\section{Concentration determination}

\subsection{method}

Henceforth only the list of molecules to be checked for their concentration, as assembled according to methods mentioned in \autoref{sec:determination of molecules} are used. At this stage the strictness of the list can be adjusted by only allowing molecules present in a certain amount or more of the previously determined regions of low p-values to be processed further. In order to process the molecules further and compare them to the measured data, the information of the molecules are first transcribed to match the format of the measured data, i.e. in wavenumber range and resolution. This comes down to scrapping all the information outside of the relevant wavelength region, and matching the wavenumber spacing as used in the measured data through interpolation. Furthermore the measured data and molecules need to be in the same physical quantity, for which in this case absorbance is the most useful. The aggregated absorbance of the gas is determined by the terms of \autoref{eq:2.2} and for a single molecule by \autoref{eq:dezehier}

\begin{equation}

A(\nu,c\_{mol}) = \epsilon\_{mol}(\nu)c\_{mol}l\_{path},

\end{equation}

where the absorbance \(A(\nu,c\_{mol})\) is determined by the concentration \(c\_{mol}\), the optical path length of the laser in the gas \(l\_{path}\), and the molar absorptivity \(\epsilon\_{mol}\). Since the path length is measured from the setup and the molar absorptivity of the molecules is obtained from the databases, the absorbance is left as a function of the concentration. All calculations are done over the set wavelength region of 832 $cm^{-1}$ to 1263 $cm^{-1}$ as determined by the range of QCL. The concentrations are determined through what is essentially a curve fitting problem as the absorbances of the molecules can be laid over the measured absorbance and then best fitted to match by tweaking the concentrations of the molecules. This curve-fitting problem can be expressed as a non-linear least squares problem as in \autoref{eq:onderstaande}:

\begin{equation}

r(\nu,C) = A\_{spectrum}(\nu) – \sum\_{\substack{c\_{mol} \in C\\

\epsilon\_{mol}(\nu) \in E(\nu)}} \epsilon\_{mol}(\nu)c\_{mol}l\_{path}

\end{equation}

where $C$ and $E(\nu)$ denote the set of all concentrations and the set of all molar absorptivities respectively of the molecules in the gas. Now take

\begin{equation}

S(C) = \sum\_{\nu=832 cm^{-1}}{1263 cm^{-1}}(r(\nu,C)^2),

\end{equation}

where \textit{r} is a residue quantity, and \texit{S} is the quantity to be minimized. This non-linear least squares problem is solved using the Levenberg–Marquardt algorithm which tweaks the concentrations from a given set of initial concentrations.

\subsection{Input and results}

The method as described in \autoref{concentration determination:method} is applied on the molecules found by way of the p-region analysis as in \autoref{app:compound\_region}, where all molecules with presence in one or more regions are checked for their concentration with the measured absorbance \autoref{app:absorbance}. The initial concentration as in \autoref{app:appendix} are used. The Levenberg-Marquardt algorithm is implemented through the \textit{lsqnonlin} function in MATLAB, with its \textit{option} argument as given in \autoref{app:appendix}. The concentrations found this way are given at \autoref{app:appendix}.

The molecules with the highest concentrations are plotted in \autoref{fig:}:

[FIGURE]