Technical Report 8: on the physical meaning of Principal Components

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Chapter 1

Introduction

The work presented in this document was performed as part of the optional phase for contract EUM/CO/10/4600000847/XC, and aims to provide EUMETSAT with evidence useful to address wether *the MTG-IRS L1 PC compression method is a valid method when performing retrievals.* Specific goal of the optional phase is to assess the *physical meaning* of individual Principal Components obtained from IASI data, by investigating the relationship between the spectral structure of the PCs and the spectral absorption structure of individual atmospheric molecular species. The intent is to verify the existence of PCs which mostly account for trace gases and have virtually little or no information on main parameters to be retrieved by the MTG-IRS level 2 processor. Spectral coefficients from such PCs could be ignored in the operational retrieval of temperature and water vapor, while could be selectively used in trace gas retrievals.

In order to achieve the scientific goal of this study, absorption spectra for 39 molecular spices were calculated, using LBLRTM [1] (version 12), by differentiating a radiance spectrum obtained from a reference atmosphere with spectra obtained from the same atmosphere but zeroing individual gas absorption properties (not amounts). The 39 simulated absorption spectra were used to derive the scalar product with real data PCs. Magnitude of the scalar products were transformed in measures of angles between the PCs and individual absorbers. Angles close to 90° indicated orthogonality between an absorption spectra and a PC, which was interpreted as low information content carried by a the PC with respect to the absorber. The closer to 0° or 180° the angle, the more information on the absorber was assumed to be embedded in the PC.

The following sections will describe in detail the procedure followed and the results obtained.

1.1   Procedure

Principal Components are simply linear combinations of individual spectral channels, and the $m-th$ element of the $n-th$ PC represents the scalar product $\tau_{m,n}$ between PC_n and the spectral channel $L(\nu_m)$. :

$$\tau_{m,n} = L(\nu_m) \times PC_n \tag{1.1}$$

and can be therefore used to calculate the angle between (or contribution of) the $m - th$ channel and (to) the $n - th$ PC in degrees:

$$\alpha_{m,n} = arccos\left(\frac{\tau_{m,n}}{\|L(\nu_m)\| \|PC_n\|}\right)\frac{180}{\pi} \tag{1.2}$$

which under the consideration that $\|L(\nu_m)\| = \|PC_n\| = 1$, becomes:

$$\alpha_{m,n} = arccos\left(\tau_{m,n}\right)\frac{180}{\pi} \tag{1.3}$$

The idea of using the angles between PCs and channels has been exploited in this study to obtain an integrated measure of the degree of orthogonality between the PCs and all the channels in which given molecular species are active absorbers. With this goal in mind, LBLRTM was used to generate a IASI radiance spectrum in the LW, MW, and SW (figure 1.1) from a reference atmosphere which contained the 39 molecular species in tbl. 1.1. Differences with reference spectrum were calculated for each molecular specie by zeroing the absorption properties of that molecule in the LBLRTM TAPE3 file, and absorption spectra, S_i, like the one showed in figure 1.2 were generated for each molecule. Each absorption spectrum represent the ensemble of channels in which a given molecular specie is an active absorber. Therefore, extending the concept of a single channel scalar product, defined in eq. 1.1, to the ensemble of absorbing channels, it was possible to calculate the scalar product $\kappa_{i,j}$, between the $i - th$ absorption spectrum, S_i, with $i = 1\ldots 39$, and the $j - th$ PC, with $j = 1\ldots 100$ (for each of the 3 spectral bands):

$$\kappa_{i,j} = S_i \times PC_j \tag{1.4}$$

Applying the concept of angles between individual channels and PCs (eq. 1.2) to the ensemble of absorbing channels, the scalar products $\kappa_{i,j}$ were then used to calculate the angles (in degrees) between the $i - th$ absorber and the $j - th$ PC using:

$$\theta_{i,j} = arccos\left(\frac{\kappa_{i,j}}{\|S_i\| \|PC_j\|}\right)\frac{180}{\pi} \tag{1.5}$$

Values of the angles $\theta_{i,j} \simeq 90^o$ indicated high level of orthogonality between the $i - th$ absorption spectra and the $j - th$ PC, which was interpreted as low information content carried by PC_j with respect to the absorber S_i. The closer to 0° or 180° the angle $\theta_{i,j}$, the more information on the absorber S_i was assumed to be embedded in PC_j.

Along with the angles, the spectral linear correlation, $r_{i,j} = \rho_{1,2} = \rho_{2,1}$, between absorption spectra S_i and PC_j was also calculated according to the following equation:

$$\rho_{l,k} = \frac{C_{l,k}}{\sqrt{C_{l,l}C_{k,k}}} \tag{1.6}$$

where $C_{l,k} = cov(X)_{l,k}$ is the element of the covariance matrix X whose two rows are respectively the absorption spectrum $S_i(\nu)$ and the $PC_j(\nu)$.
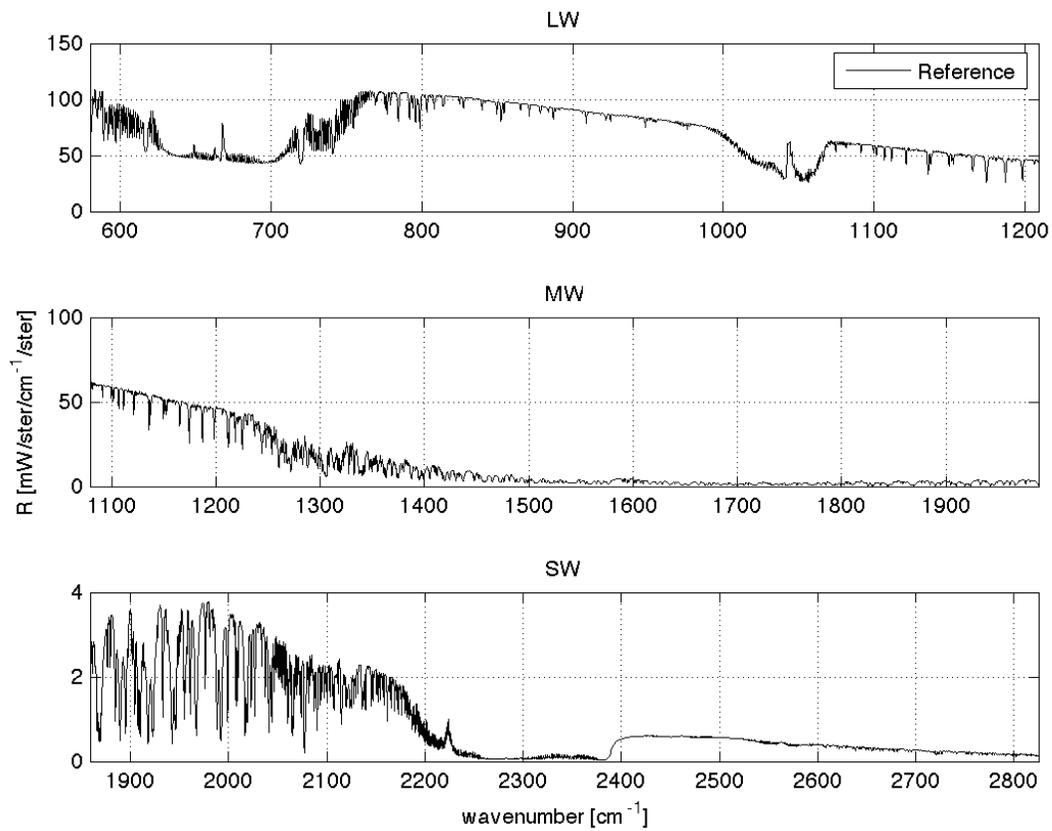
Figure 1.1: Reference spectrum

H_2O	CO_2	O_3	N_2O	CO	CH_4	O_2
NO	SO_2	NO_2	NH_3	HNO_3	OH	HF
HCl	HBr	HI	CLO	OCS	H_2CO	$HOCl$
N_2	HCN	CH_3Cl	H_2O_2	C_2H_2	C_2H_6	PH_3
COF_2	SF_6	H_2S	$HCOOH$	HO_2	O	$ClONO_2$
NO^+	$HOBr$	C_2H_4	C_3HOH			

Table 1.1: Molecular species

1.2   Results

The full matrices $\Theta_{39x100} = \theta_{i,j}$ with $i = 1 \ldots 39$, $j = 1 \ldots 100$, obtained from eq. 1.5, are color mapped in figures 1.3, 1.6, and 1.9 respectively for the LW, MW, and SW. The y-axis represents the different molecular species, while the x-axis the individual PCs. Dark red and blue colors are indicative of lower degree of orthogonality between the PCs and the absorbers. The same angles are showed in form of stackplots in figures 1.4 and 1.5 for the LW; figures 1.7 and 1.8 for the MW; and figures 1.10 and 1.11 for the SW. For each molecule (on the y-axis) the 0-line correspond to 90° angles.

