

# Final report

## 1.1 Project details

<b>Project title</b>	<b>On-line trace gas measurement technique for gasification</b>
<b>Project identification (program abbrev. and file)</b>	<b>2011-1-10622</b>
<b>Name of the programme which has funded the project</b>	<b>Forsk EL</b>
<b>Project managing company/institution (name and address)</b>	<b>DTU Chemical Engineering, Søtofts Plads 229, 2800 Kgs. Lyngby, Danmark</b>
<b>Project partners</b>	<b>none</b>
<b>CVR</b> (central business register)	<b>30060946</b>
<b>Date for submission</b>	<b>19-09-2016</b>

## 1.2 Short description of project objective and results

The main objective of the project is the development of trace gas *in situ* measurement technique which will be suitable for industrial applications on various types of gasifiers.

The technique consists from a base knowledge (selected PAH and S-compounds absorption cross section databases) and tools (high-resolution UV/FTIR spectroscopy). Results obtained in the project can be used for developing a PAH/tar/particle/etc analyzer which can be built with use of various approaches: broad-/narrow-band absorption measurements with broad/narrow-band light sources as e.g. compact UV spectrometers with Xe-pulsed light sources or UV/VIS LED's.

## 1.3 Executive summary

UV absorption spectroscopy has shown a potential for in situ/on line measurements of PAH/tar/etc. gas components. The spectra of all gases tend to change their fine structures when temperature increases: the fine structure starts to disappear and absorption bands become broader. Temperature range 250-300C is optimal for PAH/tar measurements when the absorption bands preserve their unique structures and the gas temperature is high enough to prevent condensation on the heavy tars. A DOAS approach can be used for measurements of S-and PAH/tar compounds in 220-370 nm. There are possibilities for measurement system simplification with use new (commercially available) UV/VIS LED's or Xe-pulsed light sources. An absorption pathlength for in situ/on line measurements can be few mm. This makes a system quite compact compare to IR-based one. On line measurements can be performed with or without controlled dilution and cooling of the gas. In a "clean" gasification UV absorption spectroscopy shows possibilities to track traces of PAH/VOC/tar/etc. in the producer gas while the IR does not.

In situ and on line UV absorption measurements for phenol (the major PAH in the low-temperature gasification) agree with traditional PAH sampling methods. Moreover the UV measurements give possibilities for particle (black carbon) measurements after some calibration of the system.

IR absorption spectroscopy is an excellent tool for measurements of major (CO, CH<sub>4</sub>, CO<sub>2</sub>, H<sub>2</sub>O etc.) gas components. However high water content in the LT-CFB producer gas and its high temperature makes measurements for trace components extremely challengeable. The measurements require a few meters path-length to reach a ppm detection level and a strong interference with water absorption structures makes measurements very difficult.

#### 1.4 Project objectives

The project is an experimental research project started at Risø DTU and continued later at DTU Chemical Engineering. The project consists from 5 work packages (WP).

The main original objectives in the main project were:

- to establish a vapour generation system and matched it to a hot flow gas cell (HGC). An existing HGC operated at around atmospheric pressure and temperatures up to 1000°C will be modified to keep uniform temperature flows of highly-reactive gas species.
- to build a high-temperature ultraviolet (UV) absorption cross section database gases of interest, e.g. H<sub>2</sub>S, OCS, CS<sub>2</sub>, CH<sub>3</sub>Cl, NH<sub>3</sub>, benzene and few 2-4 rings PAH suitable for *in situ* industrial applications. Absorption measurements in the HGC will be done by a UV/VIS spectrometer (nominal resolution 0.02 nm) equipped with a UV enhanced CCD camera and UV light source.
- to build a high-resolution high-temperature infrared (IR) absorption cross section database gases of interest, e.g. H<sub>2</sub>S, OCS, CS<sub>2</sub>, CH<sub>3</sub>Cl, NH<sub>3</sub>, HCN and benzene suitable for *in situ* industrial applications. Absorption measurements in the HGC will be done by a high performance FTIR spectrometer (nominal resolution 0.125 cm<sup>-1</sup>) equipped with a sensitive MCT detector and powerful IR light source (black body).
- to develop an UV/IR measurement tools suitable for *in situ* trace gas measurements in the flue gas of gasifiers. The measurements will be performed either cross-stack or with specially designed UV/IR probes equipped with UV/IR light sources at Risø DTU gasifiers operated at typical operation conditions.

