Column (2) of Table 4. So, we are self-consistent, but still within only 10% of $E_{J''}$ given by Adam et al. (1995).

TABLE 4
LOWEST ENERGY LEVELS

J''	Our Calculation of $E_{J''}$ (cm^{-1})	Adam et al.'s Calculation of $E_{J''}$ (cm^{-1})
0.5......	0.392	0.616
1.5......	1.960	2.113
2.5......	4.573	4.654
3.5......	8.231	8.196

4. CONCLUSION

We have presented a concise summary for the calculation of molecular oscillator strengths. The Franck-Condon factors are the most straightforward terms to determine. The Hönl-London factors can be determined empirically, as long as experimental data presenting the wavenumbers and angular momenta are available. The sum of the components of the electronic transition moment, R_e^2, is the most difficult term to determine. In order to find R_e^2, we must know the *band* oscillator strength, which is determined either empirically (as was the case in this paper) or theoretically.

We are in the process of incorporating the oscillator strengths, lowest energy levels, and wavenumbers of all of the VO transition bands given in Table 1 into the calculation of the synthetic spectra. In future computations, the synthetic spectra with the VO molecule included in the data set will be compared to our observed spectra of Mira variable stars.

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