Maps of the correlation values between absorbers and PCs, calculated according to eq. 1.6, are shown in figures 1.12, 1.13, and 1.14 respectively for the LW, MW, and SW. The y-axis represents the different molecular species, while the x-axis the individual PCs. Dark red and blue colors are indicative of higher degree of linear correlation (anti-correlation) between the PCs and the absorbers. Both sets of figures 1.3, 1.6, 1.9, and 1.12, 1.13, 1.14, reveal specific properties of the PCs. LW PC number 6 is a good example as it forms angles of about 110° with H_2O and O_3 absorption spectra, and an angle of about 60° with CO_2 while angles with all other absorbers are very close to 90° (figures 1.3 and 1.15). Figure 1.16 shows how LW PC number 6 (in black) is a mixture of the water vapor, carbon dioxide, and ozone absorption bands (red, purple and pink respectively), with water vapor and ozone being negatively correlated and carbon dioxide positively correlated.
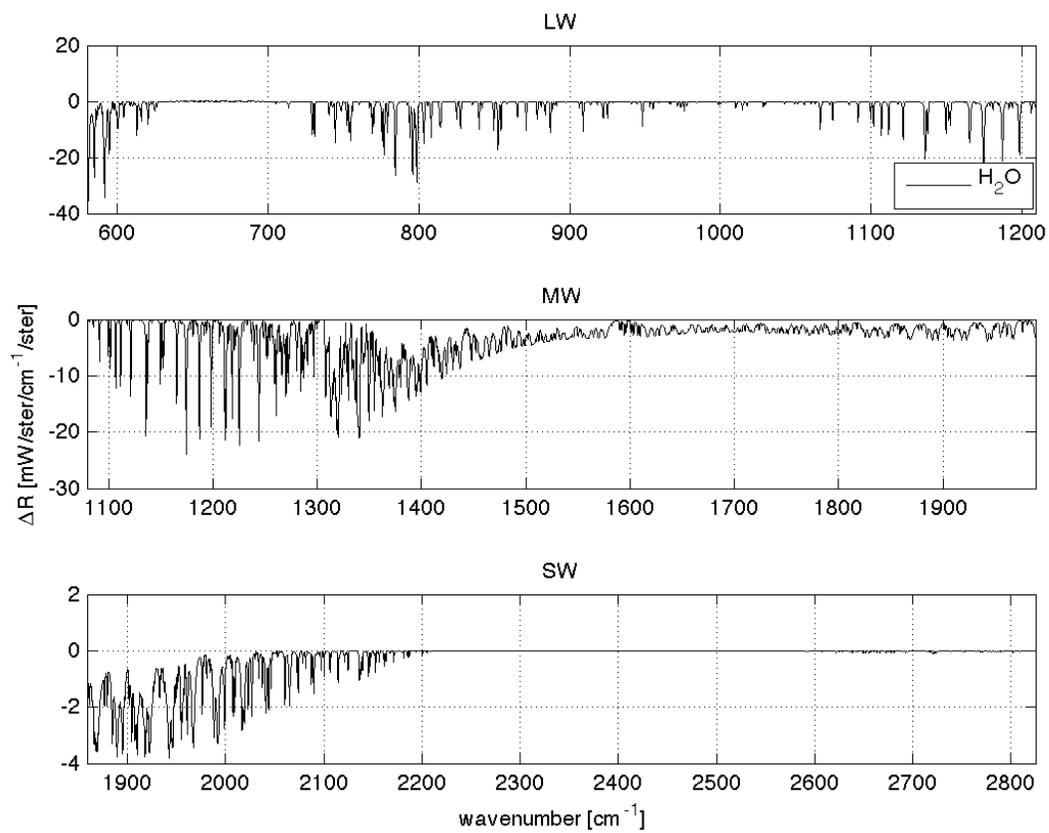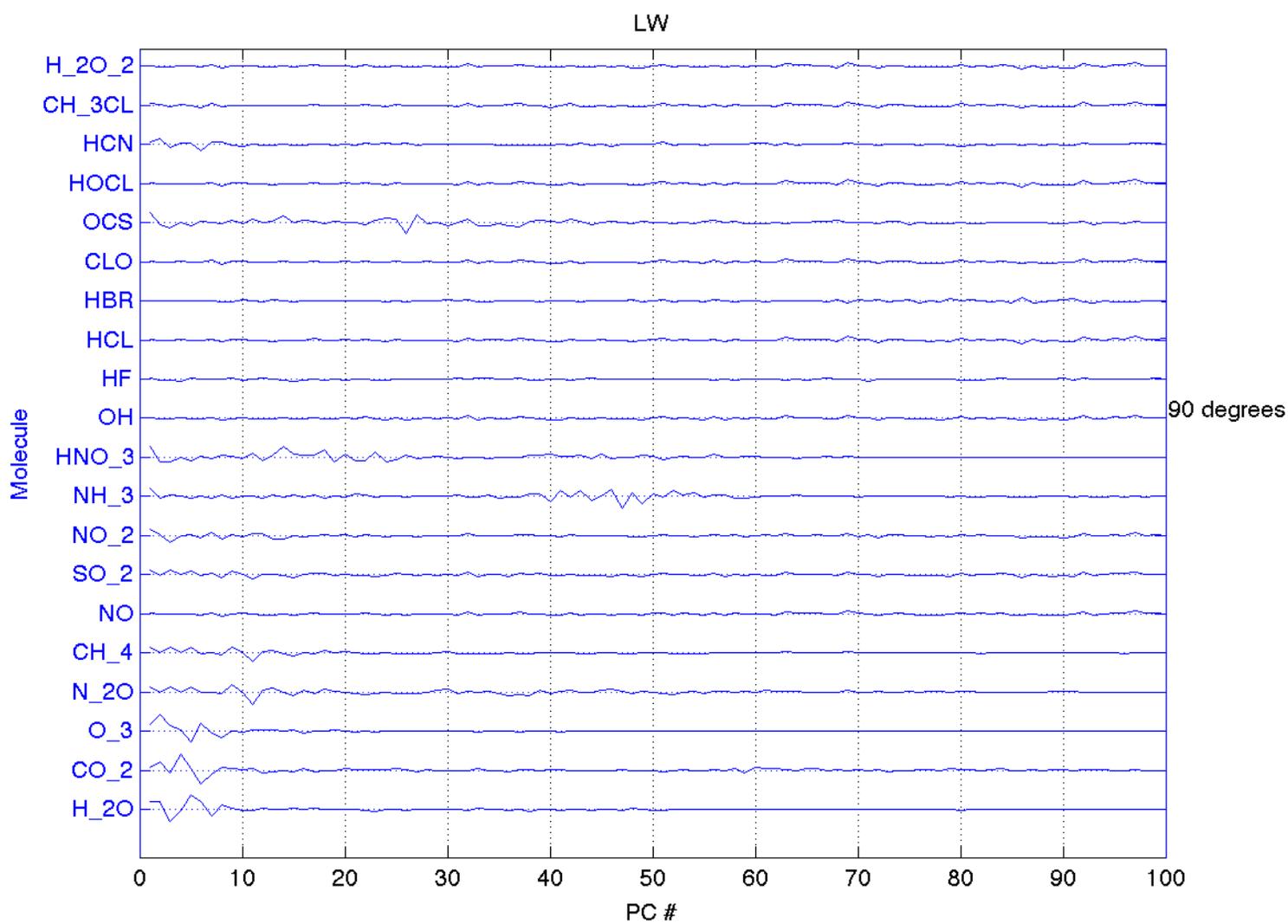
Figure 1.2: Water Vapor absorption

