Opacity Incompleteness and Atmospheres of Late-type Stars

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Abstract. The completeness of opacity data for model photospheres of late-type stars is discussed. It is concluded that for the Sun there are still indications that the ultraviolet opacity is not quite satisfactorily described by existing data; a problem that is still more pronounced for K giants. For M, N, and S stars the situation is improving rapidly, but is still far from satisfactory due to incomplete data for a number of molecules. The significance of these shortcomings is discussed in view of other, perhaps more fundamental problems in the modeling of late-type stellar atmospheres.

1. Introduction

The need for adequate opacity data to model stellar photospheres was appreciated in the 1930's (McCrea 1931, Strömgren 1932) and in fact was illustrated clearly by the demonstration of the negative hydrogen ion as the most significant opacity source for solar type stars (Wildt 1939). Later, the need for adding further opacity in modeling the ultraviolet part of the solar spectrum has been repeatedly stressed (e. g., Matshushima 1968, Gustafsson et al. 1975). This opacity source has sometimes been referred to as the “missing” or “unknown” opacity, although it has since long been argued that it could be due to a “veil” of weak metal lines (e. g., by Carbon, Gingerich & Kurucz 1968, Holweger 1970).

A zero-order effect of a missing opacity is that the model atmosphere gets too compact - the pressures become unrealistically high. This follows directly from the equation of hydrostatic equilibrium,

$$\frac{dP}{d\tau} = g \frac{\kappa}{\chi},$$

(1)

where P is the total pressure, \( \tau \) the optical depth, g the surface gravity, and \( \kappa \) the opacity per gram corresponding to the optical-depth scale. Thus, if \( \kappa \) is underestimated by a certain factor \( X \) one sees directly that the pressure of the model increases. If \( \kappa \) is roughly proportional to the pressure, as is the case for \( \text{H}^- \) absorption as well as absorption from a veil of neutral metal atoms like iron in solar-type stars, the relative pressure increase is on the order of 0.5 \( X \). A zero-order effect of such an error in the monochromatic absorption coefficient \( \kappa_\nu \) on
the calculated line spectrum is that the strength of a weak line, with an
equivalent width, proportional to \( l_r / \kappa \), where \( l_r \) is the line absorption
coefficient, will be overestimated by roughly the same factor. For inter-
mediate- and late-type stars this is often compensated for since \( \kappa \)
 itself increases with the pressure (or, really, the electron pressure). This holds true
for lines due to atoms in ionization states that dominate for the element in
question. For the majority of spectral lines in a solar-type stellar spectrum,
however, which are due to neutral atoms of elements that mainly exist in
ionized form, such as iron, there is also an effect on the neutral fraction of the
element - this fraction is approximately proportional to the pressure, i. e., to \( X \).
Thus, at an underestimated \( \kappa \), the spectral line strengths from these elements
are overestimated to a similar degree. A similar phenomenon occurs for cooler
models with underestimated opacity where the formation of certain molecules
(and thus the strength of corresponding molecular lines) is highly pressure
sensitive. This does not only affect the stellar spectra by blocking extra
radiation but it also (at a constant effective temperature, i. e. constant total
flux) forces an increase in the temperature (the so-called backwarming) of the
regions where the continuous flux is formed. What would be the quantitative
effects of this on the temperature structures?

The backwarming in the deep layers of the atmosphere (\( \tau \_\text{Ross} > 1 \))
corresponds to a temperature increase by a factor on the order of \( \eta / 4 \), where \( \eta \)
is the flux fraction blocked by spectral lines (Chandrasekhar 1935). That is, a
continuous opacity underestimated by a factor of \( \chi \) would lead to an increase
of the line blocking \( \eta \) by \( \leq \chi \eta \), with approximate equality in the case when the
blocking is due to, e. g., neutral iron lines on the linear part of the curve of
growth. Thus, the increase in the temperature in the deep layers would be
\[ \leq \frac{1}{4} \chi \eta T(\tau) \]. The same estimate applies if the line absorption is increased such
that \( \eta \) is changed by a factor \( \chi \). With typical values in the solar case (\( \chi \leq 0.1 \),
\( \eta = 0.1 \) and \( T = 6000 \) K), we get effects on the order of 20 K which is practically
insignificant. For a red giant model, however, where both \( \eta \) and \( \chi \) may be on
the order of 0.5 at least, the effects may be quite important.

