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ULTRAFINE STRUCTURE IN THE λ5797 DIFFUSE INTERSTELLAR ABSORPTION BAND[1]

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ABSTRACT

High-resolution and high-S/N observations of the strong and relatively narrow λ5797 diffuse interstellar absorption band, recorded with the Ultra–High-Resolution Facility at the 3.9 m Anglo-Australian Telescope and the 0.9 m coudé feed of the Kitt Peak National Observatory, are reported. For selected lines of sight and using resolving powers of up to 600,000, a remarkable degree of intrinsic ultrafine structure is found within the band. There exists an almost exact correspondence between the structure in the spectra recorded toward μ Sgr, ζ Per, and ζ Oph, including one particularly narrow component with a width that is comparable to the widths of atomic and molecular absorption lines along these lines of sight. The results provide a new and extremely exacting test against which theoretical or laboratory candidates can be assessed, and they point to a new approach to studies of diffuse band carrier distributions through their velocity signatures.

Subject headings: ISM: molecules — line: identification — stars: individual (μ Sagittarii, ζ Ophiuchi, ζ Persei)

1. INTRODUCTION

The unidentified λ5797 diffuse interstellar absorption band occupies a prominent position in the history of diffuse band studies. It was first noted by Heger (1922) in spectra recorded toward several B-type stars, including ζ Per. The band was further observed in 1934 by Merrill, who demonstrated the band to be interstellar in origin through observations toward the binary star Boss 6142 (Merrill 1934, 1936); it was found to be stationary in that it did not share the dynamical Doppler shift exhibited by atomic stellar lines associated with the orbital motion of the binary. Use of the adjective *diffuse* might suggest that there is little prospect of finding fine structure in the profile of a diffuse interstellar band such as λ5797. However, studies at ultra-high and high resolution over the past few years have shown that multiple peak structure is prevalent in narrow diffuse bands (Sarre et al. 1995; Ehrenfreund & Foing 1996; Kerr et al. 1996; Jenniskens et al. 1996; Krełowski & Schmidt 1997). The structure is reminiscent of partially resolved rotational branches in electronic spectra of large gas-phase molecules, but does not of itself prove that the carriers are molecular. Here we report the discovery of an even higher level of *ultrafine* structure in λ5797, one component of which has a width that is comparable to the intrinsic widths of interstellar atomic and molecular absorption lines.

The search for fine structure is motivated in part by anticipation that high-resolution spectra may yield clues as to the identity of diffuse band carriers, and that the size and symmetry of the carriers may be inferred through rotational contour modeling calculations. To date, modeling of observational data using a χ^2 minimization approach has only been undertaken for λ5797 and the related λ6614 band. This yielded a set of molecular and line width parameters, rotational temperatures, etc., consistent with the recorded spectrum of λ6614 (Kerr et al. 1996). Earlier, a set of contour calculations had illustrated the likely appearance of spectra for a range of polycyclic aromatic hydrocarbon and C_{60}-type molecules (Cossart-Magos & Leach 1990; Edwards & Leach 1993). An approximate value for a rotational constant of such carriers may be deduced by taking the separation between *P*- and *R*-branches, but a rotational temperature has to be assumed, and the geometry of the carrier is undefined in this approach (Ehrenfreund & Foing 1996). Evidence in favor of some of the sharper diffuse interstellar bands arising from electronic transitions in free molecules includes the observation that a few of the absorption bands that belong to family 3 of Krełowski & Walker (1987), including λ5797, have counterpart emission features in the Red Rectangle Nebula (Scarrott et al. 1992; Sarre, Miles, & Scarrott 1995) and the R CrB star V854 Cen (Rao & Lambert 1993).

The first evidence for intrinsic structure within a "sharp" diffuse band was presented by Herbig & Soderblom (1982), who detected an inflection in the shortward wing of the λ6614 diffuse band at resolving powers of 65,000 and 115,000. The profiles of several other diffuse bands were observed at $R \sim 100{,}000$ by Westerlund and Krełowski (1988a, b), in which account was taken of multiple velocity components along the lines of sight. The results included the demonstration that the λ5797 diffuse band is highly asymmetric, with a steep blue side and with an extended undulating red wing; the profile was described in terms of five Gaussian components.

