# Experimental and Theoretical Studies of Pressure Broadened Alkali-Metal Atom Resonance Lines

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## ABSTRACT

We are carrying out a joint theoretical and experimental research program to study the broadening of alkali atom resonance lines due to collisions with helium and molecular hydrogen for applications to spectroscopic studies of brown dwarfs and extrasolar giant planets.

## 1.   Introduction

The broadened resonance lines of sodium and potassium appear prominently in the spectra of certain classes of brown dwarfs, and are expected to be present in the spectra of certain extrasolar planets as well (Burrows et al. 2001; Sudarsky et al. 2003). Accurate line-profiles, as a function of temperature and density, will be invaluable to astrophysicists as diagnostics of the atmospheres of substellar mass objects. Our project currently consists of an experiment to measure pressure broadening of potassium resonance lines by He and by $H_2$ at about 1000 K combined with theoretical calculations for other temperatures.

## 2.   Description of the experiment

The critical elements in the absorption spectroscopy experiment include a Mach-Zehnder interferometer and a 3 m Czerny-Turner grating spectrograph with CCD camera detector ($1024 \times 256$ pixels with a size of 26 $\mu$m) for dispersing and recording spectra. The spectrometer (McPherson model 2163) covers the wavelength range from 360 to 920 nm through the use of a stepper controller enabling the rotation of a 1200 l/mm plane ruled grating at 116 different angles. As a background light source, we use a tungsten halogen lamp (250 W, 24 V) with the beam collimated through an arrangement of optics before entering the interferometer. A unique feature of the experiment is the accurate determination of the absorber atom number density, which is obtained using the "hook" (or anomalous dispersion) method.

To reproduce the conditions of the environments we want to study, the apparatus was designed to allow measurements at different noble gas pressures, from 10 torr to 700 torr, and at high temperatures (about 900 K). The cell was fabricated according to the design showed in Fig. 1. The cell body is composed of three welded tubes of grade 330 stainless steel,
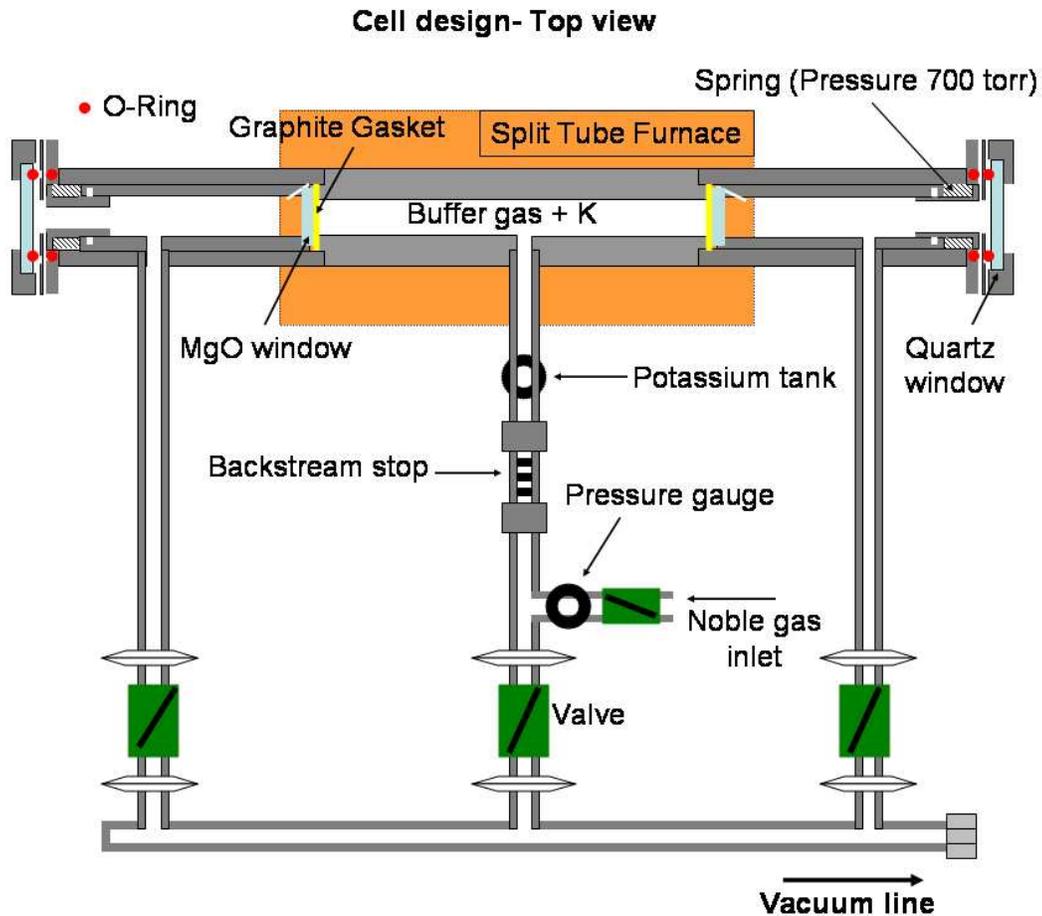
**Cell design- Top view**



Fig. 1.— Cell design.

chosen for its resistance to the corrosive effects of alkali-metal gases at high temperature. The middle tube (cold path-length $l = 20$ cm) is the gas chamber and it is closed by MgO windows sealed with graphite gaskets. Each of the two tubes on the outside of the gas chamber contains a cylinder and a spring to press the MgO window in, thereby allowing the noble gas pressure in the gas chamber to reach values as high as 700 torr. The cell ends are closed by quartz windows sealed with Viton O-rings. All of the cell body tubes are independently connected to a vacuum line. The potassium sample is placed in a 330 grade stainless steel reservoir attached to the cell by a Swagelok fitting allowing the reservoir to be removed readily for sample replacement.