In the surface layers, the temperature effects of different opacity
sources are most easily understood (following Mihalas 1978, Carbon 1979) from
the radiative equilibrium equation (assuming LTE):

\[
\int \kappa J \, dv - \int \kappa B \, dv = 0 . \tag{2}
\]

Close to the surface the angular mean intensity \( J \), departs from \( B/T \) at \( \tau \leq 1 \),
where it decreases towards \( \frac{1}{4} B/T(\tau = 1) \), since the ingoing radiation intensity
gets small. However, \( J \) may still be larger than \( B/T \) for high frequencies, since
the outward directed intensity comes from inner and hotter atmospheric
regions, and the temperature sensitivity of the source function is considerable.
In this case, adding extra opacity may enable the first integral to catch hot
radiation from below and thus heat the surface. This is particularly the case if
the absorption at high frequencies is not too strong, or occurs suddenly at the
surface, so that \( J \) is not thermalized. This may happen for molecular
absorption, e. g., by TiO in M stars. However, if the absorption added is strong and persistent to greater depths it cools the surface even when located at high frequencies in the spectrum. One example is the cooling effects when strong atomic lines are added in the blue spectral region of G and K star models. If the extra line absorption occurs at lower frequencies the second integral of Equation (2) is usually more affected than the first one since $B_\nu$ is greater than $J_\nu$. $B_\nu(T)$ and $T$ must then decrease. One example of this is the surface cooling by several hundred K in K-star models when adding the rotation-vibration bands of CO, an effect found by Johnson (1973) and verified by Gustafsson et al. (1975) with a more realistic blanketing treatment. For a general discussion of these effects, see Carbon (1979) and Gustafsson & Olander (1979).

If one corrects for an opacity error (by a factor of $X$ in $\kappa$) the relative balance between line absorption and continuous absorption will change. For solar-type models the effects on the temperature $T$ at a given optical depth only amount to a few percent of $T$ times $X$. For cooler models the effect is of the same order of magnitude. If instead a line absorption is underestimated it will, as long as it is weak and distributed across the spectrum, have similar effects. If it is concentrated towards the short wavelength side it will cool or heat the surface layers, depending on the depth distribution of the absorption, just as discussed above. Similarly, it will generally cool the surface if it occurs at long wavelengths.

An especially complex interplay between opacity changes and pressure-temperature structures occurs for spherically symmetric models of cool giants where the radiation field in the outer layers of a model that is expanded by an increased opacity is diluted. This cools the surface layers which may enhance molecular formation and further increase the opacity (cf. Gustafsson & Jørgensen 1994, and references cited therein).

It must be stressed that the discussion above is based on the, in reality very questionable, assumption of LTE in the surface layers of the photospheres. When departures from LTE are considered, new surface effects may occur, like the Cayrel mechanism of surface heating (cf., e. g., Mihalas 1978). The surface temperature may also be less affected by line absorption if LTE is not assumed; the magnitude of the effects will depend on whether the lines are collision dominated - if the line radiation is less coupled to the local temperature and, e. g., mainly formed in scattering processes, the effects will be smaller. At great depths, the effect of extra line absorption is generally further back-warming in any case.

Here, I shall now discuss the need for improvements in opacities for models of atmospheres of late-type stars, starting with solar-type stars and then proceeding towards cooler stars and ending with carbon stars. The emphasis will be on missing line absorption in model photospheres. For the continuous absorption the situation seems much more satisfactory, in particular due to the impressive efforts in the OPAL and OP projects (see Seaton 1994a and references quoted therein). Several valuable reviews and more detailed
discussions of molecules and their opacities in cool stars were presented at IAU Colloquium No. 146, and references will repeatedly be made here to the proceedings from that meeting (Jørgensen 1994a, Thejll & Jørgensen 1994). For a more general review of model atmospheres of cool stars, see Gustafsson & Jørgensen (1994).

2. Solar-Type Stars

Calculated low-resolution spectra of blanketed model solar atmospheres of the 1970's (flux-constant ones as well as semiempirical ones) were compared by Gustafsson & Bell (1979) and Kurucz (cf. Kurucz 1992a) with the Labs & Neckel (1968, 1970) observations of the solar intensity and found to fail in reproducing the solar ultraviolet flux. Typically, the models predicted too much flux throughout the ultraviolet, e.g., by 25% around 350 nm, while the agreement was found to be satisfactory around 400 nm. For the longer wavelengths the computed fluxes of the flux-constant models were, conversely, systematically low by typically 5 to 10%. Gustafsson & Bell (1979) also found, from observed scans and colours of stars, that this discrepancy increased with decreasing effective temperature and increasing metal abundance. They concluded, after an extensive discussion, that the most probable explanation for this discrepancy was incomplete blocking in the model atmospheres, due to a missing "veil" of weak spectral lines. (Their model atmospheres and synthetic spectra were based on spectral line lists which mainly consisted of lines measured in the laboratory or in the solar spectrum.) By arbitrarily increasing the weak opacity Gustafsson et al. (1975) found that a good reproduction of the uv flux with a flux-constant solar model resulted if one increased $\kappa_\nu$ (including the line absorption) by 40%, for all wavelengths shorter than 400 nm and for all $\kappa_\nu < 10 \kappa_{Ross}$. The resulting effects on the temperature structure for the solar model were about 75 K at $\tau_{Ross} > 1$, and much smaller at shallower depths. That temperature increase is approximately consistent with what is needed to produce the missing flux in the visible spectrum. For cooler stars the effects on the temperature structures were found smaller and at greater depths, reflecting the decreased significance in the stellar atmosphere of the energy transfer in the ultraviolet.