Figure 1.3: LW angles

Figure 1.4: LW angles: molecules are mapped on the y-axis and PCs on the x-axis; for each molecule the angles are calculated around the 90° line and showed as a stackplot.
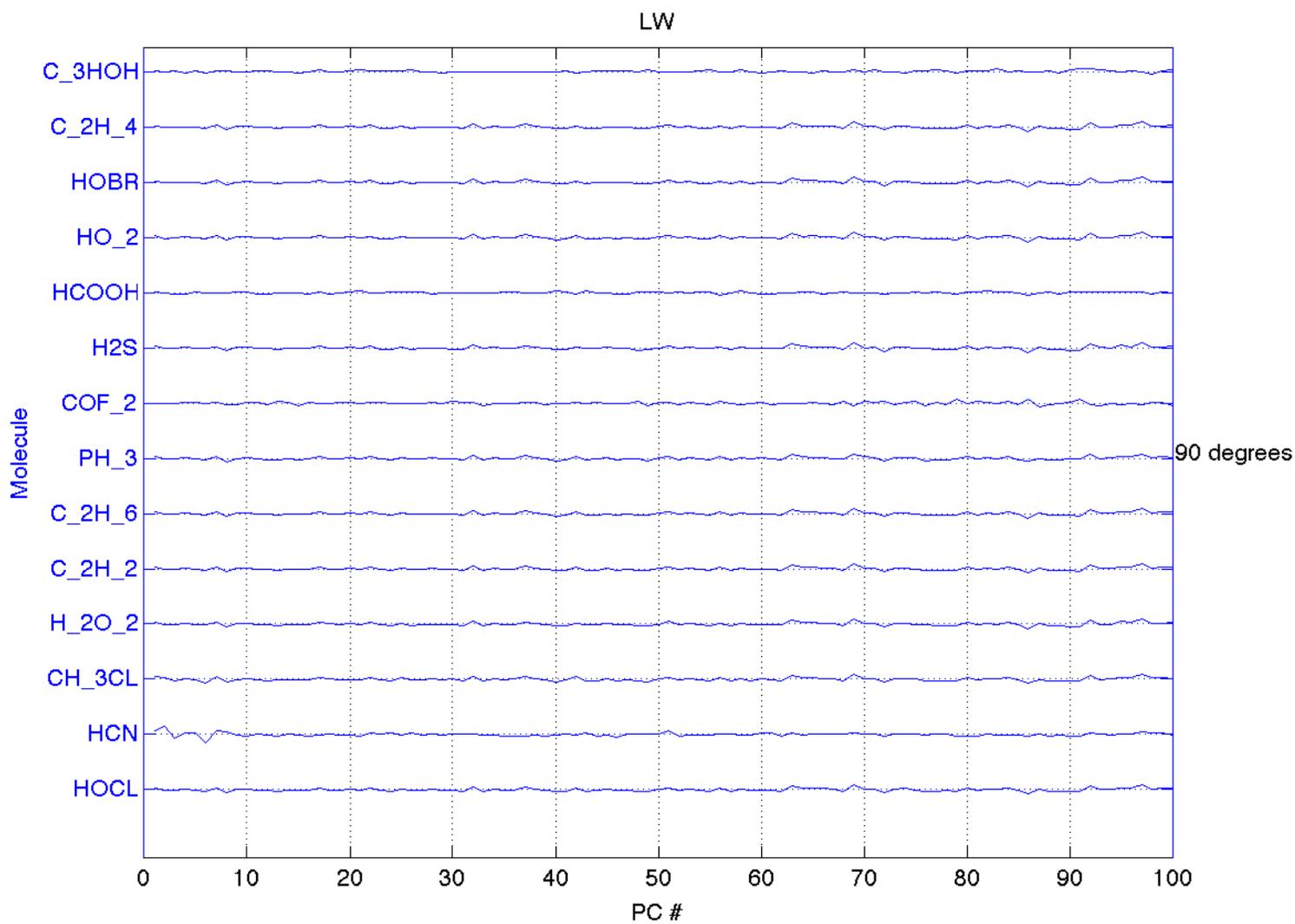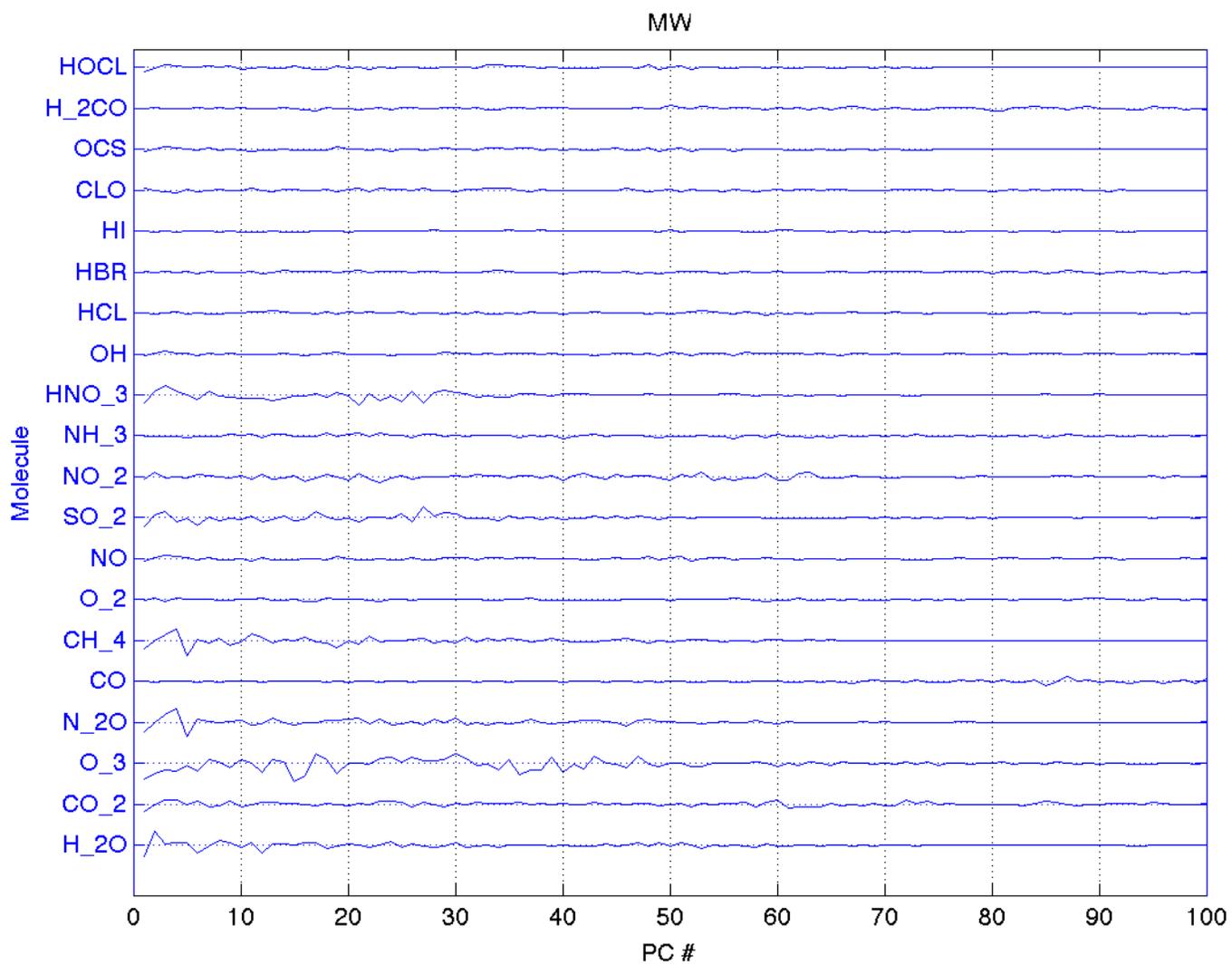