

THE BROADENING OF CALCIUM II H AND K LINES BY HELIUM

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ABSTRACT

Laboratory measurements of widths and shifts of the Ca II H and K lines have been made under conditions simulating those in the atmospheres of metallic-line white dwarfs, namely, densities of 10^{21} helium atoms cm^{-3} and temperatures of 4500° to 6000° K. There are significant differences in the shifts and damping constants of the two fine-structure components. The impact theory is evidently applicable to the Ca II/He system under these conditions, and the observed damping constants are fortuitously close to the predictions of conventional Lindholm-Foley/van der Waals theory. The widths and shifts have also been analyzed in terms of Lennard-Jones potential theory.

Subject headings: Line profiles — spectra, laboratory — white dwarf stars

I. INTRODUCTION

Early work on cool white dwarf atmospheres (Weidemann 1960) indicated that gas pressures of about 1000 atm and helium-rich compositions were necessary to produce the wide Ca II H and K lines such as those observed in van Maanen 2. It was also clear that electron pressures would be low and that the dominant line broadening mechanism would be the "van der Waals," or neutral-atom collision broadening process. To make further progress in determining compositions and effective temperatures for these metallic-line white dwarfs, we have constructed non-gray, LTE, convective, constant-flux model atmospheres for these stars (Hammond and Bell 1975). To calculate accurate line profiles for the strong Ca II lines, however, it was necessary to obtain experimental collisional damping constants for these lines because the existing line broadening theories are inadequate. This paper presents a brief review of the current status of both the theoretical and the experimental work on van der Waals broadening, a description of the experimental techniques employed here to simulate white dwarf atmospheric conditions, the results for Ca II H and K broadened by helium, and a brief analysis in terms of Lennard-Jones interaction potentials.

Nearly all stellar-atmosphere line-profile studies for spectral types F and cooler have relied on the Lindholm-Foley impact theory of line broadening (Lindholm 1942; Foley 1946) containing only the attractive van der Waals force. There is abundant experimental evidence that this standard theoretical treatment is inadequate in several respects. It yields widths often too small, shifts generally too large and often in the wrong direction for helium and other light perturbers, and a temperature dependence of $T^{3/10}$ for both shift and width that has never been observed. The van der Waals interaction constant is conventionally calculated with the Unsöld (1955) suggestion of approximating the polarizabilities of excited quantum states

by scaling with effective principal quantum numbers and hydrogenic dipole moments. This procedure does not provide for the complex fine-structure (J -dependence) effects that have been observed. The experimental work referred to here is that reviewed by Ch'en and Takeo (1957), and the more recent work by Ch'en and Garrett (1966*a, b*), Ch'en, Looi, and Garrett (1967*a, b*), Ch'en, Gilbert, and Tan (1969*a*), and Ch'en, Lewis, and Stacy (1969*b*); and the low density measurements by Hindmarsh (1959, 1960), Smith (1967), and McCartan and Hindmarsh (1969).

Recently, improvements have been made in the Lindholm-Foley theory with the substitution of the Lennard-Jones (12, 6) interaction for the van der Waals interaction (Behmenburg 1964; Hindmarsh, Petford, and Smith 1967). This substitution provides an additional parameter, the repulsive (or exchange) interaction constant, and insertion of width and shift data yields both attractive and repulsive interaction constants. A similar procedure has been derived by Dyne (1971) for an exponential-6 potential. However, the constants thus determined should be regarded only as parameters that satisfy a model potential function, whereas it is hoped that realistic interaction constants can eventually be derived from intrinsic atomic or molecular properties.

Some recent evidence suggests that higher order terms in the attractive part of the potential are important in line broadening phenomena. Hindmarsh, Duplessis, and Farr (1970) found that by including a term C_8/r^8 with the Lennard-Jones (12, 6) potential, and with C_8 calculated from dipole and quadrupole polarizabilities, the resulting C_6 van der Waals interaction constant obtained from width and shift data agreed much better with the theoretical C_6 values than did the C_6 values derived without the r^{-8} term. Theories incorporating several higher order attractive terms, but omitting the exchange interaction that contributes to the widths, have been developed by Fullerton and Cowley (1970, 1971) and by Brueckner (1971), all of whom treated the case of broadening by

hydrogen atoms as well as by rare gases. In the case of broadening by hydrogen atoms, however, a more *a priori* approach has been taken by Lewis, McNamara, and Michels (1971), who have derived damping constants for the sodium D lines broadened by hydrogen by calculating potential curves for the NaH molecule. The computational effort involved probably limits this approach to only a few simple systems at the present time, but the scheme is attractive because the only input data required are properly chosen atomic wave functions. Another approach to foreign gas broadening that also requires a minimum of input data is the work of Roueff and collaborators (Roueff and Van Regemorter 1969, 1971; Lortet and Roueff 1969; Roueff 1970, 1972) in which the interaction is taken to be that between the valence electron of the emitter, treated as a quasi-free electron, and the perturbing atom. The input data required are the polarizability of the perturber, and the scattering length for the electron interacting with the perturber, a quantity obtained from Ramsauer-Townsend effect data (O'Malley 1963) in the case of heavy rare gases, and directly calculable for helium and hydrogen. This approach yields good agreement with experiments on Cs lines broadened by helium (Rostas and Lemaire 1971).

In view of uncertainties regarding the form of the interatomic potential, the inability to calculate interaction constants directly from atomic properties, and the computational effort required for the sophisticated treatments recently developed, it seems clear that there is presently little recourse, if one wants reliable damping constants, except to laboratory measurements. However, there are currently few experimental data that can readily be applied to astrophysical problems. The emitter-perturber systems selected for laboratory studies are rarely cosmically abundant species, the temperatures of most experiments are much too cool, and there are no reliable theoretical or empirical rules for transforming laboratory data to astrophysically relevant temperatures and species. Most experimental work to date at high temperatures is largely qualitative because of difficult practical problems. If the light source is a steady state device such as a DC arc (Kusch 1958) or a flame (Behmenburg 1964), the principal causes of error are radial composition and temperature gradients. In shock-tube spectroscopy, the low densities of neutral species and high electron densities result in line widths contaminated by Stark broadening (Day 1969; Miller, Roig, and Moo-Young 1971).

However, as we shall show in more detail below, the temperatures, pressures, and chemical compositions appropriate to F, G, and K white dwarf atmospheres can be achieved in the laboratory by rapid, quasi-isentropic gas compression. This technique yields temperatures of the order of 5000° K and pressures of a few thousand atmospheres over intervals of a few hundred microseconds. Although this experimental method has been used occasionally for thermodynamic measurements (Ryabinin 1952, 1961; Price and Lalos 1957; Longwell *et al.* 1958), it has recently

come into increasing use for line broadening studies (Hammond 1962; Lalos and Hammond 1962, 1965; Takeo, Holmes, and Ch'en 1967; Holmes, Ch'en, and Takeo 1969*a, b, c*; Burgess and Grindlay 1970).

Line broadening data obtained with this technique fall generally into one of two regimes. If both emitter and perturber are light atoms with small polarizabilities, then the observed damping constant is sufficiently small to permit nearly the entire line profile to fall within the validity criteria of impact theories up to perturber densities of nearly 10^{22} atoms cm^{-3} . However, if either emitter or perturber has a large polarizability, the lines may appear distinctly asymmetric at densities as low as 10^{20} atoms cm^{-3} , and theories allowing for the effects of multiple, overlapping collisions must be considered in the analysis of such data. Line broadening theories for this so-called quasi-static regime have been developed for the van der Waals potential (Margenau 1951) and for the Lennard-Jones potential (Bergeon, Robin, and Vodar 1952; Hindmarsh and Farr 1969). Also, theories which go over asymptotically to the impact theory at low pressures and to the quasi-static theory at high pressures have been developed for the transition region between these two regimes. These theories have been developed for both the van der Waals potential (Lindholm 1945; Anderson 1952) and the Lennard-Jones potential (Behmenburg 1968; Fox and Jacobson 1969; Takeo 1970; Jacobson 1971*a, b*). As was the case for the impact theories mentioned earlier, these quasi-static and general pressure theories do not provide relations for calculating the interaction constants, and all contain the additional assumption that the multiple interactions add as scalars. Therefore it seems safe to conclude that for practical problems involving very high densities, as in white dwarf atmospheres, and metal species with large polarizabilities, such as iron or neutral calcium, one must resort to laboratory techniques such as gas compressors for reliable damping constants, collisional line shifts, and profile functions.