This empirical evidence for a missing solar opacity, relative to the line lists of the 1970's, is, however, still a bit controversial. More recently Lookwood, Tüg & White (1992) measured the solar irradiance from 330 to 850 nm relative to the spectrophotometric standard star Vega. Their results, which are not necessarily superior to the Labs & Neckel data set (cf. Neckel & Labs 1984) suggest higher solar uv fluxes (by, typically, 10%) and lower red fluxes. They thus tend to agree much better with the Gustafsson et al. (1975) model, and still better with more recent spectra calculated by Bell (1995).

As a result of the impressive and systematic efforts of Kurucz in creating very extensive line lists, based on a semiempirical approach with scaled Thomas-Fermi-Dirac and Hartree-Fock calculations, a new grid of model atmospheres could be constructed (Kurucz 1992a). The new solar model fluxes showed an improved agreement with the Labs & Neckel measurements.
and the problem of the missing opacity was declared solved (Kurucz 1992b, cf. also Edvardsson et al. 1993). However, Bell, Paltoglou & Tripicco (1994) have used the data from Kurucz's recent list and found from calculated synthetic spectra that "many strong lines are too strong" in that list, as compared with the observed line strengths. Edvardsson & Gustafsson (1994) have independently verified this result by recomputing the wavelength regions displayed in the paper by Bell et al. (1994). The discrepancies are so great that they cannot possibly be explained as results of improper damping constants, microturbulence, or non-LTE. However, a detailed look at the lines that do not match reveals that the vast majority connect atomic states with energies that are, in one or both cases, only predicted. Thus, the wavelengths may well be seriously in error. One does not, however, find in the computed spectrum a corresponding number of lines that are far too weak or missing, which one would expect if it were only a question of miscalculated wavelengths. Most of the lines that are too strong originate in highly excited states, and a minority of them end above the lowest energy level of the ionized atom. For these autoionization is important. This is further studied by Bell & Tripicco (1994) and, when taken into account, seems to improve the fit although it does not remedy the general problem with the lines that are too strong.

An interesting aspect of the study of Bell et al. (1994) is the effects on the ultraviolet colours when different line lists are used for a solar model and a model for a Population I K2 III star. A shift from the line list of Bell, mainly containing laboratory or "astrophysical" gf values for about 50,000 identified lines, to Kurucz's list with its 40 million lines leads to a change in the $U-B$ colour by 0.09 and 0.20 magnitudes, respectively, for the two models. These results are consistent with the findings by Gustafsson & Bell (1979), discussed above. However, if a line list is composed of the lines of Bell's list, which at least in the wavelength regions displayed by Bell et al. (1994) seems to match the solar spectrum better, and with the contributing weaker lines added from Kurucz's list, the effects on the $U-B$ colour are much less, as compared with a model spectrum based on the Bell list alone, the effects then being only 0.02 and 0.07 magnitudes, respectively, for the two models. From this it seems that most of the improved fit to the Labs & Neckel low ultraviolet flux of the Sun and to the colours of the orange giants is due to an excess of a relatively small number of strong lines in Kurucz's list, rather than the contribution from of a veil of numerous weak lines. If so, the problem seems to remain.

What could then be the explanation for the uv discrepancy? One possibility is that there is no severe discrepancy in the solar case, i.e., that the Labs & Neckel data are wrong, as suggested by the Lockwood et al. (1992) observations. If so, another explanation must be invoked for the problems with the red giant colours, such as erroneous transmission functions for the ultraviolet filters or incomplete molecular line lists used in the calculations of synthetic colours. Another possibility, suggested by Seaton (1994b), is that configuration interaction is not taken into account to the full extent in Kurucz's calculations. If that were done, the highly excited lines could split into several components, each being considerably weaker and thus less in conflict with the observed
solar spectrum and still preserving the total blocking as measured in the lower-resolution fluxes. Still another possibility is that the continuous absorption from iron, in particular, may be severely underestimated. It cannot be excluded that the Fe I absorption used until now, e. g., that of Dragon & Mutschlechner (1980), is grossly in error. Some further support for this explanation is offered by Short & Lester (1994) who have found that the ultraviolet flux and the profiles of strong lines in the spectrum of Arcturus (K2 III) are much better reproduced by blanketed Kurucz model atmospheres if the continuous opacity is doubled from 285 to 400 nm. Still other possibilities are incomplete lists of molecular lines or the neglect of inhomogeneities and the improper description of convection.