In a running complex project as one in question there is frequently a need for some on-go adjustments taking account gained up to date experience and targeting where the results at the end of the project are potentially going to be used. Therefore some minor changes in the objectives, not however sacrificing the main purpose of the project, have been made taking into account potential end user needs. The changes attributed to particular WP's are reported below.

The project has been started with WP1, WP2, shot after with WP4 and finally with WP3.

The project had a couple times prolongations (under however the same budget frame) to cover possibilities for in situ/on line measurements (subject of agreement and access availability with the third party).

#### 1.5 Project results and dissemination of results

The main purpose of the project is the development of trace gas *in situ* measurement technique which will be suitable for industrial applications on various types of gasifiers.

Results achieved are grouped under relevant WP's.

## **WP1: Vapour generation system and HGC**

Because 1) many of gases mentioned in the project are corrosive and 2) temperature range of a producer gas from LT-CFB gasifier is 300C-530C, it has been decided to use a quartz hot flow gas cell (qHGC, maximum temperature 525C) developed under Energinet.dk project 2010-1-10442 "*Sulphur trioxide measurement technique for energy system*". A qHGC is based on a "flow-windows" concept in order to avoid possible reaction of the reactive gases with physical windows. Mostly chemical inert materials like Teflon and quartz are used in order to minimize possible side reactions. Performance of the qHGC has been investigated and the cell has been validated in measurements with CO<sub>2</sub> and SO<sub>2</sub>.

The producer gas from high-temperature gasification (e.g. Viking gasifier) is much cleaner compare to the LT-CFB one. Moreover a temperature level of the producer gas about 500C can easily be achieved because the gas has to be cooled down for further utilization anyway (e.g. gas motors, fuel cells). The measurements performed on the Viking gasifier under WP4 have confirmed this.

The other reason to limit upper temperature range to 525C instead of 800C mentioned in the WP's2-3 was because parallel running activities at Pyroneer (6MW) gasifier in Kalundborg (DONG Energy) where the DTU Chemical Engineering was involved. The activities concerned about gas composition, particle and flow measurements. The Pyroneer gasifier was an up-scaled version of LT-CFB (100kW) gasifier at Risø. At that time DONG Energy put a large focus on the technology and had plans to build 100 MW demonstration plant with use the same LT-CFB technology. The temperature level of the producer gas with high tar load was about 500C.

Finally, UV/IR absorption spectra are changing with the temperature. Many of molecules mentioned in the project have a unique structure which can be used as a "fingerprint" for their identification. These structures are changing when the temperature increases and the fine structures start to smooth or even disappear when temperature exceeds about 500C. The spectra become also broader that increases their "mixing" with spectra of major gas components (as for example H<sub>2</sub>O and CO<sub>2</sub> in IR or (broad class) PAH's in the UV) those have extended absorption bands in the spectral ranges of interest (400-6000 cm<sup>-1</sup> and 200-400 nm).

In general 300-500C temperature range seems to be optimal for applications on various types of gasifiers because 1) the "fingerprints" of the molecules are conserved up to these temperatures and 2) these temperatures are quite above (heavy) tar dew points found in low-temperature gasification that allows one in situ/on line measurements without any condensation issues.

Therefore use of the qHGC operated at temperatures up to 525C is reasonable and sufficient to fulfil current project requirements and keeping in minds potential users/customers of the technique in Denmark and abroad.

Several pre-mixed gas mixtures has been received for the project (e.g. N<sub>2</sub>+OCS(1000 ppm), N<sub>2</sub>+CS<sub>2</sub>(1000 ppm)). Gas flow evaporation tubes for phenol and naphthalene have been established: solid crystals have been melted inside of thermally isolated quartz tubes. The gas tubes can be fitted to the gas supply system of the qHGC.

## **WP2: UV and GC/MS measurements on HGC**

An ACTON high-resolution spectrometer ( $\Delta\lambda=0.016$  nm) equipped with PIXIS UV enhanced CCD camera, special optics and D<sub>2</sub>-lamp (UV light source) have been aligned and tested for UV absorption measurements for known N<sub>2</sub>+SO<sub>2</sub> gas mixtures at room temperature. It was shown that SO<sub>2</sub> UV absorption cross sections calculated from the SO<sub>2</sub> absorption spectra are

in excellent agreement with data available from the literature (e.g. MPI-Mainz-UV-VIS Spectral Atlas of Gaseous Molecules).

