

A Principal Component Analysis of the Diffuse Interstellar Bands

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OUTLINE

- ▶ Diffuse Interstellar Bands (DIB)
- ▶ Principal Component Analysis (PCA)
- ▶ Observational Data
- ▶ PCA results
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- ▶ Conclusions

Diffuse Interstellar Bands (DIB-s)

- ▶ DIB-s - absorption lines that arise from material in interstellar clouds
- ▶ There are known for more than 100 years - Mary L. Heger letter (1922)
- ▶ There are known about 500 bands
- ▶ The carriers of most DIB-s remain unidentified.
- ▶ Very difficult identification - it is usually assumed that responsible are big molecules containing carbon.
- ▶ The only known absorber related to DIB-s is *buckminsterfullarene* (C_{60}^+) responsible for several DIB-s in the infrared (Campbell et al. 2015).

Diffuse Interstellar Bands (DIB-s) - correlation studies

- ▶ If two DIB-s arise from the same state in the same carrier, they should have the same strength ratio in all lines of sight and thus, their equivalent widths (EWs) should exhibit a perfect correlation.
- ▶ Mutual DIB-s correlations
- ▶ No perfect correlation - different carriers, but “one DIB - one carrier” is rather exaggeration (C_{60}^+ is responsible for 4 DIB-s at least)
- ▶ DIB-s families - strong correlations between EW (for λ 6196 and λ 6614 $r = 0.986$)
- ▶ Correlations between DIB-s and line-of-sight properties (E(B-V), N(H), N(HI)).
- ▶ Dependence on environmental conditions (example $W(\lambda$ 5797)/ $W(\lambda$ 5780) ratios are smaller in clouds with stronger UV exposure - effects on dust properties σ clouds and ζ clouds)

Diffuse Interstellar Bands (DIB-s) - correlation studies

The main aim of a paper: determine parameters that drive the variations in DIB spectrum.

- ▶ Perform a principal component analysis (PCA) on the data to find out how many parameters are required to describe the observed variations among the DIB-s.
- ▶ Interpret new parameters.
- ▶ Use DIB-s to determine physical parameters of their environment

Principal Components Analysis (PCA)

- ▶ Krystian Iłkiewicz introduction to PCA given at SJC 05.05.2022.
- ▶ PCA - statistical technique for reducing dimensionality of a dataset.
- ▶ We chose new parameters by linear combination of input data parameters
- ▶ New parameters form orthogonal set of vectors whereas old parameters are often strongly correlated.

Principal Components Analysis (PCA) - main steps

- ▶ n variables for m lines of sight.
- ▶ Rescaling of a data (subtract mean, divide by standard deviation)

$$z_{i,j} = \frac{x_{i,j} - \bar{x}_j}{s_{x_j}}$$

- ▶ Calculate covariation matrix ($n \times n$ matrix)

$$C_{k,l} = \frac{1}{m-1} z_{k,i} z_{i,l}$$

- ▶ Find eigenvalues and eigenvectors of covariation matrix
- ▶ Sort eigenvalues from the largest
- ▶ Corresponding eigenvectors give principal components
- ▶ Multiply transposed eigenvector matrix by rescaled data matrix to obtain a data in principal components base

$$y_i \hat{n}' = a_{i,1} x_1 \hat{n}_1 + a_{i,2} x_2 \hat{n}_2 + \dots + a_{i,n} x_n \hat{n}_n$$

\hat{n}_n - unit vectors in the original parameter space

\hat{n}'_n - unit vectors in the new reference frame - principal components

$$a_{i,1}^2 + a_{i,2}^2 + \dots + a_{i,n}^2 = 1$$

$$Y = AX$$

X - $n \times m$ matrix containing original set of data

A - $n \times n$ - transformation matrix

Y - $n \times m$ matrix containing transformed data points in the new reference frame.

Observational data - target selection

- ▶ Search for high quality, high resolution spectra in VLT/UVES and ELODIE archives for 243 stars from the study of Jenkins (2009) where are present fairly strong and narrow DIB-s possibly free of contamination from stellar lines (16 DIB-s)
- ▶ Selection of single cloud lines of sight based on examination of Na I (589.0 nm and 589.5 nm) and K I (766.5 and 769.9 nm) lines.
- ▶ Final set of 30 stars with observations characterized by 23 parameters

Target stars.