II. DESCRIPTION OF ERCA FACILITY

In this section we present a condensed description of the Naval Ordnance Laboratory (NOL) ballistic piston compressor ERCA III¹ with which the line broadening measurements were made.

The current version of ERCA has evolved from a series of earlier compressors that have been described in some detail elsewhere. (ERCA I: Price and Lalos 1957; Lalos 1962. ERCA II: Lalos and Hammond 1965.) Those compressors have been reviewed by Vodar and Saurel (1963), Griem (1964), and Tsiklis (1968).

Figure 1 shows a schematic diagram of the principal components of ERCA III. The configuration is similar

¹ An acronym derived from Experimental Rapid Compression Apparatus by analogy with ERMA, the Expansion Rate Measuring Apparatus developed by Professor Michels and three NOL scientists at the van der Waals Laboratory, Amsterdam, two decades ago (Michels, Slawsky, Jacobs 1954*a, b, c*; Seigel 1952).

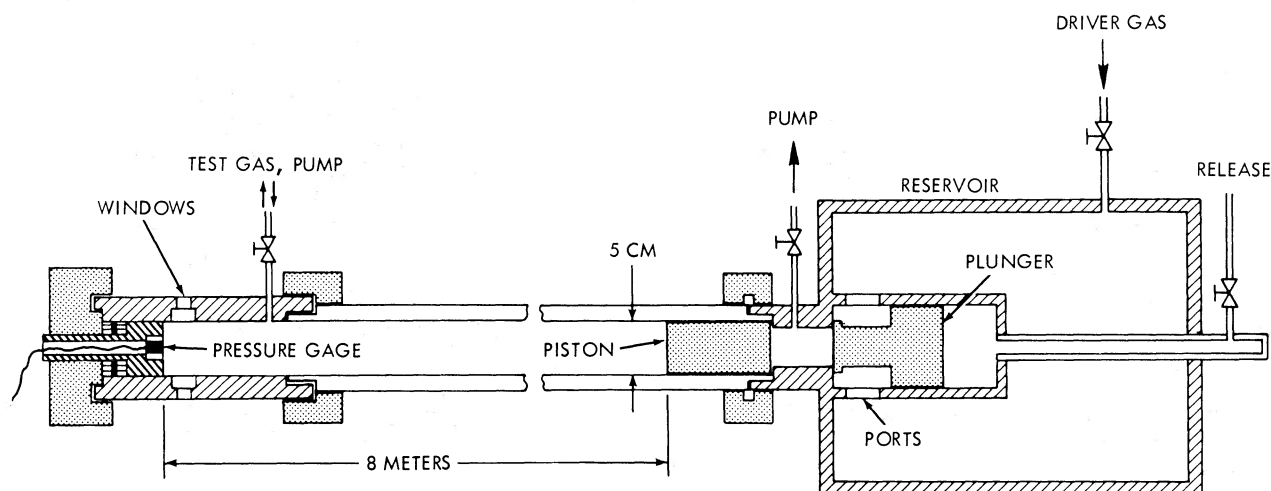


FIG. 1.—Schematic diagram of ERCA III

to a conventional shock tube. The distinguishing feature is the use of a heavy, tight-fitting metal piston that is propelled along the 8-meter tube by compressed gas released from the reservoir by the quick-release plunger valve.

If the compression process were isentropic and the equation of state were the ideal gas law, we would expect that pressures, densities, and temperatures achieved in the compression could be derived from the initial values with the ideal polytropic relations:

$$P/P_0 = (N/N_0)^\gamma = (T/T_0)^{\gamma/(\gamma-1)}, \quad (1)$$

where γ is the polytropic exponent, the ratio of specific heat capacities. These relations are illustrated in figure 2 for the case of ambient initial gas temperature, T_0 . An ideal isentropic compression and expansion cycle would traverse a straight line in figure 2 labeled by the appropriate value of initial pressure, P_0 , up to the

maximum pressure value, $P_{\max}$, and then return along the same line toward the starting point. An equation relating $P_{\max}$ to P_0 and P_r , the reservoir driving pressure, can be derived by equating the work done on the piston by the expanding reservoir gas to the work done by the piston on the test gas. The result, after assuming $(P_{\max}/P_0)^{1/\gamma} \gg 1$ and assuming a constant P_r over the compression cycle, is

$$P_{\max}/P_0 = [1 + (\gamma - 1)P_r/P_0]^{\gamma/(\gamma-1)}. \quad (2)$$

Equations (1) and (2) are sufficient to characterize the physical state of the compressed gas sample in terms of the initial conditions. However, there are several processes occurring in a real gas and in an imperfect machine that render these equations useful only as crude approximations.

In a real gas at high densities and temperatures, the equation of state is uncertain; only for helium will it

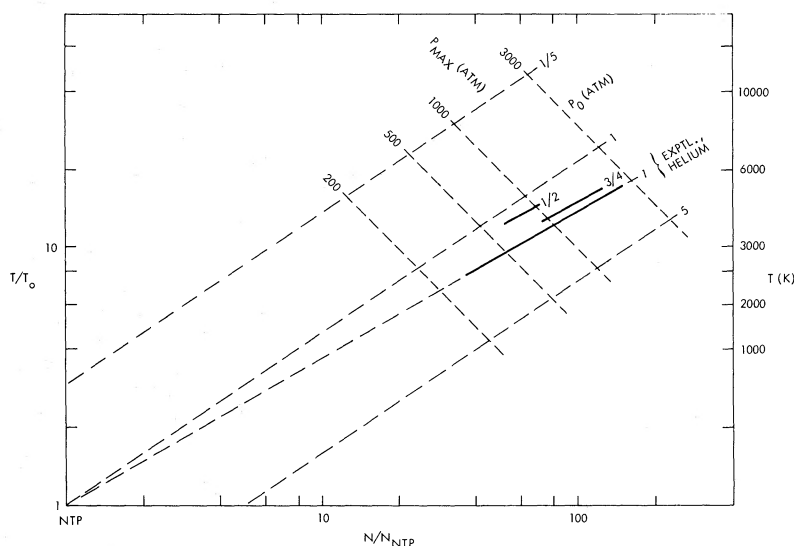


FIG. 2.—Temperature-density relations for ideal isentropic compression

be safe to use $P = NkT$. It is interesting to note that the uncertainties in the theoretical equation of state arise from the same causes as do many of the theoretical line broadening problems mentioned earlier, namely, the uncertainties in the form of the interaction potential (Klein and Hanley 1968).

Every real process is irreversible, and ERCA certainly has its share of irreversibilities. Gas leaks past the piston, frictional forces must be overcome, heat is lost to the surroundings, and shock waves and other inhomogeneities are occasionally detectable. Over the past decade of compressor development, numerous modifications have been incorporated to minimize the effects of these processes. Expanding-cup piston seals reduce gas leakage, refractory metal coatings on the inner walls and piston head reduce heat loss via conduction, and shock waves are negligible when heavy pistons are used with gases of low molecular weight. In spite of these precautions, however, considerable departure from the predictions of equations (1) and (2) has been observed.

With a reliable equation of state, a knowledge of the nature of the leakage flow past the piston, and data for viscosities, thermal conductivities, and heat capacities, the equation of motion of the piston could be solved to yield pressures, temperatures, and densities throughout the compression and expansion cycle. Such an approach has been taken by Takeo *et al.* (1967) for the University of Oregon compressor. It is difficult to assess the accuracy of that work in view of the absence of equation of state and transport properties data at the temperatures and densities achieved in these compressors. We take an alternative approach here by applying experimental diagnostic schemes to measure the state variables directly. In the following sections, some details of these schemes are presented.

a) Pressure Measurements

A commercial (Kistler) pressure transducer is mounted centrally in the end wall. This device is a quartz crystal piezoelectric transducer with an upper limit of 5000 atm pressure. Its rise time of 1.5 μ s allows it to follow accurately the test gas pressure pulse, which typically has a half-width duration of 2 ms. The calibration supplied by the manufacturer is occasionally checked by measuring the response to a step function generated by a quick release of pressure accurately measured with a dead-weight balance. These checks generally agree with the manufacturer's calibration to within 2 percent. The transducer calibration supplied by Kistler was used for all the experiments reported here.

