A new TiO line list

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Abstract. A new line list for 9 electronic transitions of TiO ($\alpha, \beta, \gamma, \gamma', \delta, \epsilon, \phi$, a-f, and E-B) is presented and made publicly available. It is the latest and much improved version of a suite of TiO line lists inaugurated in Plez et al. (1992). It includes the transition moments of Langhoff (1997) and provides a better match to both high- and low-resolution spectra of cool stars than any previous extensive TiO line list. It is shown to be adequate for most purposes in stellar atmosphere modelling and spectroscopy. The line strengths appear to match observations very well, except for a mismatch of the δ band system, when using Langhoff's transition moment. It appears too strong in the calculations. It would be very valuable to perform accurate lifetime and branching ratios measurements for the δ and ϕ transitions.

Key words: molecular data – stars: atmospheres – stars: late-type

1. Some history

The importance of opacity from the electronic transitions of TiO for the thermal structure and spectrum of cool stars need not be insisted upon once more. Strong absorption bands appearing in M-type star spectra were identified by Fowler as arising from an oxide of Ti as early as 1907. Christy (1929) summarizes the early observations and the identification of TiO in stars. The first attempt to model the absorption of some of these transitions by Collins (1975) and Collins & Faÿ (1976) resulted in a line list, recently extended and corrected by Jørgensen (1994). Investigators of stellar atmospheres used various approximations (straight mean, opacity sampling - OS), and sometimes scaled line-strengths, but allways based their work on Collins (1975) line list. Jørgensen (1994) gives an account of the effects of TiO in stellar atmospheres. Plez et al. (1992, PBN92), however, produced a new line list based on the then best available laboratory data. They computed energy levels from molecular constants, and Franck-Condon factors (FCF) and Hönl-London factors (HLF). Transitions were computed up to high v and J values. Only ^{48}Ti^{16}O was included. Average electronic transition moments were taken from Davis et al. (1986). Unfortunately only an astrophysical calibration of the ϵ transition

strength was available then (Brett 1990). That list proved to be quite adequate and was subsequently used in a variety of applications: stellar atmosphere models for cool giants (PBN92, Plez 1992) and dwarfs (Brett & Plez 1993, Brett 1995a, 1995b), and high resolution spectroscopy (Plez et al. 1993) where it was demonstrated that the line positions, although not perfect, were quite adequate for abundance analysis of cool red giants. Later, the line list was improved upon by scaling the strength of some systems according to new lifetime measurements (Doverstål & Weijnitz 1992). At that point it was used to generate new models for an investigation of the spectrophotometry and temperature scale of M giants (Fluks et al. 1994). More improvements and changes (e.g. inclusion of isotopes of Ti) were made along the years. The line list, however, was never published, and I feel it is time for a public release of this data, especially after some dramatic breakthrough by Langhoff (1997) who computed reliable ab initio electronic transition moments that I recently included. Also the possibility to include the line list in the VALD database (Piskunov et al. 1995) will ease its consultation and its inclusion in synthetic spectrum calculations. Some preliminary accounts on the present new line list and its historical predecessors are presented by Alvarez & Plez (1998) and Bessell et al. (1998). Note that Schwenke (1998) independently proposes a new line list for TiO, with a few more transitions included, based on the ab initio work of Langhoff and the available laboratory data. This list appears too late for comparisons with the present data.

2. The new line list

2.1. Method and data

The main task when producing a line list from molecular constants is the collection and evaluation of existing data. Energy levels can then be calculated using polynomial expansions (see e.g. Herzberg 1989, and references given below for the various electronic levels). Transitions between these levels are then derived taking proper account of parity and other selection rules. A line is defined as being one component of a Λ-doublet. It is only degenerate in its magnetic substates and its hyperfine structure (see Larsson 1983 for definitions and conversions between various conventions). All satellite lines were included, and Λ-doubling accounted for. This results for example in $3 \times 3 \times 3 \times 2$ lines for a transition between 2 triplet states for each combina-

tion of v', v'' and J' ($'$ and $''$ denote the upper and lower level respectively, v is the vibrational and J is the rotational quantum number). This amounts to 2.7 million lines per isotope for v up to 15 and J up to 200 for one triplet-triplet transition. Of course a number of these lines are extremely faint. After some cut is imposed in strength the number becomes more reasonable.