Table 1
Basic Target Data

Target	Alt. Name	R.A. (J2000)	Decl. (J2000)	V	$E(B - V)$	$N(H)$ (10^{21} cm^{-2})	$N(H_2)$ (10^{20} cm^{-2})	$f(H_2)$	F_*	$W(15797)$ $W(15786)$	V_{turb}^a (km s^{-1})	References ^a	Data Source
HD 15137	...	02 27 59.81	+52 32 57.6	7.86	0.24	1.29 ^{+0.37} _{-0.40}	1.86 ^{+0.26} _{-0.26}	0.22 ^{+0.09} _{-0.09}	0.37 ± 0.09	0.30 ± 0.02	...	1	ELODIE
HD 22951	40 Per	03 42 22.65	+33 57 54.1	4.98	0.19	1.10 ^{+0.35} _{-0.32}	2.88 ^{+1.48} _{-1.48}	0.35 ^{+0.27} _{-0.27}	0.73 ± 0.05	0.35 ± 0.02	12.47	1	ELODIE
HD 23180	o Per	03 44 19.13	+32 17 17.7	3.86	0.22	0.76 ^{+0.26} _{-0.23}	3.98 ^{+1.64} _{-1.26}	0.51 ^{+0.33} _{-0.24}	0.84 ± 0.06	0.65 ± 0.04	13.45	2	ELODIE
HD 23630	η Tau	03 47 29.08	+24 06 18.5	2.87	0.05	0.22 ^{+0.09} _{-0.07}	0.35 ^{+0.18} _{-0.12}	0.28 ^{+0.21} _{-0.21}	0.89 ± 0.10	0.16 ± 0.04	16.76	2	ELODIE
HD 24398	κ Per	03 54 07.92	+31 53 01.1	2.88	0.27	0.63 ^{+0.06} _{-0.07}	4.68 ^{+2.40} _{-1.59}	0.59 ^{+0.46} _{-0.31}	0.88 ± 0.05	0.55 ± 0.02	14.54	2	ELODIE
HD 24534	X Per	03 55 23.08	+31 02 45.0	6.10	0.31	0.54 ^{+0.08} _{-0.09}	8.32 ^{+0.80} _{-0.75}	0.76 ^{+0.13} _{-0.11}	0.90 ± 0.06	0.62 ± 0.04	14.5	5	ELODIE
HD 24760	ε Per	03 57 51.23	+40 00 36.8	2.90	0.07	0.25 ^{+0.05} _{-0.05}	0.33 ^{+0.27} _{-0.15}	0.21 ^{+0.25} _{-0.14}	0.68 ± 0.04	0.18 ± 0.02	7.06	2	ELODIE
HD 24912	ξ Per	03 58 57.90	+35 47 27.7	4.04	0.26	1.29 ^{+0.26} _{-0.24}	3.39 ^{+1.40} _{-0.99}	0.35 ^{+0.21} _{-0.15}	0.83 ± 0.02	0.26 ± 0.01	11.2	1	ELODIE
HD 27778	62 Tau	04 23 59.76	+24 18 03.6	6.33	0.34	0.22 ^{+0.55} _{-0.22}	5.25 ^{+1.06} _{-0.88}	0.82 ^{+0.45} _{-0.27}	1.19 ± 0.07	0.43 ± 0.03	15.22	2	ELODIE
HD 35149	23 Ori	05 22 50.00	+03 32 40.0	5.00	0.08	0.43 ^{+0.12} _{-0.11}	0.03 ^{+0.00} _{-0.05}	0.02 ^{+0.00} _{-0.02}	0.54 ± 0.11	0.20 ± 0.04	24.09	2	UVES
HD 35715	ψ Ori	05 26 50.23	+03 05 44.4	4.60	0.03	0.31 ^{+0.13} _{-0.13}	6 ± 2 × 10 ⁻⁶	4 ± 2 × 10 ⁻⁶	0.66 ± 0.11	0.10 ± 0.04	25.2	1	ELODIE
HD 36822	φ ¹ Ori	05 34 49.24	+09 29 22.5	4.40	0.07	0.65 ^{+0.11} _{-0.12}	0.21 ^{+0.09} _{-0.06}	0.06 ^{+0.04} _{-0.03}	0.74 ± 0.08	0.19 ± 0.04	25.3	1	ELODIE
HD 36861	λ Ori A	05 35 08.28	+09 56 03.0	3.30	0.10	0.60 ^{+0.16} _{-0.16}	0.13 ^{+0.08} _{-0.05}	0.04 ^{+0.04} _{-0.02}	0.57 ± 0.04	0.48 ± 0.04	25.2	3	ELODIE
HD 40111	139 Tau	05 57 59.66	+25 57 14.1	4.82	0.10	0.79 ^{+0.15} _{-0.15}	0.54 ^{+0.31} _{-0.20}	0.12 ^{+0.10} _{-0.07}	0.49 ± 0.04	0.20 ± 0.04	15.29	2	ELODIE