The signal from the transducer is amplified by a charge amplifier, displayed on oscilloscope screens, and photographed with Polaroid cameras. A calibration pulse is simultaneously displayed and photographed to provide a reference signal, thus eliminating the need for precise oscilloscope calibration. However, nonlinearities in the display introduce a maximum additional error of 1 percent.

The pressure is considered to be uniform throughout the test gas volume in these experiments with helium because transit times for sound waves across the volume are short compared with the characteristic times in the compression cycle. Corrections due to the momentum flux arising from heat conduction to the walls will be negligibly small for a thin boundary layer (Griem 1964, chap. 9).

b) Temperature Measurements

The spectroscopic "brightness-emissivity" method is employed for gas temperature measurements. This scheme previously has been applied to flames in the infrared spectral region (Silverman 1949), to internal combustion engines in the ultraviolet region (Smith and Starkman 1969), and to a variety of plasma diagnostic experiments in shock tubes (Huber and Tobey 1968; Grasdalén, Huber, and Parkinson 1969). The widely used line-reversal technique is a special case of this more general method.

The scheme is based on the solution of the radiative transfer equation for a homogeneous gas sample in local thermodynamic equilibrium (LTE):

$$I_{\lambda} = B(\lambda, T_g)[1 - \exp(-\tau_{\lambda})], \quad (3)$$

where I_{λ} is the intensity at some wavelength λ , $B(\lambda, T_g)$ is the Planck function for the gas temperature T_g , and τ_{λ} is the optical depth at that wavelength. To apply equation (3), I_{λ} and τ_{λ} are simultaneously measured, and then (3) can be solved for T_g . The optical depth is measured by passing a chopped light beam through the hot gas and into a polychromator equipped with photomultiplier detectors. Exit slits in the polychromator are positioned to allow opacity measurements at several wavelengths simultaneously. The optical depth is obtained directly from attenuation measurements via the Lambert-Beers law. During the intervals when the chopper is closed, the emission signal I_{λ} from the hot, dense gas is detected in each wavelength channel of the polychromators. The emission intensity is put on an absolute basis by passing a light beam from a radiation standard through the same optics and into the polychromator, and taking care to fill identically all apertures by the beams from both the hot gas and the standard source. A schematic diagram of the temperature optics is shown in figure 3.

The standard light source used in this work is the hot anode crater of a 12-A DC graphite arc manufactured by Mole-Richardson Company. The radiance temperature, spectral radiance, and short-time fluctuations of the Mole-Richardson arc have been determined by the National Bureau of Standards (NBS) (Lee and Lewis 1966; Hattenburg 1967; Cezairliyan 1971), and the spectral emissivity of the hot anode crater has most recently been measured by Schurer (1968). Those studies have shown that when the arc is operating within 0.5 A below the overload or "hissing" point, the radiance temperature is $3800^{\circ}\text{K} \pm 10^{\circ}\text{K}$, this temperature is constant with wavelength over the range 3000–8500 Å except in the vicinity of the CN

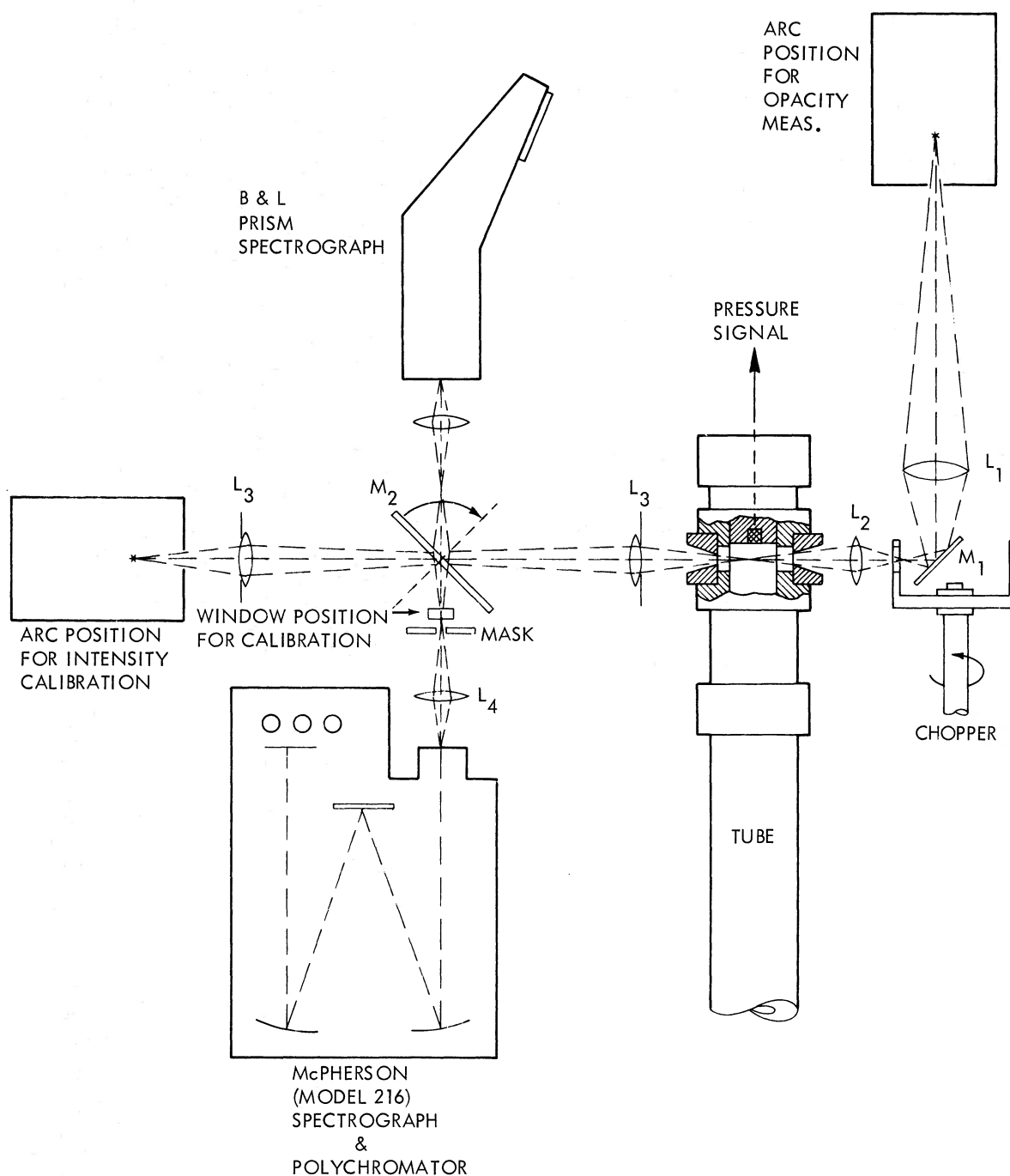


FIG. 3.—Optics for temperature measurements

molecular bands originating in the plasma column, and the emissivity over this range is greater than 0.98 and equals 0.99 from 4000–6000 Å. Thus the anode crater is very nearly a blackbody radiator in this spectral region; its true temperature is only about 19° K greater than its brightness temperature. Short-term temperature fluctuations are approximately $\pm 5^\circ$ K on a millisecond time scale.

Temperatures have been measured with the polychromator slots positioned at the peaks of several of the strong, severely broadened lines. The bandwidth of 3 Å for each channel is much narrower than the line widths, and thus the opacity and intensity over the bandwidth is nearly constant. Measurements have been made at the sodium D lines, the calcium resonance line at 4226 Å, and the neutral copper line at

5105 Å, which has its lower state 1.4 eV above the ground state. At temperatures greater than 4000° K, continuum emission is detectable and polychromator channels have been installed at line-free positions adjacent to the lines being measured. These channels allow corrections to be made for continua under the lines so that the excitation temperature of the species radiating the line can be determined. Temperature measurements have also been made at the band head of the C_2 (0, 0) Swan band at 5165 Å. This species is formed in the hot core of the gas sample from the decomposition of CH_4 which is introduced in trace amounts for thermometric studies.

The results of the temperature studies are summarized by the following findings:

1) When temperatures of more than one species are measured in a single experiment, the disagreement is less than 4 percent between resonance lines (Na D, Ca 4226) throughout the compression cycle.

2) For shots with temperatures greater than 4500° K, the C_2 band and nonresonant Cu I line yield higher temperatures than the resonance lines, but they agree with each other within 5 percent. This result is attributable to boundary layer effects on the resonance lines.