Separating the wave functions according to the Born-Oppenheimer approximation, the line strength is expressed as:

$$S_{J'J''} = | < v'_{J'}|R_e(r)|v''_{J''} > |^2 \mathcal{S}_{J'J''}, \qquad (1)$$

where $\mathcal{S}_{J'J''}$ is the HLF, R_e is the electronic transition moment, r the internuclear distance, and $< v'_{J'}|$ and $|v''_{J''} >$ are the upper and lower state vibrational wave functions derived from the effective potential energy curves for the rotating molecule. When only average $R_e^2(\bar{r})$, lifetimes, or band oscillator strengths are available, the r-centroid approximation has to be used and FCFs calculated :

$$q_{v'J',v''J''} = | < v'_{J'}|v''_{J''} > |^2.$$

This was done in previous versions of my TiO line list. In the present case, transition moments from Langhoff's investigation (1997) were used. Computer programs from Whiting (1972, 1973) and Jarmain (1971) were used for calculating HLFs and the integral in Eq. (1).

The TiO molecule has been the object of many experimental studies and, more recently, of a number of theoretical investigations. Molecular constants necessary for the computation of energy levels and line strengths were collected from a variety of sources: Amiot et al. (1995, 1996), Hocking et al. (1979), Huber & Herzberg (1979), Kaledin et al. (1995), Merer (1989), Phillips (1971, 1973, 1974), Simard & Hackett (1991). The data differs from the set of values adopted by Jørgensen (1994). Note that the T_e values for the b, c, d and f singlet levels listed in Table 2 of Jørgensen (1994) are too low by about 2760cm^{-1}. The T_e value for the a level should be 3346.34cm^{-1}, to reproduce the observations by Kaledin et al. (1995) of the forbidden $C^3\Delta_3 - a^1\Delta$ transition. Except for the inclusion of the ϵ system, Jørgensen did not improve on the molecular constants initially adopted by Collins (1975). By contrast, I included the result of more recent studies and tried to reproduce more accurately the observed line positions. This, combined with the inclusion of internuclear distance-dependent transition moments leads to a line list in much better agreement with various observations at high and low spectral resolution. I included also the a-f transition system, which absorbs in the same region as the α system, i.e. mostly around the V band. The E-B system in the IR was found to be very faint and virtually invisible but is included in the line list. All five isotopes of Ti were included, with the corresponding energy levels calculated by multiplying the molecular constants by the proper mass factor (Herzberg 1989).

The transitions were computed up to v=15, J=200, with a cut in strength defined as follows. For each line the quantity $gf \exp -(h E_l/kT)$, where E_l is the energy of the lower level, was computed for T=4000K. Lines were kept in the list if this number was at least 10^{-7} of the strongest of all lines. This

ensures that up to 4000K, no line with an intensity larger than that threshold is missing. At higher temperature extremely faint lines may be missing. This is hardly of any significance. With gf-values scaled by the solar Ti isotopic ratios, and the cut in strength of 10^{-7} the total number of lines in the 9 transitions is about 15.7 million lines.

2.2. Line positions

Line positions were compared with the Berkeley data (available at http://sumner.berkeley.edu/) for the bands they observed in the $\alpha, \beta, \gamma, and \gamma'$ systems. I computed the mean $o-c$ (observed - calculated position) and its standard deviation, as well as the maximum $o-c$ with the rotational number J where it is reached, for each band, and for the whole set of bands in each transition. The result is displayed in Table 1. The γ bands show only small deviations, even for higher v and J values. The β bands line positions are also quite good, becoming worse at higher v. The line positions in the α system are quite good, but their accuracy decreases with increasing v (esp. v'). The γ' system wavenumbers tend to deviate systematically at high J, the P2, Q2 and R2 branches being more accurate. This reflects missing higher order terms in the term-values polynomial fits. Note that newer, often more accurate line position measurements have been performed by other groups and were used to fine-tune some of the molecular constants (e.g. Amiot et al. 1995, Ram et al. 1996, Hocking et al. 1979).

