

NASA LAW, February 14-16, 2006, UNLV, Las Vegas

Metal Hydride and Alkali Halide Opacities in Extrasolar Giant Planets and Cool Stellar Atmospheres

Philippe F. Weck

Department of Chemistry, University of Nevada-Las Vegas, Las Vegas, NV 89154

`weckp@unlv.nevada.edu`

Phillip C. Stancil

Dept. of Physics & Astronomy and Center for Simulational Physics, The University of Georgia, Athens, GA 30602

`stancil@physast.uga.edu`

Kate Kirby

ITAMP, Harvard-Smithsonian Center for Astrophysics, 60 Garden Street, Cambridge, MA 02138

`kirby@cfa.harvard.edu`

Andreas Schweitzer & Peter H. Hauschildt

Hamburger Sternwarte, Universitaet Hamburg, Gojenbergsweg 112, D-21029 Hamburg, Germany

`Andreas.Schweitzer@hs.uni-hamburg.de,phauschildt@hs.uni-hamburg.de`

ABSTRACT

The lack of accurate and complete molecular line and continuum opacity data has been a serious limitation to developing atmospheric models of cool stars and Extrasolar Giant Planets (EGPs). We report our recent calculations of molecular opacities resulting from the presence of metal hydrides and alkali halides. The resulting data have been included in the PHOENIX stellar atmosphere code (Hauschildt & Baron 1999). The new models, calculated using spherical geometry for all gravities considered, also incorporate our latest database of nearly 670 million molecular lines, and updated equations of state.

The study of the spectra of cool stars requires detailed knowledge of molecular opacities. This includes important absorbers such as TiO, CO, and water vapor, which have bands that cover large wavelength ranges and are very important for the structure of the atmosphere due to their overall cooling or heating effects. In addition, there are a number of molecules that have bands covering comparatively small wavelength ranges (e.g., 10-100 Å). Many of them are trace molecules that have only small effects on the overall physical conditions inside the atmosphere but that are important for spectral classification and for the determination of stellar parameters such as effective temperatures, gravities and abundances. We have therefore started a project to update or provide for the first time molecular data of astrophysical interest for important trace molecules. These data are computed using state-of-the-art molecular physics codes and should improve our ability to model and analyze cool stellar atmospheres considerably (Weck *et al.* 2003a,b,c, 2004a,b; Homeier *et al.* 2005).

Ab initio potential energy curves and dipole moment functions have been calculated for the $X^1\Sigma^+$ and $B^1\Sigma^+$ electronic states of ${}^7\text{Li}{}^{35}\text{Cl}$ (Weck *et al.* 2004a). The line oscillator strengths were computed for all allowed transitions between the 29,370 rovibrational levels calculated neglecting spin-splitting for the $X^1\Sigma^+$ state, thus giving a total of 3,357,811 lines (Weck *et al.* 2004b).

