

## THE IMPORTANCE OF MOLECULAR OPACITIES IN STELLAR ATMOSPHERES

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### INTRODUCTION

Opacities are of vital importance in astrophysics necessary to model stellar atmospheres and interiors, and below about 6000 K diatomic molecules make an increasing contribution to that opacity. Moreover, at around 3000 K polyatomic molecules, such as  $H_2O$  for an oxygen rich solar composition, start playing an important rôle, and additionally at high pressures collision induced  $H_2 - H_2$  and  $H_2 - He$  absorption is important for late-type main sequence stars.

In order to investigate the importance of molecular opacities, in Sharp (1992) we computed and compared opacities for a solar and a three times enhanced *CNO* abundance, and some further comparisons were made in Sharp et al. (1992). Some of these results are briefly summarised here.

### RESULTS OF CALCULATIONS

In table 1, reproduced from Sharp (1992), Planck and Rosseland mean opacities are given for 104 temperature-density points for temperatures between  $kT = 0.2$  and  $1.0eV$ , and densities between  $10^{-10}$  and  $10^{-3} gm cm^{-3}$  for a Cameron (1973) solar composition with a turbulent broadening of  $1 Km s^{-1}$  in all cases. At each temperature-density point, atomic and molecular equilibria were first obtained by iterating the Saha equations of atomic ionization and molecular dissociation, then the continuous absorption on a coarse grid of a few thousand points was calculated due to scattering, free-free, bound-free and collision induced absorption. To this was added a fine grid of several hundred-thousand points on which molecular bands were calculated on an individual line-by-line bases. Diatomic molecules were calculated using the Morse oscillator approximation (Doktorov et al. 1976, Sharp, 1984 and 1988), with the Hönl-London factors for the line strengths obtained from Kovács (1969), and  $CO_2$  and  $H_2O$  were calculated using the harmonic oscillator approximation, (Auman 1966). Atomic lines were, however, neglected. Although molecules made a negligible contribution at the higher temperatures calculated, these points were included for continuity and to permit comparisons with other calculations.

In the equilibria mentioned above, calculations were performed for the 22 most abundant elements in the mixture with their associated ions, 38 diatomic molecules and 12 triatomic molecules, of which  $H_2O$  was by far the most important of the triatomics at the lowest temperatures. A subset of these molecules was included in the opacity calculations, with the most important contribu-

Table 1. Planck (upper) and Rosseland (lower) mean opacities in  $\text{cm}^2/\text{gm}$  for a solar mixture.

kT (eV)	0.2	0.25	0.3	0.4	0.5	0.6	0.8	1.0
T (K)	2320	2900	3480	4640	5800	6960	9280	11600
$\rho$ (gm/cc)								
1(-10)	1.725(-1)	8.009(-2)	4.668(-2)	3.468(-2)	1.796(-2)	2.436(-1)	3.678(1)	2.802(1)
	4.535(-4)	5.424(-5)	2.654(-4)	1.126(-3)	1.180(-2)	1.323(-1)	3.665(0)	2.756(0)
1(-9)	3.681(-1)	8.263(-2)	5.258(-2)	6.987(-2)	5.208(-2)	3.026(-1)	8.685(1)	2.180(2)
	1.428(-3)	3.311(-4)	7.743(-4)	3.537(-3)	2.633(-2)	1.951(-1)	8.378(0)	1.813(1)
1(-8)	4.753(-1)	1.075(-1)	5.822(-2)	9.806(-2)	1.684(-1)	5.176(-1)	1.184(2)	8.975(2)
	2.345(-3)	4.369(-3)	2.936(-3)	1.795(-2)	7.759(-2)	4.138(-1)	1.289(1)	7.447(1)
3(-8)	4.913(-1)	1.571(-1)	6.713(-2)	1.188(-1)	2.920(-1)	7.594(-1)	1.273(2)	1.286(3)
	2.720(-3)	1.042(-2)	6.257(-3)	4.016(-2)	1.370(-1)	6.299(-1)	1.551(1)	1.093(2)
1(-7)	5.001(-1)	2.399(-1)	9.090(-2)	1.722(-1)	5.289(-1)	1.250(0)	1.357(2)	1.630(3)
	3.150(-3)	1.945(-2)	1.626(-2)	9.426(-2)	2.665(-1)	1.033(0)	1.953(1)	1.450(2)
3(-7)	5.045(-1)	3.033(-1)	1.402(-1)	2.932(-1)	9.110(-1)	2.084(0)	1.444(2)	1.858(3)
	3.632(-3)	2.822(-2)	4.021(-2)	2.003(-1)	5.128(-1)	1.685(0)	2.507(1)	1.788(2)
1(-6)	5.079(-1)	3.478(-1)	2.436(-1)	5.938(-1)	1.680(0)	3.808(0)	1.584(2)	2.047(3)
	4.286(-3)	3.745(-2)	9.168(-2)	4.430(-1)	1.104(0)	3.009(0)	3.462(1)	2.225(2)
3(-6)	5.112(-1)	3.777(-1)	3.826(-1)	1.188(0)	3.118(0)	6.908(0)	1.804(2)	2.203(3)
	5.208(-3)	4.666(-2)	1.588(-2)	8.963(-1)	2.327(0)	5.400(0)	4.913(1)	2.800(2)
1(-5)	5.165(-1)	4.148(-1)	5.911(-1)	2.560(0)	6.659(0)	1.402(1)	2.254(2)	2.415(3)
	7.150(-3)	6.144(-2)	2.590(-1)	1.897(0)	5.412(0)	1.095(1)	7.745(1)	3.838(2)
3(-5)	5.275(-1)	4.920(-1)	1.003(0)	5.838(0)	1.533(1)	2.958(1)	3.112(2)	2.743(3)
	1.380(-2)	1.095(-1)	4.906(-1)	4.394(0)	1.282(1)	2.314(1)	1.299(2)	5.618(2)
1(-4)	5.835(-1)	8.217(-1)	2.063(0)	1.500(1)	3.942(1)	6.692(1)	4.928(2)	3.391(3)
	4.472(-2)	3.221(-1)	1.146(0)	1.165(1)	3.283(1)	5.246(1)	2.393(2)	9.188(2)
3(-4)	8.326(-1)	1.869(0)	5.483(0)	4.319(1)	1.030(2)	1.576(2)	8.724(2)	4.666(3)
	1.391(-1)	9.382(-1)	3.592(0)	3.538(1)	8.421(1)	1.220(2)	4.668(2)	1.620(3)
1(-3)	1.135(0)	2.920(0)	8.782(0)	5.865(1)	2.139(2)	6.874(2)	2.105(3)	8.350(3)
	1.982(-1)	1.358(0)	5.471(0)	4.668(1)	1.676(2)	4.269(2)	1.192(3)	3.631(3)

