Comparison Dobson and Brewer (total ozone):
Effects of Bass and Paur (1995), Malicet et al. (1995) spectral data on seasonal variation

Johannes Staehelin and Barbara Scarnato*

Institute for Atmospheric and Climate Science, ETHZ

** Present address: NASA Ames, Moffett Field, California, USA*

Part of PhD thesis of Barbara Scarnato (funded by MeteoSwiss)

Temperature and Slant Path Effects in Dobson and Brewer Total Ozone measurements

B. Scarnato, J. Staehelin, T. Peter,

J. Gröbner and R. Stübi

J. Geophys. Res., 114, D24303, doi:10.1029/2009JD012349 (2009).

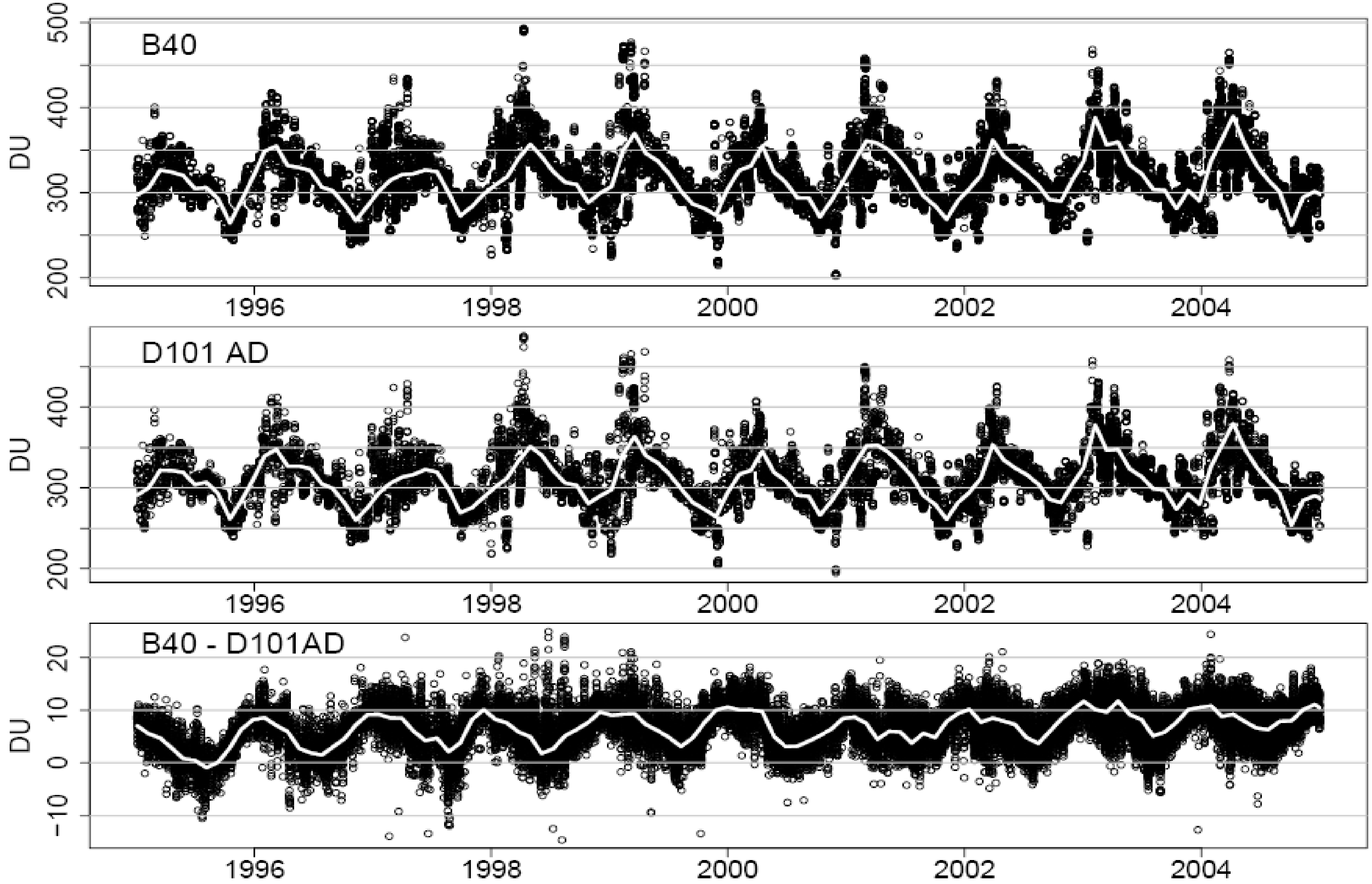
1. INTRODUCTION
Total ozone measurements by Dobson and Brewer instruments at Arosa

