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On the relation between diffuse bands and column densities of H_2, CH and CO molecules*

T. Weselak[1], G. A. Galazutdinov[2,3], F. A. Musaev[2,3], and J. Krełowski[4]

[1] Kazimierz Wielki Academy, Faculty of Physics, Weyssenhoffa Sqr. 11, 85-072 Bydgoszcz, Poland
e-mail: towes@ab-byd.edu.pl
[2] Special Astrophysical Observatory, Nizhnij Arkhyz 357147, Russia
e-mail: gala@sao.ru
[3] Isaac Newton Institute of Chile, SAO Branch
e-mail: faig@sao.ru
[4] Center for Astronomy, Nicolaus Copernicus University, Gagarina 11, 87-100 Toruń, Poland
e-mail: jacek@astri.uni.torun.pl

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Abstract. Mutual relations between column densities of H_2, CH and CO molecules as well as between the latter and strengths of the major 5780 and 5797 diffuse bands are presented and discussed. The CH radical seems to be a good H_2 tracer, possibly better than CO. It is also demonstrated that the molecular fraction of the H_2 molecule is correlated with an intensity ratio of 5797 and 5780 DIBs, suggesting the possible formation of narrow DIB carriers in denser clouds, dominated by molecular hydrogen and reasonably shielded from ionizing UV radiation by small dust grains.

Key words. ISM: molecules

1. Introduction

The possible relationship between column densities of simple two-atomic molecules and the strengths of Diffuse Interstellar Bands (DIBs), which have remain unidentified since the publication of Heger (1922), may shed some light on the origin of DIBs. It has already been suggested (Krełowski et al. 1992) that DIB intensity ratios vary from cloud to cloud together with the strengths (measured in relation to $E(B-V)$), of spectral features of simple molecules. This fact may be important as the column densities of well known molecules observed along sight-lines intersecting individual clouds can help us to determine the physical conditions that facilitate formation and survival of the carriers of strong DIBs. Possible relations between column densities of simple two-atomic molecules and DIB intensities may help identification of their carriers – the longest-standing unsolved problem in spectroscopy.

The latest surveys of DIBs (Galazutdinov et al. 2000; Tuairisg et al. 2000; Weselak et al. 2000) have shown more than 300 features of this type. Such a wealth of spectral lines (most of them very weak) is consistent with the hypothesis of large molecules as the carriers of DIBs. Ultra high resolution spectra (Sarre et al. 1995; Walker et al. 2001) showed substructures in the profiles of observed DIBs, suggesting rotational components inside molecular bands.

If the DIBs are carried by large molecules, it seems sensible to check whether their strengths correlate with those of simple, well-identified species – likely building blocks of complex ones. The first optical spectra of simple two-atomic molecules such as CH, CH^+ and CN were identified by McKellar (1940) and later spaceborne ultraviolet observations have led to the detection and study of H_2, using the Copernicus satellite (Savage et al. 1977; Bohlin et al. 1978) and FUSE (Rachford et al. 2002). A rocket spectrum by Smith & Stecher (1971) provided the first observation of CO, and further observations using Copernicus and IUE satellites led to the detection of CO in the direction of many stars (Jenkins et al. 1973; Morton 1975; Federman et al. 1980; Federman et al. 1994). Many studies have been published concerning CH: Federman (1982), Danks et al. (1984), Mattila (1986), Federman et al. (1994), Krełowski et al. (1999), H_2: Savage et al. (1977), Bohlin et al. (1978), Herbig (1993) and CO: Federman (1980), Federman et al. (1994). The CO molecule is usually considered as the tracer of the most abundant molecule in the ISM, H_2, which is formed on grain surfaces (Gould & Salpeter 1963). Abundances of H_2 (Savage et al. 1977; Bohlin et al. 1978) relate linearly to those of CH (Federman 1982; Matilla 1986) while those of CO increase with the second power of $N(H_2)$ (Federman et al. 1980). Some of the data from the above studies have been incorporated into chemical models of diffuse clouds (Federman et al. 1980; van Dishoeck & Black 1989; Federman et al. 1994).