2.3. Lifetimes and band-strengths

The transition moments of Langhoff (1997) at the IC-MRCI level were included for all transitions except the α-band system which he provides only at the CASSCF level. Langhoff's potential energy curves are different from the Klein-Dunham potentials with Morse extension used here, but the difference is small as shown by him. The lifetimes of the various levels resulting from the present computation are very close to Langhoff's values. Langhoff compared his results with laboratory determinations and with the earlier calculations of Schamps et al. (1992). He found a general good agreement with the latter and with the lifetimes measurements of Hedgecock et al. (1995) for the triplet transitions. Note the recent measurement of the lifetime of the E$^3\Pi_0$ level at $4.9 \pm 0.2\mu s$ by Lundevall (1998) within 15% of Langhoff's value of 4.3. Large differences were found by Langhoff for the δ and ϕ transitions. As is demonstrated below the use of Langhoff's transition moments is an improvement over the r-centroid approximation and past oscillator-strengths (esp. for ϵ). One notable exception is the δ band system which seems too strong by a factor of about 2 when using Langhoff's prescription. This is further discussed below, and I finally adopted half of Langhoff's strength in the line list for this system. Also, by comparison with the lifetime measurements of Hedgecock et al. (1995), Langhoff discusses the possibility that his calculations overestimate the strength of the β system by about 40%. I kept however Langhoff's value,

Table 1. Observed - calculated line positions. For each band are listed: the number of lines compared, the average $o-c$, and standard deviation, and the maximum $o-c$ with the J where it is reached. Observations from the Berkeley database, http://sumner.berkeley.edu/

Band	lines	$\overline{o-c}$ (cm^{-1})	$\sigma(o-c)$ (cm^{-1})	$(o-c)$ max (cm^{-1})	J
$\alpha(0-0)$	879	0.268	0.634	-2.954	158
$\alpha(0-1)$	865	0.319	0.566	-2.273	150
$\alpha(0-2)$	702	0.364	0.448	-1.539	142
$\alpha(0-3)$	437	0.477	0.380	1.466	61
$\alpha(1-0)$	849	0.630	0.797	3.925	155
$\alpha(1-2)$	707	0.470	0.578	2.648	125
$\alpha(1-3)$	629	0.556	0.807	5.079	120
$\alpha(2-0)$	605	0.217	0.872	2.306	103
$\alpha(2-1)$	650	0.398	1.134	4.134	126
$\alpha(2-3)$	347	-0.246	0.583	-1.524	6
$\alpha(2-4)$	578	0.736	1.866	8.612	112
$\alpha(3-1)$	628	1.416	1.782	8.256	119
$\alpha(3-5)$	464	0.815	1.161	6.260	113
$\alpha(4-2)$	437	1.205	1.104	6.001	89
α all	8777	0.537	1.054	8.612	112
$\beta(0-0)$	291	0.412	0.964	5.215	100
$\beta(1-1)$	283	0.483	1.309	-5.403	100
$\beta(2-2)$	252	1.255	0.870	3.246	79
β all	826	0.693	1.132	-5.403	100
$\gamma(0-0)$	1353	-0.115	0.254	-1.186	165
$\gamma(0-1)$	1276	-0.057	0.207	0.853	146
$\gamma(0-2)$	766	0.004	0.139	-0.934	117
$\gamma(1-0)$	1259	-0.208	0.236	-1.122	147
$\gamma(1-1)$	1308	-0.202	0.223	-1.094	149
$\gamma(1-2)$	1108	-0.103	0.155	-1.510	132
$\gamma(1-3)$	986	-0.018	0.191	1.402	142
$\gamma(2-0)$	1229	-0.218	0.251	-1.219	155
$\gamma(2-1)$	1211	-0.182	0.195	-0.951	137
$\gamma(2-3)$	1150	-0.037	0.189	0.818	147
$\gamma(2-4)$	854	-0.046	0.121	-0.715	125
$\gamma(3-1)$	1115	-0.123	0.155	-0.723	127
$\gamma(3-2)$	1155	-0.065	0.201	-0.788	137
$\gamma(3-4)$	1026	0.027	0.144	0.559	130
$\gamma(3-5)$	978	-0.020	0.130	0.549	126
$\gamma(4-2)$	1077	-0.045	0.204	1.299	135
$\gamma(4-3)$	1080	0.007	0.137	-0.450	110
$\gamma(4-5)$	1035	0.004	0.165	-0.589	132
$\gamma(5-3)$	1025	-0.035	0.129	-0.558	117
γ all	20991	-0.082	0.205	-1.510	132
$\gamma\prime(0-0)$	1574	2.455	2.152	13.298	139
$\gamma\prime(0-1)$	1515	2.385	2.033	11.096	127
$\gamma\prime(1-0)$	1478	2.225	1.316	8.052	124
$\gamma\prime$ all	4567	2.357	1.880	13.298	139

