Description of the SCAN-TIO line list.

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The computation of the SCAN-TIO line list has been described in detail in my paper "Effects of TiO in stellar atmospheres", U.G.Jørgensen, A&A, 284, 179−186, 1994, which I kindly ask you to refer to if you want to use the data. Also, I kindly ask you not to distribute the lists, but instead refer interested friends and colleagues to the ftp site where you found the data (stella.nbi.dk, anonymous login with your userid as password, cd to pub/scan). The data are occasionally updated if errors are discovered or improved molecular constants etc have become available which can influence the line list data. New lists are added to the old ones when time permits. So, to optimise the completeness and to minimise the risk of circulating data with errors, each user aught to look for his data himself at this ftp site as he wants to use them. Therefore, please try to be a bit unfriendly in sharing your data, but friendly in advising the ftp address if somebody asks you for the data. Of course I am also curious about the possible use you have of the data, so I gladly hear about your projects and results. I try to keep a list of email addresses of people to whom I send an information file if the lists I know of that they have been using are updated. I have described the whole SCAN molecular data base, and compared it to other available data, in U.G.Jørgensen, "Cool Star Models", In: E.F.vanDishoeck (ed.), *Molecules in Astrophysics: Probes and Processes* (IAU Symp. 178), Kluwer, 1997, p.441−456.

I have not computed the TiO line list from scratch, rather this list is an updated version of the original line list computed by James Collins in his Thesis work from Indiana University in 1975, which has been described by Collins & Faÿ 1974 (JQSRT, 14, 1259), Collins 1975 (J.Phys.B, 1975, 304), and Krupp et al. 1978 (ApJ 219, 963). My update of the list include computation of the epsilon system, computation of the relevant isotopic shifts, and inclusions of effects due to improved molecular constants. The most important change in molecular constants since Collins' work is a new measurement of the energy of the electronic a-level. The value adopted by Collins was $\mathrm{T_e(a)} = 581.0\ \mathrm{cm}^{-1}$, whereas I have adopted the 6 times larger value $\mathrm{T_e(a)} = 3448.32\ \mathrm{cm}^{-1}$ as described in my paper. Since the energy of all the singlet states are measured relative to the a-level, the new value of $\mathrm{T_e(a)}$ means that the excitation energies of the lines from all the singlet transitions are larger by $\Delta\mathrm{T_e(a)} = 3448.32-581.0 = 2867.32\ \mathrm{cm}^{-1}$ compared to the original line list. This in turn means that all the computed singlet transitions become considerably weaker relative to the triplet transitions, provided the same f-values are adopted. Furthermore a major revision of the partition functions turned out to be necessary, as will be described below.

The compilation consist of approximately 12 million transitions from 7 electronic systems ($\alpha(\mathrm{C}^3\Delta-\mathrm{X}^3\Delta)$, $\beta(\mathrm{c}^1\Phi-\mathrm{a}^1\Delta)$, $\gamma'(\mathrm{B}^3\Pi-\mathrm{X}^3\Delta)$, $\gamma(\mathrm{A}^3\Phi-\mathrm{X}^3\Delta)$, $\epsilon(\mathrm{E}^3\Pi-\mathrm{X}^3\Delta)$, $\delta(\mathrm{b}^1\Pi-\mathrm{a}^1\Delta)$, $\phi(\mathrm{b}^1\Pi-\mathrm{d}^1\Sigma)$) and 5 different isotopes ($^{46}\mathrm{Ti}^{16}\mathrm{O}$, $^{47}\mathrm{Ti}^{16}\mathrm{O}$, $^{48}\mathrm{Ti}^{16}\mathrm{O}$, $^{49}\mathrm{Ti}^{16}\mathrm{O}$, $^{50}\mathrm{Ti}^{16}\mathrm{O}$). The line list exist in two versions on the disk. One version list each of the elec-

tronic systems separately in pure ascii format. Each of these files fill from 5 to 70 MB on the disk. They are named scan_tio_epsilon.dat, scan_tio_gamma.dat, scan_tio_delta.dat, etc (the first two lines in the files identify the transition name and gives the number of calculated lines in the transition). Another version of the same line list is compiled such that all lines from the 7 systems are in the same file, ordered according to increasing wavenumber. This version is compressed, and needs to be uncompressed with the command gunzip by the receiver after having transfered the file. Remember to do binary ftp in this case. In both versions, each line in a file list the variables:
wn, ex, gf, el_trans, v_low, v_up, j_low, j_up, branch, nu_46, nu_47, nu_49, nu_50
in the format f10.3, f12.5, 1pe11.4, i2, 2i3, 2i4, i3, 0p4f8.3 (i.e., the line list can be read in free format), and with the following meaning of the variables:

- wn is the wavenumber in cm^{-1} of the listed transition for ^{46}TiO.
- ex is the excitation energy measured relative to the lowest electronic-vibrational-rotational level (i.e., v = 0, J = 1 in the $X^3\Delta_1$ electronic multiplet). With the adopted molecular constants this lowest energy is 396.354 cm^{-1} above the potential minimum.
- gf. The real, physical and dimensionless gf value of the spectral line is obtained from the listed variable gf by multiplying the listed value with the f-value ($f_{el}(\nu_{00})$), times the wavenumber of the line (wn), divided by the band centre wavenumber (ν_{00}) as described in my paper. Values of $f_{el}(\nu_{00})$ and ν_{00} can be found in Table 1 in my paper, or other values preferred by the user can be multiplied on the listed gf variable. Recent experimental f-values have been determined by Costes and collaborators, and recent theoretical f-values have been published by Langhoff and collaborators. The conversion factor from the computed, physical gf-values to line strengths in cm/mol is $5.33137\,10^{11}$.
- el_trans is an identification of the electronic system (1$\sim$ α, 2$\sim$ β, 3$\sim$ γ', 4$\sim$ γ, 5$\sim$ ϵ, 6$\sim$ δ, 7$\sim$ ϕ)
- v_low, v_up, j_low, and j_up designates the v and J quantum numbers of the lower and upper state
- branch designates the branch (a number between 1 and 27, see my paper or standard text books for details).
- nu_46, nu_47, nu_49, and nu_50 are the isotopic shifts in cm^{-1}, such that for example nu_50 means that $\nu(^{50}Ti^{16}O) = \nu(^{48}Ti^{16}O)$ + nu_50.

Remark that all the triplet states in TiO have total electronic orbital momentum Λ = 2 ($\sim$ Δ state) and total electronic spin S = 1 ($\sim$ triplet state). Therefore the total electronic angular momentum $\Omega = \Lambda + \Sigma$ can take the values 3, 2, 1 ($\sim$ $^3\Delta_3$, $^3\Delta_2$, and $^3\Delta_1$ states). In addition the coupling between orbital electronic motion and rotation of the molecule give rise to a Λ doubling of all Δ states (i.e., + and - rotational states). In principle therefore all vibrational-rotational levels in a given triplet state appears 6 times (but there will be more transitions than the 3 branches corresponding to $J_{up} - J_{low} = 0, \pm 1$ from each state of a given v, J quantum number, because different couplings in the upper and lower electronic states may permit transitions between states with different value of Ω too). Whereas the multiplet splitting generally is large (typically 100 cm^{-1} or more), the Λ splitting may be very small or even zero. In several cases the Λ splitting constants are not known, and in such cases they have been set to zero. This means that it may look like, at a first glance, that many energy levels are listed twice. If the the splitting is close to zero for both the upper and the lower electronic level of the transition, it may even look like that the same line is listed more than once. It should, however, be reminded that these double listings are physically correct, and one day astrophysically studies may give us new insight into the molecular structure by actually observing such splittings and their dependences on the quantum numbers in for example high resolution studies of the solar (spot) spectrum. The doublings should therefore not be treated as one line.

Remark also that the J quantum number is a sum of the electronic and nuclear angular momentums, and therefore has a minimum value, which is different for the different electronic systems, so do not necessarily expect to find transitions with J = 0. Finally, remark that the listing of the excitation energy now is relative to the lowest populated state, not relative to the potential minimum as it was in earlier versions of the list.

The number of levels with identical main quantum numbers, the minimum J quantum numbers, and the excitation energies of the levels (in particular the electronic energies, T_e) and the reference energy, should of course be treated consistently in the line list data and the partition functions adopted in order to compute correct opacities, spectra, etc, from the line list data. In my paper on TiO, I recommended the use of the partition functions from Tatum (1966) because these (as the line list data on the scan_tio line list, and in agreement with present day believe) are based on a rather high value of T_e for the a-state, contrary to what was the generally accepted value for a large number of years until recently. However, I overlooked that the reference energy in the work of Tatum and the line list was not identical. The reference energy of the partition functions computed originally by Collins in his Thesis was identical to the original line list (and presumably these were used in the earlier works on TiO), but these, on the other hand, turned out to have an error in the computation of the number of levels with a given set of main quantum numbers (each of the multiplet levels of the triplet states were presumable counted twice for each Λ doublet), and of course the lower energy of the electronic a-state was adopted according to the generally accepted value then.