Send offprint requests to: T. Weselak,
e-mail: towes@ab-byd.edu.pl

* Tables 1 and 2 are only available in electronic form at the CDS via anonymous ftp to cdsarc.u-strasbg.fr (130.79.128.5) or via
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The division of diffuse clouds into two main σ- and ζ-types is based on the behaviour of two strong diffuse bands at 5780 and 5797 Å in the spectra of σ Sco and ζ Oph (Krełowski & Walker 1987). Further observations led to the suggestion that the intensity ratios of $\lambda\lambda$ 5780 and 5797 vary in unison from cloud to cloud with the strengths (measured in relation to $E(B-V)$ of spectral features of two–atomic molecules as CH and CN (Krełowski et al. 1992). These features as well as that of the CO molecule are more likely observed in spectra of ζ–type clouds (Sikorski et al. 1998). It is also known that the CH molecule seems to be related to narrow DIBs but the relation obtained by Krełowski et al. (1999) shows a considerable scatter. The latest results of Thorburn et al. (2003) concerning the CH molecule and diffuse bands are also uncertain as the latter frequently blend, which was not taken into account by the authors. The relations between strong DIBs: 5780, 5797 and the H_2 molecule examined by Herbig (1993) showed that carriers of these DIBs are not produced by the processes based upon H_2.

H_2 as the most abundant species in the ISM may play a crucial role in the formation of DIB carriers grouped in the σ- or ζ-type environments. The aim of this work is to check whether intensities of strong diffuse 5780 and 5797 bands increase with the column densities of H_2. It is important also to check how far the column density of H_2 can be estimated if those of other two–atom molecules such as CH or CO are known, i.e. whether their ratios remain constant. In the case of diffuse bands we use the set of central depth measurements based on our observations. The molecular data were collected mostly from the literature.

2. The observational data

Our observational material, listed in Table 1, has been collected with three telescopes. The list of targets for this project was mostly chosen based on the sample of spectra acquired by one of us (JK) in 1993 at the McDonald Observatory (mcd), using the Cassegrain echelle spectrograph, fed with the 2.1-m telescope. The instrument consisted of refractive collimator and camera optics, a 23.2 per mm echelle grating with a blaze angle of 65 degrees, a prism cross-disperser and a Reticon 400×1200 CCD with 27×27 micrometer pixels. The spectra were recorded with the resolution equal to 64 000 and signal-to-noise ratio ~500. Each spectrum covers the spectral range 5600–7000 Å divided in 26 orders (McCarthy et al. 1993). The details of the method of data reduction of the spectra recorded with this instrument were described by Krełowski & Sneden (1993). The spectra from the McDonald Observatory were used to measure intensities of 5797 and 5780 diffuse bands.

Some additional spectra were used to measure $\lambda\lambda$ 5780 and 5797 intensities and equivalent widths of the CH band at 4300.321 Å. These spectra were acquired with the aid of the echelle spectrometer fed by the 2-m telescope of the Observatory on top of peak Terskol (trl). Two spectra were obtained with the spectrometer fed with the 1-m telescope of the Russsian Academy of Sciences at the Special Astrophysical Observatory (SAO). The spectrometer at Terskol is attached to the Wright Instruments 1242×1152 CCD matrix (22.5×22.5 micrometer pixels) camera. The spectrum recorded in a single exposure covers the range ~3500 Å – ~10 000 Å with the resolution $R = 45\,000$. A similar spectrometer is attached to the 1-m telescope of the Russian Special Astrophysical Observatory (Musaev 1993, 1996) and two spectra from this telescope, marked SAO, were used in our sample of target stars.

The reduction of the spectra was made using the DECH code (Galazutdinov 1992). This program allows a flat-field division, bias/background subtraction, excision of cosmic ray features, etc. The DECH code also allows a precise location of the continuum and measurements of line equivalent widths, central depths, line positions, etc.

Table 1 characterizes our sample of target stars. This is the most complete sample of reddened OB stars for which the column densities of H_2, CH and CO molecules have been published and our observations allow one to measure the major DIBs: 5780 and 5797. In Table 1 we also mark the stars whose spectra are typical for σ- or ζ-type clouds (targets where the 5797/5780 ratio is high are called zeta-type and targets with low 5797/5780 ratio – sigma-type). As demonstrated by Krełowski et al. (1997) these stars are very likely seen through single, individual clouds of σ- or ζ-type. The Sp/L estimates of our target stars as well as B, V photometry were taken from the Simbad database; the calculated colour excesses $E(B-V)$ are based on the intrinsic colours of Flower (1977) and Papaj et al. (1991).