The resolution of the problems with the uv fluxes in solar-type stars must be judged to be of very great significance from an applicational point of view, e. g., for synthetic photometry, work in galactic structure, and in the population synthesis of galaxies. More definitive measurements of the solar uv flux should be made. Improved calculations of configuration interaction and bound-free absorption from iron and other metals should be performed. An empirical way to study the problem further would be a detailed survey of the line absorption in, say, four solar-type stars, spanning a range in effective temperatures and metal abundances.

3. The M Stars

For the photospheric structures of the cool stars the problems with the atomic line opacities are smaller since the temperatures are lower (i. e., less excitation of numerous high energy states of the atoms) and less radiation is transferred in the ultraviolet and blue spectral regions, where the metal line blocking is still very considerable. Yet, in those spectral regions the metal line blocking is still very considerable, not the least in the high-pressure dwarfs and subdwarfs, where the damping wings are very broad. However, for cool stars the molecular line blanketing gets very strong all over the spectrum. What is needed, also for relatively simple-minded LTE model atmospheres with a reasonably detailed blanketing treatment, are extensive lists of all (collectively) important molecular lines, with wavelengths, excitation energies, and line oscillator strengths. The wavelengths do not have to be precise for model construction, while for synthetic spectra which are often needed, they should be accurate to a hundredth of a nm or better. The errors in the oscillator strengths should be considerably smaller than 50 %, and in particular not systematically off by much. For the most important molecules these data are not available yet; in particular oscillator strengths are missing and existing line lists are far from complete.

Already for K stars, the effects of the diatomic molecules CO, CN, and C2 are significant (cf. Alexander & Johnson 1972, Gustafsson et al. 1975, Carbon 1979) as is still the atomic line blocking. For the M stars, however, the structure of current model atmospheres is predominantly determined by molecular opacities, in particular those of TiO and H2O.
The situation as regards data for TiO has improved considerably in recent years due to the compilation and calculation of several new line lists. Of basic significance was the list by Collins (1975) for six different electronic systems, based on molecular constants from extensive and accurate laboratory wavelengths and calculated line strengths. Large improvements have occurred since then with regard to transition rates (see Davis, Littleton & Phillips 1986), data on the ε system by Simard & Hackett (1991) and the inclusion of the latter system in the stellar opacities (Brett 1990, Plez, Brett & Nordlund 1992, with an astrophyscial oscillator strength, and Jørgensen 1994b, based on lifetimes from Simard & Hackett 1991) and of the isotopic bands (Jørgensen 1994b). See also the discussion and references given by Schamp (1994).

There are still some indications that the models do not match the observed spectra for the φ and δ systems, which were found to be too strong in the calculations for giants by Alexander et al. (1989). No corresponding mismatch was reported by Plez et al. (1992) but may, in fact, be traced in their Figure 7. Allard (1994) reports a similar mismatch for M dwarf models. (Although the dissociation energy used by her is unrealistically high and changed in her later work, the resulting model spectra are probably not strongly affected by that, since the dissociation energy of TiO is anyhow so high, e. g., relative to the ionization energy of Ti I, that the determining factor for the amount of TiO found in the stars is the amount of Ti I that is available for molecule formation.)

A different type of uncertainty for TiO are the possibly significant non-LTE effects, operating through departures from the Saha equilibrium in the Ti I/Ti II balance. This matters for the molecular absorption since the atomic ionization energy is so low relative to the dissociation energy of the molecule that overionization of the atom due to hot radiative fields will be able to reduce the amount of TiO molecules considerably. For further comments on these effects, which remain to be studied in detailed calculations, see Johnson (1994). (A similar situation occurs for La and LaO in cool giants.) Also, for the formation of the TiO lines non-LTE effects may be significant in the sense that radiative transitions dominate over collisional ones, in particular in giant atmospheres. Hinkle & Lambert (1975) suggested that it may be more correct to treat lines in electronic systems like those of TiO as if they were formed in scattering processes rather than in true absorption processes. If this is true, the strong coupling between the radiation field and the local gas temperature at the surface of M stars (where TiO is a strong heating source in the LTE models; cf. Krupp et al. 1978, Jørgensen 1994b) weakens considerably, and the atmospheric structure in the surface layers of the atmospheres is much less affected than the LTE models indicate. The strong backwarming effects, however, remain, as well as the very profound effects on the spectrum (for a nice illustration of the latter, see Plez et al. 1993).