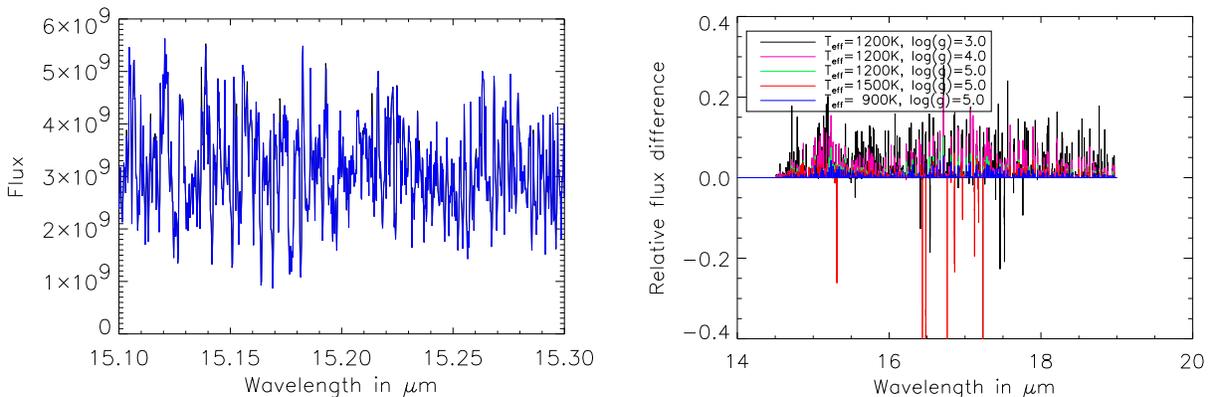


Fig. 1.— Left: LTE synthetic spectra computed with (blue) and without (black) LiCl line absorption as a function of the wavelength for $T_{\text{eff}} = 1200$ K, $\log(g) = 4.0$ and solar abundances; 2 \AA resolution, i.e. $R = 76,000$. Right: Relative flux difference for brown dwarf models with $T_{\text{eff}} = 900 - 1500$ K, $\log(g) = 3.0 - 5.0$ and solar abundances

To assess LiCl line absorption in the spectra of brown dwarfs, we have calculated LTE synthetic spectra with and without the new LiCl data. Several brown dwarf models somewhat in the L/T-dwarf regime with $T_{\text{eff}} = 900 - 1500$ K, $\log(g) = 3.0 - 5.0$ and solar abundances were considered using the PHOENIX code. The small differences shown in the left panel of Figure 1 suggest that the line opacity due to LiCl in cool brown dwarf atmospheres is relatively insignificant. The opacity in the far infrared is apparently dominated by H_2O .

As depicted in the right panel of Figure 1, relative flux differences are typically less than 20% for young ($\log(g) = 3.0, \simeq 100$ Myrs) to old ($\log(g) = 5.0, > 1$ Gyr) brown dwarfs for $T_{\text{eff}} = 900 - 1200$ K