not beeing able to test lines of this system against spectroscopic observations.

3. Comparison with Jørgensen's line list

In model atmosphere calculations very precise line positions are not a critical ingredient. Rather, the general distribution and
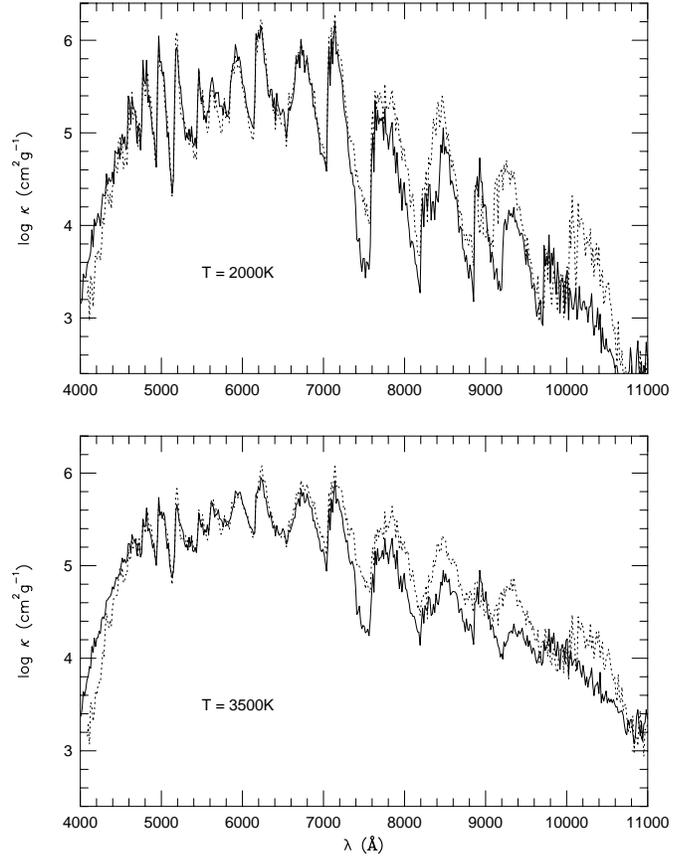
Fig. 1. TiO opacity averaged over 15Å intervals at 2000 K and 3500 K. Present line list: full line; Jørgensen's line list: dotted line.

strength of opacity over the spectrum and depth in the atmosphere needs to be well reproduced. As one of the main use of extensive line lists is opacity calculations for stellar atmospheres, it is useful to compare at low spectral resolution the present line list with Jørgensen's (1994) work. An easy way to carry out this comparison is to compute the opacity per gram of TiO on a sample of wavelengths at various temperatures, i.e to calculate an opacity sampling (OS) for each line list. These OS can then be compared, as well as model atmospheres and low resolution synthetic spectra computed with them.

