THE ASTROPHYSICAL JOURNAL, 226:931–936, 1978 December 15

ON THE IDENTIFICATION OF FeH AND CeO IN S STARS

ROBIN E. S. CLEGG AND DAVID L. LAMBERT
McDonald Observatory and Department of Astronomy, University of Texas, Austin

Received 1978 April 13; accepted 1978 June 22

ABSTRACT

Observations of stellar spectra at a resolution of 0.2 Å support the identification of FeH and CeO in S stars by resolving the rotational structure of the bands. FeH lines are also identified in 61 Cyg B (K5 V), α Tau (K5 III), and in two M giants. CeO is present in the pure S star R Gem and in R And, an S star with TiO. The possibility of measuring Fe and Ce isotope ratios is discussed.

Subject headings: line identifications — molecular processes — stars: S-type

I. INTRODUCTION

A number of molecular band heads continue to resist identification in the spectra of cool stars. In particular, the visible and near-infrared spectra of S stars contain a rich assortment of unidentified features. Wyckoff and Clegg (1978) provide a catalog of the band heads and a discussion of chemical equilibrium for conditions appropriate to S stars.

Two molecules—FeH and CeO—were recently identified in stellar spectra. Nordh, Lindgren, and Wing (1977) proposed that FeH was the carrier of the Wing-Ford (1969) band at 9910 Å which was first detected in M dwarfs and later in S stars (Wing 1972). Their identification of FeH was based upon the correspondence between a spectrophotometric scan of R Cyg near 9910 Å at a resolution of 12 Å and a smoothed laboratory spectrum of FeH. Wing, Cohen, and Brault (1977) obtained low-resolution (4 Å) image-tube spectra of S stars and late-M dwarfs. They point out that the 9910 Å band has a similar structure in all stars. The match to the smoothed laboratory spectrum of FeH is very slightly improved at their resolution. A key piece of additional evidence is their identification of individual FeH lines from both the 9910 Å and 8691 Å bands in a high-resolution sunspot spectrum. These lines are predicted to strengthen in M dwarfs and can be expected to account for the observed 9910 Å band.

A tentative identification of CeO in the spectrum of R Cyg and two other pure S stars was proposed by Wyckoff and Wehinger (1977). Fifteen stellar band heads matched laboratory wavelengths with an rms error of 0.3 Å. The CeO identification in S stars showing strong LaO bands is supported by molecular equilibrium calculations (Wyckoff and Clegg 1978).

In this paper, high-resolution spectra of cool stars are described in which the rotational lines of the FeH 9910 Å and the CeO 7236 and 7275 Å bands are resolved. The spectra provide additional evidence to support the FeH identification and fully confirm the tentative identification of CeO. The spectra also extend the identification of FeH to late K dwarfs and M giants.

The spectra discussed in this paper were obtained with the 2.7 m reflector at the McDonald Observatory and the Tull coudé spectrometer equipped with a Reticon silicon diode array detector (Vogt, Tull, and Kelton 1978). Each exposure provided a 90 Å interval at a resolution of about 0.2 Å.

II. FeH IN COOL DWARFS AND GIANTS

The S star R Cyg was observed on 1977 August 17. At this time, R Cyg was approximately 6 weeks beyond the predicted maximum light (AAVSO 1977). Exposures were centered at about 9913 Å and 10000 Å. Exposure times of 15 minutes provided a signal-to-noise ratio of about 100. Each observation was followed by one of Vega at a similar air mass. After division by the Vega spectrum, weak interference from telluric H_2O lines is effectively removed from each R Cyg spectrum. Another exposure on R Cyg was made near 9726 Å. This region contains several strong Ti I lines which are used to determine the stellar radial velocity. Inspection shows the Ti I lines to be resolvable into components separated with velocities of 45 and 69 km s^{-1}. The FeH lines are associated only with the stronger component at +45 km s^{-1}.

FeH lines were identified by using a laboratory emission spectrum (Klynning and Lindgren 1973). A representative portion of the R Cyg spectrum is shown in Figure 1. FeH lines are obviously present. The stellar and laboratory wavelengths agree to ±0.1 Å, and there is also a rough correspondence between the intensities. The reader is reminded that the FeH band has not been rotationally analyzed, and the laboratory intensities are simply measurements off the spectrum reproduced by Klynning and Lindgren.

