

# Diffuse band shifts: a possible explanation

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Abstract. We discuss the behaviour of broad and narrow diffuse interstellar bands inside the Orion association. The peculiarities, observed in this region, such as enormous weakness of some features as well as wavelength shifts of others suggest that the diffuse band carriers – most probably some sort of complex molecules – accrete onto grain surfaces. It appears that the processes which occur upon accretion make the narrow DIBs vanish while the broader features are less attenuated but always red–shifted. The observed shapes of interstellar extinction curves suggest that where this happens the small dust grains which are responsible for the FUV extinction are also reduced in numbers which naturally goes along with gas accretion and increased ratio of total to selective extinction.

**Key words:** ISM: dust, extinction – ISM: lines and bands – ISM: molecules

#### 1. Introduction

It has now become accepted that the unidentified diffuse interstellar bands (DIB's) whose existence has been known since 1922 are produced by certain varieties of large molecules. The most common view is that these molecules are some form of polycyclic aromatic hydrocarbons (PAH's), carbon chains or fulleranes and that the widths of the bands are to be associated with molecular rotation. It is also now recognized that the DIB's form not one but a number of families in the sense of differing correlations of their strength with each other. The dependence of these correlations on local conditions is to be expected if there can be a distinct difference between the sources of different families of bands.

The varying strength ratio of the two prominent DIBs: 5780 and 5797 was shown beyond a doubt by Krełowski & Walker (1987) and by Krełowski & Westerlund (1988). The varying ratios of other DIBs have also been observed (e.g. Krełowski et al. 1995). However, it remains uncertain whether some proposed DIB "families" really exist as sometimes a single case disproves any proposed division of all observed features. See the review by Herbig (1995).

Recently it has been demonstrated that not only the strength of various features may change but also their shapes (Porceddu et al. 1992). The question we shall address here is whether one can associate such shape changes with other variable interstellar features and, in particular, with some sort of interaction with interstellar dust. The evidence that the sharper (narrow) bands are more reduced in regions of high local extinction (Krełowski & Sneden 1995) has been attributed to the possibility that the molecules are relatively small and may be attacked by ultraviolet radiation after they accrete in the icy mantles of dust (Mendoza-Gomez et al. 1995). However, such an effect is less likely to occur for large molecules because they may readily disperse the absorbed energy into vibrational modes and are therefore less likely to be partially dissociated within the dust mantle. On the other hand the larger molecules responsible for DIB's are, when accreted on the dust, expected to provide broadened band shapes and the induced effects are more likely to be on the band shapes than on the strength. Such effects will be addressed in this paper and comparisons made with observations.

It is also to be mentioned that the DIB spectrum is very likely to vary together with other interstellar features. Krełowski et al. (1992) demonstrated that the varying ratio of the two prominent DIBs: 5780 and 5797 is accompanied by the varying abundances of simple molecular species (like the CN radical which seems to be more abundant when the narrow DIBs are strong) and the shapes of interstellar extinction curves as indicated, for example, by the ratio of total to selective extinction. An increase in the latter can be attributed to the accretion processes followed by molecular formation on grain surfaces. The formation of grain mantles changes the size and physical properties of the dust particles. Following this reasoning the extinction curves produced by grains covered with mantles should be characterized by a relatively weak 2200 Å feature and reduction of the far-UV extinction as the big grains do not cause any excess reddening in this spectral range.

### 2. Profiles of diffuse interstellar bands

The problem of the profile determinations of the diffuse interstellar bands could only be adequately addressed after the new solid state detectors were widely applied to record the astrophysical spectra. The first attempt was made by Snell & Van den

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Bout (1981) who determined several high resolution and high S/N spectra covering a very narrow range around the 5780 DIB at the McDonald Observatory. Their analysis was not, however, accompanied with that of other, identified, interstellar features; e.g. sodium or ionized calcium lines, which are known to be composed of many Doppler–shifted single cloud profiles. The latter apparently originate in several clouds along the same line of sight. The Doppler splitting could, in principle, also change the DIB profiles, but, this broadening is not very likely to happen in the case of the analyzed 5780 feature as this DIB is quite broad and reasonable Doppler shifts which are expected towards relatively nearby objects (high resolution and high S/N spectra are known only for bright stars), cannot change its profile substantially.