HD 110432	BZ Cru	12 42 50.27	-63 03 31.0	5.32	0.39	0.71 ^{+0.29} _{-0.29}	4.37 ^{+0.42} _{-0.29}	0.55 ^{+0.13} _{-0.11}	1.17 ± 0.11	0.25 ± 0.01	6.8	3	UVES
HD 143275	δ Sco	16 00 20.01	-22 37 18.1	2.29	0.00	1.41 ^{+0.29} _{-0.29}	0.26 ^{+0.15} _{-0.15}	0.03 ^{+0.03} _{-0.03}	0.90 ± 0.03	0.19 ± 0.02	-10.90	2	UVES
HD 144217	β ¹ Sco	16 05 26.23	-19 48 19.6	2.62	0.18	1.23 ^{+0.12} _{-0.12}	0.68 ^{+0.10} _{-0.10}	0.10 ^{+0.02} _{-0.02}	0.81 ± 0.02	0.11 ± 0.01	-8.95	2	UVES
HD 145502	γ Sco	16 11 59.74	-19 27 38.5	4.13	0.20	1.17 ^{+0.26} _{-0.25}	0.78 ^{+0.32} _{-0.25}	0.12 ^{+0.08} _{-0.08}	0.80 ± 0.11	0.18 ± 0.01	-8.49	2	ELODIE
HD 147165	σ Sco	16 21 11.32	-25 35 34.0	2.91	0.31	2.19 ^{+0.90} _{-0.87}	0.62 ^{+0.25} _{-0.18}	0.05 ^{+0.01} _{-0.03}	0.76 ± 0.06	0.13 ± 0.01	-6.26	2	UVES
HD 147933	ρ Oph A	16 25 35.10	-23 26 48.7	5.02	0.37	4.27 ^{+0.88} _{-0.80}	3.72 ^{+1.51} _{-1.09}	0.15 ^{+0.07} _{-0.07}	1.09 ± 0.08	0.27 ± 0.03	-8.02	2	UVES
HD 149757	ζ Oph	16 37 09.54	-10 34 01.5	2.58	0.29	0.52 ^{+0.02} _{-0.04}	4.47 ^{+0.75} _{-0.75}	0.63 ^{+0.22} _{-0.17}	1.05 ± 0.02	0.50 ± 0.04	-14.98	2	UVES
HD 164284	66 Oph	18 00 15.80	+04 22 07.0	4.78	0.11	0.42 ^{+0.19} _{-0.19}	0.71 ^{+1.47} _{-0.21}	0.25 ^{+0.20} _{-0.20}	0.89 ± 0.18	0.15 ± 0.02	-15.32	1	ELODIE
HD 170740	...	18 31 25.69	-10 47 45.0	5.76	0.38	1.07 ^{+0.36} _{-0.47}	7.24 ^{+1.47} _{-1.22}	0.58 ^{+0.14} _{-0.14}	1.02 ± 0.11	0.26 ± 0.01	-12.9	6	UVES
HD 198478	55 Cyg	20 48 56.29	+46 06 50.9	4.86	0.43	2.04 ^{+0.81} _{-0.63}	7.41 ^{+3.06} _{-2.17}	0.42 ^{+0.27} _{-0.27}	0.81 ± 0.05	0.24 ± 0.01	-10.04	2	ELODIE
HD 202904	v Cyg	21 17 55.08	+34 53 48.8	4.43	0.09	0.23 ^{+0.21} _{-0.23}	0.14 ^{+0.07} _{-0.05}	0.11 ^{+0.12} _{-0.10}	0.39 ± 0.11	0.13 ± 0.05	-12.90	4	ELODIE
HD 207198	...	21 44 53.28	+62 27 38.0	5.96	0.47	3.39 ^{+0.59} _{-0.59}	6.76 ^{+0.65} _{-0.59}	0.28 ^{+0.05} _{-0.05}	0.90 ± 0.03	0.53 ± 0.01	-15.28	2	ELODIE
HD 209975	19 Cep	22 01 05.08	+62 16 47.3	5.11	0.27	1.29 ^{+0.41} _{-0.41}	1.20 ^{+0.62} _{-0.41}	0.16 ^{+0.12} _{-0.12}	0.57 ± 0.26	0.31 ± 0.01	-11.39	2	ELODIE
HD 214680	10 Lac	22 39 15.68	+39 03 01.0	4.88	0.08	0.50 ^{+0.14} _{-0.14}	0.17 ^{+0.03} _{-0.03}	0.06 ^{+0.03} _{-0.03}	0.50 ± 0.06	0.34 ± 0.02	-9.2	1	ELODIE
HD 214993	12 Lac	22 41 28.65	+49 13 31.6	5.23	0.06	0.58 ^{+0.20} _{-0.20}	0.43 ^{+0.22} _{-0.22}	0.13 ^{+0.09} _{-0.07}	0.68 ± 0.10	0.17 ± 0.02	-9.44	1	ELODIE
HD 218376	1 Cas	23 06 36.82	+59 25 11.1	4.84	0.16	0.89 ^{+0.28} _{-0.26}	1.41 ^{+0.73} _{-0.48}	0.24 ^{+0.19} _{-0.15}	0.60 ± 0.06	0.28 ± 0.01	-12.65	1	ELODIE