To further improve the situation for TiO a detailed comparison between model spectra and observations would be very valuable to clarify the situation further as regards the mismatch for the φ and δ systems. Also, a detailed
intercomparison of the current line lists is recommended. A study of the non-LTE effects in the ionization balance of Ti as well as of the formation of the TiO electronic system lines is also urgently needed.

For H$_2$O the situation has also become greatly improved in recent years. Previously, stellar atmosphere calculations were based on the mean opacities for water vapour, calculated by Auman (1967), or statistical line lists calculated to match the experimental low resolution (25 cm$^{-1}$) data of Ludwig (1971), see Alexander et al. (1989) and Plez et al. (1992). Alternatively, Ludwig's data were just used as straight mean opacities, cf. Allard & Hauschildt (1994). The recent ab initio dipole and potential energy surfaces have made it possible to generate detailed and reasonably accurate line lists for the rovibrational bands. A particularly accurate method for generating the potential energy surface is the MORBID (Morse Oscillator Rigid Bender Dynamics) approach (Jensen 1989), which nevertheless demands a large amount of experimental input and therefore so far has been applied only to a small number of molecules of astrophysical interest. Jørgensen & Jensen (1993) computed a CASSCF dipole surface and used it together with the MORBID potential surface to generate a complete band list of transitions between energy levels up to the dissociation energy, finding a satisfactory agreement between the calculated and measured band strengths. This band list was later used to generate an extensive line list (Jørgensen, Jensen & Sørensen 1994). Miller et al. (1994), also using Jensen's (1989) potential surface, have calculated another list based on rovibrational wave functions calculated with the Finite Basis Representation (FBR) technique. These two, partly independent, lists still have to be intercompared. The FBR method is expected to give more accurate line frequencies, but has not resulted in a complete list, because of the larger computational task involved which would make computations up to the dissociation energy difficult. Jørgensen, Jensen & Sørensen (1994) strongly emphasize the significance of a high degree of completeness of the list: the blanketing in their M giant models is so heavy that remaining gaps between the molecular bands play a major role for the transfer of energy. Thus, if a mat of very weak lines, able to fill in these gaps, is not considered properly, the model atmosphere may be significantly in error.

Spectra of early M giant models were compared with observations by Plez et al. (1992) with a resulting acceptable over-all agreement. For the M dwarfs, models with TiO and H$_2$O have been compared with observed spectra by Allard (1994) and Allard & Hauschildt (1995). In spite of significant improvements as compared with earlier comparisons (e. g., those of Kirkpatrick et al. 1993a) considerable discrepancies still appear. For the cool dwarf VB 10 (dM8, $T_{\text{eff}}$ = 2800 K) Allard (1994) finds that her model is too faint in the infrared or too bright in the visible. This points at a possible problem with the relative strengths of TiO and H$_2$O bands, respectively, e. g., due to errors in Ludwig's H$_2$O opacities, or possibly a calibration error. Indeed, Allard, Hauschildt, Miller & Tennyson (1994) report an improved fit when a detailed line list (cf. Miller et al. 1994) is used. Further systematic comparisons with observations are needed.
For other molecules that play a role in M-type spectra the situation is less satisfactory. VO, for example, has several electronic systems of significance in the region 800 to 1200 nm (Merer et al. 1987); although detailed rotation analyses have been performed (e. g., Cheung et al. 1994) no very extensive line lists have been calculated as yet, and no reliable f values exist to my knowledge for the A-X and B-X systems (for approximate treatments of VO with "astrophysical line strengths", see Brett 1990, or Allard 1994). An interesting example of the effects of this molecule is offered by the cool dwarf GB 165B, the spectrum of which is dominated by VO bands (Kirkpatrick et al. 1993b, Davis 1994).

Turning to the hydrides, which are particularly significant for spectra of dwarfs and subdwarfs, FeH is an important opacity around 1 micron and is relatively significant for S-type stars and metal-poor stars, also as a potentially significant diagnostic (cf. Bessell 1991). For an interesting account of the identification of FeH in stellar spectra, see Lambert (1988). The green and blue bands of this molecule were studied by Carter et al. (1991), Fletcher et al. (1993), and Carter & Brown (1994), the IR F^4Δ-X^4Δ system by Phillips et al. (1987), and the fundamental rotation-vibration bands by Towle et al. (1993). The f values are uncertain - those calculated by Langhoff & Bauschlicher (1990a) are probably not correct (see Langhoff & Bauschlicher 1994) and do not match M dwarf observations (Allard 1994). Lifetime measurements for this molecule are urgently needed. The FeH^+ ion might also be a significant absorber in dwarf atmospheres, and might be expected to be abundant enough (assuming LTE) to be visible in stellar spectra; however, it is not, which could be due to photodissociation (Langhoff & Bauschlicher 1991).