Since it therefore turns out that none of the computed partition functions published in the literature are consistent with the line list in any form, I decided to compute a set of partition functions directly from the line list as a sum of all the lower levels appearing on the line list (taking into consideration the appropriate possible lambda type doubling of each level). The lower levels all originate in the electronic X-, a-, or d-state, as can be seen from the tables in my paper, and in total there is a little less than 20,000 such levels in the line list. The partition function, calculated as a sum over 2j+1 times the exponential of minus the energy of these levels (i.e., $(2j+1)\exp(-E_{low}hc/kT)$), is listed in the table below (all degenerated vibrational states are counted separately, so that no degeneration factor is multiplied in front of the factor 2J+1). For higher temperatures, levels not included as lower levels in any line on the line list (i.e., mainly states from higher electronic levels than the d-level) may play a role for the value of the partition function. I therefore include also a partition function based on all the levels which are either upper or lower level in any line on the list. In theory these partition functions should be used for synthetic spectrum calculations, whereas the former partition functions (i.e., those based only on the lower levels originating in the X, a, and d electronic states) are recommended for opacity computations. The lower value of the partition function recommended for opacity computations partly compensates for the "missing" lines by distributing approximately the missing intensity over the existing lines, whereas the more "complete" partition function is the theoretically more correct one when the aim is correct intensity of the individual spectral lines. In practice the differences between the two partition functions are however small (less than 1% below 3000 K, but increasing up to almost 10% at 5000 K and more than 25% at 8000 K). For comparison typical differences between the largest of these partition functions and the one of Tatum (1966) is around 10% at most temperatures, and the partition functions computed by Collins is typically a factor of 2 to 3 larger (which is partly due to a difference in reference state, partly due to the mentioned error, and partly due to a difference in the adopted energy of the a-state). For comparison these two latter partition functions are also listed, but it should be remembered that they are not consistent with the line list.

Table 1: Partition functions for TiO.

Temperature	X,a,d levels	all 7 levels	Tatum 66	Collins 75
200.	8.645E+02	8.645E+02		
400.	2.297E+03	2.297E+03		
600.	4.090E+03	4.090E+03		
800.	6.290E+03	6.290E+03		
1000.	8.932E+03	8.932E+03	1.027e+04	1.5752e+04
1200.	1.204E+04	1.204E+04		
1400.	1.565E+04	1.565E+04		
1600.	1.977E+04	1.977E+04		
1800.	2.442E+04	2.443E+04		
2000.	2.964E+04	2.964E+04	3.081e+04	6.9584e+04
2200.	3.541E+04	3.544E+04		
2400.	4.177E+04	4.182E+04		
2600.	4.871E+04	4.881E+04		
2800.	5.622E+04	5.642E+04		
3000.	6.432E+04	6.467E+04	6.308e+04	1.6360e+05
3200.	7.299E+04	7.358E+04		
3400.	8.222E+04	8.315E+04		
3600.	9.200E+04	9.342E+04		
3800.	1.023E+05	1.044E+05		
4000.	1.132E+05	1.161E+05	1.087e+05	3.0515e+05
4200.	1.245E+05	1.285E+05		
4400.	1.363E+05	1.417E+05		
4600.	1.486E+05	1.557E+05		
4800.	1.613E+05	1.705E+05		
5000.	1.745E+05	1.861E+05	1.707e+05	5.0897e+05
5200.	1.880E+05	2.025E+05		
5400.	2.020E+05	2.198E+05		
5600.	2.163E+05	2.379E+05		
5800.	2.309E+05	2.568E+05		
6000.	2.458E+05	2.766E+05	2.531e+05	
6200.	2.611E+05	2.973E+05		
6400.	2.766E+05	3.188E+05		
6600.	2.923E+05	3.412E+05		
6800.	3.083E+05	3.645E+05		
7000.	3.245E+05	3.885E+05	3.607e+05	
7200.	3.409E+05	4.135E+05		
7400.	3.575E+05	4.392E+05		
7600.	3.742E+05	4.658E+05		
7800.	3.911E+05	4.932E+05		
8000.	4.081E+05	5.213E+05	4.990e+05	