Reference high-resolution UV absorption measurements at 20-500C have been performed for SO<sub>2</sub>, OCS, CS<sub>2</sub>, phenol and naphthalene. The spectra show highly temperature-dependence. Thus, for example, fine structures in the spectra those can be used as molecular fingerprints in UV DOAS measurements become less pronounced with temperature rise and fully disappear at 500C. The spectra become also broader. The temperature-dependent absorption cross-sections for SO<sub>2</sub>, OCS and CS<sub>2</sub> have been calculated for 25C, 150C, 300C and 500C. Those temperatures are relevant for GC/UV, gas extraction, LT-CFB/Viking measurements, respectively. The temperature gives a positive effect on the UV OCS, CS<sub>2</sub> absorption cross-sections: they become larger. And both of them keep fine structures even at 500C that makes possible to use UV DOAS for their measurements.

Phenol and naphthalene are the most abundant organic compound in LT-CFB and high-temperature (Viking) gasification (so-called light PAH's). Measurements with phenol and naphthalene have been accompanied by simultaneous sampling for gas chromatography-mass spectroscopy (GC/MS) analysis because difficulties to control their concentrations in the carrier gas. The complete gas flow has been sampled by GC/MS gas sampling unit using a so-called Petersen column and GC/MS analysis of the sample has been performed using a gas chromatograph interfaced to a mass spectrometer. Naphthalene and phenol concentrations in the carrier gas have been determined and temperature-dependent naphthalene cross sections calculated from measured UV absorption are calculated. It should be noted that the UV measurements were very stable and highly reproducible from time-to-time and day-to-day. In opposite, sampling for GC/MS measurements and further sample handling and sample analysis was tricky and therefore it was necessarily to repeat the measurements (UV and GC/MS) several times (at various temperatures in the qHGC) in order to find a right sampling method and further data analysis procedure and finally to get good data sets.

It was also shown that all obtained low-temperature UV absorption cross sections are in excellent agreement with that available from the literature (MPI-Mainz-UV-VIS Spectral Atlas of Gaseous Molecules).

Based on gained experience obtained in various measurements on 100kW LT-CFB and 6 MW Pyroener gasifiers it was decided to skip CH<sub>3</sub>Cl, NH<sub>3</sub> and phenol UV absorption measurements on the qHGC. The CH<sub>3</sub>Cl, NH<sub>3</sub> are difficult to measure with use UV absorption technique due to their smooth broad spectral structures and strong interference with PAH compounds in 200-230 nm. In opposite, CH<sub>3</sub>Cl and NH<sub>3</sub> both have unique absorption features in IR spectral range where their detection may, in principle, be performed. Thus, for example, measurements on LT-CFB and Pyroener gasifiers show NH<sub>3</sub> content at a sub-percentage level (0.2-0.6 vol %, wet) and CH<sub>3</sub>Cl one is below 100 ppm (wet).

No benzene traces have been found in the measurements either on Viking or LT-CFB gasifiers in UV or UV DOAS absorption measurements. Therefore it was decided to skip benzene measurements on the qHGC. It should be noted that UV absorption measurements for benzene on the qHGC can easily be done with use the same concept as for phenol and naphthalene. Benzene absorption cross sections can also be obtained with use of appropriate gas sampling for further GC/MS analysis.

### **WP3: FTIR measurements on HGC**

High-resolution FTIR absorption measurements of NH<sub>3</sub> and CH<sub>3</sub>Cl have been performed in the WP3. CH<sub>3</sub>Cl has shown a quite complex structure and it is under more investigation in other followed up Energinet.dk project 2013-1-1027 in collaboration with University College London (UK) where other Cl-compounds are also included.

NH<sub>3</sub> measurements up to 500C have been performed on the qHGC and few measurements have been done at 1027C on other flow HGC. The upper temperature was chosen to be below possible NH<sub>3</sub> heterophase decomposition. The absorption cross-section spectra have been analysed by comparison to a variational line-list BYTe and experimental energy levels determined using the Marvel procedure. The work was done in collaboration with UCL who is a DTU's partner in Energinet.dk projects 2013-1-12027 and 2010-1-10442. The UCL group maintains the EXOMOL web-site ([www.exomol.com](http://www.exomol.com)) where line lists for many molecules relevant to gasification and combustion are listed. The line lists are used in the theoretical spectra calculations.

