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REJECTION OF THE C_7^- DIFFUSE INTERSTELLAR BAND HYPOTHESIS

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ABSTRACT

Using the new high-resolution (∼8 km s^{-1}) echelle spectrograph on the 3.5 m telescope at the Apache Point Observatory, we have begun a high-sensitivity survey of the diffuse interstellar bands (DIBs) in a large sample of reddened stars. Now that we are 2 years into this long-term survey, our sample includes over 20 reddened stars that show at least one of the DIBs that had been suggested to be caused by C_7^-, based on the gas-phase measurement of the C_7^- spectrum by J. P. Maier's group. The high-quality astronomical data from this larger sample of stars, along with the spectroscopic constants from the new laboratory work recently reported by Maier's group, have enabled us to examine more carefully the agreement between C_7^- and the DIBs. We find that none of the C_7^- bands match the DIBs in wavelength or expected profile. One of the DIBs (λ5748) attributed to C_7^- is actually a stellar line. The two strongest DIBs attributed to C_7^- (λ6270 and λ4964) are not correlated in strength, so they cannot share the same carrier. On the whole, we find no evidence supporting the hypothesis that C_7^- is a carrier of the DIBs.

Subject headings: ISM: molecules — line: identification — methods: laboratory — molecular data

1. INTRODUCTION

Perhaps the longest unsolved problem in astrophysical spectroscopy is that of the diffuse interstellar bands (DIBs), a series of hundreds of absorption lines present in the visible spectra of nearly all reddened stars. It is now generally believed that the DIBs are caused by free molecules in the gas phase (Herbig 1995), but despite many decades of effort by astronomers and molecular spectroscopists, there has been no match between any subset of the diffuse bands and the gas-phase laboratory spectrum of an individual molecule.

Many astronomers and molecular spectroscopists were hopeful that this impasse had finally been broken when J. P. Maier's group reported (Tulej et al. 1998) a possible match between the gas-phase spectrum of C_7^- and five DIBs in the catalog of Jenniskens & Désert (1994). The promising laboratory bands are all vibronic bands of the lowest electronic transition ($A\,^2\Pi_u \leftarrow X\,^2\Pi_g$) of C_7^-. The strongest of the reported bands, the origin (0_0^0) band at 6270.2 Å, seemed to match the strong λ6270 DIB. The other four laboratory bands that seemed to match the DIBs were the 1_0^1 band at 5612.8 Å (λ5610 DIB), 2_0^1 at 5747.6 Å (λ5748), 3_0^1 at 6063.8 Å (λ6065), and the combination band $1_0^2 3_0^1$ at 4963 Å (λ4964).

All five of these laboratory transitions seemed to agree with DIBs within about 2 Å, which is a far closer agreement than had been achieved by any previously proposed DIB carrier. Many of the astronomical observations of the DIBs were at the limit of the sensitivity, as were the laboratory observations. Because it was not possible to infer the rotational or spin-orbit constants of C_7^- from the laboratory work, it was unclear how the bands might shift in wavelength or profile as a function of temperature. For these reasons, agreement within ∼2 Å was sufficient to warrant further investigation.

Using initial data from our DIB survey (McCall, York, & Oka 2000), we confirmed the existence of four of the five DIBs but had reservations about the λ5748 band. With data from four reddened stars, it appeared that these four DIBs agreed reasonably well in both wavelength and relative intensities, given the uncertainties in the laboratory data. Additionally, in these four sources (HD 46711, HD 50064, HD 183143, and Cygnus OB2 12), the four bands seemed to vary together in intensity.

Recently, J. P. Maier's group has obtained laboratory data on the 0_0^0, 1_0^1, 2_0^1, and 3_0^1 bands of C_7^- with considerably higher resolution and sensitivity (Lakin et al. 2000). The authors performed theoretical calculations to estimate the ground- and excited-state rotational and spin-orbit constants and then varied the spin-orbit constants to best fit their experimental spectrum. Since the overall profile of the spectrum is very different as the spin-orbit constants are varied, this approach results in a fairly unambiguous determination of the molecular constants (although not as unambiguous as would be possible from a fully rotationally resolved spectrum). With the constants determined from the experiment, it is now possible to predict how the C_7^- spectrum will change with temperature. Such predictions are essential in performing a detailed comparison with the DIBs.