operated at Arosa by MeteoSwiss (Rene Stübi)

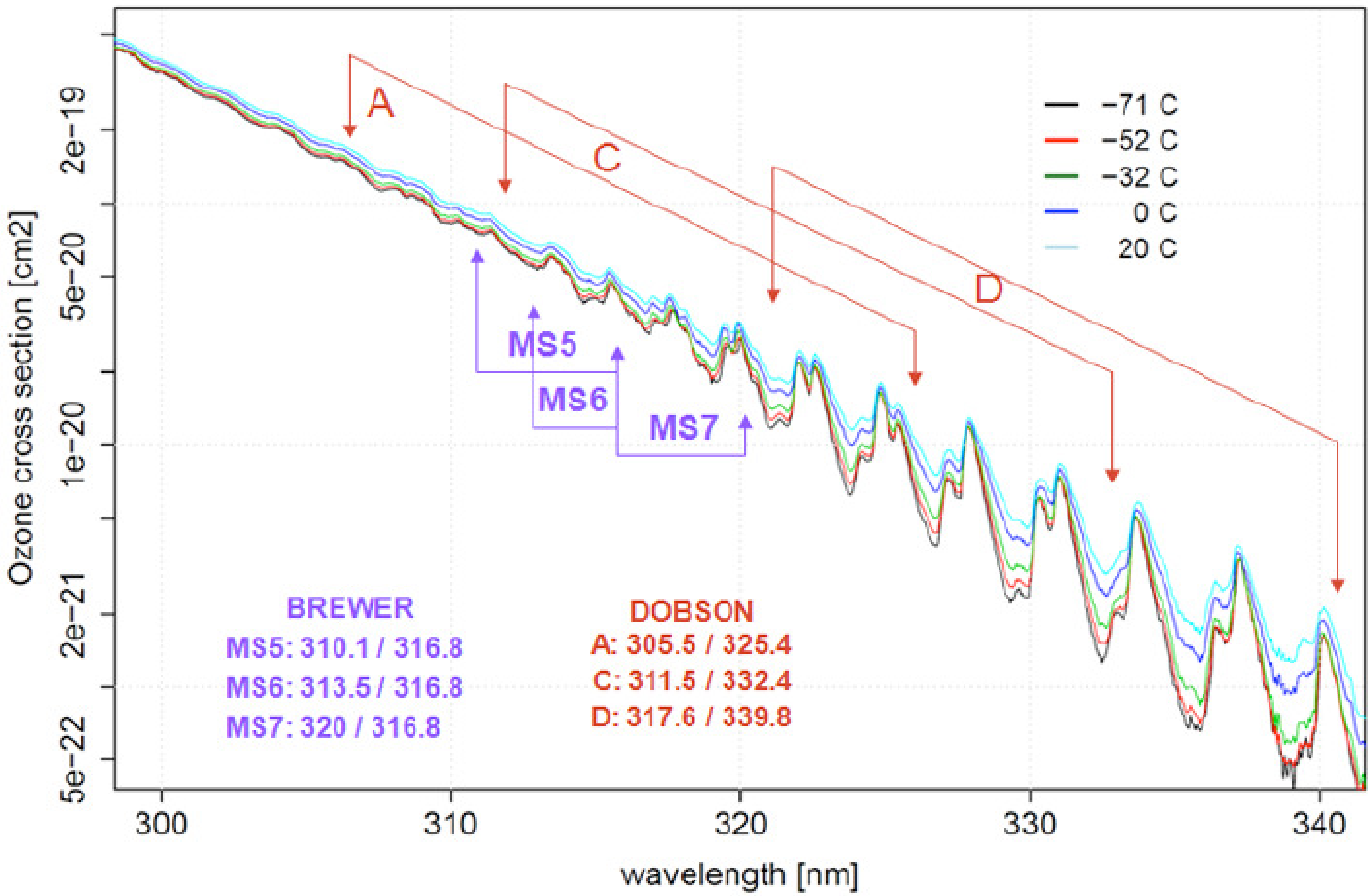
2 Dobson instruments: ***wavelength separation by 2 prisms***