We have undertaken a program of observation of several sharp diffuse interstellar bands using resolving powers from 3 to 9×10^5, i.e., where the instrumental contribution to the line width is comparable to, and generally much smaller than, the intrinsic dispersions caused by thermal and turbulent motions within individual interstellar clouds (typically less than 1 km s^{-1}; see Crawford et al. 1994; Barlow et al. 1995). The intrinsic interstellar profile of a diffuse band is obtained by observing along selected lines of sight where

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the velocity structure of the diffuse cloud components, as indicated by known atomic or molecular absorptions, is relatively simple.

Early results confirmed Herbig & Soderblom's result for λ6614 (Hibbins et al. 1995) and also suggested the existence of structure within λ5797 (see Hibbins 1996). Unambiguous detection of partially resolved components within the λ5797 and λ6614 diffuse bands was discovered in 1994 August, as described in Hibbins et al. (1994) and Sarre et al. (1995). The reproduction of similar structures for all of the targets effectively ruled out a significant contribution to the observed profiles from stellar photospheric lines. Lower resolution observations have confirmed the general nature of the structure, reported recently for some other bands (Ehrenfreund & Foing 1995, 1996; Jenniskens et al. 1996; Krełowski & Schmidt 1997). In this paper we present high-S/N spectra of the λ5797 diffuse band recorded at resolving powers of up to 600,000, using two telescopes and along different lines of sight, and find it to be highly structured, particularly within the core of the band.

2. OBSERVATIONS

2.1. *AAT/UHRF*

The observations of λ5797 toward μ Sgr and ζ Oph were obtained with the Ultra–High-Resolution Facility (UHRF) at the 3.9 m Anglo-Australian Telescope (AAT) on 1994 August 15–18 and 1995 June 26–28. The UHRF was operated at a nominal resolving power of 600,000 (Diego et al. 1995) with a confocal image slicer (Diego 1993), masked to allow scattered light to be sampled either side of the spectral order for background determination. Data were recorded with the AAO Tektronix CCD (1024 × 1024, 24 μm pixels), and the output was binned by a factor of 4 perpendicular to the dispersion direction in order to reduce the readout noise of the wide sliced spectrum.

The spectral resolution was checked by measuring the widths of (resolved) Th-Ar hollow cathode lines, which were also used for wavelength calibration. Assuming an intrinsic line width of 0.43 km s^{-1} (Crawford et al. 1994), the mean resolution at 5797 Å over 1995 June 26–28 was found to be 0.0093 ± 0.0002 Å (0.48 km s^{-1}, or $R = 620{,}000$). The UHRF spectra presented here represent a combined integration time (in poor conditions) of 7.5 hr for μ Sgr and 5.5 hr for ζ Oph. Spectra of fast-rotating unreddened standard stars were recorded on the same nights to characterize the telluric spectrum. Flat fields were obtained with a wide slit in place of the image slicer, and detector bias frames were obtained at the beginning and end of each night.

Spectra were extracted using the FIGARO data reduction package (Shortridge 1988). At the high dispersion of the UHRF, only four Th-Ar lines with well-determined wavelengths fell in the short wavelength interval ($\sim$5 Å) recorded by the detector around 5797 Å. However, the spectral dispersion over this interval is almost perfectly linear (Barlow et al. 1995; Diego et al. 1995), and linear or quadratic fits to the four lines consistently yielded rms residuals of less than 0.001 Å.

Observations of the λ7699 K I interstellar line toward μ Sgr and ζ Oph were also obtained in 1994 August in order to characterize the velocities and intrinsic dispersions of the clouds along the lines of sight. For these observations the UHRF was operated at a nominal resolving power of 300,000; the actual resolving power determined from the widths of the Th-Ar comparison arc lines was found to be $R = 460{,}000$ (0.65 km s^{-1}, or 1.4 pixels at 7699 Å; see also Diego et al. 1995).