At the same time, our DIB survey has progressed to the point where we now observe at least some of the bands attributed to C_7^- in the spectra of over 20 reddened stars. Additionally, our data reduction pipeline has improved substantially, such that the aliasing that limited the signal-to-noise ratio in our earlier work has been completely eliminated. These advances in both the laboratory and astronomical spectroscopy have prompted us to reexamine the case for C_7^- as a diffuse band carrier.

2. OBSERVATIONS AND DATA REDUCTION

The observations reported here are part of our long-term survey of the DIBs in a large sample of stars. High-resolution ($R \sim 37{,}500$) visible (4000–10000 Å) spectra have been obtained with the Astrophysical Research Consortium Echelle Spectrograph (ARCES) on the 3.5 m telescope at the Apache Point Observatory. Data reduction is performed using standard IRAF routines, as described in detail by J. Thorburn (2000).[1] A more complete description of our DIB survey will be given in a future paper.

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[1] The IRAF Data Reduction Guide for the ARCES is available at http://www.apo.nmsu.edu/Instruments/echelle.

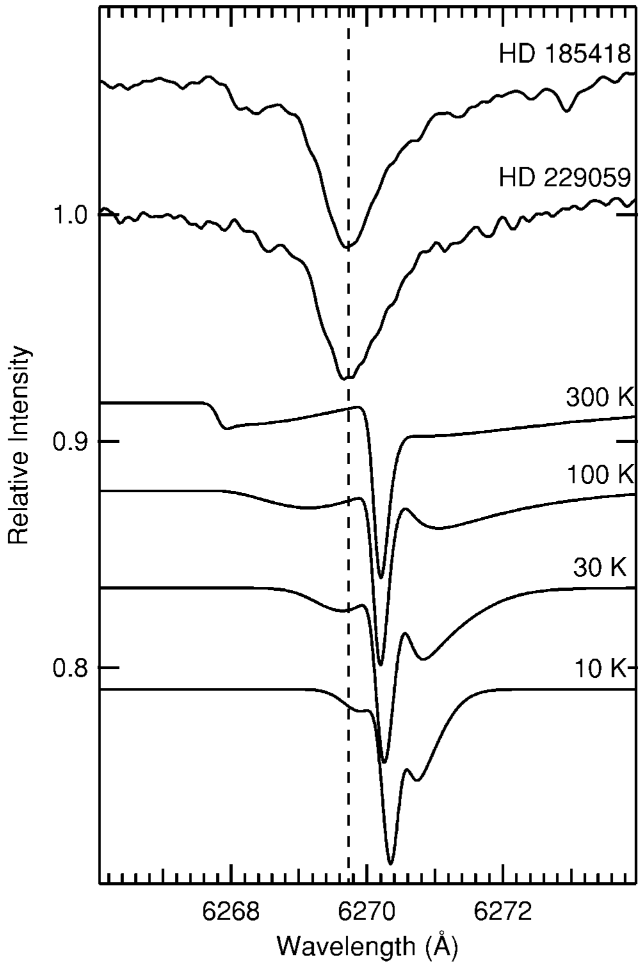

FIG. 1.—Spectra of the λ6270 DIB in two reddened stars (*upper traces*) compared with simulations of the $\Omega'' = 1/2$ component of the $A \leftarrow X\ 0_0^0$ origin band of C_7^- at various temperatures. The simulations assume a Gaussian line width of 10 km s^{-1} derived from K I λ7699 (not pictured). Note the lack of agreement between C_7^- and the DIB, both in wavelength and in profile.