I added the contribution of all lines of each list on the sample of 10912 wavenumbers used in the SOSMARCS model atmosphere code (PBN92), for temperatures from 1000K to 5000K. The step of the sampling is about 1Å below 7200Å and 2Å above. The line broadening was assumed purely gaussian with a thermal and a microturbulence contribution (2 kms^{-1}). Fig. 1 shows both opacities smoothed by averaging them over 15Å intervals. The difference is large in the red where the ϵ transition strength of Jørgensen is much larger than in the present work. His bandheads appear also shifted to the blue, as e.g around 8500Å and 9200Å. Apart from that very discrepant system, the overall shape and even strength of the opacity are quite similar, but Jørgensen's opacity becomes systematically fainter at shorter wavelengths. This appears surprising as the strength of most systems is fainter in the present line list, but may be ex-

plained by my addition of the a-f bands system, and by the redistribution of the strength of the α, γ, and $\gamma\prime$ systems towards shorter wavelengths by the inclusion of Langhoff's transition moments.

I computed model atmospheres of three representative red giants of solar composition with T_{eff} of 3200 K, 3650 K and 3900 K. The difference in temperature on the τ_{12000}-scale around $\tau = 10^{-5}$ is less than 5 K at T_{eff}=3900 K, less than 10 K at T_{eff}=3650 K, and 20 to 30 K at T_{eff}=3200 K, decreasing inwards. Models computed with Jørgensen's TiO opacity are warmer. The pressure differs by a few percents only. This reflects the similarity of the OS underlined above. Although the thermal structure of the models computed with the 2 data sets are quite similar, the spectra differ by larger amounts. The maximum differences in flux are of the order of 5% for $\lambda > 6500$Å at T_{eff}=3900 K, around 20% at T_{eff}=3650 K, and more than 50% at T_{eff}=3200 K. At shorter wavelengths the respective differences are 10 to 20%, 50%, and a few 100 %, the flux of the models computed with Jørgensen's TiO being generally larger.
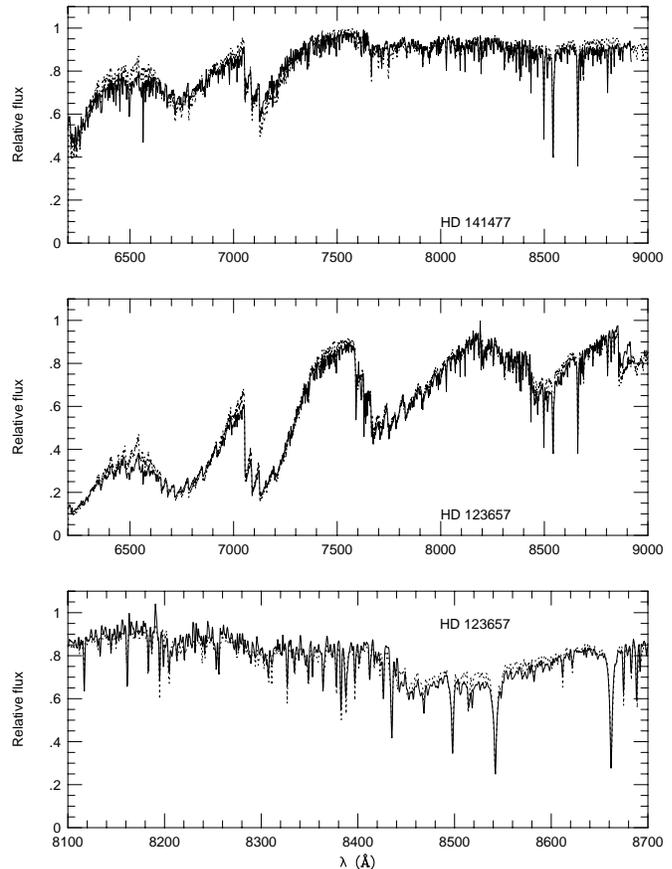
4. Comparisons to observations