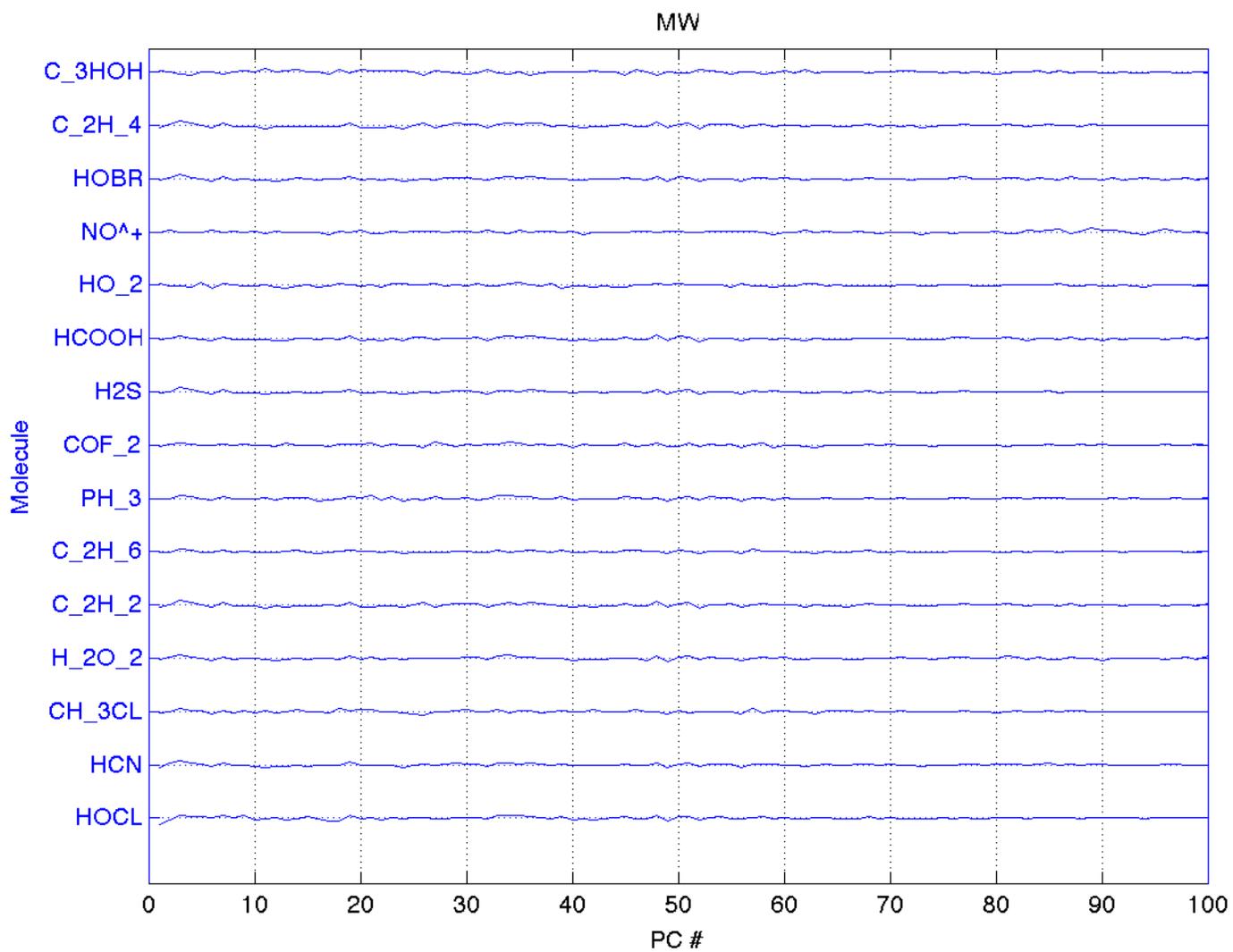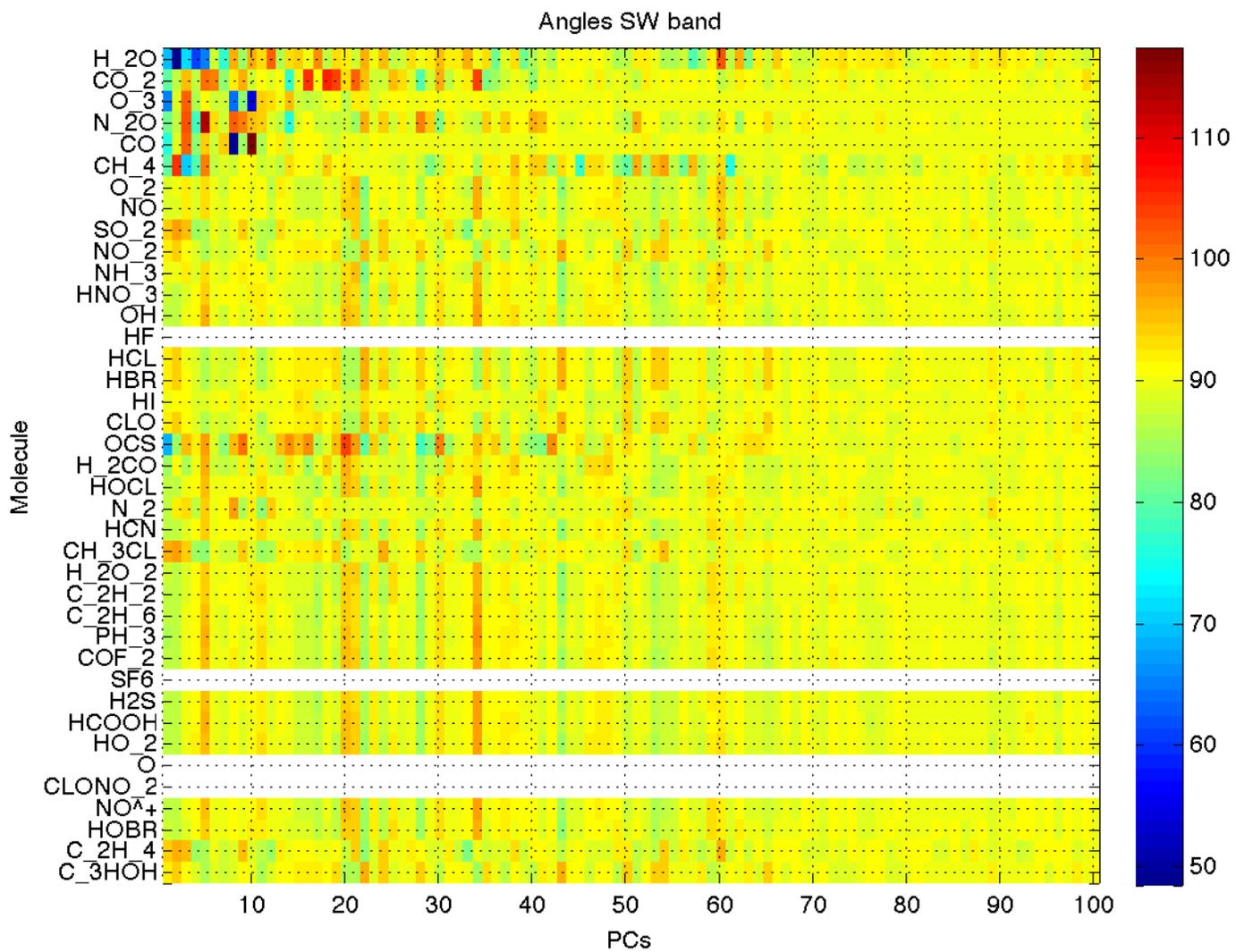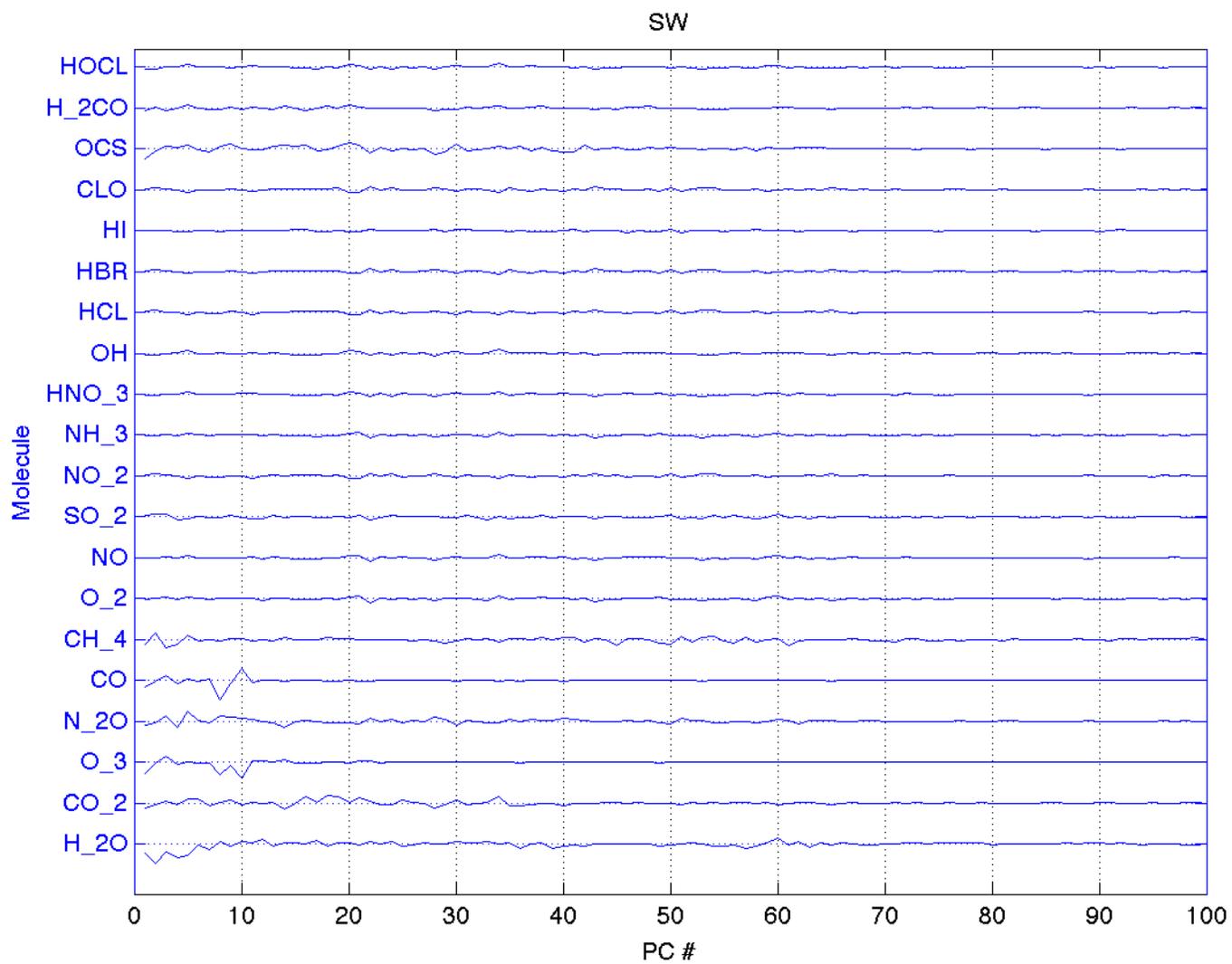
Figure 1.5: LW angles: molecules are mapped on the y-axis and PCs on the x-axis; for each molecule the angles are calculated around the 90° line and showed as a stackplot.