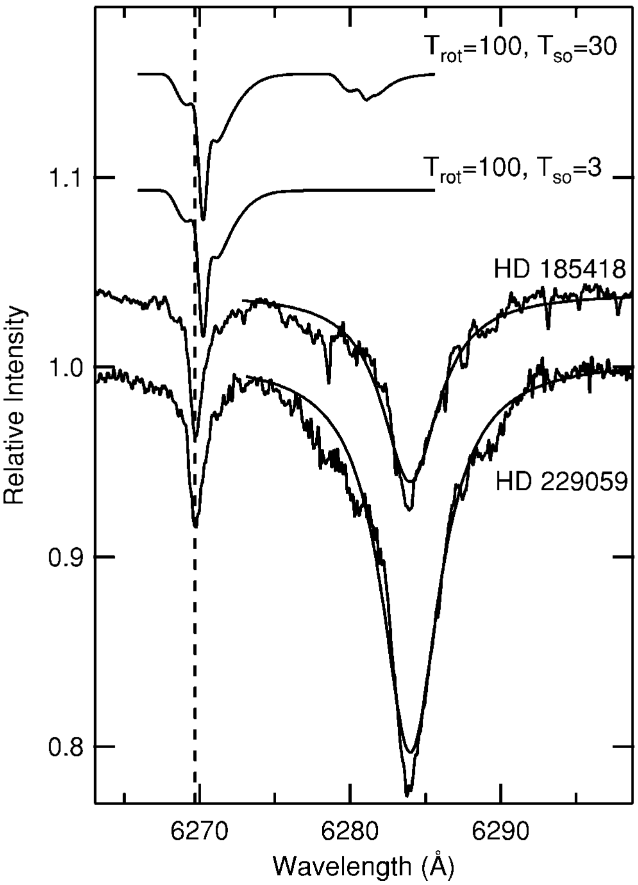

FIG. 2.—Simulations of the $\Omega'' = 1/2$ (*left-hand side*) and $\Omega'' = 3/2$ (*right-hand side*) components of the C_7^- origin band (*upper traces*). In this figure, the simulations were performed assuming an (unreasonably large) ad hoc line width of 30 km s^{-1} in order to better match the width of λ6270 for comparison. The lower traces show the spectra of HD 185418 and HD 229059. These spectra have been divided by standard stars (HD 149757 and HD 176437, respectively) in order to remove atmospheric absorption lines of O_2. The smooth curves are Lorentzian fits to the unrelated λ6284 DIB.

3. RESULTS AND DISCUSSION

3.1. *Simulation of* C_7^- *Spectra*

Given the constants from Lakin et al. (2000) ($B'' = 897$ MHz, $B' = 887$ MHz, $A''_{so} = 27.4\ \mathrm{cm}^{-1}$, and $A'_{so} = 0.6\ \mathrm{cm}^{-1}$), we used the method of Hill & Van Vleck (1928) to calculate the energy levels of C_7^- and the intensity factors for the individual rotational lines within a given vibronic band. (We assumed the same constants for each vibronic band since the vibrational dependence of the constants is expected to be smaller than the uncertainty in the determined constants.) The populations of the individual levels of C_7^- were then calculated using a Boltzmann expression assuming an effective temperature for the rotational distribution (T_{rot}) and for the population of the two spin-orbit levels $\Omega'' = 1/2$ and 3/2 (T_{so}). T_{rot} may be higher than the kinetic temperature of the gas because C_7^- cannot rotationally relax through spontaneous emission. We have therefore performed simulations at $T_{rot} = 10$, 30, 100, and 300 K. On the other hand, T_{so} may be considerably lower than the kinetic temperature because the lifetime for spontaneous emission from $\Omega'' = 3/2 \rightarrow 1/2$ ($\sim 3 \times 10^6$ s) due to the magnetic dipole moment is shorter than the (magnetic) collision time. We have performed simulations for $T_{so} = 3$ and 30 K. For the line width of each transition, we assumed a Gaussian profile with FWHM = 10 km s^{-1}, which is the FWHM of the observed K I lines in HD 185418 and HD 229059, two stars we have chosen for the comparison because of their narrow K I lines.