Spectra of 61 Cyg B and α Her A are shown in Figures 2 and 3. The FeH lines are weakly present in the K7 dwarf 61 Cyg B. Figure 2 shows a one-to-one correspondence between the FeH laboratory spectrum

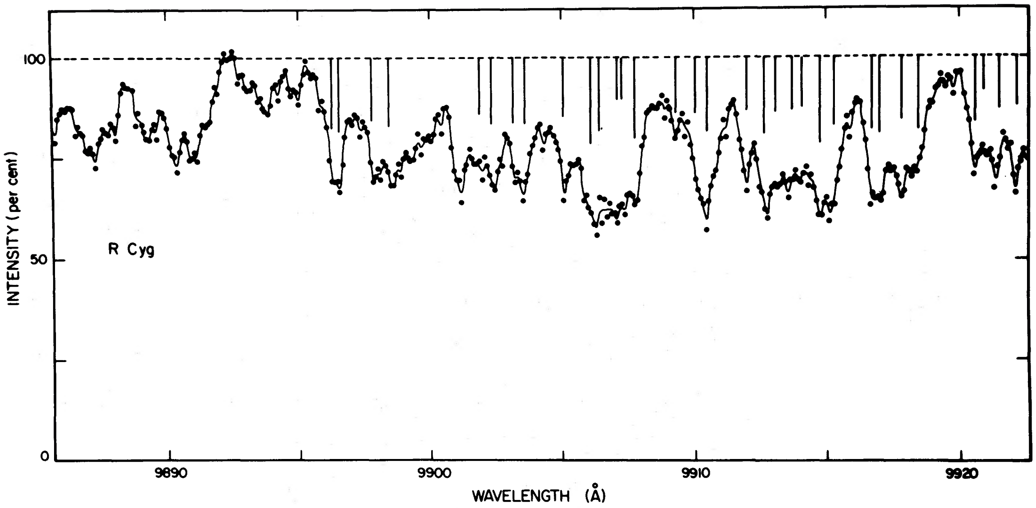

FIG. 1.—The spectrum of R Cyg between 9885 and 9922 Å. The observed spectrum has been corrected for interfering telluric water vapor lines. The positions and approximate relative intensities (see text) of the FeH lines are shown by the vertical lines.

and the stellar spectrum. Indeed, the stellar spectrum in this and adjacent regions (~120 Å) is almost a pure FeH spectrum. Another spectrum shows the FeH lines in the K5 dwarf companion 61 Cyg A. Figure 3 shows that FeH is also present in the M5 giant α Her A.

On examination of the several factors controlling the strength of a molecular line, the identification of FeH in late-type dwarfs and giants is not a surprise. To illustrate this remark, FeH and another hydride, MgH, are compared. Spectra of 61 Cyg B show that the equivalent widths of the FeH lines are quite similar to those of the MgH lines near 5600 Å which are members of the weak $\Delta v = -1$ sequence of the $A\,^2\Pi$–$X\,^2\Sigma^+$ transition. (The $\Delta v = 0$ MgH lines near 5160 Å are strong and saturated in the 61 Cyg B spectrum.) The FeH-to-MgH comparison suggests a band oscillator strength for the 9910 Å FeH band of $f \sim 0.01$ for $D_0{}^0 = 2.4$ eV to $f \sim 0.4$ for $D_0{}^0 \sim 1.3$ eV. The dissociation energy $D_0{}^0$ of FeH is unknown. Theoretical work by Walker, Walker, and Kelly (1972) suggests $D_0{}^0 = 2.4$ eV, but Carroll, McCormack, and O'Connor (1976) suggest that $D_0{}^0$ could be closer to 1 eV. There is no experimental or theoretical work on the band oscillator strength. The f-value estimates are reasonable values and quite consistent with the f-value sum rule. In short, the appearance of FeH in cool stars is expected.