Note. R.A. and decl. are taken from SIMBAD. V , $E(B - V)$, $N(H)$, $N(H_2)$, and F_* values are from Jenkins (2009), where we assume an uncertainty of ± 0.02 mag on the $E(B - V)$ values. $f(H_2) = 2N(H_2)/[N(H) + 2N(H_2)]$ is the fraction of molecular hydrogen.

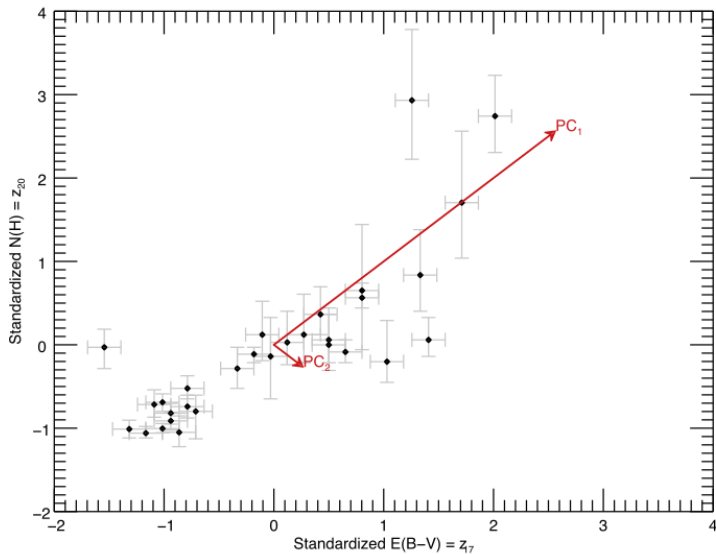
^a Value and reference refer to the velocity of the dominant interstellar component.

Observational parameters.

Table 2
Input Variables Used in the PCA, and Their Mean Values and
Standard Deviations

Variable Name (x_i)	Mean (\bar{x}_i)	Standard Deviation (s_{x_i})
$x_1 = W(\lambda 4428)$	645.9	350.9
$x_2 = W(\lambda 4964)$	6.8	5.7
$x_3 = W(\lambda 5494)$	5.6	4.1
$x_4 = W(\lambda 5513)$	3.9	3.9
$x_5 = W(\lambda 5545)$	5.9	4.3
$x_6 = W(\lambda 5546)$	2.8	2.2
$x_7 = W(\lambda 5769)$	2.6	2.2
$x_8 = W(\lambda 5780)$	131.5	77.0
$x_9 = W(\lambda 5797)$	37.7	27.8
$x_{10} = W(\lambda 5850)$	15.6	13.6
$x_{11} = W(\lambda 6196)$	13.5	8.3
$x_{12} = W(\lambda 6270)$	20.7	13.9
$x_{13} = W(\lambda 6284)$	149.4	84.1
$x_{14} = W(\lambda 6376)$	9.3	7.4
$x_{15} = W(\lambda 6379)$	24.7	18.0
$x_{16} = W(\lambda 6614)$	52.5	35.2
$x_{17} = E(B - V)$	0.20	0.13
$x_{18} = N(H_1)$	1.0×10^{21}	9.2×10^{20}
$x_{19} = N(H_2)$	2.4×10^{21}	2.6×10^{20}
$x_{20} = N(H)$	1.5×10^{21}	1.2×10^{21}
$x_{21} = f(H_2)$	0.27	0.23
$x_{22} = F_*$	0.75	0.21
$x_{23} = \frac{W(\lambda 5797)}{W(\lambda 5780)}$	0.2907	0.1567