Figure 1.6: MW angles

Figure 1.7: MW angles: molecules are mapped on the y-axis and PCs on the x-axis; for each molecule the angles are calculated around the 90° line and showed as a stackplot.

Figure 1.8: MW angles: molecules are mapped on the y-axis and PCs on the x-axis; for each molecule the angles are calculated around the 90º line and showed as a stackplot.
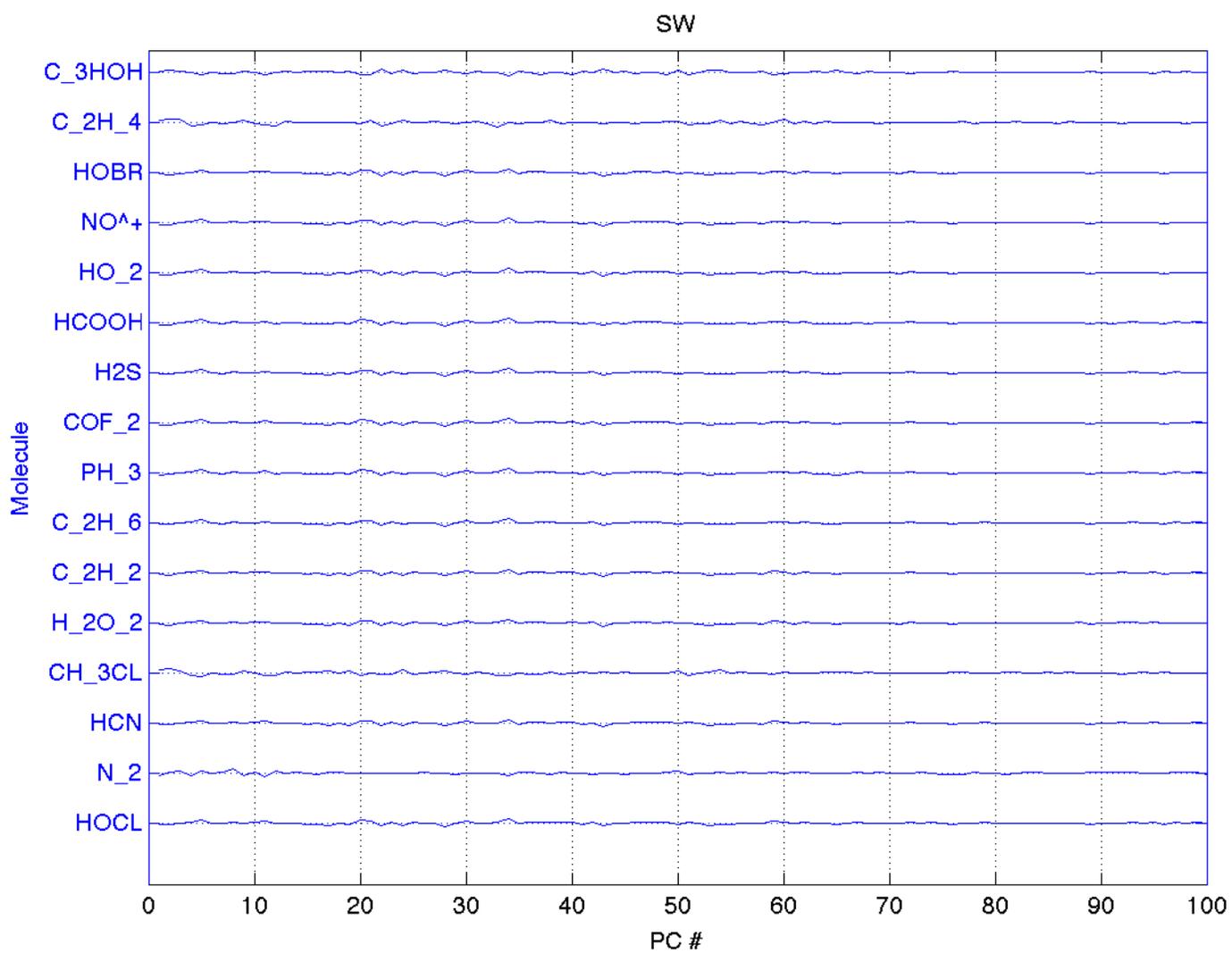
Figure 1.9: SW angles

Figure 1.10: SW angles: molecules are mapped on the y-axis and PCs on the x-axis; for each molecule the angles are calculated around the 90° line and showed as a stackplot.