H<sub>2</sub>S measurements have been performed at 0.1-0.5 cm<sup>-1</sup> nominal spectral resolution in 400-6000 cm<sup>-1</sup> (MIR) at 25C and 500C in the qHGC. H<sub>2</sub>S has very low IR absorption cross-sections. Therefore the measurements have been performed at high H<sub>2</sub>S concentrations (60-90%) in N<sub>2</sub>. The results at 25C have been compared with PNNL high-resolution database and it was found an excellent agreement between our data and the data from PNNL. It should be noted that PNNL data are limited by 25C or 50C only.

Few impurities like C<sub>2</sub>H<sub>6</sub> and CH<sub>4</sub> has also been observed in the H<sub>2</sub>S spectra at around 3000 cm<sup>-1</sup>. H<sub>2</sub>S spectrum changes significantly at higher temperatures: the bands become broader and maxima in absorption cross-sections spectra decrease. Modelling of the H<sub>2</sub>S spectra with use of UCL's line list shows in general a good agreement with experiment for H<sub>2</sub>S strong lines, although many of weaker (hot) H<sub>2</sub>S lines are missing in the calculations.

Measurements at T>500C can be affected by heterophase decomposition of H<sub>2</sub>S into H + HS with the final products as H<sub>2</sub> and S<sub>x</sub> (x=6-8). This effect can be handled by measurement of the products in the other cell connected to the HGC in series. However one can expect that H<sub>2</sub>S absorption will become weaker and broader than that at 500C. Measurements in far IR (FIR) can be useful because H<sub>2</sub>S absorption cross-sections are higher in the FIR than that in the MIR. Measurements in FIR are however outside of the project scope.

Taking into account temperature variations in the H<sub>2</sub>S absorption cross-sections and that H<sub>2</sub>S concentration in the producer gas is far below a percentage level no more H<sub>2</sub>S measurements have been conducted. The H<sub>2</sub>S data obtained under the WP3 will be used by UCL group for further H<sub>2</sub>S hot line list development.

Benzene has unique absorption features in UV (240-270 nm) and one the strongest one in the IR (673 cm<sup>-1</sup>). The UV (MPI-Mainz-UV-VIS Spectral Atlas of Gaseous Molecules) and IR (PNNL) absorption cross sections at 25C are quite similar on their maxima levels. Because no benzene has been detected either in UV gas extraction or UV in situ measurements on LT-CFB gasifier it was decided to skip benzene IR measurements on the qHGC and save more time for measurements under the WP4 and data analysis under the WP5.

In the last few years several improvements in HCN line lists have been made by the UCL group. The line list seems to be in good agreement with available experimental data. Therefore for the time being the HCN measurements were skipped (require customized HCN preparation).

Analysis of PNNL's infrared absorption cross-sections for OCS, CS<sub>2</sub> at 25C shows that the cross sections are about 20-100 times lower than the UV ones. Therefore OCS, CS<sub>2</sub> in situ IR absorption measurements require a longer absorption pathlength in order to reach a ppm-level detection level. In situ measurements made under WP4 on LT-CFB gasifier have shown that most of IR light has been absorbed by H<sub>2</sub>O, CO<sub>2</sub> and C<sub>x</sub>H<sub>y</sub> because of their high concentrations in the producer gas and there is a strong interference between H<sub>2</sub>O, CO<sub>2</sub> and OCS, CS<sub>2</sub> making measurements of the last two very challengeable. Therefore for the time being the OCS, CS<sub>2</sub> IR measurements on the qHGC have been skipped in favour for data analysis in the WP5.

#### WP4: UV/IR on-line measurements in gasifiers

Most of the measurements have been performed in 2012 on 100kW LT-CFB gasifier (Risø Campus) and 6MW Pyroneer gasifier in Kalundborg. The purpose was to get an experience with the measurements, get into the possible problems and find hints for future developments of the on-line trace component measured technique. It should be noted that any optical measurements on gasifiers are quite rare and mainly concern major gas components like CO, CO<sub>2</sub> or CH<sub>4</sub>.

The measurements have successfully been performed with several techniques:

- gas extraction UV/IR absorption measurements with N<sub>2</sub> controlled dilution (150C, 50 cm), T<sub>gas</sub>= 300C;
- cross-stack UV/IR measurements (T<sub>gas</sub>= 300C, 3 mm);
- cross-stack IR measurements (T<sub>gas</sub>= 290C, 550 cm);

Results and discussion of the all measurement campaigns in 2012 can be found in the Report attached<sup>1</sup> (Appendix). In the Report measurements at 100 kW LT-CFB gasifier are compared with that at 6 MW Pyroneer one as well. It is interesting that in situ measurements on a wood stove smoke and on a LT-CFB producer gas show some similarities.