3.2. *Comparison between DIBs and Simulated* C_7^- *Spectra*

We begin by considering the $\Omega'' = 1/2$ spin-orbit component of the origin (0_0^0) band of C_7^-, in comparison with the λ6270 DIB. The origin band is naturally the strongest of the laboratory features, and λ6270 is also by far the strongest of the DIBs suggested to correspond to C_7^-. Figure 1 shows the spectra of λ6270 toward HD 185418 and HD 229059 along with the simulations of the C_7^- origin band at $T_{rot} = 10$, 30, 100, and 300 K. As can be seen from the figure, neither the central wavelengths nor the profiles of the C_7^- spectra agree with the λ6270 diffuse band. This disagreement argues strongly against the assignment of λ6270 to C_7^-. Note that the position of the absorption maximum is determined by an *R*-head at 6270.2 Å for high T_{rot}—consequently, agreement with λ6270 is not improved by raising T_{rot} further.

In Figure 2, we examine both the $\Omega'' = 1/2$ (*left-hand side*) and $\Omega'' = 3/2$ (*right-hand side*) components of the C_7^- origin band. Because $\Omega'' = 3/2$ is higher in energy, the intensity of the right-hand component increases with T_{so}, as evident in the

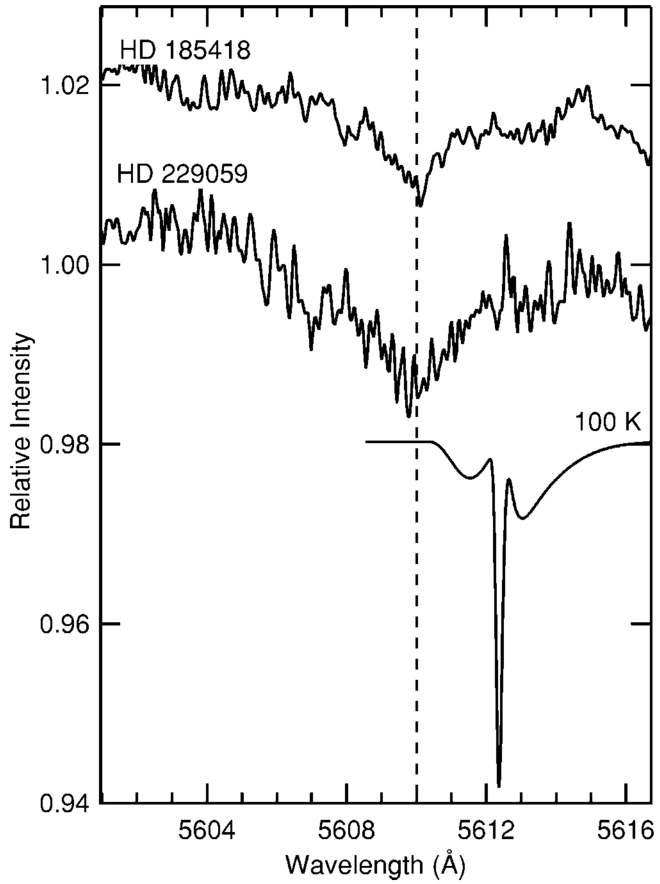

FIG. 3.—Spectra of the λ5610 DIB in HD 185418 and HD 229059 compared with a simulation (10 km s^{-1} line width) of the $\Omega'' = 1/2$ component of the 1_0^1 band of C_7^- at 100 K. Note the disagreement in wavelength and profile between C_7^- and the DIB.

simulations at $T_{\rm so} = 3$ and 30 K (in these simulations, $T_{\rm rot} = 100$ K). In Figure 2, an (unreasonably large) ad hoc Gaussian line width of 30 km s^{-1} has been assumed in order to improve the agreement with λ6270. It appears that there is little evidence for the $\Omega'' = 3/2$ component in the astronomical spectra, but this may not be surprising if $T_{\rm so}$ is low. In the remainder of this section, we consider only the $\Omega'' = 1/2$ components.

Figure 3 compares the simulated spectrum of the 1_0^1 vibronic band of C_7^- with the λ5610 DIB. In this case, the wavelength discrepancy between the C_7^- band and the DIB is particularly egregious, over 2 Å. In addition, the profile is considerably different—the simulated spectrum shows a sharp band head, while the DIB has a fairly Gaussian profile. There is no reason to attribute the λ5610 DIB to C_7^-, and no evidence for any astronomical feature resembling the 1_0^1 band of C_7^-.