3) The maximum temperatures occur approximately 100 μ s after $P_{\max}$; at these times the pressure has decreased less than 2 percent from $P_{\max}$. This delay can be attributed to the mass leakage out of the

test section past the piston during the high-pressure portion of the compression cycle.

4) A strong correlation exists between $P_{\max}$ and $T_{\max}$ over the pressure range 400–2500 atm and temperature range 2600°–5200° K. Figure 4 illustrates this correlation for a plot of $\log(T_{\max}/T_0)$ versus $\log(P_{\max}/P_0)$, where $T_0 = 298^\circ$ K. A linear least-squares fit to these data yields a correlation coefficient of 0.985, and a rms vertical deviation from the best fit line corresponding to 7 percent of $T_{\max}$. The equation for the best fit line is

$$\log(T/T_0) = 0.360 \log(P/P_0) + 0.015. \quad (4)$$

Referring to equation (1) for comparison with an ideal isentropic process, the coefficient 0.360 in equation (4) should be compared with 0.400 corresponding to $\gamma = 1.667$ for the ideal isentropic process. The small temperature axis intercept of 0.015 is only 10° above the NTP initial conditions. Therefore, we interpret equation (4) as one of polytropic form with an exponent $\gamma' = 1.563$. The data used to determine equation (4) were those for $P_0 = 1$ atm. Some temperature measurements on shots with $P_0 = 3/4$ and $P_0 = 1/2$ atm have been made (see fig. 4), and the results indicate a weak dependence of γ on P_0 . This dependence has been taken into account for spectroscopic data taken on shots with $P_0 \neq 1$ atm. Since $T_{\max}$ occurs well within the interval centered at $P_{\max}$

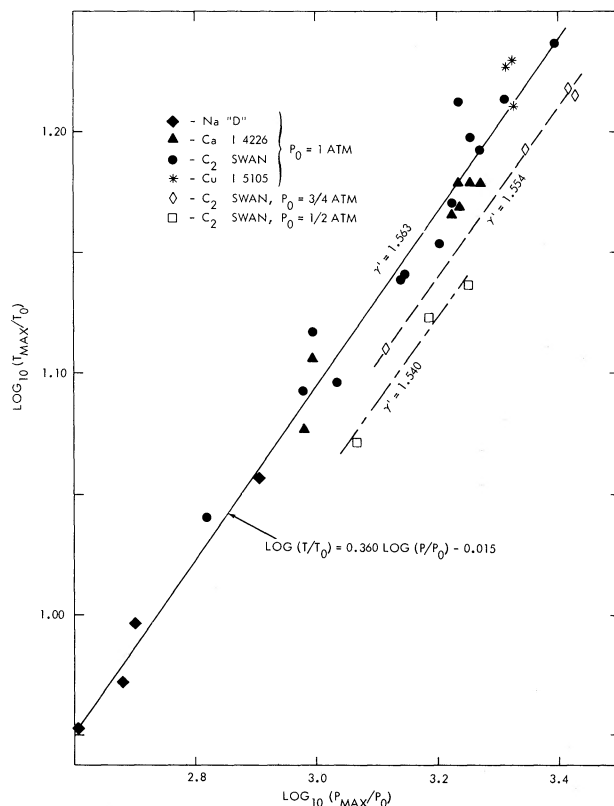


FIG. 4.—Correlation between measured temperatures and pressures

during which spectroscopic observations are made, we conclude that equation (4) provides an adequate temperature calibration for helium over these pressure and temperature ranges. We have used it for all spectroscopic data reported here because it was not feasible to make both spectra and temperature measurements simultaneously.

The existence of LTE in ERCA hinges on excitation rates for atom-atom collisions. As a rule of thumb, the collisional excitation rate should exceed by a factor of 10 the radiative decay rate for the energy level under consideration (Griem 1963). For helium densities of 10^{21} cm^{-3} , relative velocities of 10^6 cm s^{-1} , and transition probabilities of 10^8 s^{-1} appropriate for resonance lines of Ca I and Na I, the excitation cross section for helium collisions should be greater than 10^{-18} cm^2 for LTE. From the meager experimental data available for alkali-rare gas collisional excitation (Faizullov and Sobolev 1961; Dodd, Enemark, and Gallagher 1969, who also reference earlier work), we can infer that these cross sections certainly are not much larger than 10^{-18} cm^2 . The observed agreement in temperatures obtained with species of differing excitation cross sections is taken to be the best available evidence for the existence of LTE in ERCA.

Very little experimental evidence for chemical and thermal homogeneity exists. Boundary layer effects have already been mentioned. The existence of a uniform, hot gas core interior to a thin (approximately 1 mm) boundary layer is postulated upon consideration of helium thermal diffusivity under ERCA conditions. The C_2 and nonresonant Cu I temperatures are expected to be representative of the hot core temperature, the C_2 molecules are expected to be uniformly distributed in the hot core, and the optically thin emission lines of Ca II under study originate in the hot core.

c) Density Measurements

In ERCA I, volume measurements were made by photographing the leading edge of the piston through a side window positioned near the end wall. Uncertainties concerning gas leakage past the piston prevented accurate density calculations. In ERCA II, an optical scheme based on the variation of refractivity with density failed due to opacity at the continuum wavelengths chosen (Hammond and Lalos 1971). Presently, ERCA III has no density diagnostic scheme, and recourse must be made to the equation of state to calculate the density from pressure and temperature measurements. For the present experiments with helium, however, this procedure introduces a negligible error compared with the 3 percent pressure error and 7 percent temperature error. The ideal-gas equation of state, $P = NkT$, is appropriate for helium at ERCA temperatures and pressures; $(P/NkT) - 1 = 0.006$ at $N_{\text{He}} = 3 \times 10^{21} \text{ cm}^{-3}$ and 400° K (Michels and Wouters 1941) and will become even smaller at higher temperatures, and ionization effects are completely negligible up to $15,000^\circ \text{ K}$ at 1000 atm pressure (Lick and Emmons 1962). Therefore, the helium

densities calculated in this work are accurate to within 10 percent.

III. DATA TECHNIQUES

The line broadening measurements reported here consist of half-widths and frequency shifts of the Ca II H and K lines over a range of helium perturber densities and temperatures. In this section, we describe the data collection and data reduction techniques employed that yield the collisional damping constants reported in the next section.

a) Spectroscopy

The ERCA III emission spectra are recorded photographically with the spectrograph-polychromator mentioned above in the temperature measurement discussion. In the spectrograph mode, the polychromator exit slots at the focal plane are replaced with a $2'' \times 8''$ film cassette. The instrument is a McPherson model 216, 1-m focal length spectrograph with a $600 \text{ groove mm}^{-1}$ plane grating in a Czerny-Turner mount. The nominal reciprocal dispersion is 16 Å mm^{-1} , and the effective aperture ratio is f/9. The optical components between the spectrograph and ERCA are fused quartz lenses and an aluminized front-surface mirror as shown in figure 3, except that lens L_4 is moved slightly to focus the ERCA exit window on the entrance slit jaws.

In order to admit light into the spectrograph only during moments of maximum compression, a high-speed electromechanical shutter system has been designed and mounted at the spectrograph entrance slit. This shutter (Kendall 1968) consists of a slotted plate driven horizontally past the entrance slit. The shutter operation is controlled to allow light emitted during the interval centered at and within 95 percent of P_{max} . The gas density and temperature vary only 3 percent and 2 percent, respectively, over this interval. The open times used in these experiments ranged from 250 to 500 μs .

The spectra were recorded on Kodak 103-F and 103-O plates. After the ERCA exposure was made, wavelength calibration exposures were made without moving the plate cassette or changing the entrance slit width. Emulsion calibration exposures were then made on each plate, and the plate was immediately processed. Development in D-19 at 20° C for 4.0 minutes in a temperature-regulated Jarrell-Ash processing machine was followed by a water bath; the plate was then fixed for 8 minutes and washed for 30 minutes.

