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Quadratic temperature parametrization of ozone X-sections

Recently, Johanna Tamminen made available various ozone X-sections at URL: http://igaco-o3.fmi.fi/ACSO/cross_sections.html as a part of the IGACO-Ozone effort. The data available there are from several laboratory measurements for various sets of temperature. Only Bass-Paur, as we discovered, must have already come from a quadratic equation with respect to temperature. So, the Bass-Paur X-sections at the IGACO-Ozone URL are not from measurements. Our objective was to create a quadratic parametrization for each data set and provide annotation and documentation to maintain a clear chain of data custody.

We downloaded the files on November 2nd and performed the parametrizations by generating wavelength dependent coefficients $c_0(\lambda)$, $c_1(\lambda)$ and $c_2(\lambda)$ that minimize the sum of squared residuals (no weights)

$$\sum_k \left(X(T_k) - X_k(\lambda) \right)^2$$

where

$$X(T) = c_0(\lambda) + c_1(\lambda) \cdot T + c_2(\lambda) \cdot T^2$$

and T is temperature in Celsius and $X_k(\lambda)$ is measured X-section at temperature T_k.

The generated files in the directory *Xsec_T_Parametrized* contain wavelengths in vacuum and air, $c_0(\lambda)$, $c_1(\lambda)$, $c_2(\lambda)$ coefficients, relative residuals in percent

$$rr_k(\lambda) = 100 \cdot [X(T_k) - X_k(\lambda)] / X_k(\lambda)$$

and absolute residuals in optical depth for 300DU

$$ar_k(\lambda) = 10^{20} \cdot 0.26868 \cdot 0.3 \cdot [X(T_k) - X_k(\lambda)]$$

and $RMS(\lambda)$ values of relative and absolute residuals.

The names of files with parametrization coefficients and graphs are listed in the Table 1.

Plots of residuals are available in *Figures* directory. Also two plots of $RMS(\lambda)$ of absolute and relative residuals for all five X-sections were generated: (see *ResidSummary.png* and *ResidSummary.png*).

Note 1: Small residuals of Bass-Paur fits and their behavior (truncation errors oscillations) indicate that the input data from the IGACO-Ozone URL were already generated from a quadratic parametrization.

Note 2: We have also included a file with Bass-Paur quadratic coefficients that is of unknown (to us) provenance. However, we suspect that this file has been widely used within the community of ozone research. No comparison between this file and the newly generate parametrization of IGACO-Ozone Bass-Paur data was performed.

Note 3: Daumont-Brion-Malicet data were parametrized once with all available temperature and once with 273K data removed. The latter approach was suggested by *Liu et al., Atmos. Chem. Phys., 7, 971–993, 2007* who claimed that the 273K data are an outlier. The comparison of residuals in available graphs may verify the severity of this claim.

Note 4: We provided both vacuum and air wavelengths. When input files were in vacuum wavelength we generate wavelength in air and vice versa when the input files were in air wavelength. For conversion we used the modified Edlen formula from NIST at http://emtoolbox.nist.gov/Wavelength/Documentation.asp. We defined the air wavelength as that at 20°C, 101.325 kPa and 0% RH.

Note 5: In some cases the input X-sections for different temperatures were at slightly different wavelength grids. Then we defined the common grid as the grid of the X-section that had the narrowest spectral range. Then the X-sections for other temperatures were interpolated with a cubic spline algorithm into the common grid. The interpolator did not change values of X-sections at the wavelengths also belonging to the common grid.

Note 6: VOB parametrization was performed on 1000mb data only as they appear to be less noisy than 100mb data. Still the noise level in the VOB data is high enough to question the validity of parametrization VOB data at 5cm^{-1} resolution. We think that the VOB data should be smoothed to a lower resolution prior to parametrization. This has not been done.

Table 1. Ozone X-sections from IGACO -Ozone URL and file names (in this directory) with parametrization coefficients and with plots of residuals

Origin	**Acronym**	**Temperatures**	***Xsec_T_Parametrized***	***Figures***
Bogumil-Orphal-Burrows	BOB	203, 223, 243, 273, 293	*O3_XofT_BOB.txt*	*ResidBOB_290_345.png*
Bass-Paur	BP	203, 223, 246, 273, 276, 280	*O3_XofT_BP.txt*	*ResidBP.png*
		Unknown temperatures	*O3_XofT_BP_unknown.txt*	
Daumont-Brion-Malicet	DBM	218, 228, 243, 273, 295	*O3_XofT_DBM.txt*	*ResidDBM_195_345.png* *ResidDBM_290_345.png*
		218, 228, 243, 295	*O3_XofT_DBM_4T.txt*	*ResidDBM_4T_195_345.png* *ResidDBM_4T_290_345.png*
GOME Flight Model (Burrows et al.)	GMFM	202, 221, 241, 273, 293	*O3_XofT_GMFM.txt*	*ResidGMFM_290_345.png*
Voigt-Orphal-Burrows (1000mb)	VOB	203, 223, 246, 280, 293	*O3_XofT_VOB.txt*	*ResidVOB_290_345.png*