PCA for two parameters: $E(B-V)$, $N(H)$



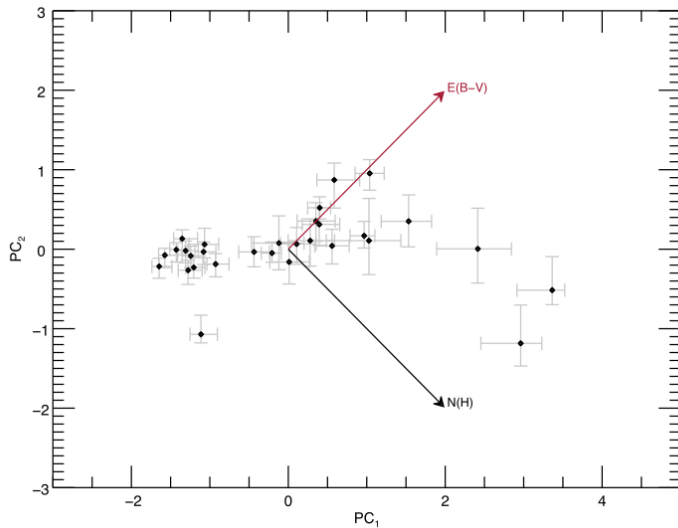
PCA for two parameters: $E(B-V)$, $N(H)$

Table 3

Principal Components, Eigenvalues, and Relative Importance of Each PC for a 2D Example Involving $E(B - V)$ and $N(H)$

PC	Eigenvalue	% Variation	Cumulative %	Eigenvector
1	1.813	90.63	90.63	(0.707, 0.707)
2	0.187	9.37	100.00	(0.707, -0.707)

PCA for two parameters: $E(B-V)$, $N(H)$



PCA for all components

Table 4
Principal Components, Eigenvalues, and Relative Importance of Each PC

PC	Eigenvalue	% Variation	Cumulative %
1	15.248	66.30	66.30
2	3.158	13.73	80.03
3	1.801	7.83	87.86
4	1.139	4.95	92.81
5	0.355	1.54	94.35
6	0.262	1.14	95.49
7	0.192	0.84	96.33
8	0.186	0.81	97.14
9	0.157	0.68	97.82
10	0.117	0.51	98.33
11	0.096	0.42	98.75
12	0.074	0.32	99.07
13	0.066	0.29	99.35
14	0.055	0.24	99.60
15	0.032	0.14	99.74
16	0.025	0.11	99.85
17	0.012	0.05	99.90
18	0.008	0.03	99.93
19	0.006	0.03	99.96

Screeplot for principal components

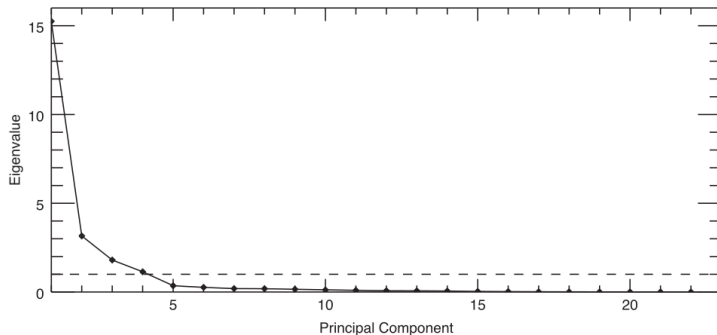
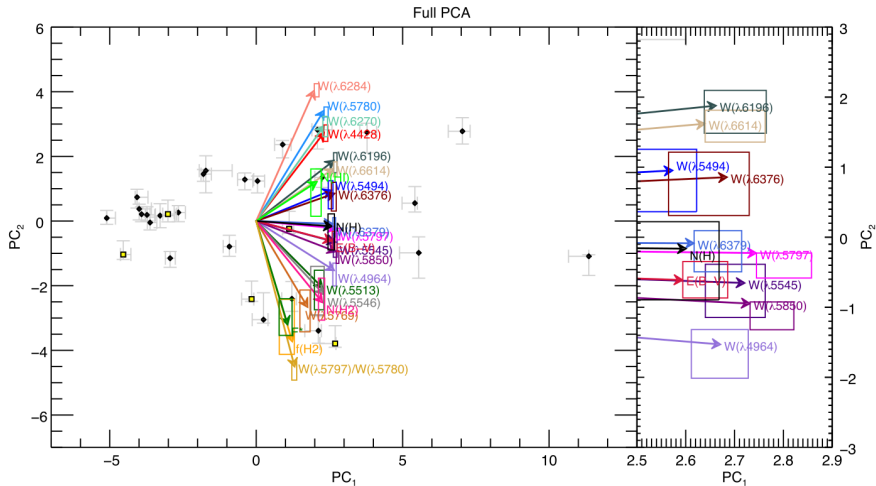