3 Brewer instruments (2 single and 1 double Brewer):
wavelength separation by 1 or 2 holographic gratings

Seasonal variation of difference between Dobson and Brewer at Arosa



Wavelengths of Dobson and Brewer instruments: (main) reason for difference in seasonal variation (e.g. Kerr et al., 1988) ?



2. MEASUREMENT PRINCIPLE OF DOBSON AND BREWER INSTRUMENTS

Intensity at Earth's surf.	Intens. outside atmosph.	Absorption ozone	Rayleigh scattering	Aerosol scattering

$$I(\lambda) = I_0(\lambda) exp(-\alpha(\lambda) X \mu - \beta(\lambda) \frac{p_s}{p_0} m_R - \delta(\lambda) m_a)$$

$$\alpha(\lambda) = \frac{1}{X} \int_{z_0}^{\infty} \sigma(\lambda, T(z)) \rho(z) dz$$

Ozone Absorpt. Coefficient

$$X = \frac{kT_0}{p_0} \int_{z_0}^{\infty} \rho(z) dz$$

Determination Total Ozone

Intensity outside Atmosphere (calibration): Langley Plot Method

Dobson retrieval:

temp. fixed at -46^{o}C

$$X_{A,D} = \frac{N_A - N_D - (\Delta\beta_{AD})\frac{p_s}{p_0}m_R - (\Delta\delta_{AD})m_a}{\mu(\Delta\alpha_{AD})}$$

$$N_A = \ln[\frac{I_0(305.5)}{I_0(325.4)}] - \ln[\frac{I(305.5)}{I(325.4)}]$$

$$N_D = \ln[\frac{I_0(317.6)}{I_0(339.8)}] - \ln[\frac{I(317.6)}{I(339.8)}]$$

$$\Delta\beta_{AD} = [\beta(305.5) - \beta(325.4)] - [\beta(317.6) - \beta(339.8)]$$

$$\Delta\delta_{AD} = [\delta(305.5) - \delta(325.4)] - [\delta(317.6) - \delta(339.8)]$$

$$\Delta\alpha_{AD} = [\alpha(305.5) - \alpha(325.4)] - [\alpha(317.6) - \alpha(339.8)]$$

N: Instrumental Readings: wavelength pair

α_{AD}: absorption coefficient at -46^o

Notation: $w_{i,D}$: (+1,-1, +1,-1) (difference of wavelengths A and D)

Brewer retrieval: temp. fixed at -44^{o}C

$$X = \frac{MS9 - B_1}{\Delta\alpha\mu}$$

$$MS9 = MS5 - 0.5MS6 - 1.7MS7 =$$

$$= \ln[I(310.0)] - 0.5\ln[I(313.5)] - 2.2\ln[I(316.8)] + 1.7\ln[I(320)]$$

$$= F_3 - 0.5F_4 - 2.2F_5 + 1.7F_6$$

$$MS5 = F_5 - F_3$$

$$MS6 = F_5 - F_4$$

$$MS7 = F_6 - F_5$$

$$\sum_i w_i = 0$$

$$\Delta\tau^{aod} = \sum_i w_i \tau_i^{aod} = \sum_i w_i (a\lambda_i) \approx 0$$

$$\Delta\alpha^{SO_2} = \sum_i w_i \alpha_i^{SO_2} = 0$$

W_i: (+1,-0.5, -2.2,+1.7): wavelengths of network (nominal)

$w_{i,ri}$: Instrument related coefficients (in sum. report of calibr. test)