4.1. High-resolution stellar spectroscopy

An earlier version of the present line list was used by Plez et al. (1993) to carry out a chemical analysis of AGB stars in the SMC. High-resolution spectra ($R = \lambda/\Delta\lambda = 20000$) in the range 6500 to 7900Å were compared to detailed synthetic spectra. The overall agreement was quite good (e.g. bandheads position and depth), with however discrepancies in the detailed structure of the spectra (see figures in Plez et al. 1993, which provide a good idea of the performances of the list). In earlier similar studies, using more limited TiO line lists, some fudge pseudo-continuous opacity had to be advocated. With the present extensive list this becomes superfluous and the spectra are well modelled thanks to the veil due to the numerous faint lines. When possible, replacing the calculated wavenumbers by the Berkeley, or other laboratory measured wavenumbers should further improve the fit to observations. Preliminary test calculations by Piskunov for warmer M dwarfs in the near-IR and by Pavlenko around the Li I lines at 6707Å and 8126Å in cool M dwarfs tend to indicate that the TiO band strengths in these regions better match the observations than other lists. The case of dwarfs is delicate however, as other, less well-known, opacities like hydrides interfere in the spectrum. Further, uncertainties about the pressure broadening coefficients for TiO (and other molecules) complicate the comparison between observations and synthetic spectra.

4.2. Spectrophotometry of M-giant stars

Recently, Bessell et al. (1998) used models and model spectra calculated with the present line list to compute synthetic colours (BVRIJHK) and bolometric corrections, and compared them to observations. They found a better fit than with the older models of PBN92. A large part of the improvement is due to the new TiO opacity data, but part of it is also caused by better VO and H_2O

Fig. 2. Comparison of synthetic spectra (dotted line) with observations from Serote Roos et al. (1996, full line). The spectra were degraded to a resolution of about 4Å, in the upper 2 panels.

opacities. Bessell et al. find also good agreement with observed colours for cool dwarfs, except for some IR bands. Unsolved problems with other opacities, e.g. H_2O, may well be the cause of these discrepancies. It is therefore difficult at present to assess the quality of the TiO line list using M-dwarfs.

Alvarez & Plez (1998) computed narrow-band photometry in the 7500-11000Å range for M giants and miras and found very good agreement with observations. Also there, significant improvement was achieved by including the lifetimes from Langhoff (1997), except for the δ band (see Sect. 4.3).

Serote Roos et al. (1996) present carefully calibrated spectra of cool stars at a resolution of up to 1.25Å. Fig. 2 shows a comparison of their spectra for HD 141477 (M0 III) and HD 123657 (M5 III) with synthetic spectra including the present line list as well as a line list for VO (PBN92, Alvarez & Plez 1998), CN (Jørgensen & Larsson 1990), and atoms from Kurucz (1994). Spherically symmetric solar abundance models were computed with SOSMARCS (PBN92) for T_{eff}=3800 K, logg=1.5, and T_{eff}=3500 K, logg=0.9, both for 1.5 $M_\odot$. Synthetic spectra were calculated with a 0.1Å step and then degraded to about 4Å resolution, as well as the observed spectra. A blow-up at the original resolution of the observations is also shown. The calculations were made with the TurboSpectrum package, sharing most

of its routines with SOSMARCS. The chemical equilibrium is solved for more than 300 molecules using dissociation energies and partition functions from Sauval & Tatum (1984) and Irwin (1988), with some updates (Sauval 1996, private comm. and Irwin 1996, private comm.). The dissociation energy of TiO seems now firmly established with the recent determination of $D_0 = 6.87^{+0.07}_{-0.05}$ eV by Naulin et al. (1997) in agreement with the value of 6.87 recommended by Huber & Herzberg (1979).

The agreement in Fig. 2 is very good, with the exception of an absorption band which appears in the observations around 6500Å but is not present in the synthetic spectra. Part of the differences may be due to calibration problems in the observations. Serote Roos et al. find residuals of up to 10% when comparing their K-type spectra to Silva & Cornell (1992) observations. The abundance pattern of the two stars may not be solar, and fine tuning of the stellar parameters may provide a better agreement. We can however not exclude that some opacity source is missing at 6500Å or that the present TiO line list is defectuous in this region. Closer scrutiny at high spectral resolution in more stars is necessary. Despite these small local disagreements, Fig. 2 illustrates the overall good match provided by the new TiO line list at spectral resolution typical of population synthesis work.