Figure 1.11: SW angles: molecules are mapped on the y-axis and PCs on the x-axis; for each molecule the angles are calculated around the 90° line and showed as a stackplot.
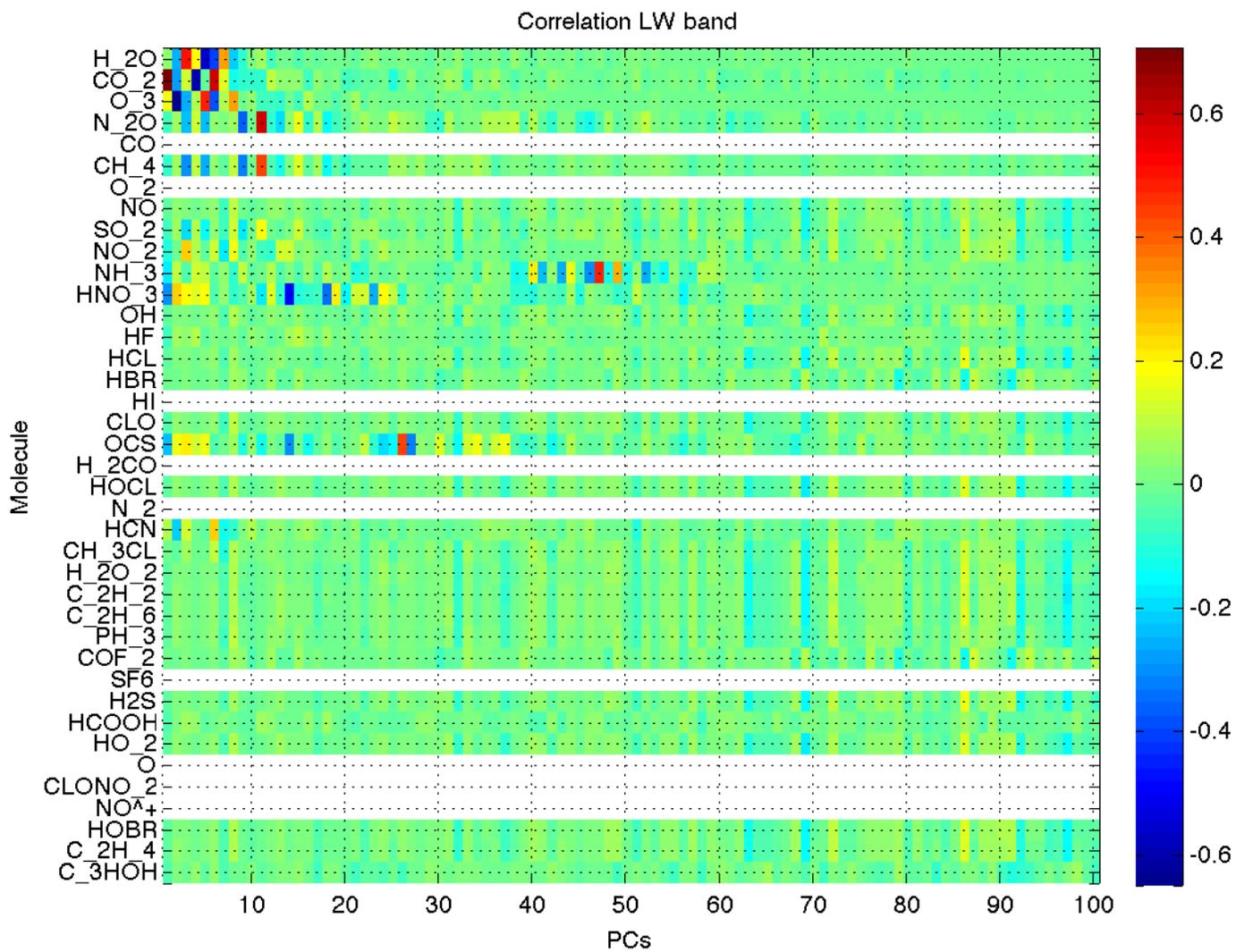
Figure 1.12: LW correlations
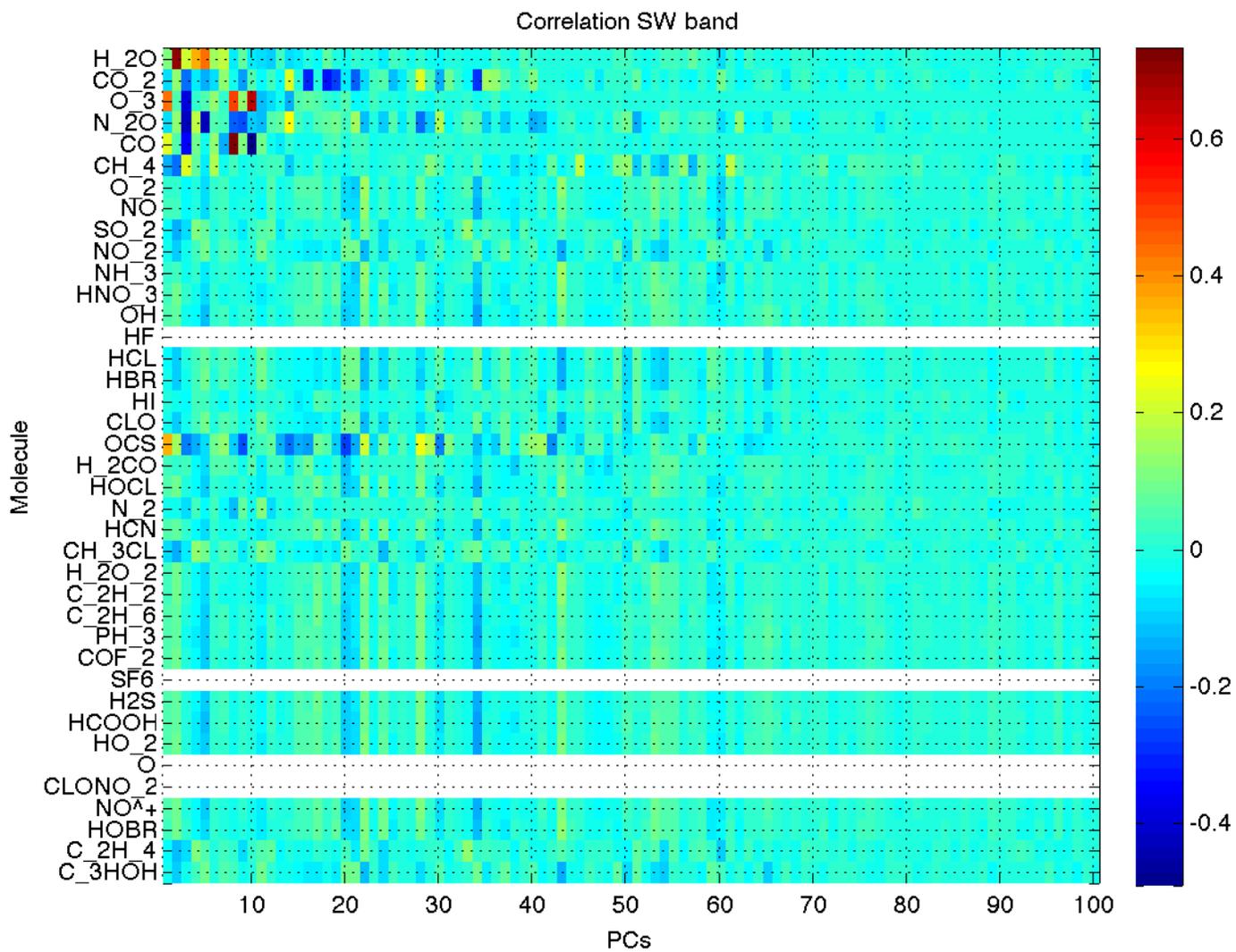
Figure 1.13: MW correlation
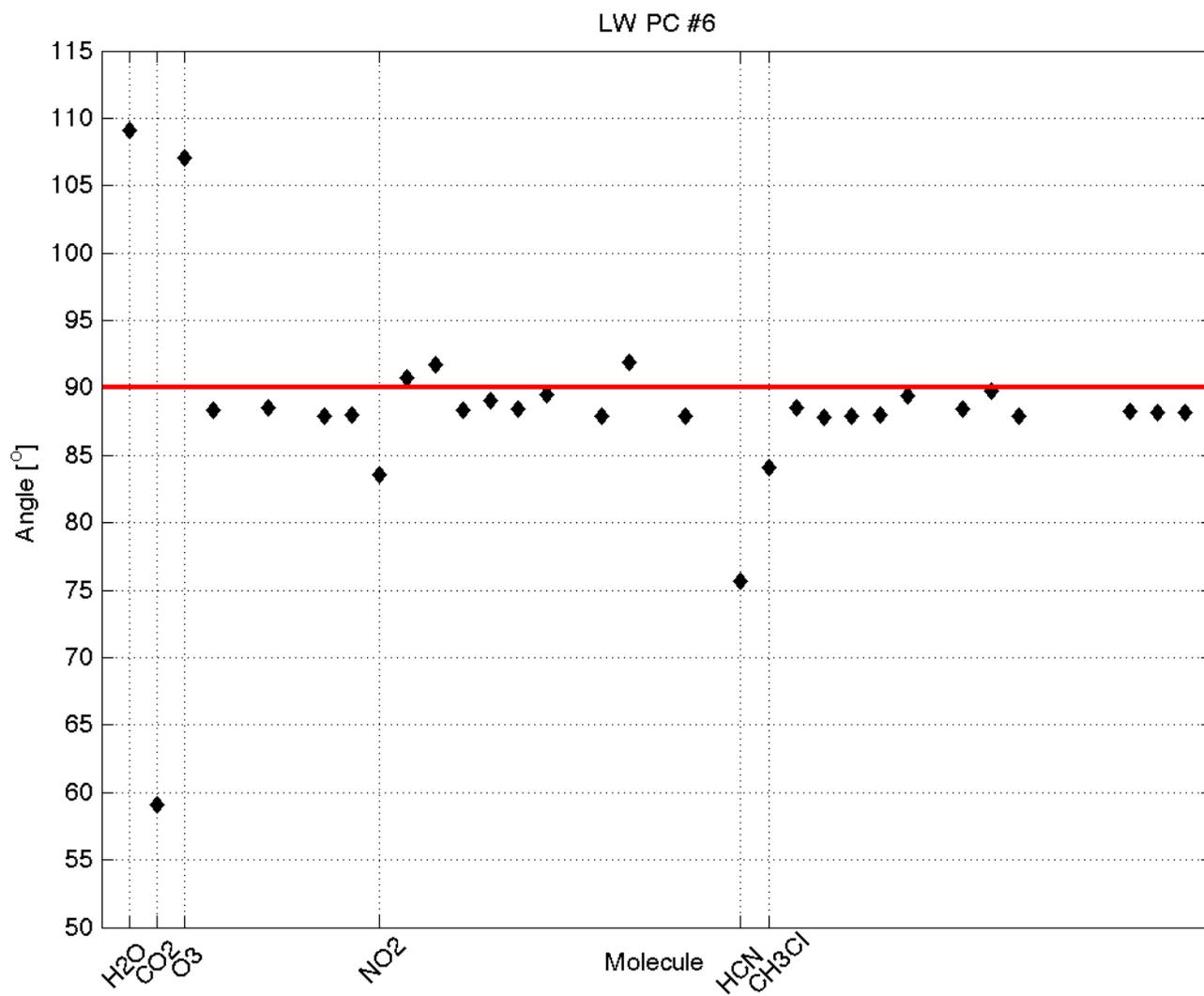
Figure 1.14: SW correlation