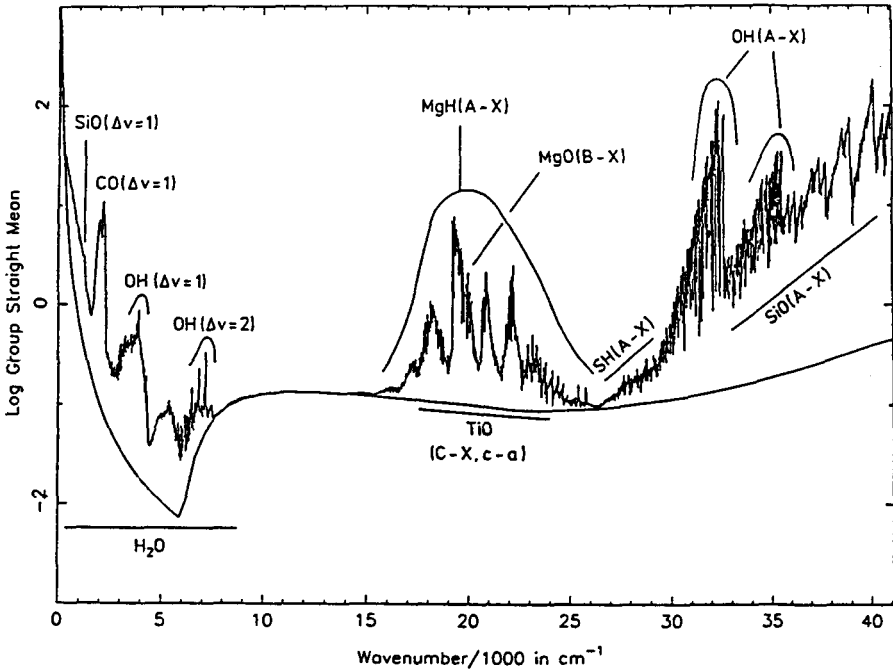


Figure 1. Plot of the group straight mean absorption coefficient at  $kT = 0.3\text{eV}$ ,  $\rho = 10^{-6}\text{gm cm}^{-3}$  and a turbulent velocity of  $1\text{Km s}^{-1}$  for a solar composition. The absorption due to molecular bands plus continuum is shown superimposed on the continuum alone.

tors at a representative temperature-density point being indicated in figure 1 from Sharp (1992). In this figure for  $kT = 0.3eV$  and a density of  $10^{-6}gm^{-3}$ , the group straight mean absorption coefficient over 3400 intervals in  $cm^2gm^{-1}$ , where the mean from the fine grid in each interval is represented, is plotted against the photon energy in units of  $1000 cm^{-1}$ , with the lower curve being the continuum alone, (the minimum is at the  $H_{bf}^-$  absorption threshold). The vibration-rotation bands in the infrared, and the electronic systems in the visible and ultraviolet regions are identified.

At this temperature the maximum in the Rosseland weighting function is not far above in frequency from the minimum of the  $H^-$  opacity, so the contribution molecular bands make in this region is particularly important. At lower temperatures  $H_2O$  completely dominates this region and additionally the maximum of the weighting function is closer, resulting in  $H_2O$  increasing the Rosseland mean opacity by about a factor of 100 at the lowest temperatures tabulated. As discussed in Sharp (1992) and Sharp et al. (1992), a number of diatomic molecules and their ions, at least for  $CO^+$ , appear to be still important at  $kT = 0.6eV$ , however a number of important atomic processes were neglected.

## CONCLUSIONS

Some extensive molecular opacity calculations discussed in Sharp (1992) are briefly summarised here. Scattering and some important atomic and molecular continuous opacity sources were included to obtain a background continuum, then molecular bands were calculated on a detailed line-by-line basis. As expected, it was found that molecular bands can make a very substantial contribution to the Rosseland mean opacity, and the graphs, one of which is included here, are particularly instructive in showing the importance of molecular bands.

However, we have had to make a number of important approximations in neglecting several atomic processes, calculating line strengths and assuming Gaussian profiles, together with using some relatively old data. Some of these problems are currently being addressed, and it is hoped that these improvements will be incorporated into later work.

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