The wavelength calibration exposures were made with cesium and potassium Osram lamps. The Cs I 3888.56 Å line and the K I 4044.13 Å line fell in line-free regions of the ERCA spectrum, and linear interpolation between these line positions on the plates was used to determine the wavelengths of the peaks and half-intensity points of the Ca II H and K lines, which have unshifted wavelengths of 3968.47 Å and 3933.67 Å, respectively. The interpolation scheme was

checked on test plates made with the Cs and K calibration exposures and the aluminum resonance lines at 3944.02 Å and 3961.53 Å emitted by a hollow-cathode lamp.

b) Emulsion Calibration and Microphotometry

The emulsion calibration exposures were made through a stepped slit placed at the spectrograph entrance slit. The stepped slit was made from steel shim stock by a photochemical etching process, and contained eight slit apertures ranging from 100 μ to 1.15 mm width. The widths were chosen to yield a constant increment in the logarithm of the transmitted intensity. The light source used was a Honeywell miniature electronic flash unit commonly used for amateur photography. The plastic color balance filter was removed and neutral density gelatin filters installed to control film exposure. This xenon flash unit emitted a line-free continuum in the 3900–4000 Å region for approximately 500 μ s, a duration comparable to the ERCA exposures, and thus reciprocity law failure effects were avoided. Test exposures were made to insure uniform intensity over the stepped slit array.

An emulsion calibration curve for the 3950 Å region was constructed and assumed to be valid for the 3900–4000 Å interval over which relative intensity measurements were made. The conventional H and D curve (Sawyer 1963) was linearized by a variation due to Arrak (1957) of the Seidel transform. (See Margoshes and Rasberry 1969, for a comprehensive review of such transforms; de Vaucouleurs 1968, 1969; and Margoshes 1969.)

The plates were scanned with the digitized Joyce-Loebl microphotometer of the Astronomy Department at the University of Maryland. The magnetic tapes were processed with a program containing the emulsion calibration transform (Bell *et al.* 1968). This program calculates wavelengths for each data point, subtracts plate background fog densities, calculates relative intensities, smooths out some plate grain noise, corrects for sloping background continua under the emission lines, and produces a CALCOMP plot of relative intensity versus wavelength. Shifts and widths are measured directly from the CALCOMP plots. One of these plots is shown in figure 5. To avoid some uncertainties due to grain noise in locating the peak of the line profile, averages of the midpoints of the 9/10, 3/4, and 1/2 intensity widths were taken to determine shifts. The shift and width measurements were converted to vacuum wavenumber (cm^{-1}), $\Delta\bar{\nu}_m$ and $\Delta\bar{\nu}_{1/2}$, respectively, with the NBS conversion table (Coleman *et al.* 1960), to conform to neutral line broadening practice.

It is difficult to assess the accuracy of intensity measurements made with the above scheme because some of the variables enter in nonlinear ways. The most careful spectrophotometry yields at least 10 percent intensity errors (Wright 1962). The additional presence of possible thermal drifts, Joyce-Loebl density wedge calibration errors, and grain noise effects are estimated to result in total errors in relative intensities of 15 percent.

A systematic error of 0.1 Å blue shift was found in the apparent wavelengths of the aluminum lines on CALCOMP plots of the test plates mentioned earlier. This error was allowed for in the shift and width measurements. The random errors of wavelength measurement due to grain noise, metrological screw nonlinearities, and scale errors in plot reading are estimated to be a total of ± 0.2 Å, or $\pm 1.3 \text{ cm}^{-1}$. This error is negligibly small compared with the observed line widths and does not contribute significantly to the damping constant errors.

c) Self-Absorption Effects

A problem that often affects the accuracy of line profile measurements in emission spectroscopy experiments is distortion of line shapes from self-absorption effects. Since these are not always obvious from visual inspection of the spectra, especially when the functional form of the profile is not known, it becomes necessary to measure the opacity at the line peaks. A series of experiments was made to measure this opacity before the data runs were performed.

The calcium is present in ERCA III as an ever-present contaminant. The Ca I and Ca II lines do not seem to vary appreciably from shot to shot if care is taken to clean the tube, piston, and test-section components by means of standard procedures before each shot. It was hoped that the opacities at the peaks of Ca II H and K were small enough that special procedures would not be necessary.

For these opacity experiments, the “temperature optics” shown in figure 3 were used. Exit slots in the spectrograph focal plane were placed at the peak of the Ca II K line (3933 Å) and at line-free positions in the far-blue wing (3906 Å) and the far-red wing of the Ca II H line (3995 Å). Linear interpolation between the opacities at these latter two positions yielded the continuum opacity under the K line. Photographic spectra were also taken simultaneously with these photoelectric measurements with a quartz prism spectrograph that viewed the radiation emerging from a side window port at the top of the test section. These prism spectra were scanned with the Joyce-Loebl microphotometer and converted to relative intensity CALCOMP plots. A plot of K line opacity versus K line peak intensity revealed a good positive correlation. The K line opacity ranged from 0.07 to 0.15 for a series of five consecutive shots at 4500° K and $N_{\text{He}} = 3 \times 10^{21} \text{ cm}^{-3}$. We consider this opacity variation to arise only from random calcium impurity variations. Since it was not feasible to measure the K line opacity photoelectrically and the line profiles photographically on the same ERCA shot, this correlation was used to determine the opacity for data shots.

In order to apply this correlation to observations at other temperatures and densities, we derived scaling factors from the Saha ionization equilibrium relation. At temperatures of 5000° K, all electrons come from impurities with low ionization potential, and at these temperatures and estimated typical electron densities

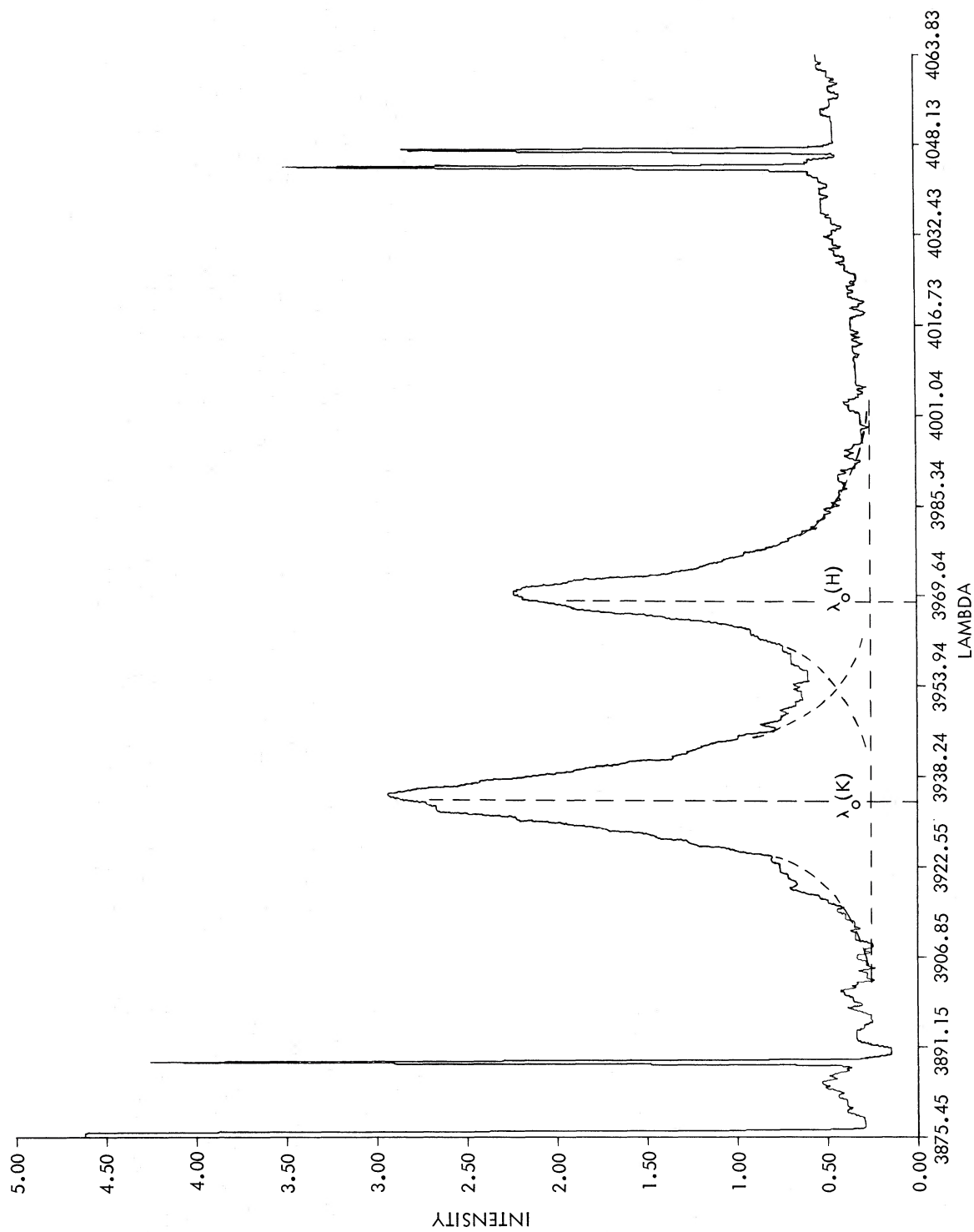


Fig. 5.—CALCOMP plot of Ca II spectra from shot C-114

of $5 \times 10^{13} \text{ cm}^{-3}$, ionization of these species will be more than 95 percent complete. For roughly constant impurity abundances, the electron density will then be proportional to the helium carrier gas density. For small optical depths, the opacity at the K line peak will be proportional to the calcium ion density. We allow for increased impurity vaporization at the higher temperature with a T/T_0 factor, where the subscript denotes the value at the opacity measurement experiments. The result is a correction of about 30 percent increase in optical depth at the low end of the density range where the H and K peak opacities are largest due to the smaller broadening.