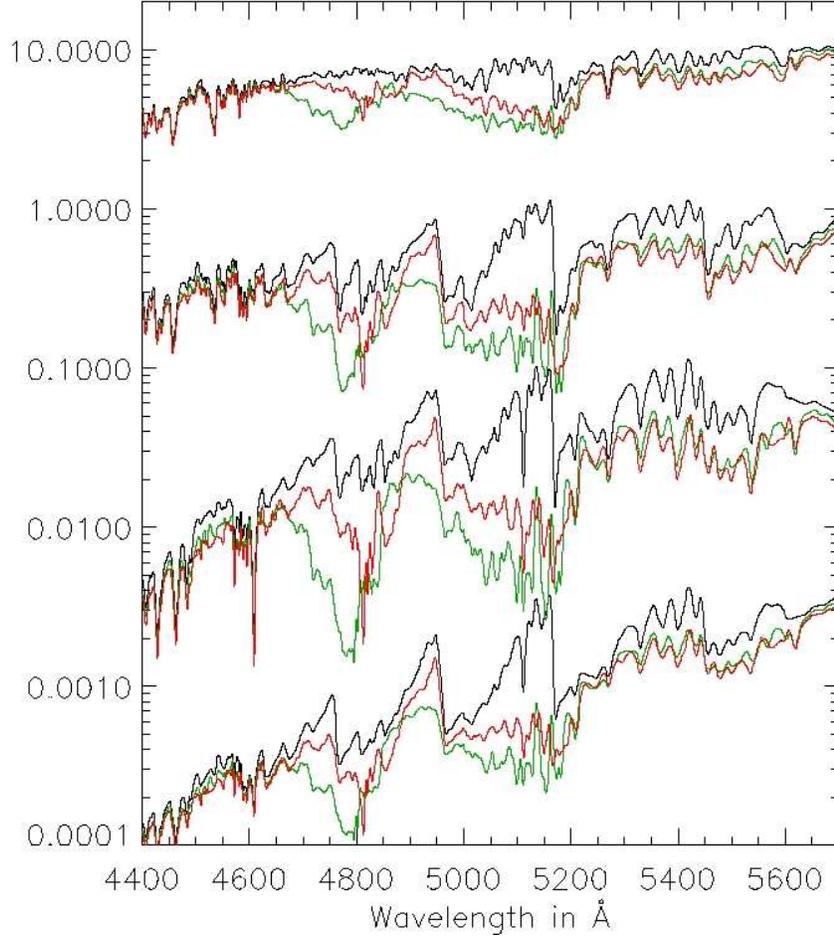


Fig. 2.— Spectra of the strongest MgH bands (log scale for flux in 10^{13} erg/cm²/s/cm) for models with $T_{\text{eff}} = 4000, 3000, 2000$ K (AMES-Cond model) and $T_{\text{eff}} = 2000$ K (AMES-Dusty model) (from top to bottom). The 2000 K AMES-Cond models have an artificial offset of +1.0 dex for better legibility. All models have $\log(g)=5.0$ and are AMES-Cond unless noted otherwise. Black: no MgH data; red: new MgH data; green: MgH data calculated with a model Hamiltonian.

In Figure 2 we show comparisons between spectra, in the spectral region where the MgH bands are most prominent, from models using: a) no MgH data, b) our new MgH line list (Weck *et al.* 2003b), and c) the Kurucz (1993) MgH line list. The comparisons have been done at $T_{\text{eff}} = 2000$ K, 3000 K, and 4000 K to sample the temperature range in which MgH is visible in the spectrum. As can be seen, the line list calculated with a model Hamiltonian

overestimates the opacity obtained with our new MgH line list. The differences between the spectra with the new and model Hamiltonian MgH line lists are very similar for the AMES-Cond and AMES-Dusty models although the overall flux level and the overall flux shape are different for AMES-Cond and AMES-Dusty in the optical. As can be seen, there are significant differences spreading among both the $A - X$ and the $B' - X$ transitions.

Conclusion

We have calculated theoretical spectra for different stellar models of brown dwarfs including our latest metal hydride and alkali halide molecular data obtained from *ab initio* calculations. The present synthetic spectra generated for stellar models somewhat in the M/L/T-dwarf regime clearly illustrate the current needs for accurate molecular data to improve our ability to identify, characterize and classify the increasing number of cool stellar objects as well as extrasolar giant planets found in recent observational surveys.

This work was supported by NASA grants NAG5-12751, NAG5-8425, NAG5-9222, and NAG5-10551 as well as NASA/JPL grant 961582, and in part by NSF grants AST-9720704 and AST-0086246 (and a grant to the Institute for Theoretical Atomic, Molecular & Optical Physics, Harvard-Smithsonian CfA). Some of the calculations were performed on the IBM SP2 of the UGA EITS, on the IBM SP “Blue Horizon” of the San Diego Supercomputer Center, with support from the NSF, and on the IBM SP of the NERSC with support from the DoE.

REFERENCES

- Hauschildt, P. H., & Baron, E. 1999, *J. Comput. App. Math.*, 102, 41
Homeier, D., Allard, N. F., Allard, F., Hauschildt, P. H., Schweitzer, A., Stancil, P. C., & Weck, P. F. 2005, *ASP Conf. Series*, 334, 209
Kurucz, R. L. 1993, CD-ROM No.15 Diatomic molecular data for opacity calculations (Harvard-Smithsonian Center for Astrophysics)
Weck, P. F., Stancil, P. C. & Kirby, K. 2003a, *J. Chem. Phys.*, 118, 9997
Weck, P. F., Schweitzer, A., Stancil, P. C., Hauschildt, P. H., & Kirby, K. 2003b, *ApJ*, 584, 459
Weck, P. F., Schweitzer, A., Stancil, P. C., Hauschildt, P. H. & Kirby, K. 2003c, *ApJ*, 582, 1263
Weck, P. F., Kirby, K., & Stancil, P. C. 2004a, *J. Chem. Phys.*, 120, 4216
Weck, P. F., Schweitzer, A., Kirby, K., Hauschildt, P. H., & Stancil, P. C. 2004b, *ApJ*, 613, 567