2.2. *KPNO* 0.9 m *Coudé Feed*

The data toward ζ Per were recorded with the 0.9 m coudé-feed telescope and 2.1 m coudé spectrograph at the Kitt Peak National Observatory (KPNO) on 1995 December 20. The spectrograph was operated with the 31.6 g mm^{-1} echelle grating with Camera 6 at a resolving power of $\sim$300,000. The total integration time on ζ Per was 4.3 hr; the bright standard star β Ori was observed to record telluric features. Reductions were performed using standard IRAF routines.

The properties of the program and standard stars are listed in Table 1.

3. SPECTROSCOPIC DETAILS

In order to ensure that the fine structure within the profile of the λ5797 diffuse band is genuine, it is essential to consider possible contributions from stellar photospheric and telluric lines, and the continuum definition. Also, given that the rest (laboratory) wavelength(s) of the band are not known, the question of the appropriate velocity reference frame must be addressed.

3.1. *Stellar Photospheric Lines*

In general, stellar photospheric lines are very broad with respect to the resolution of the spectra presented here, and cannot be confused with fine structure within the diffuse band. However, the presence of photospheric lines may affect the determination of the continuum level local to the 5797 Å band and complicate the interpretation of extended line wings.

TABLE 1

PROPERTIES OF THE PROGRAM AND STANDARD STARS

Star	HD	V	Spectral Type	$E(B-V)$	$v \sin i$ (km s^{-1})	S/N	Instrument
μ Sgr.....	166937	3.86	B8 Iap	0.25	$\leq$54	730	UHRF
ζ Oph.....	149757	2.56	O9.5 V[a]	0.33	372[a]	580	UHRF
ζ Per.....	24398	2.85	B1 Ib	0.32	67[a]	680	CF
α Gru.....	209952	1.74	B7 IV	0.00	236	...	UHRF
α Eri.....	10144	0.46	B3 Vpe	0.04	251	...	UHRF
β Ori	34085	0.12	B8 Ia	−0.01	33	...	UHRF, CF

NOTES.—All data are taken from Hoffleit & Jaschek (1982), except where indicated; CF indicates coudé feed at KPNO. Values of $E(B-V)$ are derived from the intrinsic colours given by Schmidt-Kaler (1982).

[a] Howarth et al. 1997.

The unreddened B8 supergiant β Ori is a good spectroscopic match to μ Sgr (Table 1). As seen in Figure 1, no photospheric features are found to fall near the 5797 Å band. No observations of unreddened early B supergiants were available for comparison with the spectrum of ζ Per, but synthetic spectra presented by Krełowski & Schmidt (1997) show only one significant feature, at 5799.933 Å (Fe III), which lies just outside the redward wing of the diffuse band. The early spectral type and rapid rotation of ζ Oph mean that the photospheric spectrum is featureless across the short wavelength interval observed with the UHRF.

3.2. *Telluric Lines*

The identification and removal of narrow telluric features must be carried out to avoid confusion with real intrinsic fine structure within the 5797 Å diffuse band. Unreddened fast-rotating stars were used as standards in order to obtain a featureless photospheric spectrum across the short wavelength interval recorded with the UHRF. For the KPNO data, the unreddened standard star β Ori was used. Figure 1 illustrates the removal of telluric lines in the spectra of μ Sgr (Fig. 1*a*) and ζ Per (Fig. 1*b*), which was done by scaling the template telluric spectrum in optical depth and dividing the diffuse band spectrum by the result. The same procedure was applied to the ζ Oph spectrum.