Also, CaH and CaOH are clearly visible in M dwarf spectra. For CaH, line lists for the A-X and B-X systems were published by Berg & Klynnig (1974), but existing lifetime measurements (Klynnig et al. 1982, Doverstål & Weijnitz 1991) are not sufficient for the needs of detailed model-atmospheres and synthetic spectroscopy. Recent progress for these molecules includes analyses of the rotation-vibration (IR) bands of CaH (Petitprez et al. 1989, Frum & Picket 1993) and of the A-X bands of CaOH (Coxon et al. 1991). "Astrophysical oscillator strengths" were derived for the A-X and B-X systems of CaH by Barbuy et al. (1993). The situation for MgH may be somewhat more satisfactory - acceptable fits to observed spectra of the A-X system bands have been reported for K stars by Bonnell & Bell (1993, and references cited therein) with data based on laboratory measurements and by Allard (private communication) for M dwarfs with data according to Kurucz (1994). The significance of SiH should be explored (for a discussion, see Bell & Tripiccio 1991) but is reduced below 3000 K as a result of the formation of SiO. Other molecules of some significance as absorbers in cool M stars are AlOH and AlH, HS and H2S, SiS, HCl, and CrH. However, with the exception of CrH their stronger electronic bands are located in the blue-ultraviolet spectral regions and are probably only significant at analyses of stellar spectra in these spectral regions. CrH has a strong system in the near IR (for a recent reference see Ram, Jarman & Bernath (1993)).
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At high densities and low temperatures CH$_4$ takes over relative to CO as the main carbon carrier in M stars. Tsuji (1994) has pointed out that bands from this molecule fill in gaps between the H$_2$O bands in the spectra of the coolest M dwarfs, so that it might be of significance for the structure of the atmospheres. At the moment mainly low-resolution measurements are available for this opacity, but high-resolution studies are forthcoming.

Another opacity source which is quite important at high pressures and low temperatures (perhaps of particular significance for brown dwarf stars) is the collision-induced absorption, in which dipole interaction during the transient phase of the “collision” between two atomic systems becomes possible and gives rise to very broad absorption features. The rovibrational transitions of H$_2$--H$_2$ and H$_2$--He interactions have been studied recently in considerable detail, but the overtones and three-body interactions need further study, as does the H$_2$--H collision (cf. Borysow 1994 for a review).

A general problem with the blanketing effects from molecular lines, in particular of significance for M dwarfs, is that the collision damping constants, describing the effects on the line profiles from interactions between the molecules and hydrogen atoms/molecules as well as helium atoms, are practically unknown. Here, data are most urgently needed, in particular for hydrides and H$_2$O. Please note that these data are partly accessible observationally, with contemporary spectrometers, through systematic comparisons between line profiles observed in dwarfs, subgiants, and giants of similar spectral types.

4. The S and C Stars

For the molecule most characteristic of S star spectra, ZrO, one also finds that considerable improvements have taken place in recent years as regards line lists, molecular constants, and band strength data (Simard et al. 1988, Langhoff & Bauschlicher 1990b, Littleton et al. 1993, Jonsson 1994). A comprehensive and detailed line list for model-atmosphere work has, however, to my knowledge, yet to be computed. We note, in passing, that at certain temperatures and densities Alexander & Ferguson (1994) find that significant fractions of the ZrO molecules should be ionized (e.g., at $T = 2500$ K, $\rho = 10^{-10}$ cm$^{-3}$ the abundance of ZrO may be depleted by a factor of 4 when ZrO$^+$ is included in the calculation). ZrO$^+$ is expected to show strong bands around 760 to 820 nm (Balfour & Lindgren 1980).

Also for another characteristic of S star spectra, LaO, some improvements have been made relative to earlier lifetime measurements (Carette & Bencheikh 1994, Behere & Bhartiya 1991) but more work remains before a line list satisfactory for model-atmosphere calculations may be compiled for this molecule. For YO also modern lifetime measurements are needed. (Note that the abundances of both LaO and YO decrease when the temperature drops below 3000 K as a result of formation of the dioxides, at least as long as the oxygen abundance is greater than the carbon abundance.) Also, for ZrS, another important molecule in S-type spectra and contributing most of the
famous "Keenan-bands" and the additional bands found later by Wing (see Lambert 1988 and references quoted therein, and Jonsson 1995 and Jonsson & Lindgren 1995 for rotation analyses), lifetime data are missing. This is also true for TiS, a molecule recently identified in the near-infrared spectrum of S-type Miras (Jonsson, Laurila & Lindgren 1992) and with rotation analyses of three different systems by Jonsson & Laurila (1993).