Spectra of the M5 giant α Her A (Fig. 3), the M2 giant β Peg, and the K5 giant Aldebaran show that FeH lines are present in a region rich in lines. Luck (1978) has suggested that FeH lines from the weaker 8691 Å band are present in spectra of the K Ib supergiants. Although these detections cannot be ex-

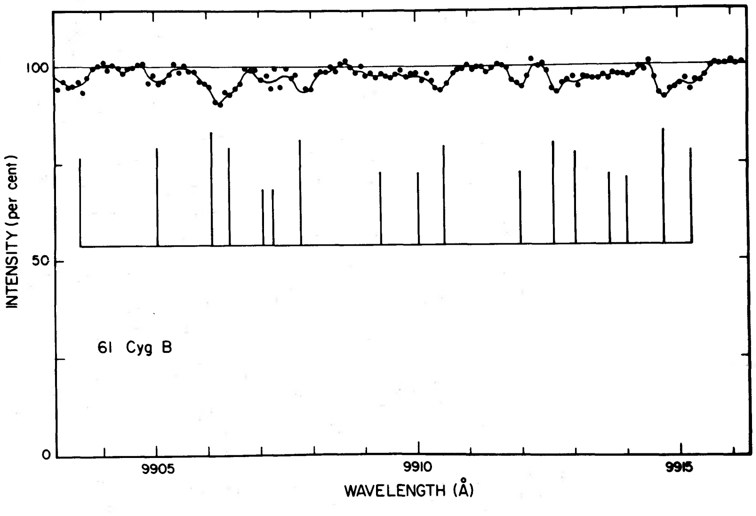

FIG. 2.—The spectrum of 61 Cyg B, a K7 dwarf, between 9903 and 9916 Å after correction for telluric water-vapor lines. The FeH lines in this interval are indicated below the stellar spectrum. It should be noted that FeH can account for all of the weak stellar lines in this interval.

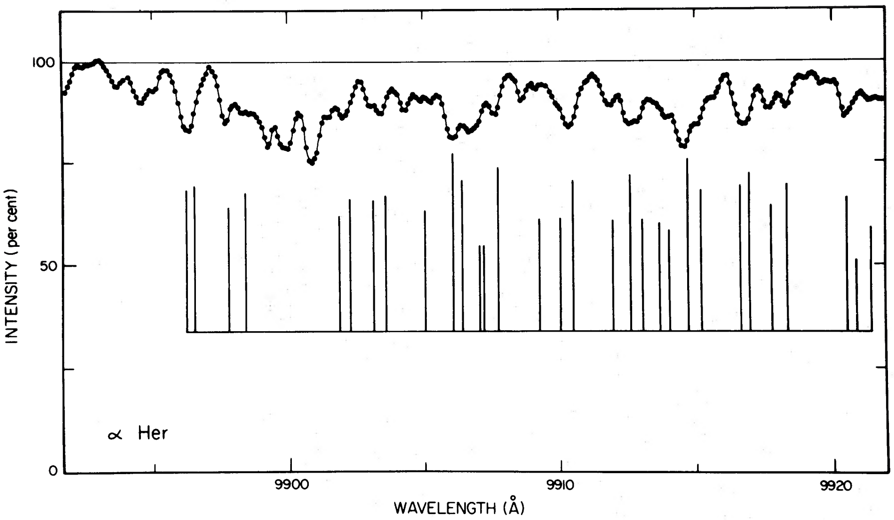

FIG. 3.—The spectrum of α Her A, an M5 giant, between 9892 and 9921 Å. This spectrum has not been corrected for the weak telluric water-vapor lines. The FeH lines, which are indicated below the stellar spectrum, are present in the stellar spectrum and account for a majority of the lines in this interval.

ploited until the FeH transition is fully analyzed and basic data (the dissociation energy and the oscillator strengths) are available, a cautionary note should be sounded: the FeH molecule is likely to be a rich contributor of weak lines to the near-infrared spectra of late-type giants. At present, the majority of these lines may be unidentified. A complete catalog of the FeH spectrum is needed.

When the FeH analysis is extended, it would be of interest to attempt a determination of the isotopic abundance of Fe. In terrestrial samples the relative abundances of the four stable isotopes are

$$^{54}\mathrm{Fe}:^{56}\mathrm{Fe}:^{57}\mathrm{Fe}:^{58}\mathrm{Fe} = 5.8:91.7:2.2:0.3 \,.$$

A rotational analysis may not be necessary in order to estimate the relative abundance of the Fe isotopes. A crucial prerequisite is an accurate measurement of the small isotopic wavelength shifts.