Figure 1 presents the spectral region of two strong diffuse bands 5780 and 5797 in the targets of ζ- and σ-type: HD 149757 and HD 144217. The profile of the strong 5780 DIB (blended with the broad λ 5778 in the spectrum of HD 144217) is slightly asymmetric with the blue side being steeper. In the case of 5797 DIB its profile is strongly asymmetric and additionally blended with the broad diffuse band λ 5795 of different origin (Krełowski et al. 1997). The continuum placement in the case of strong diffuse bands blended with broad features such as λ 5778 or 5795 can affect their intensities as measured by different authors. Figure 1 shows the continuum level (marked with dots) used to measure the central depths of strong 5780 and 5797 DIBs blended with broad λ 5778 and λ 5795 features in the spectra of HD 144217 and 149757. As presented by Krełowski & Sneden (1995) the strength ratio of 5797 and 5780 DIBs may be an indicator of cloud type (σ or ζ).

Table 2 presents the compilation of published and measured data. The molecular column densities were collected from the literature. These of the CH molecule are taken from Krełowski et al. (1999) and supplemented with the observations of additional stars (SAO, trl), for which the measurements of H_2 column densities were already published. The equivalent widths of CH molecule published by Krełowski et al. (1999) were averaged. The conversion of the CH equivalent width to the column density N(CH) was made using the relation $N(\mathrm{CH}) = 1.20 \times 10^{12}\ W_\lambda\ \mathrm{cm}^{-2}$ of Danks et al. (1984). The column densities of the H_2 molecule and H I are the ones published by Bohlin et al. (1978), Rachford (2002) and Diplas & Savage (1994). The published column densities of CO are also given in Table 2 indicating the sources. The last three columns present the data for diffuse 5780 and 5797 bands after our new

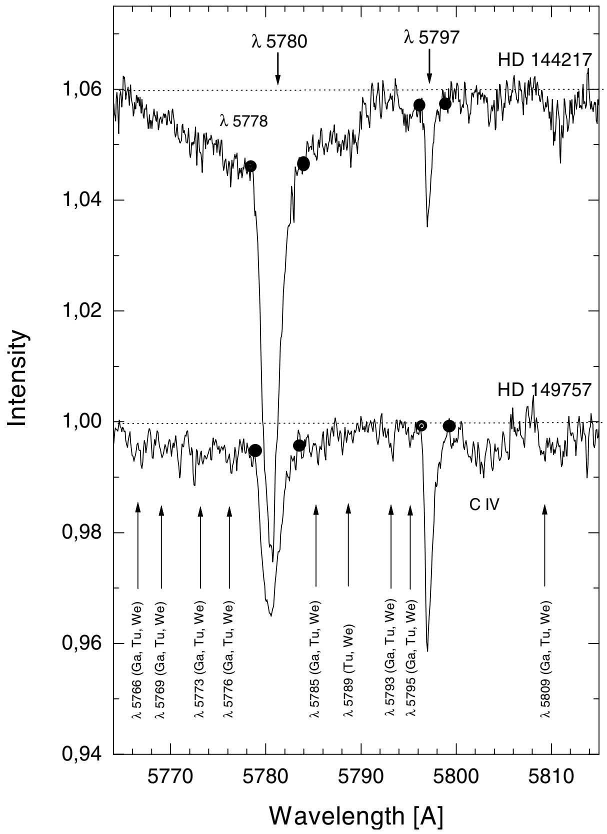

Fig. 1. The spectra of HD 144217 and HD 149757 (ζ Oph) in the wavelength range of two strong 5780 and 5797 DIBs. With two dots we mark the continuum level used to obtain the central depth of 5780 and 5797 DIBs blended with broad λ5778 and λ5795 ones. The intensity of broad λ5778 DIB in the spectrum of HD 149757 is lower than in the case of the σ-type object HD 144217. The weak and narrow diffuse bands after three surveys of DIBs (Galazutdinov et al. 2000 – Ga, Tuairisg et al. 2000 – Tu, Weselak et al. 2000 – We) are also presented. Note their higher intensities in the spectrum of the ζ-type object HD 149757. The broad stellar line of C IV in the spectrum of HD 149757 is also seen.

central depth measurements (with standard error estimated by multiple measurements) which allow us to obtain the ratio of the major 5797 and 5780 DIB intensities.