Figure 4 shows the region where the 2_0^1 band of C_7^- is expected as well as the λ6270 DIB (which has been suggested to correspond to the origin band). In this figure, the spectra have been shifted in wavelength in order to co-align the Si III stellar line at 5740 Å. It is easily seen from the figure that with this wavelength shift, the feature at 5747 Å is also aligned, whereas the DIB λ6270 is no longer aligned. This implies that the feature that Jenniskens & Désert (1994) claim as a "certain" DIB at 5748 Å is, in fact, a stellar line. This is particularly clear from the strength of the feature in the unreddened star HD 91316 (ρ Leo) that shows no trace of the λ6270 DIB. Since "λ5748" is not of interstellar origin, it cannot be assigned to C_7^-.

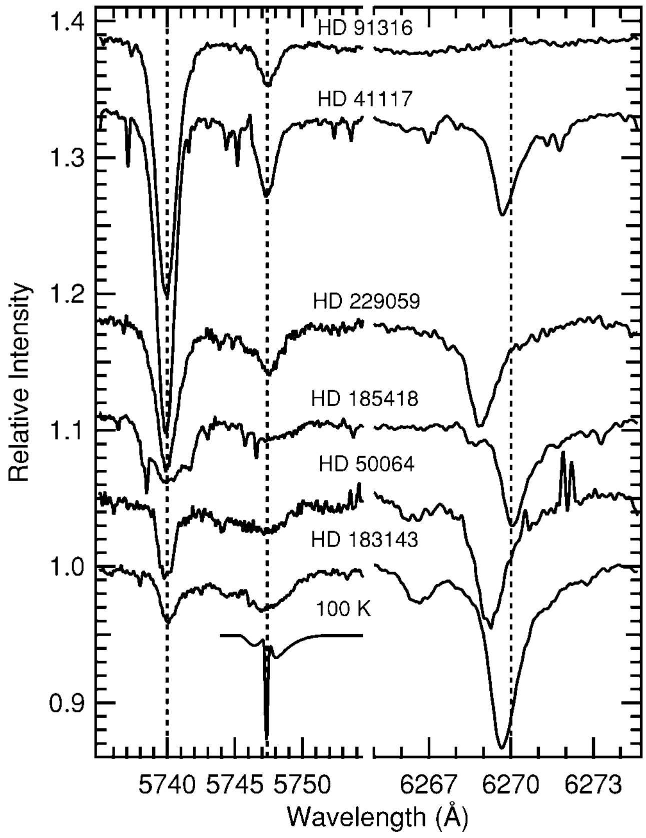

FIG. 4.—Spectra of the region near 5747 Å (*left-hand side*) and 6270 Å (*right-hand side*) in one unreddened star (HD 91316) and several reddened stars. The spectra have been shifted in wavelength to align the Si III stellar line at 5740 Å. Note that the feature at 5747 Å now has the same wavelength from star to star, in contrast to λ6270. This, along with the fact that the 5747 Å feature is seen in the unreddened star HD 91316 where the diffuse bands are absent, shows that the 5747 Å line is a stellar feature rather than a DIB, and only λ6270 is of interstellar origin. For reference, a simulation of the C_7^- 2_0^1 band (10 km s^{-1} line width) is also displayed.

Figure 5 examines the case of the 3_0^1 band of C_7^- compared with the λ6065 DIB. Here we see that again there is a pronounced wavelength discrepancy of $\gtrsim 1$ Å between C_7^- and the DIB. Once again, there is no evidence to support assigning λ6065 to C_7^-. (It is interesting to note that in our present sample of stars, λ6065 and λ6270 appear to be correlated in intensity. Thus, while these bands are not due to C_7^-, they may share a common or closely [chemically] related carrier.)

3.3. *Other Bands of* C_7^-

The combination band $1_0^2 3_0^1$ is surprisingly strong in the laboratory spectrum of Tulej et al. (1998), and it was suggested that this band may correspond to the λ4964 DIB. Since the $1_0^2 3_0^1$ band was not revisited in the experiment of Lakin et al. (2000), we cannot examine in detail its agreement with the λ4964 DIB. However, with our substantially larger sample of stars, we are in a position to reexamine the correlation between the intensities of λ4964 and λ6270 (supposedly the origin band of C_7^-). If these two bands are due to the same species, they must have the same intensity ratio from star to star since this ratio is determined solely by the Franck-Condon factors.