The first analysis of the profiles of diffuse bands taken along with that of the ionized calcium lines were conducted by Herbig & Soderblom (1982). They have shown composite profiles of 6196 and 6614 DIBs and proved that the Doppler splitting may alter the profiles of these rather narrow diffuse bands. Westerlund & Krełowski (1989) determined the intrinsic; i.e., free of any Doppler splitting, profiles of five diffuse bands. They have observed a small sample of targets characterized by a variable strength ratio of the major DIBs: 5780 and 5797. The profiles of the analyzed DIBs: 5780, 5797, 6196, 6284 and 6379 proved to be identical in all targets where the sodium lines were free of the Doppler splitting. The authors concluded that the intrinsic; i.e., Doppler free DIB profiles are constant in all environments.

However, a few years later, Porceddu et al. (1992) found three exceptionally broad 5780 profiles in the spectra of the stars belonging to the Orion Trapezium. The bands were also reported to be very weak in relation to  $E_{B-V}$ . The effect of broadening in these cases could not have been created by the Doppler effect as the weak, Doppler shifted sodium line components seen in the spectra of observed stars, could not be responsible for such a substantial broadening of the feature which is already broad. The "peculiar" profiles are also available through the WWW: http://caosun.ca.astro.it/database/main.html.

The effect has been confirmed by Krełowski & Sneden (1995) and, in this case, one more interesting factor has been observed. In the spectrum of HD 37022 the 5780 DIB is broader than expected but also very weak whereas the even broader 6284 DIB is of "normal" strength relative to  $E_{B-V}$ . It is interesting that the 6284 is the only DIB in the HD 37022 spectrum, being stronger than the same feature in HD 24398, the star characterized by a very similar colour excess. All other DIBs are much stronger towards the latter object. This effect was fully confirmed by Jenniskens et al. (1994) who proved also that the 6205 and, most probably, also 6177 broad DIBs are of normal strength in the spectrum of HD 37022. However, they have not compared the shapes of these profiles with those observed in other stars.

The existing, published material clearly suggests that the interior of the Orion Association is a very special place in which one can expect the physical conditions to be quite different from "average" or "typical". Both the ultaviolet radiation and dust properties are atypical. This makes the observations of the Orion stars very attractive.

#### 3. The observational material

The observations have been made by one of us (JK) in February, May and November 1993 at the McDonald Observatory. The spectra were formed with the aid of the Cassegrain echelle spectrograph, used with the 2.1 m telescope. Their resolution is R = 60,000 and the S/N ratio usually exceeds 500 because of multiple exposures of our targets. For the details of the acquisition of the spectra and the raw data reduction procedures see Krełowski & Sneden (1993). The observed stars are listed in Table 1. It contains five objects from the Orion Association as well as four standards; i.e., the objects characterized by narrow and symmetrical interstellar sodium lines and the lack of visible Doppler components inside them. We attempted to find standards either matching the depths of the DIBs or the  $E_{B-V}$ 's of the Orion stars.

The diffuse bands which can be seen in our Ori OB1 stars spectra are: 5705, 5780, 5797 (sometimes), 6010, 6196, 6203/6205, 6270, 6284, 6379 and 6614. All the spectra contain the sodium doublet which allows an estimate of the Doppler shifts of the interstellar features as well as bringing them to the rest wavelength scale. The narrow and symmetrical profiles of the NaI lines prove that any substantial broadening of the interstellar spectral features, caused by the Doppler splitting, is not to be expected. In our echelle spectra usually one order is severely contaminated with the dispersed light (the picket fence effect) and, in the spectra observed in February 1993, it happened to spoil the broad 6284 feature which is thus not to be extracted from those spectra. Table 1 shows also which of the spectral features have been observed twice i.e. both in February and November 1993.

All our figures present the segments of the spectra, shifted to the interstellar rest wavelength scale; i.e., to the laboratory wavelengths using the sodium  $D_1$  and  $D_2$  doublet. We must mention that while there is no direct evidence that DIBs are formed in exactly the same places as NaI lines these are the only identified and sharp interstellar features in our spectra and, moreover, in no case has it been found that the wavelength scales for DIBs and sodium lines are different.