3. Results

3.1. Molecular column densities and E(B – V)

The left panel of Fig. 2 presents the correlation plots between column densities of H_2, CH, CO molecules and colour excess $E(B-V)$, which characterizes the dust abundance in the direction of our target stars.

The relation between abundances of H_2 molecules and $E(B-V)$ is known to undergo a sharp transition from small to large values at $E(B-V) \sim 0.08$, due to the fact that H_2 molecules becomes self-shielding at that point, thus preventing their destruction in cloud interiors. From $E(B-V) \sim 0.08$ the abundance of H_2 steadily increases inside the range of observed reddenings as already stated by Savage et al. (1977). This is seen at the top of the left panel of Fig. 2, where the linear relation between abundances of H_2 molecules and colour excesses is presented with the correlation coefficient equal to 0.84.

The relation between column densities of the CH molecule and colour excesses is known to show a scatter (Gredel et al. 1993). This scatter may follow the presence of different clouds along the considered sightlines (the central plot in the left panel of Fig. 2). Generally, the CH column density correlates very well with $E(B-V)$ (the correlation coefficient equal to 0.90). Only the star HD 146175 (σ Sco) with a small abundance of CH (Danks et al. 1984) escapes the relation. Figure 2 suggests this relation to be different for σ- and ζ-type objects.

The relation between column densities of the CO molecule and $E(B-V)$ (the left panel of Fig. 2 – at the bottom) seems to be quadratic but the number of data points is small in this case which makes any conclusion uncertain.

3.2. Molecular column densities normalized to E(B – V) and intensity ratio of $\lambda\lambda$ 5797 and 5780

The right panel of Fig. 2 presents the correlation plots between column densities of H_2, CH, CO molecules normalized to $E(B-V) = 1$ and intensity ratios of two diffuse 5797 and 5780 bands. The relation in the case of H_2 and CH molecules seems to be linear with the correlation coefficients equal to 0.78 and 0.82, respectively. The similarity of the above coefficients may suggest a good relation between column densities of H_2 and CH (see also Fig. 3).

The lowest plot in the left panel of Fig. 2 presents the relation for the CO molecule which suggests a quadratic relationship with the $\lambda\lambda$ 5797/5780 ratio, but the sample of stars in this case is smaller than in the case of H_2 and CH.

3.3. Relations between molecular column densities of H_2, CH and CO

The top panel in Fig. 3 presents the correlation between column densities of H_2 and CH molecules. This relationship is known to be linear (Danks et al. 1984; Mattila 1986). The CH formation is predicted to be controlled by gas-phase reactions with H_2 resulting in the abundance proportionality between these two molecules (Black & Dalgarno 1973). The correlation coefficient of the relation between column densities of H_2 and CH molecules is equal to 0.94 with a small scatter of points which suggests that the CH molecule is a better H_2 tracer than CO, for which the spectral features are accessible only to space-born instruments.

In the central and bottom panels of Fig. 3 we show the correlation plots between column densities of H_2, CH and CO molecules. These suggest quadratic relations. This result is consistent with the previous one of Federman et al. (1980, 1994) and with the chemical models of van Dishoeck & Black (1988, 1989).