Figure 6 displays the spectra of λ4964 and λ6270 in a sample of 12 reddened stars. While it appeared in our original work (McCall et al. 2000) that these bands were correlated, this was

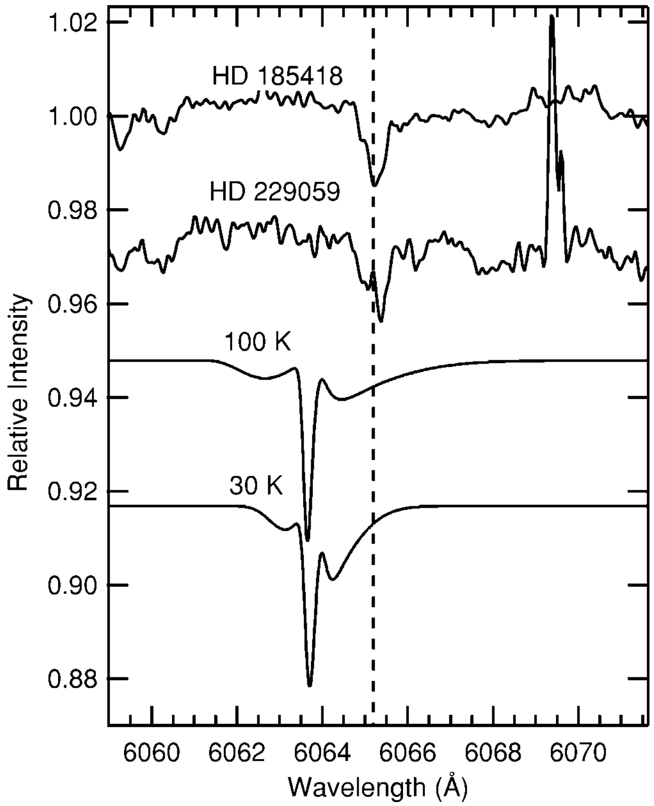

FIG. 5.—Spectra of the region near 6065 Å in HD 185418 and HD 229059, along with simulations (10 km s^{-1} line width) of the C_7^- 3_0^1 band at 30 and 100 K. Note the poor wavelength agreement between C_7^- and the DIB.

apparently due to the small sample (four) of stars considered in that work. From this figure, it is evident that in some stars (e.g., HD 183143 and HD 20041), λ6270 is much stronger than λ4964, while in other stars (e.g., HD 147888 and HD 147889), the situation is reversed. This clearly rules out the possibility that both bands can be due to the same carrier, and therefore they cannot both be due to C_7^-.

There are two other weak vibronic bands of the $A \leftarrow X$ transition of C_7^- that were reported by Tulej et al. (1998). These both happen to be doublets: 1_0^2 at 5089.5 and 5095.7 Å and $1_0^1 3_0^1$ at 5449.6 and 5456.7 Å. We were not able to detect these bands in our astronomical spectra, but because of the intrinsic weakness of these bands (compared with the origin band), we were not able to set useful upper limits on them either. Similarly, we were not able to obtain a useful limit for the origin band of the $B \leftarrow X$ band, which has a very small central depth because of its intrinsic broadness.

4. CONCLUSIONS

The hypothesis that C_7^- is a DIB carrier has been very attractive on spectroscopic grounds alone—no previously proposed carrier has come so close to providing a wavelength match to any set of the diffuse bands. There are strong chemical arguments against this hypothesis: chemical models (Ruffle et al. 1999) are unable to reproduce the necessary abundance of C_7^-, even with the most favorable assumptions. This is due in large part to the destruction of C_7^- by hydrogen atoms, which has recently been confirmed to proceed with a fast rate coefficient (Barckholtz, Snow, & Bierbaum 2001). In spite of these chemical arguments, the approximate coincidence between the C_7^- and DIB wavelengths has been too close to ignore, given the uncertainties inherent in the previously available laboratory and astronomical work.