The reservoir and the tube leading to the gas chamber are heated by homemade heaters regulated through a commercial temperature controller. The gas chamber is inserted in a specially designed split tube furnace that fits within our experimental size constraints. The oven ensures that there is a uniform temperature along the path-length of the gas chamber and facilitates the removal of the cell from the apparatus.

The system oven plus gas cell is situated in one branch of a Mach-Zehnder interferometer whereas a pair of MgO windows and a pair of quartz plates are placed in the other arm to compensate the windows of the gas cell. Then, the interferometer is adjusted at optical zero path difference to produce a set of horizontal interference fringes at each wavelength present in the light source. The fringe pattern is focused by a lens on the entrance slit of the spectrometer. As each arm of the interferometer can be blocked by a shutter, we are able to measure the spectrum arising from the gas cell, a reference spectrum and the fringe pattern.

The association of the interferometer and the spectrometer is essential to apply the so called "hook" method (Rozhdestvenskii 1912), which provides a measurement of the atomic number density of the absorbers vaporized in the gas chamber. This technique uses the change in the refractivity in the vicinity of a resonance line which induces a distortion of the fringe profile. By inserting an additional compensation plate into one of the interferometer arms, the fringes are shifted to higher orders. Consequently, the fringes will appear slanted in line-free spectral regions, whereas close to absorption lines the anomalous dispersion produces maxima and minima in the fringe positions with wavelength, giving the characteristic hook appearance near the lines. As the shape of the fringes is closely related to the number density of absorbers, fitting the fringe distortion near the potassium doublet at 770 nm leads to the determination of the potassium density number.

## 3.    Theoretical work

Accurate calculations of the opacities due to pressure broadening in the wings of resonance lines require accurate potential energy curves and transition dipole moments for the alkali-metal atom and perturber gas atom (or molecule) interactions. Because satisfactory data were not available in the literature for the K-He and K-$H_2$ systems, the "Molpro" quantum chemistry codes implementing a Multi-Reference Configuration Interaction method were used to compute, at an unprecedented level of accuracy, all of the molecular states involved in the line-broadening of the resonance lines (Santra and Kirby 2005).

The pressure broadening of Li, Na, and K by He in the wings of the resonance lines was investigated using fully quantum-mechanical methods (Zhu et al. 2005, 2006) and the calculated reduced absorption coefficients at several temperatures for Na-He and K-He are presented in Fig. 2. Future experimental and theoretical work will focus on the K-$H_2$ system.
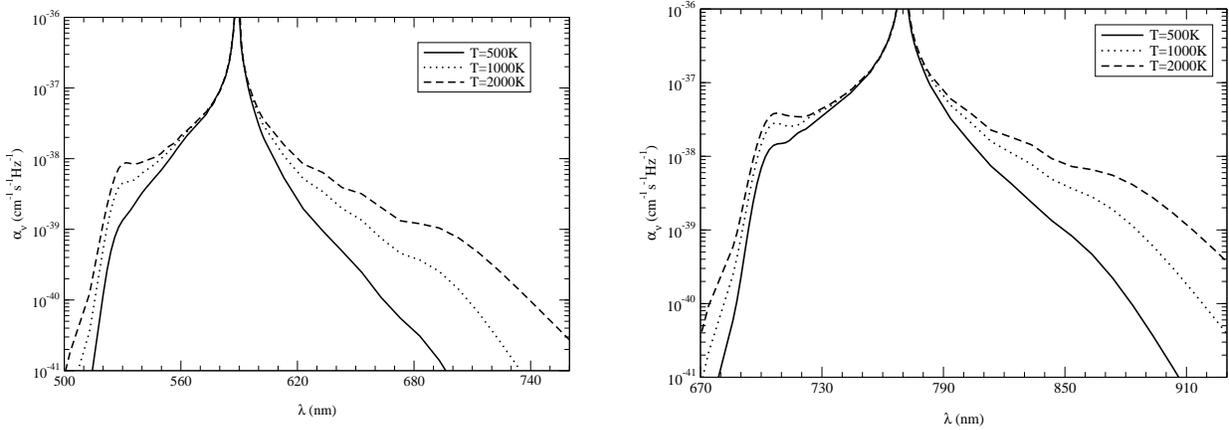
Fig. 2.— Absorption coefficients for a) (left view) Na-He and b) (right view) K-He at temperatures of 500 K, 1000 K, and 2000 K.

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