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Molecular line widths for stellar atmospheres

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Abstract. Molecules are the dominant opacity source in the atmospheres of cool stars, brown dwarfs and planets. As with rapidly decreasing electron pressure at the temperatures of the lowest-mass stars almost no true continuum opacity sources remain, the pseudo-continuum of molecular bands obtains a decisive impact on radiative transfer, and thus thermal structure of the atmosphere. To correctly include molecular opacities in stellar atmosphere calculations, therefore both complete and reasonably accurate lists of line strengths and positions, and correct treatment of line broadening is required. Classical recipes for calculating Van der Waals broadening e.g. by Unsöld, and their extension to non-hydrogenic atoms, can at best give a crude estimate of molecular interactions. For a realistic treatment of collisional damping therefore measured widths or more sophisticated theoretical broadening constants of molecular lines are required.
In this contribution I give an overview of experimental and theoretical studies on line widths and their potential application in model atmospheres for low-mass stars, brown dwarfs and giant planets. The main difficulty in finding realistic line widths for stellar models is the paucity of measurements both for the temperature conditions, and for collisions with the dominant perturbers in these atmospheres, H_2 and He. Also, theoretical models still struggle to explain observed variations of the width with rotational and vibratonal quantum numbers. The effect of the uncertainty in the resulting Voigt profile widths is studied in model atmospheres computed with the PHOENIX code.

1. Introduction

Ultracool dwarfs, starting at the low-mass main sequence stars of spectral class M and continuing through the newly defined spectral classes L (Martin et al. 1997; Kirkpatrick et al. 1999) and T (Geballe et al. 2002; Burgasser et al. 2002) into the regime of substellar objects, are characterised by molecular absorption forming most of the prominent spectral features and increasingly shaping the entire spectral energy distribution (SED) with wide and deep absorption bands. This effect is enhanced by the diminished continuum opacity of H_2^- and other negative ions, owing to the lack of free electrons. In L dwarfs molecular bands are less preeminent due to the presence of a high-reaching cloud layer (Allard & Hauschildt 1995; Tsuji et al. 1996), until with the transition from L to T dwarfs the clouds are settling into regions of larger optical depth, revealing a cool and dense atmosphere again dominated by molecular absorption (Allard et al. 2001; Ackerman & Marley 2001; Tsuji 2002). The effect of the strongly wavelength-dependent opacity is evidenced in the SED of T dwarfs, which is shifted from the maximum of the Planck function for the corresponding $T_{\rm eff}$ at $2-4\,\mu$, far to the blue to peak in the J-band around $1.2\,\mu$ instead. The blanketing effect has been shown (e. g. Allard et al. 1994) to have a similarly strong impact on the T/P structure within the atmosphere. Theoretical modelling of the coolest dwarfs therefore requires accurate data on the opacities of a variety of molecular species for different temperatures and densities.

2. Molecular Opacity

Great advances in cool stellar models over the past 10 – 15 years have been facilitated by the availability of extensive data bases for molecular line strengths, and the numerical capacity to include them in detailed physical models. For application to model atmosphere codes opacities can either be precomputed from the list of individual line strengths in opacity distribution tables or related methods (e. g. Burrows et al. 2001), or directly be included in a line-by-line calculation such as the dynamical opacity sampling method (dOS) employed in the `PHOENIX`[1] code (Hauschildt & Baron 1999). The current set of brown dwarf models, considering up to several 10^8 lines for H_2O, TiO, CH_4 and other species, was described in detail by Allard et al. (2001), with some updates given in Homeier et al. (2004). A general discussion of opacity sources at different temperatures is given by Ferguson et al. (2005). The strongest blanketing effects are generally found for bands with dense coverage of wavelength space, such as produced by the complex vibrational spectra of polyatomic molecules. In comparison, the more regularly space lines of diatomic molecules (in BDs most notably FeH, CrH and CO) allow more flux to escape between the lines (Alexander et al. 2003). Consequently, model structures are much more sensitive to having sufficiently complete data for the former species, here especially H_2O (Allard et al. 1994, 2000) and CH_4 (Homeier et al. 2003, 2005), than to the most accurate positions, shapes and strengths of individual transitions. Since in these bands several lines overlap at almost every wavelength point, simple approximations of the damping profile or even just the Doppler core of the lines can be used without introducing great errors (Schweitzer et al. 1996).

