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

Philippe F. Weck*

February 3, 2006

Abstract

The lack of accurate and complete molecular opacity data for a large number of metal hydrides and alkali halides has been a serious limitation to developing atmospheric models of cool stars and extrasolar giant planets. In fact, sophisticated modeling programs require high quality opacity data in order to produce synthetic spectra and predict important physical parameters (surface chemical composition, effective temperature, etc). Typically, atmosphere models include molecular bands with hundreds of millions of spectral lines, mostly derived from molecular band models.

In this work, we report our progress on the calculations of line opacities resulting from the presence of CaH and LiCl. Fully quantum-mechanical techniques have been applied to compute comprehensive and complete transition energies and absorption line oscillator strengths for all possible allowed transitions from the electronic ground state. *Ab initio* potential energies and dipole transition moment functions have been used, with the former adjusted to account for experimental data.

For calcium monohydride, line lists for the electronic transitions from the $X\ ^2\Sigma^+$ ground state to the $A\ ^2\Pi$, $B/B'\ ^2\Sigma^+$, $C\ ^2\Sigma^+$, $D\ ^2\Sigma^+$ and $E\ ^2\Pi$ bound excited states have been calculated using electronic structure calculations from the literature. The spectrum of CaH is characterized by strong perturbations of various types, from local shifts to large interactions between electronic states [1]. For lithium chloride, we have obtained the potential curves and dipole transition moment functions between the $X\ ^1\Sigma^+$ ground state and the purely dissociative $B\ ^1\Sigma^+$ and $A\ ^1\Pi$ excited states [2]. Using these data for LiCl and CaH, we have calculated synthetic spectra for cool dwarf test models with the `PHOENIX` stellar atmosphere code [3, 4, 5].

This work was supported in part by NSF grants AST-9720704 and AST-0086246, NASA grants NAG5-8425, NAG5-9222, and NAG5-10551 as well as NASA/JPL grant 961582. Some of the calculations were performed on the IBM SP2 of the UGA EITS, on the SP *Blue Horizon* of the San Diego Supercomputer Center, with support from the NFS, and on the IBM SP of the NERSC with support from the DoE.

1. P. F. Weck, P. C. Stancil and K. Kirby, J. Chem. Phys. **118**, 9997 (2003).

2. P. F. Weck, P. C. Stancil and K. Kirby, J. Chem. Phys. **120**, 4216 (2004).

3. P. H. Hauschildt and E. Baron, Journal of Computational and Applied Mathematics **102**, 41 (1999).

4. P. F. Weck *et al.*, Astrophys. J. **613**, 567 (2004).

5. D. Homeier *et al.*, ASP Conf. Series **334**, 209 (2005).

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