# 4. The observational results

In the following figures we will consider as examples two of the Orion stars, listed in Table 1: HD 37022 and HD 37061. The first one is probably the extreme case, i.e., the object in which many DIBs are below the level of detection. The second was selected as the heavily reddened object in which we can trace most of the strong DIBs. Fig. 1 presents the comparison of their spectra in the range of the two major DIBs 5780 and 5797 with those of the nearby, bright stars: HD 144217, already selected by Westerlund & Krełowski (1989) as a "standard" object without any apparent Doppler splitting in the interstellar lines and HD 203064 – the object with the same reddening as

Table 1. The list of selected targets and features with their depths

HD	Sp/L	$E_{B-V}$	5705	5780	5797	6010	6196	6203/05	6270	6284	6379	6614	Remarks
37020	07	0.26	1.0:	1.6	0.6	?	1.1	1.1	0.5	4.7	0.0	0.0	obs. twice
37022	06	0.31	1.0	2.6	?	0.9	0.7	1.2	0.0	7.2	0.0	?	obs. twice
37023	B0.5Vp	0.33	1.0:	2.5	0.4	?	1.8	n/a	n/a	n/a	?	0.6:	obs. Feb. 93
37042	B1V	0.14	0.0:	1.0	n/a	0.0:	0.6	0.7	0.3:	1.1:	0.0	0.7	obs. Nov. 93
37061	B1V	0.50	1.0	6.0	1.3	1.0	1.5	1.8	1.0	8.2	0.0	1.7	obs. Nov. 93
24760	B0.5V	0.10	1.1	3.2	1.5	?	2.4	n/a	n/a	n/a	?	4.0	standard
144217	B0.5V	0.17	1.1	7.3	2.0	0.8	2.7	1.5	1.9	6.9	2.1	5.3	standard
203064	08	0.28	2.0	7.5	5.0	1.0	3.9	3.9	2.4	7.8	2.7	7.2	standard
207198	O9IIe	0.49	1.7	11.1	16.0	1.2	6.3	5.0	3.6	8.9	11.7	12.4	standard





HD 37022. The major DIBs are of the same depths in HD 37061 and HD 144217 despite the fact that the colour excess  $E_{B-V} =$ 0.50 for HD 37061 and only 0.17 for HD 144217. In the other pair the 5780 is weaker by a factor ~3 in HD 37022 than in HD 203064 while the narrower neighbour feature is below the level of detection; the  $E_{B-V}$ 's are practically identical. When both spectra are shifted to the rest wavelengths of the NaI lines the DIBs do not overlay each other. It is clear that both DIBs are red–shifted and their profiles are evidently broader in the spectrum of HD 37061.

Fig. 2 compares the narrow (6270) and very broad (6284) features in the spectra of HD 37061 and HD 207198 as well as HD 37022 and HD 203064. In the presence of the same reddening (colour excess) the broad feature is of the same strength. However, in the spectra of HD 37061 and HD 37022 it is evidently red–shifted as well as 5780. The narrow DIB, 6270, is hardly visible in the spectrum of our Orion stars – it behaves more or less like 5797.



**Fig. 2.** The very broad 6284 DIB in the spectra of Orion stars and comparison objects. This DIB is not attenuated but redsifted as well as other ones.

Below we demonstrate the behaviour of the weaker features, first described by Herbig (1975). Fig. 3 compares the range of three different DIBs: 6196, 6203 and 6205 in the spectra of HD 37061 and HD 207198 – the stars of the same reddening. It has already been shown that the two blended features: 6203 and 6205 are not of the same origin (Porceddu et al. 1991). Fig. 3 shows the case in which the 6203 DIB is below the level of detection whereas the neighbour, broad 6205 feature is of "normal" strength i.e. the same as in another spectrum of the same reddening.

It seems to be of importance that the very shallow but broad DIB: 5705 can also be seen in our example Orion objects (Fig. 4). It seems a bit weak relative to the colour excess but clearly visible. In the same spectra we can hardly detect such normally strong narrow features as 5797 or 6379.

The same effect can be found in the case of the 6010 DIB (Fig. 5). However, the latter figure suggests one more comment. The band is quite weak in the spectrum of HD 207198 – the relatively heavily reddened object. Apparently this band is hardly



**Fig. 3.** The lack of the narrow 6203 DIB in the spectrum of HD 37061; the broad neighbour 6205 is of normal strength.



Fig. 4. The broad 5705 DIB in the spectra of Orion and comparison stars.

seen in "zeta" type clouds as shown by Krełowski et al. (1995) so that the HD 207198 object is apparently of the "zeta" type. In "sigma" type objects (like HD 144217) it can be easily seen even in cases of low reddening.