4.3. The δ(0-0) bandhead at 8860Å

Alvarez & Plez (1998) already noted that the δ band around 8900Å appeared too strong when computed with Langhoff's (1997) strength. The observations of the δ(0-0) bandhead of Ramsey (1981) are a useful test of the strength of that band in model spectra. Ramsey measured the bandhead depression relative to the local continuum in giant stars of spectral types K4 to M6. The spectral types were translated to T_{eff} using the Ridgway et al. (1980) calibration. I computed a series of SOSMARCS model atmospheres spanning the same range of T_{eff} and derived the bandhead depression from high resolution spectra degraded to the same resolution as Ramsey's spectra. The calculation was first done with Langhoff's value of the transition moment, then with half that strength. Fig. 3 shows the loci of the calculated depressions on top of Ramsey's measurements. The δ bandhead as calculated with Langhoff's transition moment is obviously too strong for all temperatures, whereas half that strength provides a good fit down to 3400K, where observations level off while the synthetic band-depth continues to increase. This may have various causes, e.g. uncertain scattered-light correction in the observations, depression of the local continuum by additional opacity not accounted for in the synthetic spectrum, as well as increasing uncertainties in cooler star models. It must be stressed that a shift of the T_{eff} scale by 100K, which would place the full-strength calculation in coincidence with the observations is excluded. The temperature scale of the new SOSMARCS models was carefully checked by Fluks et al. (1994) by comparing synthetic spectra to spectrophotometric data, and more recently by Bessell et al. (1998) using broad-band photometry, and in both cases an excellent agreement with the Ridgway et al. scale was found. Alvarez & Plez (1998) used the half-strength to model M-giant spectra in
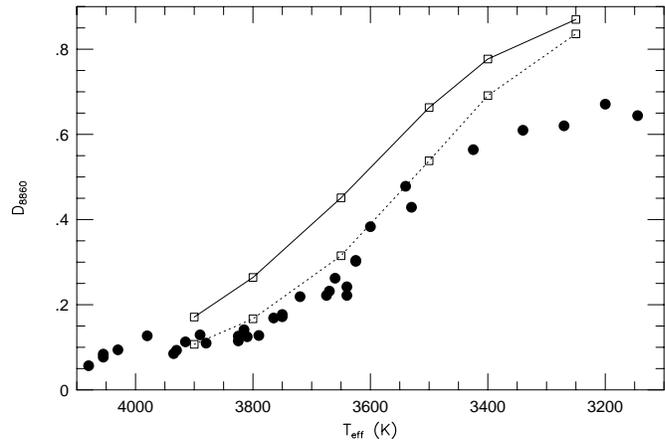
Fig. 3. δ(0-0) R-bandhead depression at 8860Å vs. T_{eff}. The full line is drawn from synthetic spectra using Langhoff's transition moment, and the dotted line using half that value. The circles are Ramsey's (1981) observations.

the far-red and found excellent agreement with observations. I therefore decided to divide by 2 the gf-values of all the lines of the δ band-system as computed with Langhoff's transition moment. Note that the band oscillator strength is then approximately Davis et al. (1986) value, whereas it is not the case for most of the other bands (see Alvarez & Plez 1998). The cause of that mismatch is unexplained, as there is no particular reason for Langhoff's calculations to be in large error for just that transition. It would be worth performing similar comparisons for other bandheads, especially the singlets, and to carry out lifetime measurements of the $b^1\pi$ electronic state and of branching ratios between the δ and φ transitions.

5. Summary

A new line list for 9 electronic transitions of TiO was presented. It is based on the best available laboratory data and recent ab initio calculations of electronic transition moments. It includes lines for all five stable isotopes of Ti. It was shown to be better than existing data through comparison with high- and low-resolution spectroscopic observations and photometry. It appears very well suited for opacity calculations and inclusion into model stellar atmospheres. Small line position adjustments may be needed for accurate high-resolution spectroscopic analysis of cool stars. A mismatch in the δ band strength remains unexplained and I decided to adopt half the transition moment of Langhoff (1997). I recommend therefore that reliable lifetimes and branching ratios be determined for the singlet levels and transitions.

The line list will be made available through the VALD database (Piskunov et al. 1995), as well as through ftp access on the Uppsala opacity database (www.astro.uu.se).

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