This situation changes somewhat for the coolest BDs detected to date, T dwarfs of $T_{\mathrm{eff}} < 1000\,\mathrm{K}$, and when analysing spectra in the mid- or far-IR. Transitions tend to be more numerous at shorter wavelengths, and at lower temperatures, fewer ro-vibrational levels are populated. Thus at longer wavelengths and in very cool objects the band opacity is shaped by fewer, but stronger lines. Similarly, when calculating synthetic spectra at high resolution, e. g. for abundance analysis, individual lines may become more important. One example is the signature of CO, which has little effect on the thermal structure in cool BD atmospheres, where it is mostly substituted by CH_4 as the main carbon-bearing species. Yet the 0 – 1 fundamental band at $4.55\,\mu$ continues to be visible at least in early T dwarfs and could be used as a temperature tracer for these atmospheres due to the temperature sensitivity of the CO/CH_4 equilibrium. Additionally, evidence exists that CO might survive in excess of chemical equilibrium abundances in cooler T dwarfs due to mixing from warmer layers (Noll et al. 1997; Saumon et al. 2003). For such studies knowledge of the line profile out to several cm^{-1} will be relevant.

3. Experimental and Theoretical Line Widths

Although laboratory measurements of line widths exist for a variety of molecular absorbers and perturbers, and are in many cases incorporated into spectroscopic databases such as HITRAN (Rothman et al. 2003), these experimental data are usually not directly applicable to stellar atmosphere models. Being designed mainly for Earth atmosphere studies, the tabulated widths for individual transitions generally are for air broadening (N_2 and/or O_2) at 296 K. These databases also lack transitions at higher temperatures, for which only theoretical predictions are available. Theoretical models to determine line widths for arbitrary per-

[1] http://www.hs.uni-hamburg.de/phoenix/

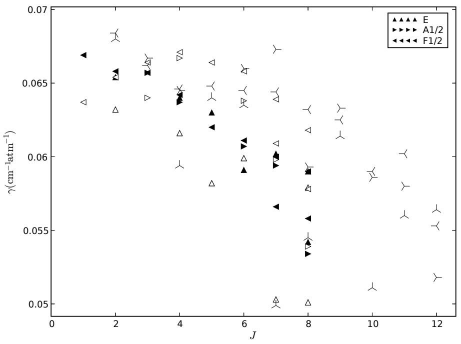

Fig. 1. Half-widths for Q-branch transitions of CH_4 at 296 K as a function of lower level rotational quantum number and symmetry. Full triangles are broadening widths calculated by Neshyba et al. (1994), open triangles experimental widths due to Pine (1992), both for the ν_3 band with N_2 as perturber. The tripod symbols show experimental H_2 widths for the ν_4 band from Margolis (1993)

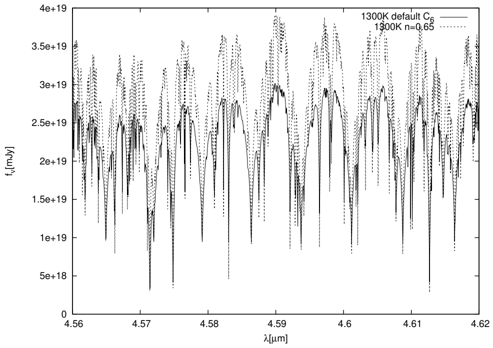

Fig. 2. AMES-Cond (Allard et al. 2001) model spectra for a 1300 K, log $g = 5$ T dwarf showing the CO fundamental with (solid) standard broadening from Schweitzer et al. (1996) and (dashed) laboratory half-widths from Sung & Varanasi (2004), extrapolated from 300 K using a scaling with $T^{-0.65}$. The latter model uses ~ 5 times smaller damping constants than the former.

turbers and temperatures would therefore be most desirable.

A number of attempts have been made to model measured widths using the theory of Anderson (1949) and its extensions, or more advanced models of impact broadening such as Robert & Bonamy (1979), e. g. by Neshyba et al. (1994). Even in the latter case a full explanation of broadening as a function of rotational and vibrational quantum numbers is usually not possible (cf. Fig. 1), but one may hope to obtain reasonable extrapolations from measured widths at 296 K to 1000 K and more. The half-width in this case can be expressed as

$$\gamma_0 = \frac{n_2}{2c}\langle v\rangle\sigma_{12}^2 = \frac{n_2}{c}\sqrt{\frac{2kT}{\pi m}}\sigma_{12}^2 \propto \frac{P_2}{\sqrt{kT}}\sigma_{12}^2(T)$$

with n_2 the perturber density, $\langle v\rangle$ taken as the mean thermal speed of the perturbing molecules, and an optical collision diameter σ_{12}. For H_2- and helium-broadening, σ_{12} can often be assumed to show little variation with T, and the half-width therefore follows the simple temperature dependence $\gamma_0 \propto T^{-n}$ with n close to $1/2$ (e. g. Varanasi et al. 1973; Margolis 1993), although Varanasi (1988) reports a range of temperature exponents from $0.3 \lessapprox n \lessapprox 0.7$. Experimental determinations of n are also mostly based on comparison with *low* temperature measurements (at 70 –200 K for solar system gas giants' atmospheres), so some caution should be exercised when using them for extrapolation to hot gases. When estimating σ_{12} from measurements at 296 K, an uncertainty of a factor 2 – 3 for widths at 1000 – 2000 K can thus be conservatively assumed. As a comparison of PHOENIX models (Fig. 2) demonstrates, such errors introduce only moderate changes in the emergent spectra even for rather strong lines. This example also shows that single molecular lines do not dominate the spectrum beyond a range of a few cm^{-1}, well below the limit where deviations from a pure Lorentzian wing shape may be found (Hartmann et al. 2002).