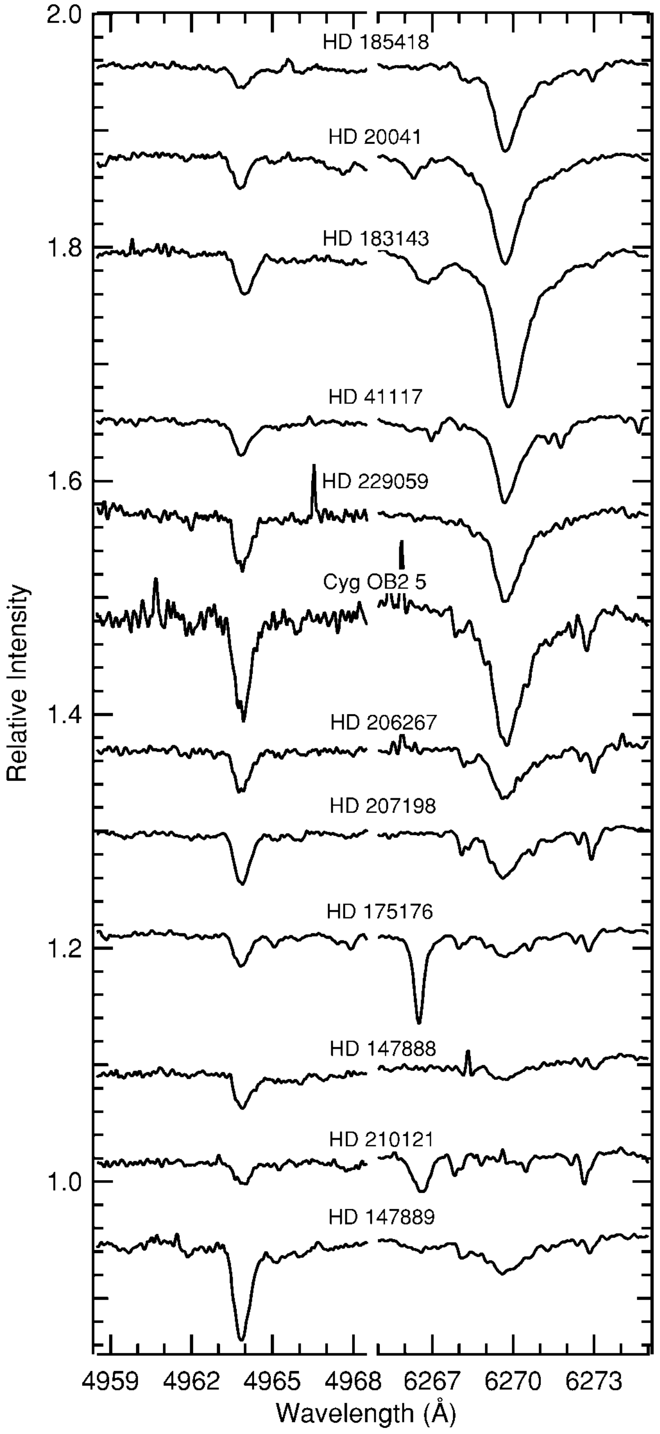

FIG. 6.—Spectra of the λ4964 (previously attributed to C_7^- $1_0^2 3_0^1$) and λ6270 (C_7^- 0_0^0) DIBs in several reddened stars. Note the lack of correlation between the intensities of the two bands, indicating that they do not have a common carrier.

Armed with the spectroscopic constants of C_7^- from Lakin et al. (2000) and our improved sample of DIB observations, however, it is now clear that C_7^- fails the stringent tests enabled by high-resolution spectroscopy. The origin band does not match λ6270 in wavelength or profile. The 1_0^1 band is way off in wavelength from λ5610 (∼2 Å) and also does not agree with the profile of the DIB. The DIB attributed to the 2^1_0 band turns out to be a stellar line. The 3^1_0 band does not match λ6065 in wavelength or profile. Finally, the DIBs attributed to the $1^2_0 3^1_0$ band (λ4964) and the origin band (λ6270) do not vary together in intensity and therefore do not share a common carrier. Close as the wavelength match appeared to be at first sight, there now seems to be no evidence to support the hypothesis that C_7^- is a carrier of the DIBs.

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