3.4. Molecular fraction and intensity ratio of diffuse 5797 and 5780 bands

Figure 4 presents the relation between hydrogen molecular fraction defined as $f_{\rm H2} = 2N({\rm H_2})/(2N({\rm H_2}) + N({\rm HI}))$, and the intensity ratio of diffuse 5797 and 5780 bands. The relation between the molecular fraction of hydrogen and the intensity

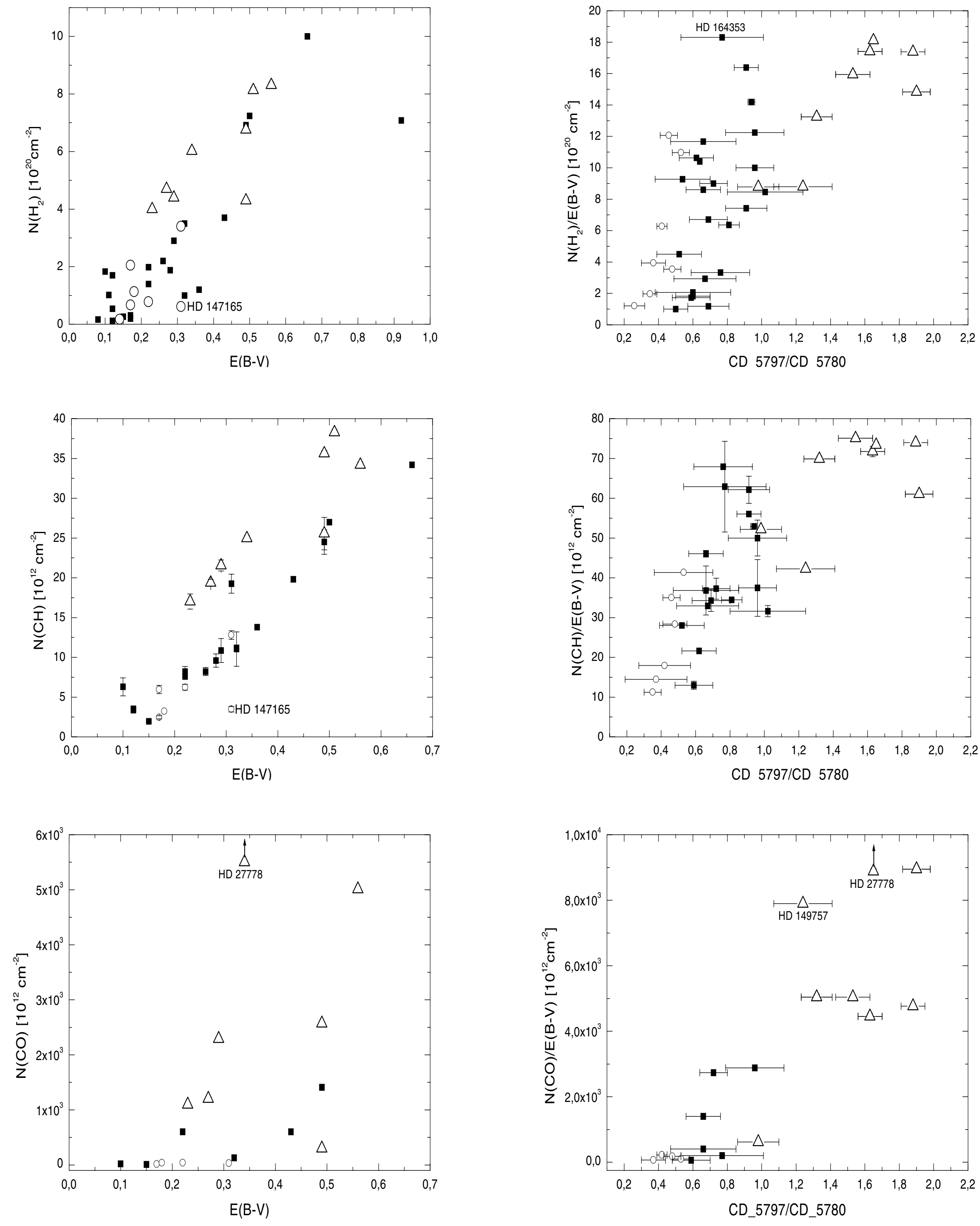

Fig. 2. At left: correlation plots between column densities of H_2, CH, CO molecules and colour excess $E(B-V)$. Note the relations in the cases of H_2 and CH molecules with the correlation coefficients 0.84 and 0.90, respectively. The relation between column density of CO molecule and $E(B-V)$ seems to be quadratic (at bottom). At right: correlation plots between column densities of H_2, CH, CO molecules normalized to $E(B-V) = 1$ and the intensity ratio of two major DIBs: 5797 and 5780. Note the similar relation in the case of H_2 and CH molecules with correlation coefficients equal to 0.78 and 0.82. Individual objects designated as follows: σ-type objects are marked with circles and ζ-type objects with triangles in each plot. Intermediate targets are marked with filled squares.