Figure 6. Screeplot illustrating the relative importance of each PC. The dashed line indicates an eigenvalue of one. The first four PCs lie above this limit.

Biplot for principal components PC1 and PC2



Biplots for principal components PC1 and PC2 for partial analysis $z_{17} - z_{23}$ and $z_1 - z_{16}$

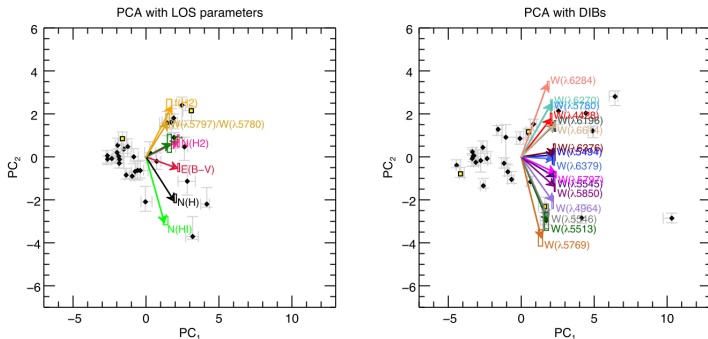


Figure 7. PC_1 - PC_2 biplots for (top) all variables, (bottom left) line-of-sight parameters only (excluding DIBs), and (bottom right) DIBs only, excluding line-of-sight parameters. The 23-dimensional vectors corresponding to the original variables are projected onto the PC_1 - PC_2 plane. The rectangular outlines surrounding the vectors indicate the uncertainty range for each projection, obtained through an MC simulation. Note that the vectors have been scaled by a constant factor for better visualization (as was done in Figure 4). Be stars are indicated by yellow squares. To help with clarity, a zoomed-in and rescaled portion of the full PCA results is presented next to the main figure. The same color scheme is used for all figures.

Interpretation of PC1

- ▶ Largest projections on PC1 is related to equivalent widths of DIB-s
- ▶ PC1 - traces amount of DIB-s producing material in gas phase ($W(\lambda 5797)$ has correlation 0.96 with PC1).

$$N_{DIB} = 0.136(PC1) + 0.90$$

$$N_{DIB} \approx 0.0185W(\lambda 5797) + 0.19$$

Correlation between $W(\lambda 5797)$ and PC_1

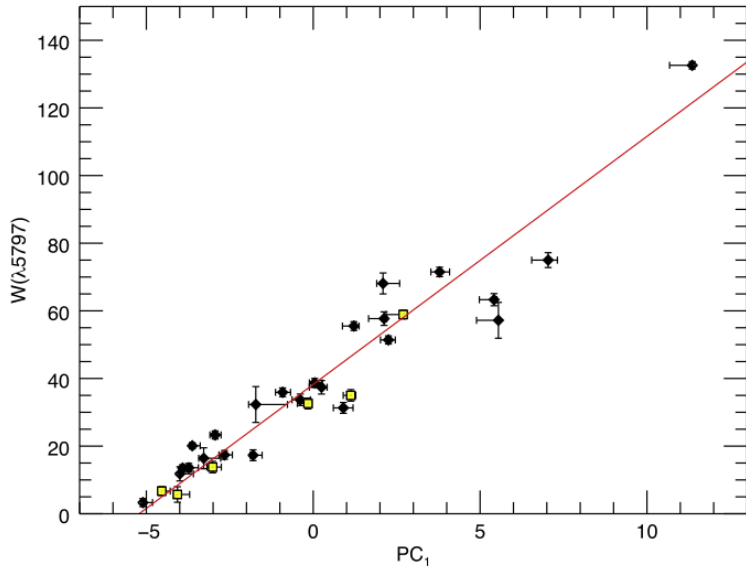


Figure 8. $W(\lambda 5797)$ and PC_1 have a very strong correlation ($r = 0.957$). The equation of the best-fit line is $W(\lambda 5797) = 7.31(PC_1) + 38.25$. Be stars are