III. CeO IN S STARS

Spectra of the pure S star R Gem were obtained on 1977 November 30. The star was then about 130 days beyond the predicted date of maximum light (AAVSO 1977) and at phase 0.35: its visual magnitude was about 11. The spectra covered the wavelength regions 7200–7295 Å and 7518–7595 Å. A hot star (α Gem) was observed with exactly the same grating setting. The strong telluric lines in the 7200 Å region were removed by dividing the spectrum of R Gem by that of α Gem. Since the α Gem spectrum has a signal-to-noise ratio of several hundred and does not contain detectable stellar lines, the division does not introduce a significant additional uncertainty into the spectrum of R Gem. In the 7200–7300 Å region, the stellar wavelength scale was set by using eight atomic lines (Ba I, La I, Ce I, Ti I), while four atomic lines (Ce I and Zr I) were used in the 7500 Å region. The stellar and laboratory wavelengths are in good agreement, with the rms difference being less than 0.1 Å. The CN red system lines are not detectable in these spectra.

Table 1 compares the laboratory and stellar wavelengths of the nine cleanest band heads thought to be due to CeO. There is excellent agreement between the stellar and laboratory band head wavelengths. The quality of the spectra is sufficiently high that the identification can be confirmed through a comparison of individual absorption features.

Since almost all CeO absorption lines are blends of several lines, a synthetic spectrum was constructed for comparison with the stellar spectrum. A line list and rotational analysis (Clements 1969) are available for the 7235 and 7275 bands which are now tentatively classified as the (0, 0) bands of a $^3\Gamma_4$–$^3\Phi_3$ system. This system appears as B_2–X_2 in the literature. The 7235 and 7275 heads are the *R* heads of the (0, 0) and (1, 1) bands, respectively. Other band heads at 7241 and 7277 Å were earlier listed as the *Q* heads of the (0, 0) and (1, 1) bands, but a reinvestigation (Dr. R. F Barrow, private communication) recognizes them as the (0, 0) and (1, 1) *R*-branch heads of a different electronic transition which is classified as a $\Omega = 3 \rightarrow 2$ transition. A rotational analysis is not available for this latter transition, and hence the lines cannot be included in the synthetic spectrum. The $\Omega = 3 \rightarrow 2$ transition (see Table 1) is present in the stellar spectrum.

The synthetic spectrum is constructed from a crude model for molecular line formation. Calculations (Wyckoff and Clegg 1978) show that CeO is abundant only in the surface layers of S stars. Hence the model assumes that line- and continuum-forming layers do not overlap. A uniform photosphere with a source function $S_\nu{}^C$ provides the continuum flux which must traverse the line-forming layer of optical depth τ_ν in which the line source function $S_\nu{}^L$ is assumed to be

1978ApJ...226..931C

TABLE 1

BAND-HEAD MEASUREMENTS (R GEMINORUM)

Feature	λ (lab)	λ (star)	Degraded	Laboratory Source
B_2–X_2 $R(0, 0)$..................	7235.65	7235.55	R	Barrow
"$\Omega = 3 \rightarrow 2$" $R(0, 0)$...........	7241.59	7241.47	R	Barrow
	7249.5	7250.0	R	Gatterer
B_2–X_2 $R(1, 1)$..................	7275.51	7275.3	R	Gatterer
"$\Omega = 3 \rightarrow 2$" $R(1, 1)$...........	7277.86	7277.8	R	Gatterer
	7522.8	7523.0	R	Gatterer
?–X_1.........................	7561.3	7561.3	R	Barrow, Harris, and Jenson
?–X_1.........................	7562.4	7561.9	R	Barrow, Harris, and Jenson
?–X_1 $Q(0, 0)$....................	7572.77	7572.57	V	Barrow, Harris, and Jenson

REFERENCES.—R. F. Barrow 1978, private communication; Barrow, Harris, and Jenson 1978; Gatterer *et al.* 1957.

depth-independent. Then, the emergent (astrophysical) flux in a CeO line of optical depth τ_ν is

$$F_\nu = S_\nu{}^L[1 - 2E_3(\tau_\nu)] + 2S_\nu{}^C E_3(\tau_\nu) .$$

The residual intensity can be written

$$R_\nu = r + 2(1 - r)E_3(\tau_\nu) ,$$

where $r = S_\nu{}^L/S_\nu{}^C$.