The correction to the line profile required to recover the optically thin profile is obtained from the expansion of equation (3) for small τ_λ :

$$I_\lambda \approx B(\lambda, T_g) \tau_\lambda, \quad \tau_\lambda \ll 1.$$

Dividing this relation by equation (3) yields a correction factor to recover the optically thin intensity (Wiese 1965):

$$I_\lambda (\text{optically thin}) = \left[\frac{\tau_\lambda}{1 - \exp(-\tau_\lambda)} \right] I_\lambda (\text{obs}). \quad (5)$$

This relation was used with the CALCOMP plots to obtain a width at half-intensity values corresponding to the optically thin peak intensities of H and K.

d) Instrumental Distortion

The narrow, unbroadened wavelength calibration lines superposed on the ERCA exposures also provide data for the instrumental slit function. These lines were scanned and CALCOMP plotted on the same tracings as the ERCA spectra. Measurements of these sharp lines on the CALCOMP plots yielded the result for the triple convolution of the spectrograph slit function and the instrumental functions of the microphotometer and CALCOMP plotter. The instrumental width was less than 10 percent of the narrowest profile observed in the Ca II ERCA spectra, and because the instrumental profile could be closely approximated by a Lorentzian function, the instrumental width was subtracted from the observed width.

IV. RESULTS

A temperature-density plane is shown in figure 6 illustrating the experimental conditions of the 10 data shots that yielded acceptable spectra of the Ca II H and K lines. The data form two sets, one with a roughly constant temperature of approximately 5200° K and covering a helium density range from 1.6×10^{21} to $3.1 \times 10^{21} \text{ cm}^{-3}$, and the other at a constant helium density of $2.9 \times 10^{21} \text{ cm}^{-3}$ and covering a temperature range from 4400° K to 6000° K. These data sets allow determination of both the damping constants and their temperature dependences. Table 1 is a compilation of the important shot data that includes ERCA III initial conditions and diagnostic information.

Inspection of the "constant temperature" data set in figure 6 revealed a scatter of almost $\pm 300^\circ$ about the average of 5200° K. Therefore, before plotting the final results, the temperature dependence of the broadening was determined from the data at 4400° and 6000° K, and then the "constant temperature" data were adjusted to the value expected for the average temperature. The temperature dependence was cast into exponential form as is predicted by conventional impact broadening theory.

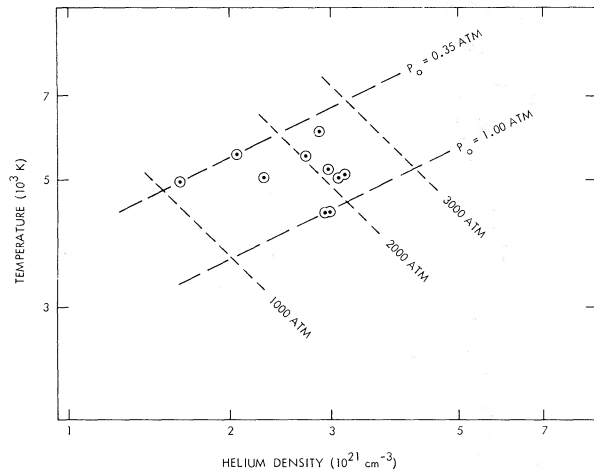


FIG. 6.—Temperatures and densities of the data shots in table 1.

TABLE 1
SHOT DATA AND DIAGNOSTIC RESULTS

Shot No.	P_0 (atm)	P_r (atm)	$P_{\max}$ (atm)	$T_{\max}$ (K)	N_{He} (10^{21} cm^{-3})	ρ/ρ_{STP} (Am)	Emulsion	Exposure time (μs)
109.....	0.750	32.5	2130	5060	3.09	115	103-F	300
110.....	0.750	32.5	2180	5090	3.14	117	103-F	300
111.....	0.504	24.9	2020	5510	2.69	100	103-F	250
112.....	0.500	22.5	1580	5060	2.29	85	103-F	400
113.....	0.350	16.1	1100	4960	1.63	61	103-O	450
114.....	0.350	18.0	1550	5560	2.05	76	103-O	250
115.....	0.650	29.2	2100	5200	2.98	111	103-O	300
117.....	1.000	35.5	1780	4410	2.96	110	103-O	500
118.....	1.000	35.5	1760	4400	2.93	109	103-O	500
119.....	0.450	24.4	2350	6080	2.84	106	103-O	200

TABLE 2
WIDTHS, SHIFTS AND CORRECTIONS

Shot No.	Line	ω (cm^{-1})*	Instr. Corr. (cm^{-1})	Optical Depth, τ †	W (cm^{-1})‡	(5200/T) exp 0.23§	$\Delta\bar{\nu}_{1/2}$ (cm^{-1})	Shift (cm^{-1})
117, 118.....	H	79.0	4.0	0.07	73.0	...	...	4.6
	K	101.0	4.0	0.09	91.1	...	...	-0.8
119.....	H	86.4	4.0	0.10	78.6	...	...	4.7
	K	110.8	4.0	0.13	98.1	...	...	1.9
113.....	H	53.0	4.0	0.17	42.1	1.01	42.5	7.3
	K	74.9	4.0	0.20	57.8	...	58.5	2.0
114.....	H	66.9	4.0	0.20	53.8	0.98	52.7	7.9
	K	85.9	4.0	0.24	72.1	...	70.6	4.2
112.....	H	69.9	4.0	0.08	62.3	1.01	63.0	5.5
	K	#	4.0	...	...	...	...	...
111.....	H	78.8	4.0	0.14	69.0	0.99	68.3	3.8
	K	106.7	4.0	0.15	96.5	...	95.5	-2.2
115.....	H	83.1	4.0	0.07	77.1	1.00	77.1	9.5
	K	106.7	4.0	0.11	95.0	...	95.0	2.7
109.....	H	85.0	4.0	0.13	72.6	1.01	73.4	5.4
	K	114.4	4.0	0.16	101.0	...	102.0	0.4
110.....	H	89.0	4.0	0.09	77.4	1.01	78.2	7.0
	K	113.1	4.0	0.10	99.4	...	100.4	1.9

* Observed width without corrections.

† (I , τ) correlation for K line assumed correct for H line also.

‡ Width corrected for instrumental and optical depth effects.

§ Temperature scaling factor; 0.23 exponent derived from 4400° and 6080° K width data.

|| Negative shift is toward higher frequencies.

Plate blemish prevented measurements of this line.

Table 2 presents the width and shift data obtained from the shots listed in table 1. To obtain adequate exposure of the H and K lines at 4400° K, the exposures of shots 117 and 118 were superposed on a single plate. Corrections for instrumental slit function, optical depth, and the above temperature adjustment are also listed in table 2.

The final results are plotted in figures 7 and 8. The straight lines drawn in figure 7 are the best fits to the data that also pass through the origin. The slopes of these lines are the desired damping constants. The shift data shown in figure 8 are too small and scat-

tered to determine any density dependence, but the H line definitely exhibits a small redshift and the K line appears unshifted.

