**ESA SEOM-IAS – Measurement and ACS database SO2 UV region – Readme**

**Scientific Exploitation of Operational Missions – Improved Atmospheric Spectroscopy Database**

**ESA/AO/1-7566/13/I-BG, http://www.wdc.dlr.de/seom-ias/**

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# General information

Measurements for generation of absorption cross sections (ACS) of SO2 in the spectral range 23000-36000 cm-1 (435-278 nm) within the framework of the ESA project SEOM-IAS were performed by means of Fourier-Transform Spectroscopy (FTS) at the German Aerospace Center. The aim of the measurements was an improved ACS database according to the needs of the TROPOMI instrument aboard the Sentinel 5-P satellite. In this document, all information necessary for further use of the spectra and the resulting ACS are given. A peer-reviewed publication is in preparation, containing all details about the measurement and the analysis. This document will be updated with the reference when available.

## Measurements

FTS transmittance measurements were performed using a Bruker IFS 125 HR high resolution spectrometer (41.8 cm focal length) in combination with a 22.15 cm coolable single pass cell with a maximum optical path difference of 0.3 cm. Details on the cell can be found in [1]. To cover the required spectral range with sufficient S/N two detectors (InGaN (28000-36000 cm-1, as loan courtesy Bruker company), GaP diode (23000-34000 cm-1)) were applied. Measurements of absorption spectra were performed under sealed-off conditions. SO2 was supplied by Linde with a specified purity of 99.98%.

Since SO2 is stable number densities could be derived from absolute pressure measurements. The absorption cross sections have a large dynamic range from 1e-24 – 1e-18 cm^2/molec, requiring a pressure range from 1.0 – 1000 mbar. In total 87 spectra were measured. A calibration factor of 1.000003905 was applied, deduced from the calibration factor of a CH4 measurement around 6000 cm-1 with a correction accounting for the different input aperture diameter.

## Analysis

A multispectrum fitting approach as described in [1] was applied for each of the 6 temperatures in the range 193 – 293 K. Uncertainties in the baseline were reduced by fixing the ACS in the ranges <23500 cm-1 and 24000 – 24400 cm-1 to zero. Uncertainties for each spectral point were propagated from the noise in the transmittance spectra.

In contrast to ozone SO2 showed high resolution features with widths down to the Doppler limit. An error free ACS database would require air broadened measurements with sub-Doppler instrumental resolution. To avoid self broadening SO2 pressures must be below 10 mbar which in turn requires multireflection cell measurements. In principle this could have been done but would have exceeded the resources by far. Thus, it was decided to measure pure SO2 up to 1000 mbar with a moderate resolution of 1.7 cm-1. In order to assess the systematic errors associated with this approach Doppler limited measurements have been carried out as well as self broadened measurements with sufficient instrumental resolution to have monochromatic spectra (not provided here). The impact under conditions relevant to the project was found to be small within the requirements.

Polynomials of 2nd order in temperature (in K) were then fitted to the ACS for each spectral point in the range 25000-36000 cm-1 (400-278 nm). This fit reveals systematic errors and improves the statistical uncertainty. Indeed, a 4th order offset polynomial had to be fitted for the 213 K ACS in the range 25000-30900 cm-1 to reduce the residuals of the temperature dependence fit. The statistical errors of the ACS were propagated into the polynomial coefficients errors and are used together with the chi^2 of the polynomial fit to calculate ACS at about measurement temperatures (see section 1.3).

## Absorption cross sections

The polynomial coefficients in temperature for each spectral point were applied to calculate absorption cross sections at about the measurement temperatures. For each spectral point a statistical uncertainty is given, calculated from the covariance-variance-matrix of the polynomial fit and multiplied by chi. 2% systematic error bars have to be added to account for self broadening/low resolution error.

# Format

## Measurements

Each transmittance spectrum is compiled as a single ASCII file. The filename contains a unique spectrum identification number as well as the filename used in the file system and principal metadata (SO2 pressure (mbar) and temperature (K)). The detector is denoted by the strings “gap” (GaP diode) and “AKE” (InGaN) found in the filename.

The files contain tab-separated values for wavenumber (cm-1), transmittance and noise level (RMS). In the header section the file name and column descriptions with units are given. Each value is given with 10 decimal places.

Example of spectrum file content:

16\_180709so2\_200mb\_3res\_100scans\_ake\_208.052\_234.00.dat

wavenumber (cm-1) transmittance noise(RMS)

28000.3977795892 0.9929888493 0.0001542164

28001.3620138184 0.9924274415 0.0001542533

...

A metadata file associated with each spectrum is provided. The metadata file name is given in the same way as the spectrum with the filename extension \_info.

Example of metadata filename:

[#]\_[orig\_filename]\_[pTarget]\_[T]\_info.dat  
 16\_180709so2\_200mb\_3res\_100scans\_ake\_208.052\_234.00\_info.dat

The metadata file contains as header information the spectrum file name. The metadata is given as follows.

[#]\_[orig\_filename]\_[pTarget]\_[T].dat  
target=[mol]  
partpressure=[pTarget]mb  
totalPressure=[pTotal]mb  
absPath=[absPath]m  
temperature=[T]K  
mopd=[mopd]cm  
aperture=[dInputAperture]mm  
spectral range=[lower limit]-[upper limit] cm-1

## Absorption cross sections

Absorption cross sections at discrete temperatures together with statistical uncertainties are given. The files contain blank-separated values for wavelength (nm), ACS (cm^2/molec) and noise level (RMS, cm^2/molec). In the header section the file name and column descriptions with units are given. The file names contain the temperature in K.

Example of ACS file content:

SO2\_ACS\_233K.asc

wavelength[nm] absorption cross section[cm^2/molecule] uncertainty[cm^2/molecule]

277.7791 7.1688e-019 9.7130e-021

277.7866 7.4233e-019 1.0150e-020

…

Furthermore, in order to allow users to calculate ACS at any desired temperature polynomial coefficients are given, too. The file “ACS\_SO2\_Tpoly\_2nd\_order\_0%\_2nolambda\_213Kbasefit.asc” contains wavelength and polynomial coefficients in the sequence of increasing order in temperature.

277.779124 1.056360e-018 -2.520743e-021 4.565520e-024

277.786564 1.237942e-018 -3.671035e-021 6.626440e-024

…

# References

[1] Wagner G, Birk M. New infrared spectroscopic database for bromine nitrate. J. Molec. Spectrosc. 326, 95-105, 2016. http://dx.doi.org/10.1016/j.jms.2016.03.007