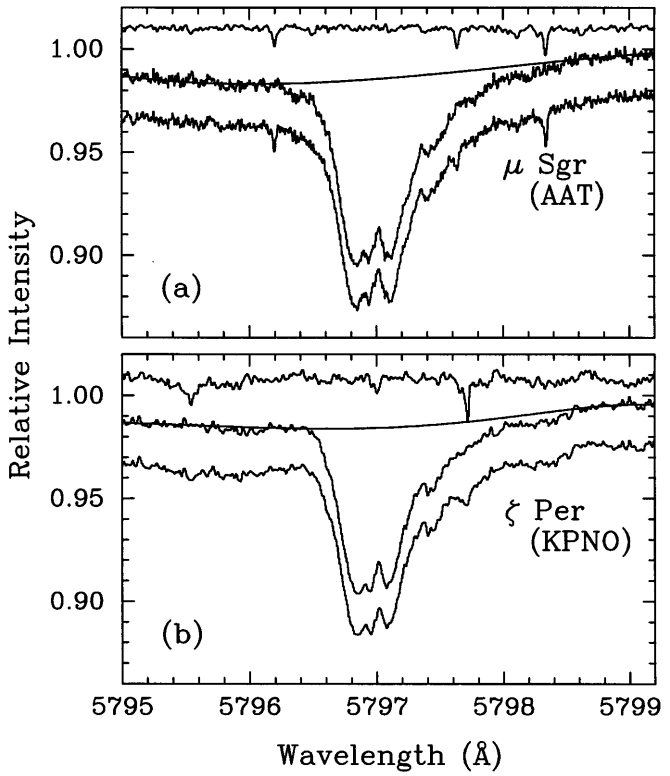


FIG. 1.—Telluric correction and continuum rectification of the λ5797 diffuse band in (*a*) μ Sgr (1995 data) and (*b*) ζ Per. The telluric-corrected spectrum is normalized to unity near 5799 Å in each case; for clarity, shifts in relative intensity of +0.01 and −0.02 have been applied to the telluric and original spectra, respectively. All spectra are presented in the interstellar reference frames described in the text. The telluric spectrum in (*a*) is the combined spectrum of α Gru and α Eri and that in (*b*) is β Ori. In order to rectify the local continuum to unit relative intensity, a polynomial was fitted to the regions $\lambda < 5796.2$ Å and $\lambda > 5798.6$ Å and divided into the telluric-corrected spectra; the polynomial fit is illustrated for each star.

3.3. *Continuum Rectification*

Accurate definition of the continuum on either side of the λ5797 diffuse band is not straightforward: the band has an extended red wing, and weaker diffuse bands near 5796 Å have been observed in some stars (Herbig 1975; Krełowski & Sneden 1993; Jenniskens & Désert 1994), interfering with the blue wing of the λ5797 band.

A relative photometric calibration was first performed by dividing each diffuse band spectrum by a polynomial fit to the continuous spectrum of a standard star obtained on the same night. A broad feature centered near 5796 Å was found to be present in μ Sgr and ζ Per, but was weak or absent in the ζ Oph spectrum, in agreement with published spectra obtained at lower resolution (e.g., see Fig. 4 of Krełowski & Sneden 1993; Krełowski et al. 1992). The continuum local to λ5797 was rectified to unit relative intensity by fitting a polynomial to each telluric-corrected spectrum (see Fig. 1). The continuum rectification of the ζ Oph spectrum, which does not suffer from interference by the broad λ5796 band, provides a check on the overall profile of λ5797 and the derived extent of the long-wavelength wing.

3.4. *Velocity Reference Frames*

It has been shown that some narrow diffuse bands share similar velocity shifts to those of neutral atomic species such as K I (e.g., Herbig & Soderblom 1982) or Na I (e.g., Westerlund and Krełowski 1988a, b). Moreover the three main components resolved in the core of the 6614 Å diffuse band (Sarre et al. 1995) observed along four different sight lines were found to be aligned when corrected to the rest frames of the principal interstellar K I lines. Here we consider the results of high-resolution studies of atoms and diatomic molecules in order to define an appropriate rest frame for λ5797 observed toward μ Sgr, ζ Per, and ζ Oph.

In Figure 2*a* we show spectra toward μ Sgr (*upper*) and ζ Per (*lower*) recorded at the AAT and KPNO, respectively. For these lines of sight the measured heliocentric velocities of the strongest components of neutral atomic and molecular species are consistent within observational error. For μ Sgr we obtain -5.8 km s^{-1} for K I, which may be compared to -5.7 km s^{-1} for CH and CH$^+$ (Crane, Lambert, & Sheffer 1995), and this was adopted for the λ5797 rest frame; for ζ Per, Crane et al. obtained a velocity of $+14.1$ km s^{-1} for CH$^+$ and discerned two almost equal components in the CH profile at $+14.0$ and $+14.3$ km s^{-1}. We have taken a velocity of $+14.15$ km s^{-1} as the rest frame for the 5797 Å band toward ζ Per; this value is consistent with an earlier value for K I ($+14.5$ km s^{-1}) determined by Hobbs (1974).