An alternative simple slab (i.e., $r = 0$) model does not fit the observed spectrum (see Fig. 5).

The relative absorption coefficients of the CeO lines were calculated from the Hönl-London factors for Hund's coupling case (*a*) (see Kovács 1969) and excitation energies estimated from the molecular constants (Ames and Barrow 1967). A rotational temperature of 2000 K was assumed. The factor r and the optical depth at the band head were adjusted to obtain a reasonable match to the band-head profile.

Figure 4 shows the region just shortward of the (1, 1) heads and contains the rotational lines $Q(59)$ to $Q(79)$, $P(33)$ to $P(51)$, and $R(105)$ to $R(119)$ of the (0, 0) band of the ${}^3\Gamma_4$–${}^3\Phi_3$ transition. Lines of the $\Omega = 3 \rightarrow 2$ system are present in the stellar spectrum but are not included in the synthetic spectrum. Of particular note is the close correspondence between the observed and predicted absorption features near 7273 Å and the "beating" effect between P and Q lines. Figure 5 shows the region near the ${}^3\Gamma_4$–${}^3\Phi_3(0, 0)$ band origin including the R-branch band head at 7242 Å. The Q-branch origin is masked by the R-branch head of the $\Omega = 3 \rightarrow 2$ (0, 0) band. In this figure (and also Fig. 4) the synthetic spectrum was calculated with τ_ν (band head) = 3 and $r = 0.63$. The slab's model with $r = 0$ cannot be fitted to the band-head profile; i.e., the shallow band head is apparently quite saturated.

The high value for r demands a comment. If the CeO lines were formed by pure absorption, the value of r would be set by the ratio of the Planck functions for the temperature of the continuum layer, T_C, and the boundary temperature, T_0, i.e., $r = B_\nu(T_0)/B_\nu(T_C)$. The value $r = 0.63$ corresponds to a temperature ratio $T_0/T_C = 0.93 \pm 0.01$ for $T_C = 3000 \mp 500$ K. Model atmosphere calculations suggest a much lower ratio. Observations of the CO vibration-rotation lines which should be formed by pure absorption (Thompson 1973; Hinkle and Lambert 1975) confirm that the boundary temperatures are low for S stars. In short, the high value of r for optically thick lines is incompatible with line formation by pure absorption.

A high value of r suggests that the CeO lines are formed by scattering. The line source function for a weak (optically thin) line is equal to the mean continuum intensity. The CeO lines occur at frequencies above the peak in the continuum Planck function such that the mean continuum intensity (i.e., the source function for weak lines formed by scattering) will exceed the Planck function for the boundary temperature (i.e., the source function in the pure absorption case). Therefore, scattering allows a high value of r to be explained. Of course, when the lines are highly optically thick, the line source function will be depressed and fall below the local Planck function.

An investigation (Hinkle and Lambert 1975) of the relative collisional and radiative rates shows that scattering is the appropriate line-formation mechanism

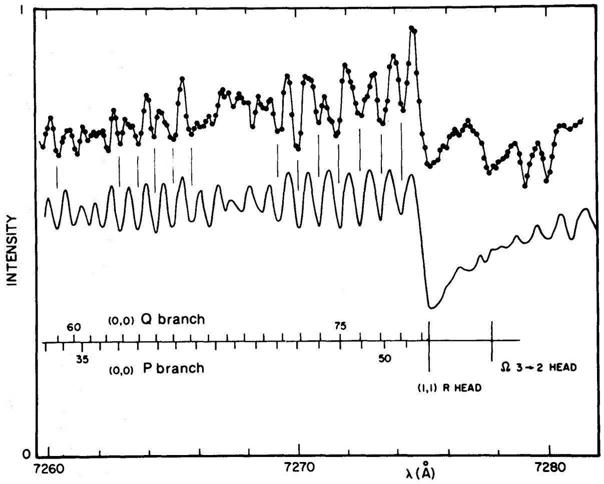

FIG. 4.—Synthetic CeO spectrum (*thin solid line*) is compared with the observed spectrum of R Gem (*line joining dots*) between 7260 and 7280 Å. The positions of (0, 0) band P- and Q-branch lines are marked, as are two (1, 1) band-head positions. Positions for the weak R-branch lines are not indicated. The synthetic spectrum has been shifted down by an arbitrary amount.