In February 2015 few measurements on a producer gas from Viking gasifier have been done by gas extraction at 150C. The gas was taken before solid fuel cell set up used for producer gas utilization. IR measurements have shown that the gas is very clean (only main gas compounds like CH<sub>4</sub>, CO etc.), no visible trace components have been found. The UV measurements have however shown some small traces of PAH/tar components in the gas.

In the 2013 report it was mentioned about very high phenol concentration (7000 ppm/306C, DOAS approach) found in in situ measurements. As it was discussed in the PhD thesis of Helge Grosch this might be caused by opened designed of the optical set up where a part of the producer gas could be diluted and cooled by N<sub>2</sub> purge gas. The measurements have been repeated in Marts 2016 with improved designed avoiding any gas penetration in the measurement path. The measurements have shown a possibility of in situ PAH/tar/particle measurements. Unfortunately the gas temperature was about 400C which was not in the favour for phenol measurements because phenol UV absorption spectra are becoming smooth with temperature increase as it was shown in the WP2. DOAS absorption spectra have shown that phenol concentration is about 500 ppm that is in the range as one can expect for this gasifier. This phenol concentration is in a better agreement with the previously reported phenol data.

#### WP5: Data analysis and reporting

The WP deals with data analysis of the measurements in the lab and on the gasification units.

The results of the project have been disseminated in a PhD thesis of Helge Grosch and several publications in peer-reviewed journals and conferences (as oral or poster presentations):

Papers:

- H Grosch, A Fateev, KL Nielsen and S Clausen "Hot gas cell for optical measurements on reactive gases", *Journal of Quantitative Spectroscopy and Radiative Transfer*, 2013, 130, p. 392-399

<sup>1</sup> A Fateev and H Grosch "Optical diagnostics in gasification: application to LT-CFB gasifier. Measurements in 2012", DTU Chemical Engineering, Report April 2013.

- H Grosch, A Fateev, S Clausen, "UV absorption cross-sections of selected sulfur-containing compounds at temperatures up to 500°C", *J Quant Spectroscopy and Radiative Transfer*, 2015, 154, pp. 28-34
- H Grosch, Z Sarossy, A Fateev, S Clausen, "UV absorption cross-sections of phenol and naphthalene at temperatures up to 500 degrees C", *J Quant Spectroscopy and Radiative Transfer*, 2015, 156, pp. 17-23

#### Posters

- EGATEC 2013, European Gas Technology Conference, Paris, France, 30<sup>th</sup>-31<sup>rd</sup> May 2013 (H Grosch and A Fateev "*In situ quantification of gas components in gasification*");
- 21<sup>st</sup> European Biomass Conference and Exhibition 2013 (EU BC&E), Copenhagen, 3<sup>rd</sup> – 7<sup>th</sup> June 2013 (Z Sárossya, H Grosch, H Egsgaard, A Fateev, J Ahrenfeldt, U Birk Henriksen, B Gøbel "*Comparative study of aromatic gasification products by GC-MS and UV spectroscopy*")

#### Oral presentations:

- 4<sup>th</sup> GERG Academic Network Event, Brussels, Belgium, 14<sup>th</sup>-15<sup>th</sup> June 2012 (PhD Helge Grosch "*Trace gas analysis in biomass gasification*")
- 11<sup>th</sup> ASA and 12<sup>th</sup> HITRAN Conferences, University of Reims, France, 29<sup>th</sup>-31<sup>st</sup> August 2012
- 13<sup>th</sup> Biennial HITRAN Conference, 23-15 June 2014, Boston, USA
- Spectroscopy of Exoplanets, Cumberland Lodge, Great Park, Windsor, 2015 July 24-26, UK

## 1.6 Utilization of project results

The results obtained in the project can be used for developing in situ/on line measurement analyzer which can be built with use of various approaches: absorption measurements with broad-/narrow-band light sources as e.g. UV spectrometers with UV/VIS LED's or Xe-pulsed light sources.

There are no plans to take out patents from DTU's side directly from the project. However DTU applies for a patent for an UV sensor for tar/particle measurements with use of UV/VIS LED's. The patent application is based on investigations of the tar/soot/particle reach gas produced in combustion process on wood stoves. At certain combustion conditions (lean combustion) the exhaust gas from the wood stoves contains high concentrations of PAH/VOC and tar which has some similarities with e.g. gas from low-temperature gasification.