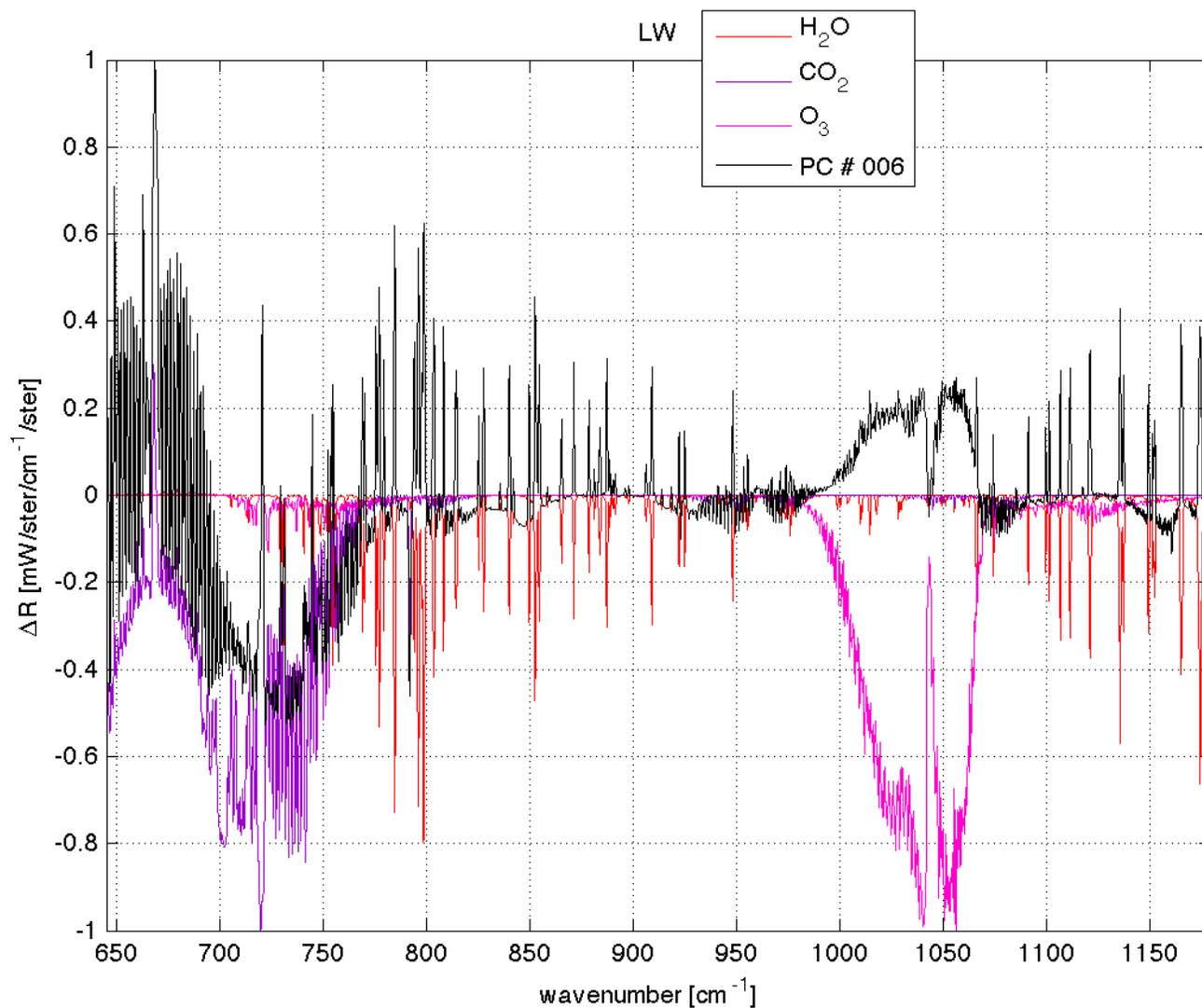Figure 1.15: Angles between PC # 6 (black diamonds) and the 39 molecules.

Figure 1.16: Principal Component 6 (in black) is showed to be mostly a mixture of water vapor, carbon dioxide, and ozone absorption bands (red, purple and pink respectively).

By assessing the relevance of each PCs for individual absorbers and by using the angles $\theta_{i,j}$, it is possible to identify those PCs which are highly orthogonal to the water vapor and the carbon dioxide absorbers and might therefore be source of uncertainty for the level 2 processor, as they carry most of their information on trace gases rather than on the main atmospheric parameters to be retrieved (moisture and temperature). An analysis of the angles θ_{H_2O,PC_j} and θ_{CO_2,PC_j} showed that LW PCs [19 24 34 35 37 39 43 46 52 54 63 67 69 72 74 75 82 83 85 86 88 89 90 91 92 93 96 97 98 99 100] are simultaneously orthogonal within 1° with water vapor and carbon dioxide absorption spectra, which means that these PCs might be dropped in the pc-based inversion process (or in the reconstruction). It is worth noting that:

1. the PCs generated form real data account also for clouds, surface properties, aerosols, instrument artifacts (correlated noise), absorption continua, CFCs, etc. and those dependencies were not explicitly investigated at this stage;

2. the threshold of 1° to identify PCs which might be neglected is, at this stage, arbitrary and should be intended as a simple indication.

A few example of PCs which could be neglected because of close-to-orthogonal with respect to water vapor an carbon dioxide are shown in figures 1.17, 1.18, and 1.19, which indicate that PC number 19 is highly correlated with HNO_3, while PC number 39 is mostly correlated with NH_3 and HNO_3, and finally PC number 96 has generally close-to-orthogonal angles (close to 90^0) with all the absorbers, and in particular with water vapor and carbon dioxide.

1.3   Conclusions

Relevance of this study was based on verifying the existence of PCs which could mostly account for trace gases and had virtually no or little information on main parameters to be retrieved by the MTG-IRS level 2 processor (temperature and moisture). Principal component coefficients from such PCs could, in fact, be ignored in the retrieval of temperature and water vapor, while could be selectively used in trace gas retrievals. The approach followed was based on the idea that the magnitude of the angles between the PCs and individual absorption spectra (generated differentiating a radiance spectrum obtained from a reference atmosphere with spectra obtained from the same atmosphere but zeroing individual gas
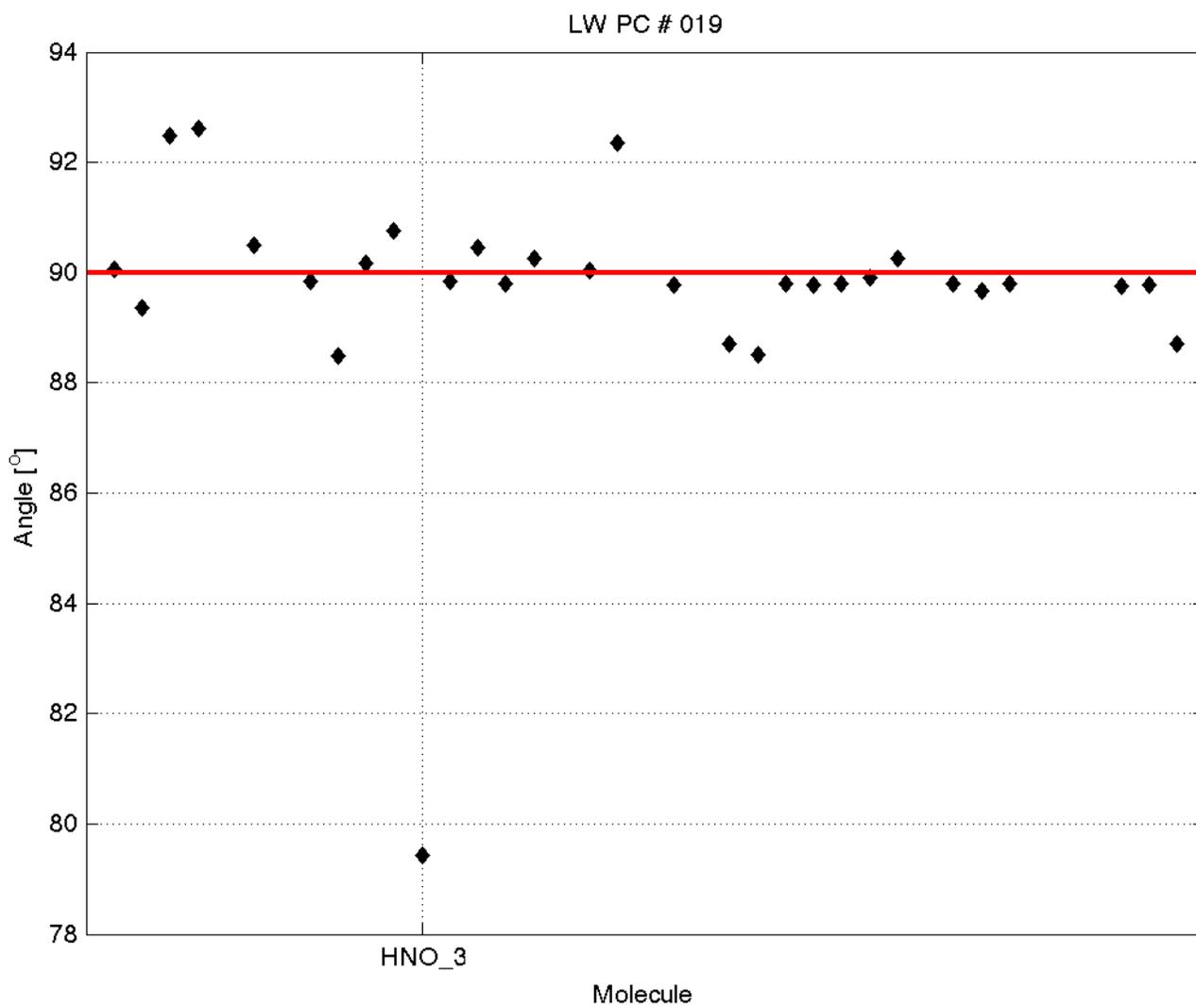
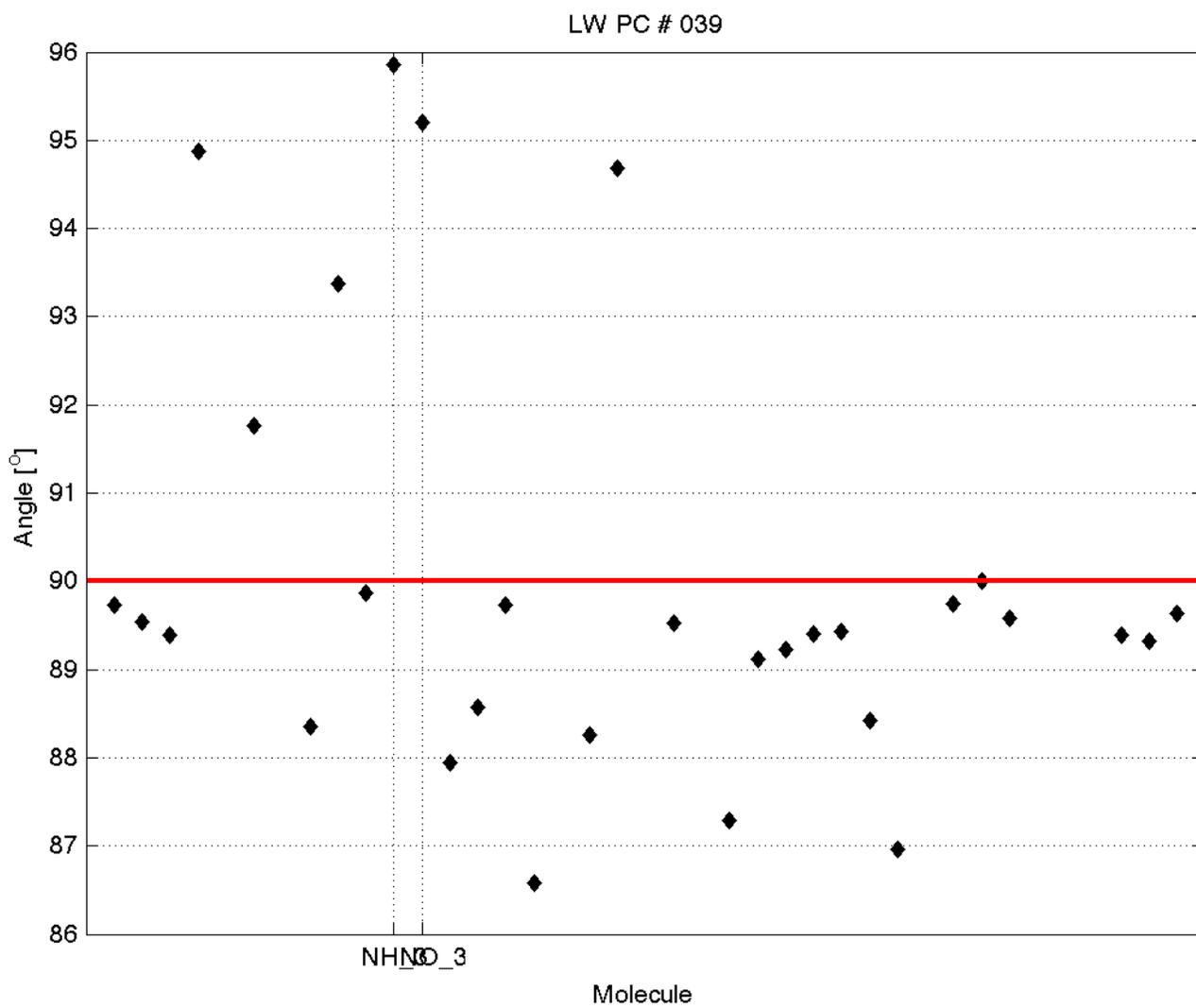Figure 1.17: LW PC 19: angles as function of absorbers