4. Conclusions

Correct modelling of molecular line absorption is essential for studying the atmospheres of the lowest mass stars, brown dwarfs and gas giant planets. The progress made in theoretical predictions of transition strengths and energies is not currently reflected in theoretical models for pressure broadening and shifts of molecular lines. Highly accurate simulations for line shapes in astrophysical objects therefore remain a challenge. Using available experimental data and theoretical insights, however a reasonably accurate description of molecular absorption is possible, sufficient to characterise the essential properties of ultracool atmospheres. Further progress in both theory and experiment is nonetheless desirable to improve our understanding of physical and chemical processes in these objects, in particular in view of improving capabilities for high-resolution spectroscopy observations in the infrared.

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References

Ackerman, A. S., & Marley, M. S. 2001, ApJ, 556, 872
Alexander, D. R., Ferguson, J. W., Tamanai, A., et al. 2003, in: Stellar Atmosphere Modeling, eds. I. Hubeny, D. Mihalas, & K. Werner, ASP Conference Series vol. 288, 289
Allard, F., Hauschildt, P., Alexander, D., Tamanai, A., & Schweitzer, A. 2001, ApJ, 556, 357
Allard, F., & Hauschildt, P. H. 1995, ApJ, 445, 433
Allard, F., Hauschildt, P. H., Miller, S., & Tennyson, J. 1994, ApJ, 426, L39
Allard, F., Hauschildt, P. H., & Schwenke, D. 2000, ApJ, 540, 1005
Anderson, P. W. 1949, Phys. Rev., 76, 647
Burgasser, A. J., Kirkpatrick, J. D., Brown, M. E., et al. 2002, ApJ, 564, 421
Burrows, A., Hubbard, W. B., Lunine, J. I., & Liebert, J. 2001, Reviews of Modern Physics, 73, 719
Ferguson, J. W., Alexander, D. R., Allard, F., et al. 2005, ApJ, 623, 585
Geballe, T. R., Knapp, G. R., Leggett, S. K., et al. 2002, ApJ, 564, 466
Hartmann, J.-M., Boulet, C., Brodbeck, C., et al. 2002, J. Quant. Spec. Radiat. Transf., 72, 117
Hauschildt, P. H. & Baron, E. 1999, J. Comp. Applied Math., 109, 41
Homeier, D., Allard, F., Hauschildt, P., Barman, T., & Schweitzer, A. 2004, in: High Resolution Infrared Spectroscopy in Astronomy, ESO Astrophysics Symposia, eds. H. Käufl, R. Siebenmorgen, & A. Moorwood; Springer, Heidelberg, in press
Homeier, D., Allard, F., Hauschildt, P., & Boudon, V. 2003, in: Modelling of Stellar Atmospheres, IAU Symposium 210, eds. N. Piskunov, W. Weiss, & D. Gray; ASP Conference Series, San Francisco, CD-ROM supplement
Homeier, D., Allard, F., Hauschildt, P., Boudon, V., & Champion, J. 2005, A&A, in prep.
Kirkpatrick, J. D., Reid, I. N., Liebert, J., et al. 1999, ApJ, 519, 802
Margolis, J. S. 1993, JQSRT, 50, 431
Martin, E. L., Basri, G., Delfosse, X., & Forveille, T. 1997, A&A, 327, L29
Neshyba, S. P., Lynch, R., Gamache, R., Gabard, T., & Champion, J.-P. 1994, J. Chem. Phys., 101, 9412
Noll, K. S., Geballe, T. R., & Marley, M. S. 1997, ApJ, 489, L87
Pine, A. S. 1992, J. Chem. Phys., 97, 773
Robert, D. & Bonamy, J. 1979, J. de Phys. (Paris), 40, 923
Rothman, L. S., Barbe, A., Benner, D. C., et al. 2003, J. Quant. Spec. Radiat. Transf., 82, 5
Saumon, D., Marley, M. S., Lodders, K., & Freedman, R. S. 2003, in: Brown Dwarfs, IAU Symposium 211, ed. E. Martín; ASP Conference Series, San Francisco, 345
Schweitzer, A., Hauschildt, P. H., Allard, F., & Basri, G. 1996, MNRAS, 283, 821
Sung, K. & Varanasi, P. 2004, JQSRT, 85, 165
Tsuji, T. 2002, ApJ, 575, 264
Tsuji, T., Ohnaka, K., Aoki, W., & Nakajima, T. 1996, A&A, 308, L29
Varanasi, P. 1988, JQSRT, 39, 13
Varanasi, P., Sarangi, S., & Pugh, L. 1973, ApJ, 179, 977