ratio of two major 5797 and 5780 DIBs, with the correlation coefficient equal to 0.83, suggests that H_2 molecules are spatially correlated with the carriers of 5797 and (most probably) other, narrow DIBs, populating spectra of ζ-type objects. The relation seen in Fig. 4 may also suggest the linear relationship between abundances of HI and intensities of 5780 DIB. This is consistent with the previous result of Herbig (1993).

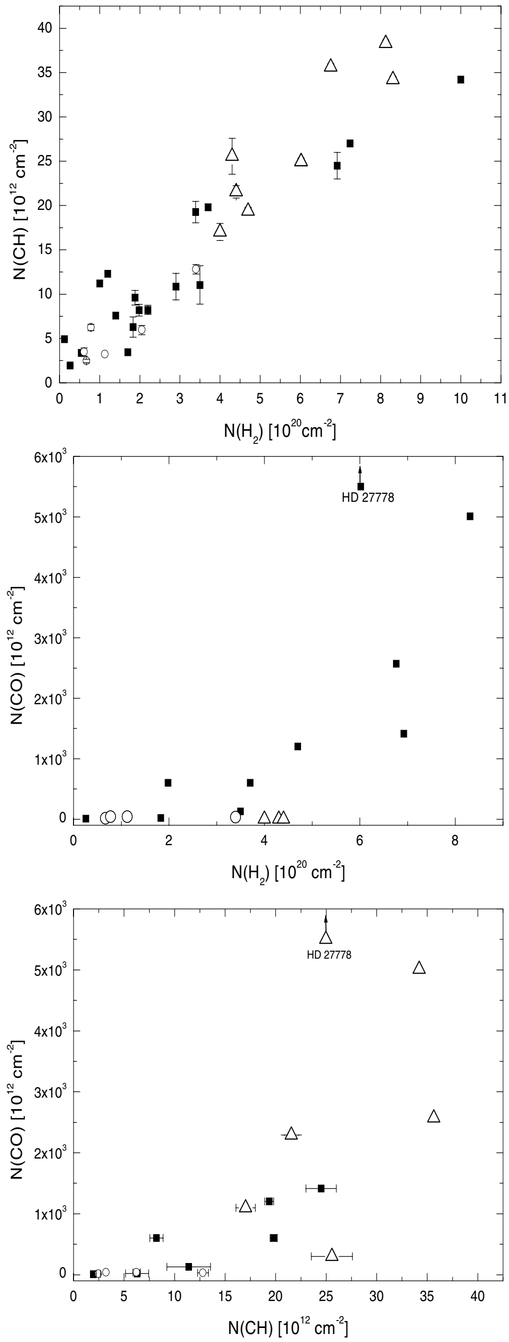

Fig. 3. Correlation plots between column densities of H_2, CH and CO molecules. Correlation coefficient in the case of a linear relation between column densities of H_2 and CH (seen at the top) is equal to 0.94. Quadratic relation in the case of N(CO) vs. $N(H_2)$ and N(CO) vs. N(CH) is seen in the central and bottom plots. Star HD 27778 with a high value of N(CO) is designated with arrow. Each object designated as in Fig. 2.

4. Discussion

The relations between intensities of different absorption features measured in the spectra of interstellar clouds are not very tight. The cause of this phenomenon is rather complicated and was already mentioned by Herbig (1993) in the case of DIBs. The measurements of their intensities by different authors differ despite the signal-to-noise of the detectors used. We also observe this phenomenon while compiling the measurements of molecular and diffuse features. In the case of the latter the