Interpretation of PC2

- ▶ Important negative contribution to PC2 comes from $W(\lambda 5797)/W(\lambda 5780)$ projection.
- ▶ $W(\lambda 5797)$ has small projection on PC2 whereas $W(\lambda 5780)$ correlates strongly
- ▶ PC2 - depend on radiation environment at place of DIB formation

$$G_{DIB} = PC2$$

$$G_{DIB} \approx -9.07[W(\lambda 5797)/W(\lambda 5780)] + 2.55$$

PC2 (G_{DIB}) as a function of $W(\lambda 5797)/W(\lambda 5780)$

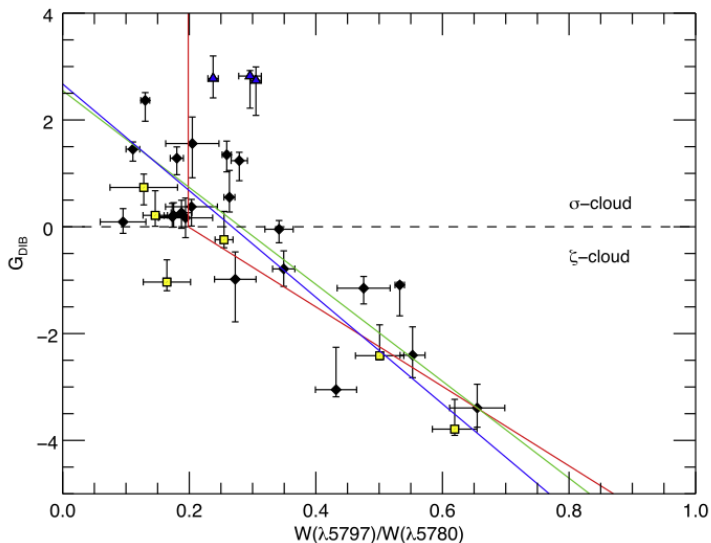
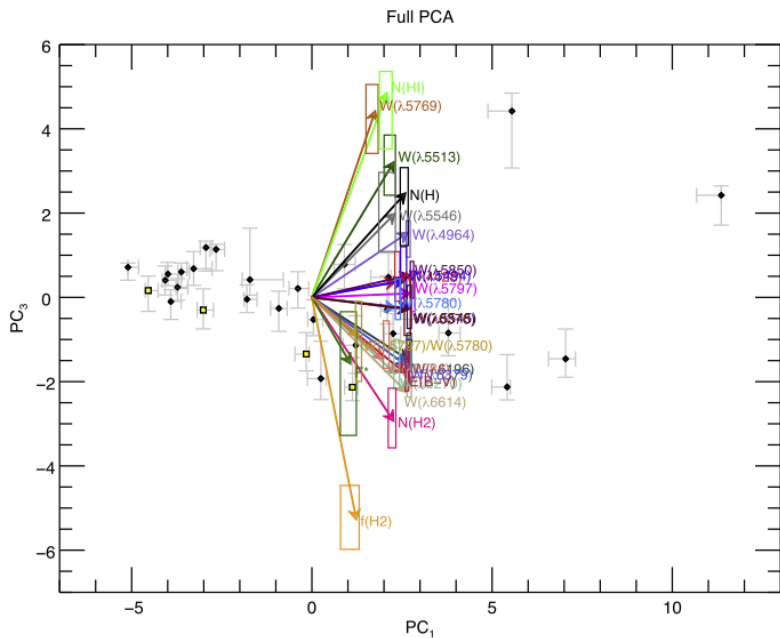


Figure 9. G_{DIB} as a function of $W(\lambda 5797)/W(\lambda 5780)$. Be stars are indicated by yellow squares; three possible outliers (HD 15137, HD 198478, and HD 209975; located at $G_{DIB} \approx 3$) are shown as blue triangles. We show the three fits discussed in the text: Equation (18) in green; the fit without outliers

Interpretation of PC2

- ▶ There is a good correlation between PC2 and $W(\lambda 5797)/W(\lambda 5780)$ for ζ clouds, but there is unclear situation for σ clouds.