The slopes of the straight lines in figure 7 yield the following damping constants per helium atom:

$$\gamma_K/N_{\text{He}} = \frac{0.5\Delta\bar{\nu}_{1/2}^K}{N_{\text{He}}} = 1.71 \times 10^{-20} \text{ cm}^{-1}/\text{cm}^{-3}, \quad (6)$$

$$\gamma_H/N_{\text{He}} = \frac{0.5\Delta\bar{\nu}_{1/2}^H}{N_{\text{He}}} = 1.28 \times 10^{-20} \text{ cm}^{-1}/\text{cm}^{-3}. \quad (7)$$

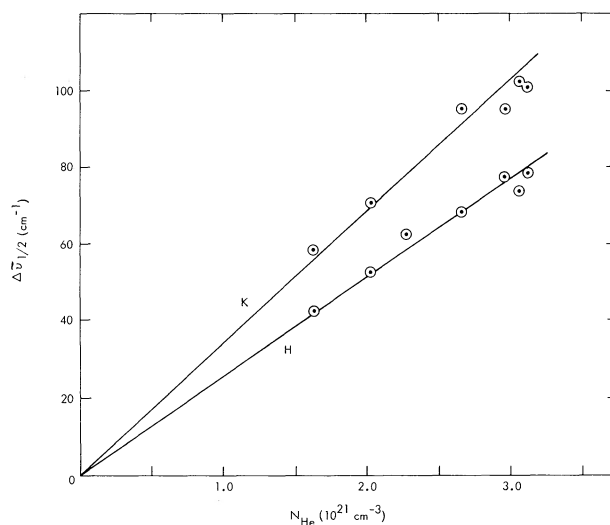


FIG. 7.—Ca II half-widths versus helium density

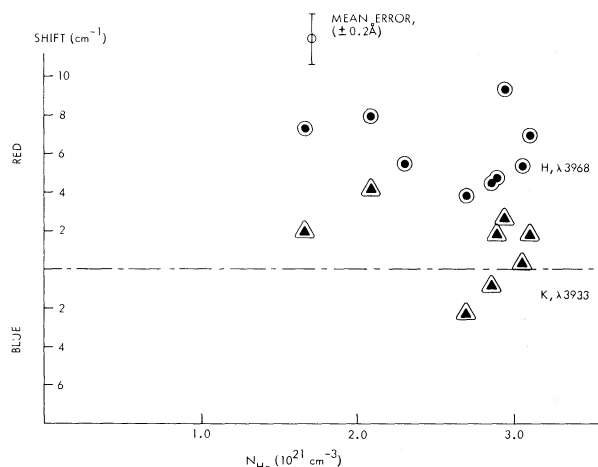


FIG. 8.—Ca II shifts versus helium density

The temperature dependence is nearly identical for both lines:

$$\frac{W_{6080}}{W_{4400}} = \left(\frac{6080}{4400} \right)^\alpha; \quad (8)$$

$$\alpha_K = \frac{\log(98.1/91.1)}{\log(6080/4400)} = 0.229, \quad (9)$$

$$\alpha_H = \frac{\log(78.6/73.0)}{\log(6080/4400)} = 0.228. \quad (10)$$

In the worst possible case where the intensity measurement errors are such that the peak intensity is underestimated and the intensity at the half-width points is overestimated, half-width error will be approximately twice the intensity error. Since this estimate is unnecessarily conservative, we assign a probable error of 20 percent to the half-width measure-

ments. The width errors are independent of the helium density error of 10 percent, and we conclude, therefore, that these damping constants are accurate to ± 30 percent. The temperature dependence exponent is far more uncertain because of poor statistics, and any comparison with theoretically predicted values should be discouraged.

A few of the observed line profiles have been analyzed, but only in a rather crude fashion to date. For a Lorentzian profile, $I(\Delta\bar{\nu}) \sim [1 + (\Delta\bar{\nu}/\Delta\bar{\nu}_{1/2})^2]^{-1}$; for a Gaussian profile, $I(\Delta\bar{\nu}) = \exp[-(\Delta\bar{\nu}/\Delta\bar{\nu}_{1/2})^2]$; and for a power-law frequency dependence appropriate to van der Waals interactions at very high densities (Margenau 1951), $I(\Delta\bar{\nu}) \sim (\Delta\bar{\nu}/\Delta\bar{\nu}_{1/2})^{-3/2}$. Plots of $\log I(\Delta\bar{\nu})$ versus $\log [1 + (\Delta\bar{\nu}/\Delta\bar{\nu}_{1/2})^2]$ should, therefore, yield straight lines only for Lorentzian profiles. These quantities have been plotted in figure 9 for the blue wings of the K lines and the red wings of the H lines for two shots which yielded the most intense exposures and thus the least grain noise in the wings. No allowance for self-absorption or instrumental broadening was made; these effects are important only near the line peak. However, errors in background continua location become important in the wings. From figure 9 we conclude that a Lorentzian profile hypothesis is not unrealistic, but a more detailed analysis (with Voigt profile techniques) with more accurate data is required to confirm it.

V. DISCUSSION AND ANALYSIS

The linear extrapolation of the width data to the origin, and the possibility of Lorentzian profiles, suggest an analysis in terms of impact theories. Impact theories are valid when the duration of a collision is short compared with the time between collisions. In classical collision damping theory, the line width is the reciprocal of the collision frequency and is proportional to a collision cross section, $\pi\rho_{\min}^2$, where $\rho_{\min}$ is

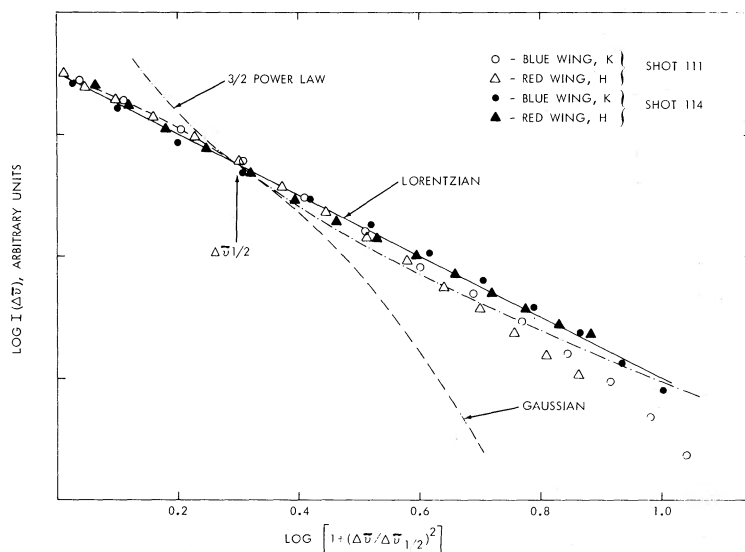


FIG. 9.—Line profile tests showing the fit to various profile functions out to three half-widths from the line center

the optical collision radius,

$$\Delta\omega_{1/2} = 2\pi c\Delta\bar{\nu}_{1/2} = \frac{2}{\tau} = 2\pi\rho_{\min}^2\langle v\rangle N, \quad (11)$$

where $\langle v\rangle$ is the mean relative velocity, $\omega_{1/2}$ is the full half-width in circular frequency units, and N is the perturber density. The collision duration is approximately $\rho_{\min}/\langle v\rangle$. Therefore, impact theory validity requires

$$(\rho_{\min}/\langle v\rangle) < (\pi\rho_{\min}^2\langle v\rangle N)^{-1} \quad (12)$$

or

$$N < (1/\pi\rho_{\min}^3). \quad (13)$$

At 5200° K, $\langle v\rangle = 5.5 \times 10^5 \text{ cm s}^{-1}$, and averaging the H and K widths yields $\rho_{\min} = 4.0 \text{ Å}$. This yields in equation (13) $N < 5 \times 10^{21} \text{ cm}^{-3}$. In more detailed theories, $\rho_{\min}$ is a weak function of interaction potential parameters, and the result is not significantly different. Although the density range of these experiments satisfies equation (13), it is uncomfortably close to the critical density. A point in the line wing can be calculated that satisfies a relation

$$\tau\Delta\omega = 1. \quad (14)$$

At the highest density obtained in these experiments, equation (14) yields $\Delta\bar{\nu} = 45 \text{ cm}^{-1}$ for $\rho_{\min} = 4 \text{ Å}$. Margenau and Lewis (1959) have shown that quasi-static theories are valid for $\tau\Delta\omega \gg 1$, and, therefore, applicable to those portions of the line wings well beyond the half-width points in these experiments. Consequently, we can proceed with a discussion of the observed widths and shifts in terms of impact theories.