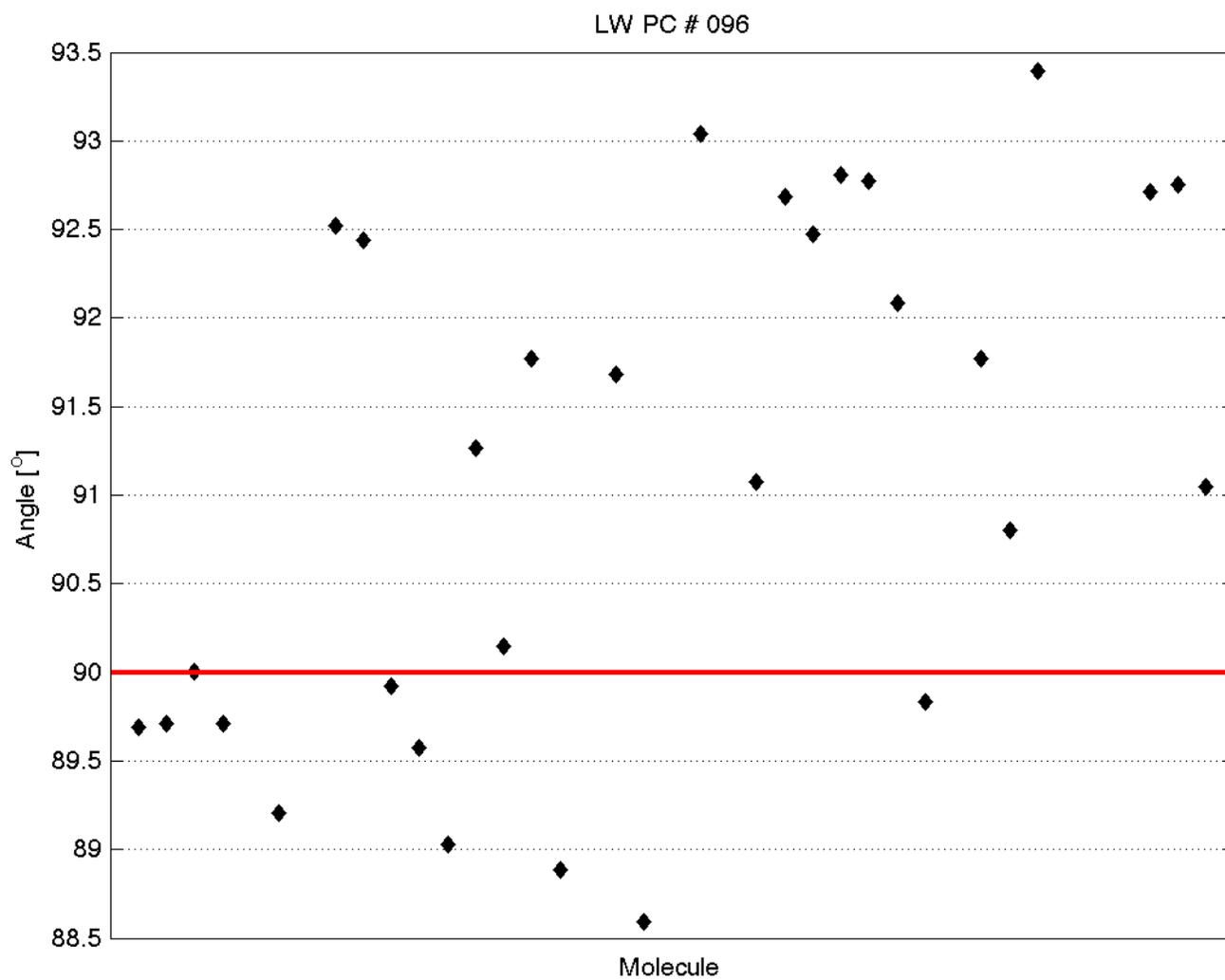Figure 1.18: LW PC 39: angles as function of absorbers

Figure 1.19: LW PC 96:angles as function of absorbers

absorption properties) could provide a simple approach to discriminate between PCs which should be retained in the inversion process and PCs which could be neglected. Angles close to 90°, which indicated orthogonality between an absorption spectra and a PC, were interpreted as the PC being potentially not informative with respect to the absorber. The closer to 0° or 180° the angle, the more information on the absorber was assumed to be embedded in the PC. Looking at LW PCs, it was found that 31 PCs (out of the first 100) were orthogonal within 1° simultaneously to water vapor and carbon dioxide (also 14 MW PCs were found to have the same properties) and could potentially be ignored in the retrieval. Since no PCs where found to account for CO_2, O_3 or H_2O only, it can be argued that it would not be possible to remove completely the effect of the trace gases in the retrieval. However by removing the PCs which have little information about all these three molecules, the effect of trace gases could be significantly mitigated.

Bibliography

[1] S.A. Clough, M.W. Shephard, E.J. Mlawer, J.S. Delamere, M.J. Iacono, K. Cady-Pereira, S. Boukabara, and P.D. Brown. Atmospheric radiative transfer modeling: a summary of the aer codes * short communication*. *J Quant. Spectrosc. and Radiat Transfer*, 2004.