Toward ζ Oph there are two principal components in absorption and emission lines near -14 km s^{-1} that are separated by ~ 1.1 km s^{-1} (Crawford et al. 1994; Barlow et al. 1995; Sembach, Danks, & Lambert 1996; Liszt 1997). We find that when the ζ Oph spectrum is corrected to the stronger of the components of, e.g., CH (-14.7 km s^{-1}; Crawford et al. 1994) or Na I λ3302 (-14.8 km s^{-1}; Barlow et al. 1995), the band is noticeably displaced with respect to that obtained from the other two lines of sight. Assuming that the (almost identical) rest frames derived for λ5797 from the μ Sgr and ζ Per analysis are correct, a rest frame of -13.1 ± 0.3 km s^{-1} is required to bring the λ5797 spectrum in ζ Oph into alignment. Within observational error, this velocity is (just) consistent with the diffuse band absorption arising in the redder of the two components, as

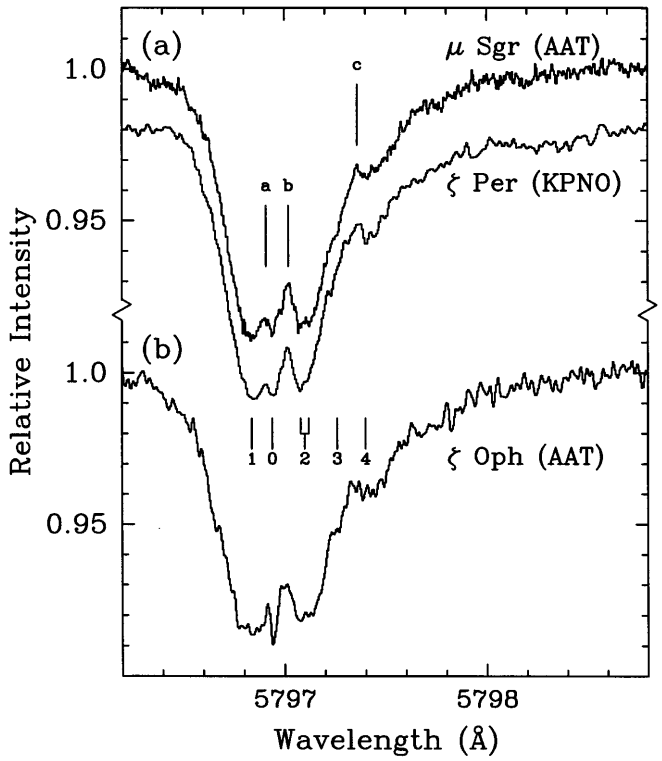


FIG. 2.—Ultra–high-resolution spectra of λ5797 (*a*) toward μ Sgr (AAT) and ζ Per (KPNO), presented in the rest frames of the main cloud components; and (*b*) toward ζ Oph, where the profile has been aligned under the spectra of Fig. 1*a* (see text). All spectra are corrected for telluric contamination, rectified, and scaled to the same optical depth at the center of the line. The scaled spectrum of ζ Oph has been smoothed to an effective resolution of ~400,000 to improve the signal-to-noise ratio.

observed, for example, in CH (-13.6 km s^{-1}) or Na I (-13.9 km s^{-1}).

4. THE PROFILE OF THE 5797 Å DIFFUSE INTERSTELLAR BAND

Considering the spectra of all three program stars in Figure 2, the two most striking results are the high level of structure within the band and the consistency between the profiles, most particularly between the two lines of sight μ Sgr and ζ Per that were studied using different telescopes. This provides very strong evidence that the observed detail is real. Table 2 lists the principal features that can be identified within the profile, where the relative wavelengths are given with respect to the sharp feature near 5796.94 Å.