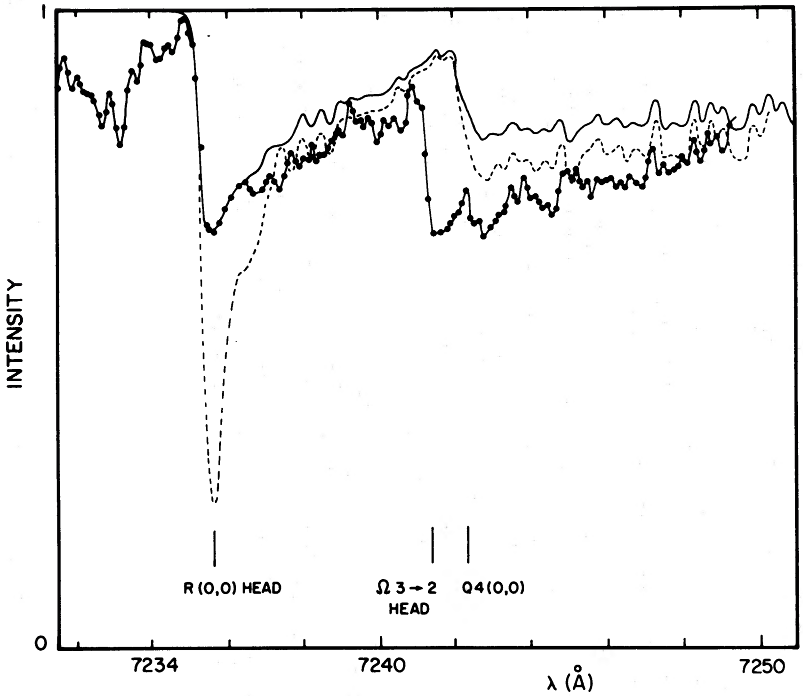

FIG. 5.—Spectrum of R Gem (*line joining dots*) near the (0, 0) *R*-branch band head at 7235 Å. The origin of the (0, 0) *Q* branch is indicated, but it is blended with lines from $\Omega = 3 \rightarrow 2$ band. The thin solid line shows a synthetic CeO spectrum calculated by using a model with $r = 0.63$, τ (band head) = 3 (see text). The dashed line shows the results for a slab model ($r = 0$; see text).

for electronic transitions in the atmospheres of giant stars. The possibility of scattering is enhanced for CeO because the molecule is concentrated toward the outer layers of the atmosphere (Wyckoff and Clegg 1978).

A spectrum of R And, an S star with TiO bands, in the region 7500–7590 Å has been examined. The star was observed on 1976 December 5, 9 days before predicted maximum light (AAVSO 1977). The violet-degraded CeO head at 7572 Å and the red-degraded feature at 7562 Å are both clearly visible. In addition to a number of identified LaO heads in this spectrum, an unidentified red-degraded band head was noticed: its measured wavelength is 7509.5 (±0.3) Å. The Vatican Atlas (Gatterer *et al.* 1957) does not indicate an LaO feature near this wavelength, but there is a CeO feature at 7509.2; Barrow (private communication) reports this feature at a measured wavelength of 7509.5 Å. A search through the Vatican Atlas and the wavelength tables of Kopp, Lindgren, and Rydh (1974) suggested no other likely identification. This head is tentatively assigned to CeO. The appearance of LaO and CeO bands so close to maximum light is noteworthy. Keenan (1954) has also reported the presence of infrared LaO bands at maximum light in this star.

Finally, the possibility of measuring the isotope ratios for Ce can be discussed. Of the four stable isotopes, only ^{140}Ce (88%) and ^{142}Ce (11%) have significant terrestrial abundance. Truran and Iben (1977) have predicted enhancements of ^{140}Ce after an *s*-process episode. The intervening nucleus ^{141}Ce is unstable to β-decay with a half-life of 32 days; thus, unless the neutron capture time scale on ^{141}Ce was much shorter than 32 days, only ^{140}Ce would be enhanced. Hence the ^{140}Ce/^{142}Ce ratio should be increased above the terrestrial value in S stars. The isotopic shifts are small: for the *Q*(75) line in the $^3\Gamma_4$–$^3\Phi_3$ (0, 0) band studied here the shift is only 0.05 Å. A (0, 1) band for this system has been reported by Watson (1938) at 7718 Å: the isotopic shift for this band head is 0.3 Å with the ^{142}CeO head lying to the blue of the red-degraded ^{140}CeO head. The (0, 1) band has not yet been identified in stellar spectra. Successful extraction of the isotopic abundance ratio will require access to a complete catalog of the CeO lines.