Biplot for PC1-PC3



Biplot for PC2-PC3

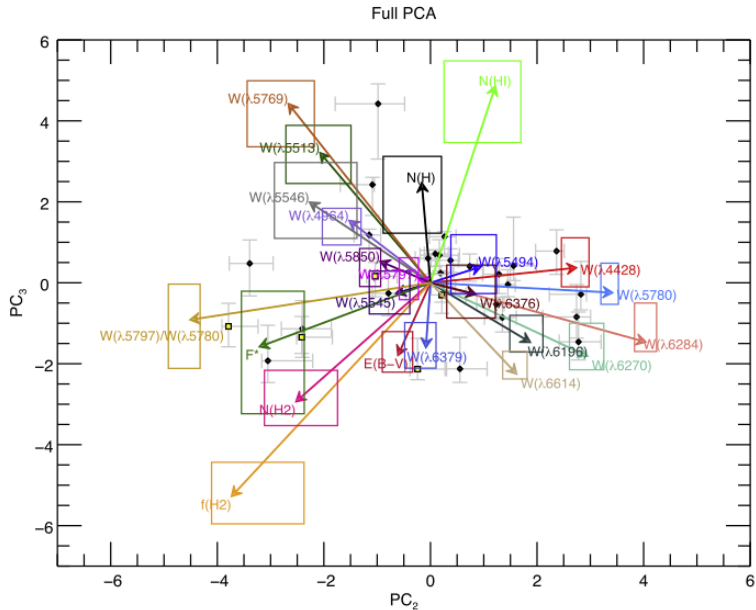


Figure 10. (Top) PC₁–PC₃ biplot. (Bottom) PC₂–PC₃ biplot. Be stars are

Interpretation of PC3

Interpretation of PC3 is uncertain, but there are two good candidates

- ▶ Dust grains size, which should be inversely correlated to $E(B-V)$ and $f(H_2)$ fraction
- ▶ Gas to dust ratio measured as $N(H)/E(B - V)$

$N(H)/E(B - V)$ as function of PC3

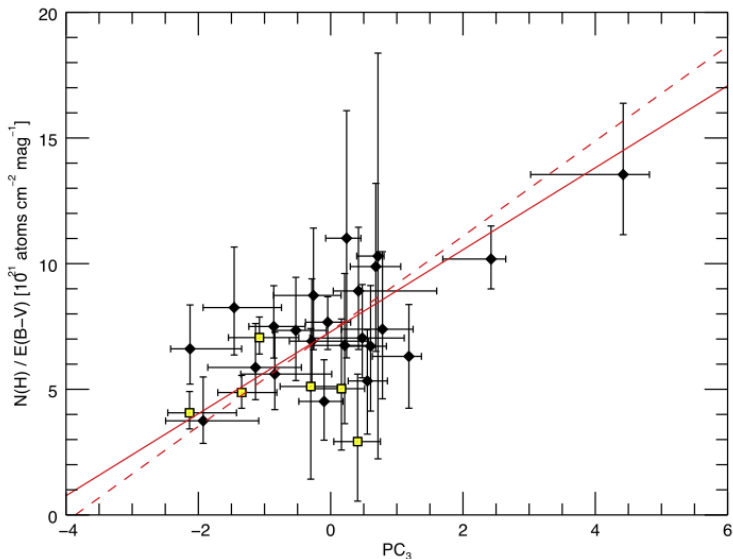


Figure 12. Total column of hydrogen per unit reddening as a function of PC₃. Yellow squares are used to indicate Be stars, which mostly fall below the trend line. The solid red line represents a straight line fit through all data points

Interpretation of PC3

$$\frac{N(H) \times 10^{-21}}{E(B - V)} = 7.31 \pm 0.27 + PC3 \times (1.89 \pm 0.26)$$

When we assume that mean interstellar value of $N(H)/E(B - V)$ is $5.8 \times 10^{21} \text{ atoms/cm}^2/\text{mag}$ and $GTD = 1$ for this value one can obtain

$$GTD = 0.318 \times PC3 + 1.29$$

Conclusions

- ▶ PCA analysis of DIB-s equivalent widths and line-on-sight properties for single cloud sightlines gives main parameters important for DIB-s formation and properties.
- ▶ PC1 - amount of DIB producing material
- ▶ PC2 - the level of UV radiation at place of DIB formation
- ▶ PC3 - related to dust properties or gas to dust ratio
- ▶ It is possible using DIB-s to determine physical parameters of their environment - even without identifying the carriers.