In all profiles of the diffuse bands seen in the Orion association we observe both broadening and red–shift. In most cases the DIBs are attenuated in comparison with  $E_{B-V}$  when compared with other places in the Galaxy. This is evidently not true in the case of 6284. Let us emphasize that this band is almost twice as broad as 5780. Our spectra clearly suggest that the narrow bands like 5797 are the first to disappear, whereas those of intermediate width, while weakened, still remain visible. The 6284



Fig. 5. The broad 6010 DIB in one Orion and two comparison objects.

and, as we may expect, other very broad DIBs, show changes in the profile shape and are red–shifted, but their depths remain the same in comparison with  $E_{B-V}$  while observed in spectra of stars seen through diffuse interstellar clouds.

The spectra, depicted in the figures above, have all been shifted to the interstellar rest wavelength scale using the radial velocities determined from the sodium  $D_1$  and  $D_2$  lines. The latter are sometimes quite broad and almost saturated which may create doubts whether the measured radial velocities are precise enough. However, the recent observations of the Orion targets, made with the aid of the telescopes and spectrometers of the Russian Special Astrophysical Observatory fully confirm the above discussed wavelength shifts of broad DIBs when the radial velocities are based on the much weaker KI 7699 Å line (for the description of the data see Krełowski et al. 1998).

### 5. Discussion

# 5.1. General remarks

The Orion association is well known as a place in which the interstellar matter is far from the "galactic average". The extinction curves derived from the IUE spectra of the Trapezium stars (Fitzpatrick & Massa 1990) show many peculiarities such as a very weak 2200 Å bump and a very flat, horizontal, far-UV branch. These, together with the above described behaviour of the diffuse interstellar bands, demonstrate some interesting consequences of the complexity of the physical processes which take place in the young Orion OB1 association. The diffuse, relic matter inside this nearby region of star formation apparently evolved after the young stars, like those of the Orion Trapezium, were formed. The aggregate has passed quite recently through the dense and cold phase which should facilitate sticking of atoms or molecules to cold grain surfaces. After the hot stars are formed this matter is strongly irradiated with UV photons.

Conceivably the mantles which are formed could have trapped the carriers of diffuse interstellar bands which are almost certainly some large, carbon bearing molecules – possibly PAHs. The smallest ones are most likely to produce the narrowest and most numerous DIBs. They apparently lose their identity immediately after they stick to the grain surfaces so that the narrowest DIBs are not observed in the Orion OB1 association. The intermediate broad DIBs have their strengths reduced as their carriers are more slowly incorporated into the grain mantles but they are weaker and red–shifted. It is to be emphasized that all DIBs observed in the Orion OB1 association are red–shifted. The broadest DIBs, created presumably by the largest molecules are not attenuated. They are, however, red–shifted which may suggest that their carriers are also residing on grain surfaces.

## 5.2. Accretion of absorbers on dust grains and band shape effects

Accretion of gas phase species on dust grains in molecular clouds is a well observed phenomenon as attested to by the infrared absorption of many solid phase molecules such as  $H_2O$ and CO. With the assumption that the DIBs are produced by large molecules in the gas we have to accept that some accretion of the species must accompany the formation of icy mantles. One possibility is that the DIB molecules are somehow modified or even destroyed in this process. If the narrowest DIBs are produced by the smallest molecules of the suggested PAH variety the latter may be likely. This would follow from the results of laboratory experiments in which it has been demonstrated that the effect of ultraviolet on coronene deposited in  $H_2O$  at 10 K is to eliminate all its characteristic infrared absorption features (Mendoza-Gomez et al. 1995). However larger PAHs are less likely to be destroyed because they can distribute the absorbed UV energy into many more modes without dissociating and are well known to be very resistant to destruction by ultraviolet so that they may be expected to accrete without losing their physical and chemical identity.

In fact they are so large that if they are plate-like and up to  $\sim 20$  Å in diameter, as frequently assumed for large PAH's, they would tend to lie flat on the surface of the large grain as they are accreted. They are also quite numerous, constituting about 20% of the available carbon (Li & Greenberg 1997, Dwek et al. 1997) so that they could make up a major fraction of the mantle surface (and volume). This is something intermediate between being embedded in an icy matrix and bulk material. It is not clear how to calculate how this affects the band absorption. What we can do is show, using Mie theory for core-mantle particles (Greenberg & Hong 1976), that by adding their absorptivity to the ice grain mantle there can be produced a possible shift as large as  $\Delta \lambda \sim 1$  Å as well as a broadening (see Fig. 6). However, this is accompanied by a distortion of the band with an effective emission wing at the short wavelength side. The latter does not appear to occur or at least is too small to be detected. In any case the concept of accretion leading to both the disappearance of the narrow DIBs (if due to small PAHs) and the shift and broadening of the broader DIBs (if due to large PAHs)