The project partly supported a DTU PhD student (Helge Grosch) who was involved in all WP's in the project. The PhD student has spent about one week at TU Berlin in the group of Dr. York Neubauer where he made a presentation about his work at a seminar. The group at TU Berlin is active about diagnostics in gasification processes. During PhD studies Helge Grosch learned about use of applied high-resolution UV/IR spectroscopy in such complex process as gasification.

The generated UV absorption cross section databases are available for free download from the MPI-Mainz UV-VIS Spectral Atlas of Gaseous Molecules of Atmospheric Interest - web site ([http://satellite.mpic.de/spectral\\_atlas](http://satellite.mpic.de/spectral_atlas)).

## 1.7 Project conclusion and perspective

The results obtained under the project show that UV/IR absorption measurements with reactive gases require careful gas handling and measurements itself. A gas cell for these kind measurements should be based on a "flow-windows" concept in order to avoid possible reaction of the reactive gases on windows surfaces. Mostly chemical inert materials like Teflon and quartz should be used in order to minimize SO<sub>3</sub> side reactions. In some cases (PAH's) the experimental set up can be supplied with a sampling system for further GC-MS analysis. In this way there are possibilities to quantify the amount of the reactive components in the gas stream. This is particularly important for measurements with compounds with low vapour pressure.

UV absorption spectroscopy has shown a potential for in situ/on line measurements of PAH/tar gas components. The spectra of all gases tend to change their fine structures when temperature increases: the fine structure starts to disappear and absorption bands become broader. Temperature range 250-300C is optimal for PAH/tar measurements when the absorption bands preserve their unique structures and the gas temperature is high enough to prevent condensation on the heavy tars. A DOAS approach can be used for measurements of S-and PAH/tar compounds. The UV absorption extends towards longer wavelengths. This gives possibilities for measurement system simplification and use new (commercially available) UV/LED LED's or Xe-pulsed light sources. Because strong UV absorption an absorption pathlength for in situ/on line measurements can be kept relatively short (few mm). This makes a system quite compact compare to IR-based one. On line measurements can be performed with or without controlled dilution and cooling of the gas. In a "clean" gasification (e.g. high-temperature Viking gasifire) UV absorption spectroscopy shows possibilities to track traces of PAH/VOC/tars/etc. in the producer gas.

In situ and on line UV absorption measurements for phenol (the major PAH in the low-temperature gasification) agree with traditional PAH sampling methods. Moreover the UV measurements give possibilities for particle (black carbon) measurements after some calibration of the system.

At certain combustion conditions (lean combustion) the exhaust gas from the wood stoves contains high concentrations of PAH/VOC and tar which has some similarities with e.g. LT-CFB gasification process.

IR absorption spectroscopy is an excellent tool for measurements of major (CO, CH<sub>4</sub>, CO<sub>2</sub>, H<sub>2</sub>O etc.) gas components. However high water content in the LT-CFB producer gas and its high temperature makes measurements for trace components extremely challengeable. The measurements require a longer path-length (few meters) to reach a low (ppm) detection level. However a strong interference with water absorption structure makes the measurements very difficult.



## Annex

Main papers:

**Hot gas cell for optical measurements on reactive gases:**

<http://www.sciencedirect.com/science/article/pii/S0022407313002835>

**UV absorption cross-sections of selected sulfur-containing compounds at temperatures up to 500°C:**

<http://www.sciencedirect.com/science/article/pii/S0022407314004713>

**UV absorption cross-sections of phenol and naphthalene at temperatures up to 500 degrees C:**

<http://www.sciencedirect.com/science/article/pii/S0022407315000400>

Web sites with UV/IR databases and line lists:

**EXOMOL** web site: [www.exomol.com](http://www.exomol.com)

**HITRAN** web site: <http://www.hitran.org/>

**HITEMP**, high-temperature extension of HITRAN: <http://www.hitran.org/hitemp/>

**MPI-Mainz UV-VIS Spectral Atlas of Gaseous Molecules of Atmospheric Interest:**

[http://satellite.mpic.de/spectral\\_atlas](http://satellite.mpic.de/spectral_atlas)

**Pacific Northwest National Laboratory (PNNL):**

<https://secure2.pnl.gov/nsd/nsd.nsf/Welcome>