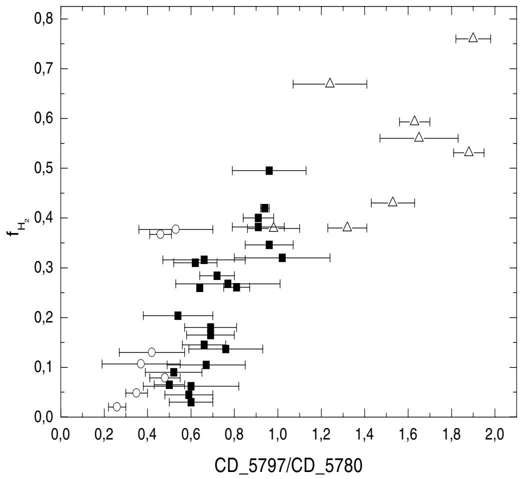

Fig. 4. Correlation plot between molecular fraction and intensity ratio of diffuse 5797 and 5780 bands. Correlation coefficient for this relation is equal to 0.83. Individual objects designated as follows: σ-type objects are marked with circles and ζ-type objects with triangles. Intermediate targets are marked with filled squares.

central depth measurements were applied in this work due to the fact that central depths can be measured more precisely than equivalent widths. Errors originating in the continuum displacement in the case of equivalent width measurements have higher values than those for central depths (Moutou et al. 1999; Weselak et al. 2001).

The another reason for the observed scatter is probably of physical origin. The correlations between interstellar absorption features are tight when sightlines probe the general interstellar medium. The differences arise when different clouds are observed along the considered sightlines, e.g. inside of OB associations where dense clouds are strongly irradiated by the neighbouring stars.

Positive correlations between molecular fraction and extinction curve parameters (the 2175 Å bump width and the strength of the far-UV curvature) have been recently found by Rachford et al. (2002). The far-UV curvature is also known to be associated with smaller than normal dust grains (Cardelli et al. 1989). The possible link between the carriers of narrow DIBs and dust grains can be also found in the publication of Megier et al. (2001). The correlation of $\lambda\lambda$ 5797/5780 with the colour excesses measuring the far UV-rise of the extinction curve suggests that the particles responsible for the far UV-rise of the extinction curve are related in some way to the 5797 diffuse band carriers. Possibly the formation of narrow DIB carriers is catalyzed by small dust particles expected to cause the UV-rise of the extinction curve.

It seems that the processes that determine abundances of molecular hydrogen and CH molecules take place in the same relatively dense clouds. Abundances of many simple molecules in σ- and ζ-type clouds are very different (Snow & Krełowski 1994). In the spectrum of the ζ Oph cloud we observe many diatomic molecules (CO, CN, CH) and narrow DIBs. In the case of σ Sco the column density of H_2 is smaller (see Fig. 2), and thus, the spectrum of diatomic molecules and diffuse bands is not as rich as in the case of the ζ Oph cloud.

The hydrogen molecular fraction (f_{H2}) apparently grows in environments rich in small dust grains. The relation between the hydrogen molecular fraction and the intensity ratio of diffuse 5797 and 5780 bands suggests that f_{H2} grows with the abundance of the λ 5797 carrier and HI is well correlated with the abundance of the λ 5780 carrier. The ζ-type clouds are not penetrated by UV-photons as intensely as σ-type ones which apparently facilitates formation of narrow DIB carriers. Thus narrow DIB carriers are possibly formed in the denser parts of clouds which are more shielded from UV, and H_2 begins to dominate over the atomic hydrogen.

5. Conclusions

The above considerations allow us to infer the following conclusions:

1. The abundance of H_2, CH and CO molecules is relatively high in ζ-type environments. The same applies to the vast majority of narrow DIBs.
2. The column densities of H_2 and CH molecules are closely related, suggesting that the CH molecule may be used as an H_2 tracer, better than CO. Its features are easily accessible.
3. The hydrogen molecular fraction (f_{H2}) is correlated with the intensity ratio of 5797 and 5780 DIBs, suggesting the formation of narrow DIB carriers in denser clouds shielded from UV and that are H_2 dominated. The 5780 DIB carrier is probably destroyed in such regions.

The results found here are compelling indications that abundances of simple two-atom molecules are connected to those of the carriers of narrow DIBs. This kind of information obtained also in the case of other molecules may be essential in identifying the carriers of DIBs, as they may lead to an understanding of the physical conditions facilitating formation of DIB carriers.

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