**Fig. 6.** Calculated variation of the shape of an absorption feature made up of both free molecules and of molecules accreted in an ice mantle. In descending sequence of increasing fraction of embedded molecules: 0, 0.25, 0.50, 0.75, 1.0. Grain core radius  $a_c = 0.1 \,\mu$ m, ice thickness delta a = 0.01  $\mu$ m,  $V_{PAH}/V_d$  = volume ratio of large molecules to the dust.

is suggestive particularly as it appears to correlate both with an increase in the value of R (total–to–selective extinction ratio) and the reduction in the ultraviolet to visual extinction. Finally, while in the Orion region, there is an enhanced ultraviolet flux as well as a unique extinction curve, we are not aware of how the ultraviolet could produce a shift or broadening of the wider DIBs.

Are the effective emission wings of broad DIBs really absent in Orion or just difficult to be observed? The implication that the large, carbon bearing DIB molecules are accreted on grain surfaces adds to the idea of organic grain mantles which should already exist on all evolved grains. However, the diffuse band spectrum is very complicated and most of the strong DIBs overlap with some other ones. The well-known 5780 DIB is observed at the background of the much broader 5778 feature as described by Herbig (1975). The feature is apparently of normal strength in relation to the colour excess in HD 37022 (see Fig. 7). A possible "blue emission wing" of the deeper 5780 feature apparently coincides with the bottom of the broader 5778 DIB and thus it may be hardly detectable. It is of importance to note that the weak interstellar features, seen on top of the 5778 broad DIB are below the level of detection in the spectrum of HD 37022 as well as the also narrow 5797 DIB. The broad 5778 DIB and (probably) also the shallow 5795 feature seem to be of normal strength in HD 37022.

In the profile of the broad 6284 DIB we can see some weak emission close to 6274 Å (see Fig. 2). This feature is, however, severely contaminated with the telluric lines and its profile can hardly be determined precisely. It is of importance to remark that this weak blue emission at 6274 Å is also seen in the spectra of Jenniskens et al. (1994). It is thus real and may be related





**Fig. 7.** The spectra of two stars of similar reddening. Note the lack of all narrow features in that of HD 37022 (5797 and the weak features seen usually inside the 5778 profile). The 5780 DIB is weak in HD 37022 but the broad 5778 and (probably) 5795 are of normal strength. Note the possible "blue emission" of 5780 coinciding with the bottom of the 5778 DIB. The variable width feature to the right is the stellar CIV line.

to the expected "blue emission wing". It is impossible to check the same phenomenon around the broad features such as 6177 or 5778 because they are very shallow and the continuum level around them is uncertain due to the fact that such features occupy always a substantial part of an echelle order. An additional observational project using a traditional spectrograph is clearly necessary in the case of very broad DIBs.

The above described processes apparently take place inside young stellar aggregates where the diffuse matter which has just passed a very cold and dense phase is being irradiated with the photons emitted by young, hot stars. It is very likely that the newly formed stars are accompanied with the circumstellar dense disks which contain only very large, core–mantle grains, in which the matter is heavily photoprocessed. Recently Krełowski & Wegner (1996) demonstrated that the DIB carriers apparently do not exist at all inside the circumstellar shells. The shapes of extinction curves, observed in stars showing the disk type line profiles seem to be the next step beyond that of the above discussed Orion stars – they do not show the 2200 Å bump at all (Wegner & Krełowski 1996). The circumstellar matter seemingly contains only very large grains which involve the processed material formerly responsible for the DIB formation.

#### 5.3. Conclusions

The above considerations seem to allow the following conclusions:

 the Ori OB1 association, the nearby young stellar aggregate, is filled with relic matter; the latter differs strongly in physical and chemical properties from that, observed in diffuse interstellar clouds

- the spectral properties of the intraassociatory clouds are peculiar in the continuous spectrum (extinction curves) as well as in discrete spectral features (diffuse interstellar bands)
- the behaviour of the diffuse interstellar bands depends on their widths: the broader the band the stronger it is relative to  $E_{B-V}$ ; the narrowest DIBs are below the level of detection even in high S/N spectra
- all the observed DIBs are red-shifted
- the selective DIB attenuation together with the observed red-shift (which can be interpreted in terms of the mattrix effect while a molecule is frozen into a grain) and the shape of extinction curves observed towards the Orion stars may suggest the grain mantle growth during the phase of gravitational collapse followed by the UV irradiation.

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