A long-standing opacity problem for the coolest (i.e., the N-type) carbon stars has been the nature of the ultraviolet-violet opacity, which produces the very drastic fall-off of the flux when approaching the ultraviolet in the spectrum. Essentially this problem was solved by Johnson, Luttermoser & Faulkner (1988) who pointed out that the contributions from several different opacity sources were significant: bound-bound and bound-free opacities from Na, Mg, Ca, and Fe, and CH and C$_3$. Further, a simple effective temperature effect occurs - the N stars were often compared with early-type M giants and supergiants, which are considerably hotter.

The line data for the diatomic molecules of significance in carbon-rich red giants are in satisfactory state as regards CO (Goorvitch & Chackerian 1994) and CN (Jørgensen & Larson 1990). The latter study demonstrates again the significance of completeness. Thus, it may be important to calculate improved and extended line lists of the Swan bands and the infrared Ballik-Ramsey & Phillips bands of C$_2$ (current models are based on line lists by Querci et al. 1974 or by Kurucz, cf. Kurucz 1994). Also, existing data for CH are worth revising and extending, and the role of CS as an opacity source should be explored.

However, the real difficulty for the cool carbon stars of spectral type N are the polyatomic molecules, which seem to play a significant role, at least when $T_{\text{eff}}$ decreases below 3000 K. In addition, possibly at slightly lower temperatures dust formation may affect the photospheric structure and the visible spectrum.

The effects on HCN for N-type model photospheres were found by Eriksson et al. (1984) to be very extensive and with considerable effects on abundance analyses (Lambert et al. 1986). The basic mechanism was the "blowing up" of the outer photosphere as a result of an opacity, widespread through the part of the spectrum where energy was transferred, i.e., essentially an effect on the pressure according to Equation (1). The results of Eriksson et al. (1984) were based on early very approximate data by Jørgensen (1982) on HCN strengths. Later Jørgensen et al. (1985) carried out extensive $ab\ initio$ CASSCF calculations and the resulting line list has been used in more recent studies. At present, Jørgensen & Jensen are recalculating this list, using a much larger set of basis functions in the CASSCF computations of the dipole function, and the MORBID method for determining the band strengths (from the CASSCF dipole surface) and more accurate band centre frequencies than what can be obtained from the CASSCF potential surface.
Another important molecule in N star atmospheres, in particular for stars with relatively large C/O abundance ratios, is C₂H₂. For modeling of photospheres only a very rough semiempirical line list exists (Jørgensen 1982), and a less extensive semiempirical list by Sharp (referred to by Brown et al. 1989), while experimental data accumulate. New calculations of higher quality are urgently needed!

Also, the C₃ molecule has been found to have considerable effects on the photospheric structure of carbon-rich N stars (Jørgensen et al. 1989). These results were based on CASSCF line lists; recently more detailed calculations based on a combination of the CASSCF and the MORBID approach were carried out by Jensen et al. (1992), although only to such low energies that an actual line list for stellar purposes cannot directly be generated from the calculations. The situation may be regarded better than that for C₂H₂, but there is still room for considerable improvement. The very low energy of the bending vibration provides an extra challenge in the \textit{ab initio} computations compared to HCN, for example, because small errors in the wavefunctions of the many combination bands can lead to relatively large errors in the band strengths, which in practice results in a number of artificially very strong combination bands which dominate the opacity if not empirically corrected.

A most problematic molecule from our point of view is the ethynyl radical, C₂H, which is a very abundant species in N-type atmospheres, especially at high carbon abundances. The identifications proposed for this molecule in carbon-star photospheric spectra are highly uncertain. Overlapping electronic states and very complex spectra seem to make \textit{ab initio} calculations similar to those successfully carried out for HCN very difficult (cf. Peric et al. 1992, Peyerimhoff 1994). For references to recent experimental data on this interesting molecule, with bands from the ultraviolet to the infrared, see Yan & Amano (1993).

Additional molecules that may play important roles in N stars are C₃H (to my knowledge its dominant linear isomer is only studied in the microwave region, see Gottlieb et al. 1985), SiC (with two electronic transitions in the infrared and one in the blue-ultraviolet (cf. Ebbern, Drabells & ter Meulen 1991 and references cited therein) and SiC₂ (see, e. g., Ross et al. 1994 for references). None of these have been explored in detail as opacity sources. In addition, for the cooler stars heavier molecules may also be of significance like the polyaromatic hydrocarbons (PAHs). Here, more data are needed, in particular laboratory measurements of intensities of individual bands and measurements of the monochromatic absorption coefficients at stellar temperatures. A full \textit{ab initio} calculation of their absorption coefficients is beyond the capacity of contemporary computers.