TABLE 2

OBSERVED COMPONENTS IN THE λ5797 DIFFUSE BAND

Wavelength Offsets (Å)	μ Sgr	ζ Per	ζ Oph
λ_0	5796.942	5796.945	5796.942
$\Delta\lambda_1$	−0.10	−0.09	−0.11
$\Delta\lambda_2$	+0.16	+0.15	+0.17
$\Delta\lambda_3$	+0.32	+0.29	+0.31
$\Delta\lambda_4$	+0.46	+0.46	+0.50
$\Delta\lambda_a$	−0.035	−0.035	−0.035
$\Delta\lambda_b$	+0.075	+0.07	+0.06
$\Delta\lambda_c$	+0.42	+0.43	+0.38

NOTES.—Wavelength offsets $\Delta\lambda_n$ from λ_0 are given, where $\Delta\lambda_n = \lambda_n - \lambda_0$ for component n is measured relative to the sharp absorption feature λ_0 at 5796.942 and 5796.945 Å for μ Sgr and ζ Per, respectively; the components for ζ Oph are defined with respect to the rest frame adopted for μ Sgr (see text). The symbols $\lambda_{0,1,\ldots}$ refer to absorption (peak) components, the mean of a possible doublet $\Delta\lambda_2$ being quoted; $\Delta\lambda_{a,b,c}$ refer to measurable valley positions.

The 5796.94 Å feature is the sharpest yet detected within a diffuse band. We cannot rule out the possibility that it is a chance alignment of an absorption caused by an unrelated atomic or molecular species. However, the apparent splitting of the feature marked as a doublet in both μ Sgr and ζ Per supports the suggestion that the sharp absorption is indeed intrinsic to the diffuse band itself. Defined with respect to local continua immediately adjacent to it, the widths (*b*-values) of the 5796.94 Å feature are estimated to be 1.2, 1.4, and 1.0 km s^{-1} for μ Sgr, ζ Per, and ζ Oph, respectively; these values are within the range of intrinsic dispersions determined for neutral atomic and molecular species such as K I and CH in these clouds.

5. DISCUSSION AND SUMMARY

Structure within the profiles of diffuse bands has generally been interpreted in terms of the molecular hypothesis, and there is certainly a strong similarity both qualitatively and, to a degree, quantitatively, between the observational data and calculated molecular rotational contours. The high level of extra detail described here places additional constraints on any proposed interpretation including molecular rotational contours, isotopic fine structure (Webster 1996), or the specific case of H_2 (Sorokin & Glownia 1996). The very narrow component has the appearance of a *Q*-branch nestling between *R* and *P* features, but there are additional features that do not naturally fall within this simple "triplet" picture, as is also the case for λ6614 (Kerr et al. 1996). It is striking that the separations between the three most prominent features of λ5797 (0.77 and 0.89 cm^{-1}) and λ6614 (0.74 and 0.69 cm^{-1}; Sarre et al. 1995) are very similar in magnitude.

The choice of velocity reference frame is difficult, as it is not certain that the diffuse band carriers share the same spatial distribution and motion as the atoms and diatomic molecules observed along the same lines of sight. Adopting the rest frame of the strongest assigned components does not lead to a consistent alignment of the structures within the band in all three lines of sight. The results for ζ Oph suggest that the λ5797 carrier is associated principally with only one of the two main clouds, described as the "red" cloud (Sembach et al. 1996). It is of interest that the relative column densities of various diatomic molecules are not the same for the two clouds. The molecules CH and CN are more abundant in the "blue" cloud (Crawford et al. 1994), whereas C_2 is reported to be approximately equally abundant in the two clouds (Sembach et al. 1996) or more abundant in the "red" cloud (Crawford 1997). One interpretation of this difference in chemical composition is that the red cloud is exposed to a more intense radiation field (Sembach et al. 1996). A diffuse band distribution skewed to this cloud would not be inconsistent with the recent results for C_2.

We comment that this work has demonstrated the very considerable value of conducting diffuse band studies at the highest possible resolving power as new structure is revealed. There is a remarkable consistency between the λ5797 profiles along the three lines of sight, and these data

provide a clear benchmark for future studies. The high precision with which the component wavelengths are determined opens the opportunity of tracing the spatial distribution of the carriers through their signatures in velocity space with greater discrimination than hitherto attained.

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