The spectra of S stars are so complex that an accurate determination of the abundance ratio will be difficult.

IV. CONCLUDING REMARKS

The spectroscopic studies reported here demonstrate the value of high-resolution spectra in establishing the identifications of complex bands in late-type stellar spectra. At the McDonald Observatory, the program of high-resolution near-infrared spectroscopy of S stars continues. Primary goals include the resolution and identification of the enigmatic Keenan bands and a search for other abundant molecules which are predicted to attain detectable column densities, e.g., HfO, TaO, and NbO (see Sauval 1978).

We thank Dr. R. F. Barrow for much helpful correspondence on the spectrum of the CeO molecule. We are indebted to Dr. J. Tomkin and Mr. G. Ferland for assistance with the acquisition and analysis of the observations. This research has been supported in part by the National Science Foundation (grants AST 75-21803 and AST 77-23213) and the Robert A. Welch Foundation of Houston, Texas.

REFERENCES

AAVSO 1977, *AAVSO, Bull.*, no. 40.

Ames, L. L., and Barrow, R. F. 1967, *Proc. Phys. Soc.*, **90**, 869.

Barrow, R. F., Harris, S. M., and Jenson, P. P. 1978, *Ap. J.*, submitted.

Carroll, P. K., McCormack, P., and O'Connor, S. 1976, *Ap. J.*, **208**, 903.

Clements, R. M. 1969, D. Phil. thesis, Oxford University.

Gatterer, A., Junkes, J., Salpeter, E. W., and Rosen, B. 1957, *Molecular Spectra of Metallic Oxides* (Vatican City: Specola Vaticana).

Hinkle, K. H., and Lambert, D. L. 1975, *M.N.R.A.S.*, **170**, 447.

Keenan, P. C. 1954, *Ap. J.*, **120**, 484.

Klynning, L., and Lindgren, B. 1973, University of Stockholm Institute of Physics, Report 73-20.

Kopp, I., Lindgren, R., and Rydh, B. 1974, *Table of Band Features of Diatomic Molecules* (Stockholm: University of Stockholm Institute of Physics).

Kovács, I. 1969, *Rotational Structure in the Spectra of Diatomic Molecules* (New York: American Elsevier).

Luck, R. E. 1978, *Ap. J.*, **219**, 148.

Nordh, H. L., Lindgren, B., and Wing, R. F. 1977, *Astr. Ap.*, **56**, 1.

Sauval, A. J. 1978, *Astr. Ap.*, **62**, 295.

Thompson, R. I. 1973, *Ap. J.*, **181**, 1039.

Truran, J. W., and Iben, I., Jr. 1977, *Ap. J.*, **216**, 797.

Vogt, S. S., Tull, R. G., and Kelton, P. K. 1978, *Appl. Optics*, **17**, 574.

Walker, J. H., Walker, T. E. H., and Kelly, H. P. 1972, *J. Chem. Phys.*, **57**, 1094.

Watson, W. W. 1938, *Phys. Rev.*, **53**, 639.

Wing, R. F. 1972, *Mém. Soc. Roy. Sci. Liège*, 6th ser., **3**, 123.

Wing, R. F., Cohen, J., and Brault, J. W. 1977, *Ap. J.*, **216**, 659.

Wing, R. F., and Ford, W. K. 1969, *Pub. A.S.P.*, **81**, 527.

Wyckoff, S., and Clegg, R. E. S. 1978, *M.N.R.A.S.*, **184**, 127.

Wyckoff, S., and Wehinger, P. A. 1977, *Ap. J.* (*Letters*), **212**, L139.

R. E. S. Clegg and D. L. Lambert: Department of Astronomy, University of Texas, Austin, TX 78712