Finally, for carbon stars as well as for cool oxygen-rich stars, the effects of dust must be considered. Although dust presumably forms rather far out, at temperatures below 1500 K, the effects due to backscattered radiation onto the photosphere, on the structure and dynamics of the outer layers, and thus on the
formation of strong photospheric lines may be profound. In spite of recent great progress in grain formation theory and chemistry (see, e. g., Sedlmayr 1994) more data are needed, not the least in grain optics. For oxygen-rich compositions, the properties of high-temperature condensates like TiO in solid form, CaTiSi ... minerals, and Al₂O₃ should be measured, and not only for bulk material but also for dust. Similarly, the properties of Fe dust, as well as of dirty silicates are important to study further.

5. Conclusions

It should be clear from the preceding sections that the need for improved and additional data for atmospheric absorption in cool stars is considerable. A condensed wish list would contain a settling of the uv-opacity problem for solar-type stars, improved data for FeH and VO for M stars as well as a resolution of the remaining problems with TiO, collision damping parameters for water vapour, hydrides and oxides, a detailed ZrO line list systematically investigated for S stars, and data for C₂H as well as improved calculations for C₂H₂ for N-type stars.

One may, however, ask whether these needs have not been over-emphasized in this review - expressing the ambitions of a perfectionist in classical photospheric modeling rather than those of astrophysicists who strive to understand real stars. That is, are the foundations of model making strong enough to warrant bothering about these details in the absorption coefficients? That this question is not simply rhetorical may be seen from the fact that the role of radiative transfer in spectral lines of different strength and origin is qualitatively different in a plane-parallel solar model atmosphere and a more realistic 3-d convection model of Nordlund & Stein (cf. Nordlund 1985). Even though one may always argue that we must learn to creep before we can walk, it is not obvious that we should develop a most advanced mastership in creeping before taking our first steps. No doubt, great efforts to calculate, e. g., red giant models with convection, inhomogeneities, and departures from LTE should be made, and efforts to observe corresponding phenomena are obviously of very great significance. They may have higher scientific priority than items on the above wish list, although some improvements of opacities discussed here could lead to changes of surface temperatures by several hundred degrees, of theoretical radii for giant stars by a factor of two, and of characteristic photospheric densities by an order of magnitude. These estimates are just taken from previous experience when adding new opacity sources; in addition to that one also must remember that qualitatively new and astrophysically very significant phenomena may appear when new opacities are added (just to mention one example: the possibility that the outer photospheric layers become unstable against radiative levitation). It is impossible to say if these phenomena would be more or less significant than, e. g., the wealth of new phenomena that could be described by more appropriate hydrodynamics.
At any rate, however, the opacity data are urgently needed! Model atmospheres are not only, not even primarily, calculated to understand the basic physics of stellar atmospheres but rather to connect the basic physical properties of the star (mass, age, angular momentum, chemical composition, ...) with the observable spectrum. To represent the spectrum as well as we can, and not only account for the more or less complex physical structure of the stellar atmosphere and the transfer of energy in it, we do need these improved opacity data. True enough, we also need better models. But there is no way around the necessity to get the basic atomic and molecular data right.

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Discussion

Carson: When you exclude H2O is only the absorption of H2O excluded and not the chemistry? What are the knock-on effects on the formation and absorption of other molecules containing H and O?

Gustafsson: In all our more recent models H2O molecules are included at least at the calculation of the molecular equilibrium and the thermodynamic quantities. H2O is an important oxygen "consumer" in cool M stars.

Bessell: A recent paper accepted by A&A by Brett on M dwarfs using the Plez et al. (1992) opacity-sampled models indicates very good agreement between observations and synthetic spectra and good agreement for most of the TiO bands in 4000 K to 3000 K models.

Kurucz: I think you are being unfair to me in describing Bell’s use of my data. I do not know what line list he used. My impression is that he has included both observed and predicted lines. I do not know how he treated the damping. I give out my data and my programs and my solar atlas so anyone can run these tests for herself. Also in my line list most of the strong lines are from laboratory measurements.

Gustafsson: We have tried to reproduce the Bell et al. (1994) results with your recent line list and found a close agreement with them. We included both observed and predicted lines and argue that those predicted lines that seem to come out with unrealistically great individual strengths may contribute
significantly to the agreement in low-resolution solar uv fluxes and also affect the ultraviolet colours considerably.

Bell: My calculations were based on the list of $42 \times 10^6$ lines given me by Kurucz. It is quite possible that some changes could occur as a result of different damping constants. However, the results published in MNRAS, 268, 711 show that numerous lines in this list have gf values which are wrong by factors of 10 or 100. These lines are used in many of Kurucz’s work since no lab data exist for them.