Following the development given by Hindmarsh *et al.* (1967), we sketch below the elements of the Fourier integral theory of impact broadening. This theory yields a Lorentzian profile of the form

$$I(\omega) = \frac{\gamma/\pi}{[(\omega - \omega_0 - \beta)^2 + \gamma^2]}, \quad (15)$$

where ω_0 is the unperturbed angular frequency, and γ , the damping constant, is equal to one-half of the full half-intensity width. The theory predicts an angular frequency shift, β , of the peak of the broadened profile from the unperturbed frequency. This shift is given by

$$\beta = 2\pi N\langle v\rangle \int_0^\infty \rho \sin \eta(\rho) d\rho, \quad (16)$$

and the damping constant is given by

$$\gamma = 2\pi N\langle v\rangle \int_0^\infty \rho [1 - \cos \eta(\rho)] d\rho, \quad (17)$$

where $\eta(\rho)$ is the phase shift produced in the emitted radiation by a collision with impact parameter ρ between the radiating and perturbing atoms. We assume the collision shifts the energy levels of the radiating atom according to the variation of the inter-

action potentials with interatomic separation. This is the adiabatic approximation. The total phase shift, found by integrating over the collision duration, is related to these level shifts by

$$\eta(\rho) = \int_{-\infty}^\infty \Delta\omega dt, \quad (18)$$

where $\Delta\omega$ is the difference between the frequency shifts of the upper and lower levels. For the Lennard-Jones interaction potential,

$$\Delta\omega = \frac{1}{\hbar} [C_{12}/r^{12} - C_6/r^6] \quad (19)$$

where r is the interatomic separation at time t , and the interaction constants C_{12} and C_6 are in $\text{erg} \cdot \text{cm}^{12}$ and $\text{erg} \cdot \text{cm}^6$, respectively. These constants are differences between the values for the upper and lower levels, and it is possible, therefore, for either or both constants to be negative, although C_6 is usually taken positive.

The integral in (18) is readily done with the aid of the straight line path approximation:

$$r = (\langle v\rangle t^2 + \rho^2)^{1/2} \quad (20)$$

and yields

$$\eta(\rho) = \frac{63\pi}{256} \frac{C_{12}}{\hbar\langle v\rangle\rho^{11}} - \frac{3\pi}{8} \frac{C_6}{\hbar\langle v\rangle\rho^5}, \quad (21)$$

using

$$C_i' = C_i/\hbar, \quad x = \rho \left(\frac{3\pi}{8} \frac{|C_6'|}{\langle v\rangle} \right)^{-1/5},$$

and

$$\alpha = 0.536\langle v\rangle^{6/5} C_{12}' / |C_6'|^{11/5}, \quad (22)$$

then

$$\eta(\rho) = \alpha x^{-11} - x^{-5}.$$

Equations (16) and (17) can now be integrated to yield

$$\beta = 2\pi N \left(\frac{3\pi}{8} \right)^{2/5} \langle v\rangle^{3/5} |C_6'|^{2/5} S(\alpha), \quad (23)$$

$$\gamma = 4\pi N \left(\frac{3\pi}{8} \right)^{2/5} \langle v\rangle^{3/5} |C_6'|^{2/5} B(\alpha), \quad (24)$$

where

$$S(\alpha) = \int_0^\infty x \sin(\alpha x^{-11} - x^{-5}) dx, \quad (25)$$

and

$$B(\alpha) = \int_0^\infty x \sin^2 \frac{1}{2}(\alpha x^{-11} - x^{-5}) dx. \quad (26)$$

Values for $S(\alpha)$, $B(\alpha)$ and $S(\alpha)/2B(\alpha)$ are tabulated by Hindmarsh *et al.* (1967) for α values ranging from 10^{-4} to 10^4 for both positive and negative α , and at intervals sufficiently small for interpolation.

To derive C_6 and C_{12} from the experimental data, we note from (23) and (24) that

$$(\beta/\gamma) = S(\alpha)/2B(\alpha) = \Delta\bar{\nu}_{\max}/0.5\Delta\bar{\nu}_{1/2}. \quad (27)$$

For the Ca II H line, this shift/width ratio is taken to be $-6/31 = -0.193$ (the values at $N_{\text{He}} = 2.4 \times 10^{21} \text{ cm}^{-3}$), but this ratio is clearly very uncertain in view of the scatter in the shift measurements. From graphs of $B(\alpha)$ and $S(\alpha)/2B(\alpha)$ versus α , interpolation yields $\alpha = 1.63$, and $B(\alpha) = 0.258$. With $\langle v \rangle = 5.5 \times 10^5 \text{ cm s}^{-1}$, equation (24) yields:

$$C_6[\text{Ca II (H)/He}] = 3.4 \times 10^{-59} \text{ erg} \cdot \text{cm}^6, \quad (28)$$

and (22) yields:

$$C_{12}[\text{Ca II (H)/He}] = 2.1 \times 10^{-103} \text{ erg} \cdot \text{cm}^{12}. \quad (29)$$

For the Ca II K line, we take the shift to be zero. This yields $\alpha = 4.09$, and $B(\alpha) = 0.316$, and the interaction constants for the K line become

$$C_6[\text{Ca II (K)/He}] = 4.1 \times 10^{-59} \text{ erg} \cdot \text{cm}^6, \quad (30)$$

and

$$C_{12}[\text{Ca II (K)/He}] = 8.4 \times 10^{-102} \text{ erg} \cdot \text{cm}^{12}. \quad (31)$$

It should be reiterated here, in view of the assumptions made regarding the form of the potential, the algebraic sign of the interaction constants, the straight line paths, the velocity averaging (see Reck and Hood 1970, 1972, for discussions of this effect), and the adiabatic approximation, that these constants should only be regarded as parameters which, when inserted into the model potential function, will reproduce the experimental observations.

Finally, we compare the experimental damping constants with the predictions of the conventional Lindholm-Foley/van der Waals theory commonly used in most astrophysical calculations. The damping constant, in circular frequency units, is given by

$$\gamma = 17.0 C_6'^{1/2} \langle v \rangle^{3/5} N. \quad (32)$$

The interaction constant, C_6' , is calculated from emitter and perturber dipole polarizabilities, and a hydrogenic approximation (Unsöld 1955) is used for both upper and lower states of Ca II:

$$C_6 = \frac{e^2}{h} \alpha_{\text{He}} a_0^2 [R^2(4^2P) - R^2(4^2S)] \text{ cm}^6 \text{ s}^{-1}, \quad (33)$$

where the helium polarizability, $\alpha_{\text{He}} = 1.384$ (Dalgarno and Kingston 1961), a_0 is the Bohr radius, and

$$R^2(n^*, l) = \frac{n^{*2}}{2Z^2} [5n^{*2} + 1 - 3l(l+1)], \quad (34)$$

where $n^{*2} = Z^2 R_{yd}/T$, $Z = 2$ for Ca II, T is the binding energy of the state with orbital quantum number l , and R^2 is the mean square radius of that state. We find $R^2(4^2P) = 20.33$, $R^2(4^2S) = 13.68$, and $C_6' = 1.33 \times 10^{-33} \text{ cm}^6 \text{ s}^{-1}$, or

$$C_6 = \hbar C_6' = 1.41 \times 10^{-60} \text{ erg} \cdot \text{cm}^6, \quad (35)$$

a value much smaller than the "experimental" Lennard-Jones values. However, when inserted into (32), this interaction constant yields, for $\langle v \rangle = 5.5 \times 10^5 \text{ cm s}^{-1}$,

$$(\gamma/N)_{\text{vdw}} = 3.34 \times 10^{-9} \text{ rad/s}^{-1}/\text{cm}^{-3}, \quad (36)$$

or

$$\begin{aligned} (\gamma_v/N)_{\text{vdw}} &= (\gamma/N)/2\pi c \\ &= 1.77 \times 10^{-20} \text{ cm}^{-1}/\text{cm}^{-3}, \end{aligned} \quad (37)$$

a value nearly identical to the experimental value for the Ca II K line (eq. [6]). This fortuitous agreement arises from the neglect of repulsive interactions in the conventional theory.

The Lindholm-Foley/van der Waals theory predicts redshifts of approximately one-third the full half-width, whereas we observed a shift/width ratio of less than 0.1. Therefore, although we find rough agreement with the broadening predicted by the conventional theory, both the fine-structure (J-dependent) effects observed and the magnitude and direction of the shifts observed play important roles in understanding cool white dwarf spectra (Hammond and Bell 1975).

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