3. DIFFERENCE IN SEASONAL VARIATION

a. Temperature dependence along light path: Ozone effective temperature

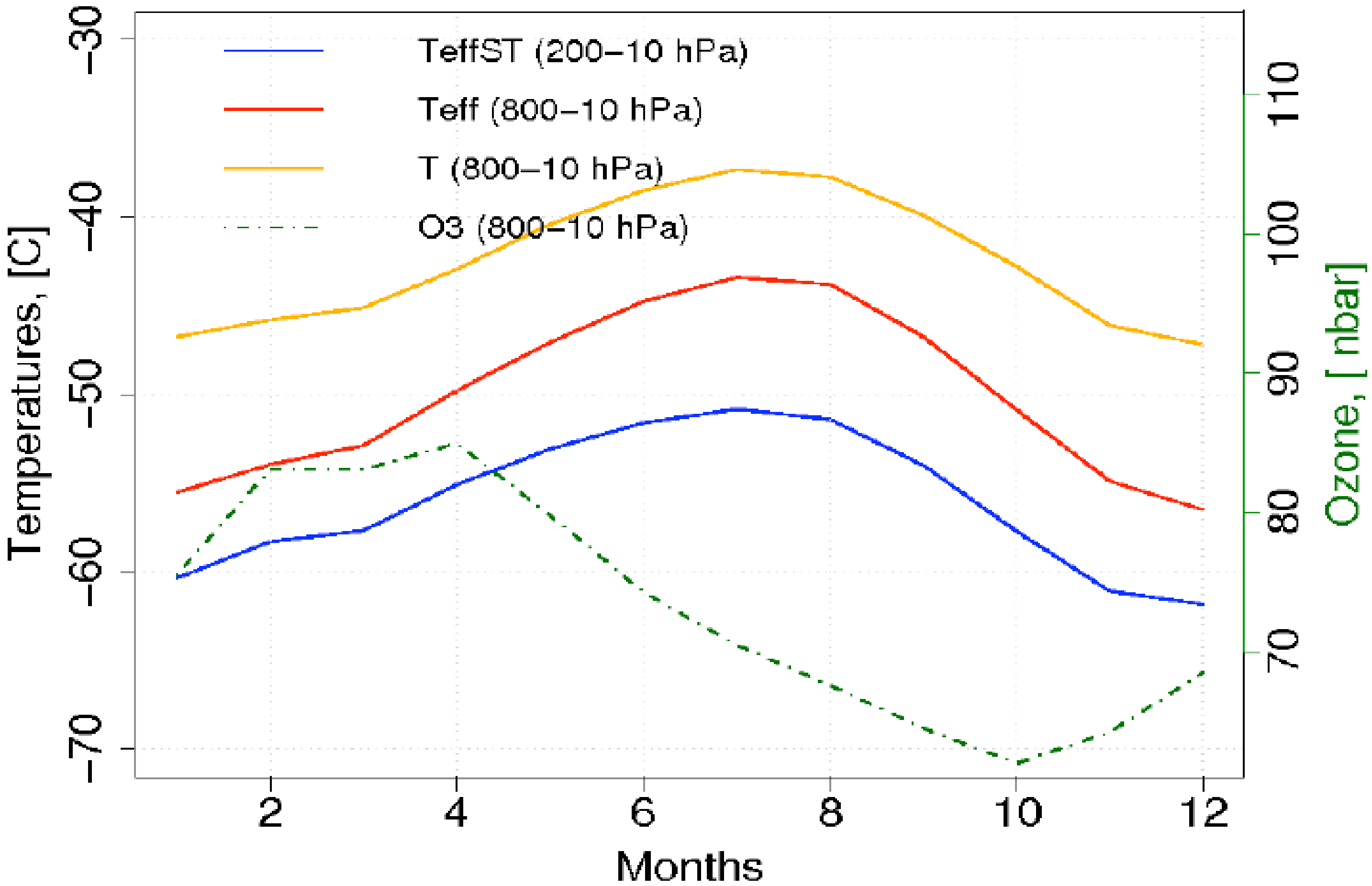
$$T_{eff} = \frac{\int_{800hPa}^{10hPa} T(p) \cdot O_3(p)dp}{\int_{800hPa}^{10hPa} O_3(p)dp}$$

From ozone sondes (Payerne)

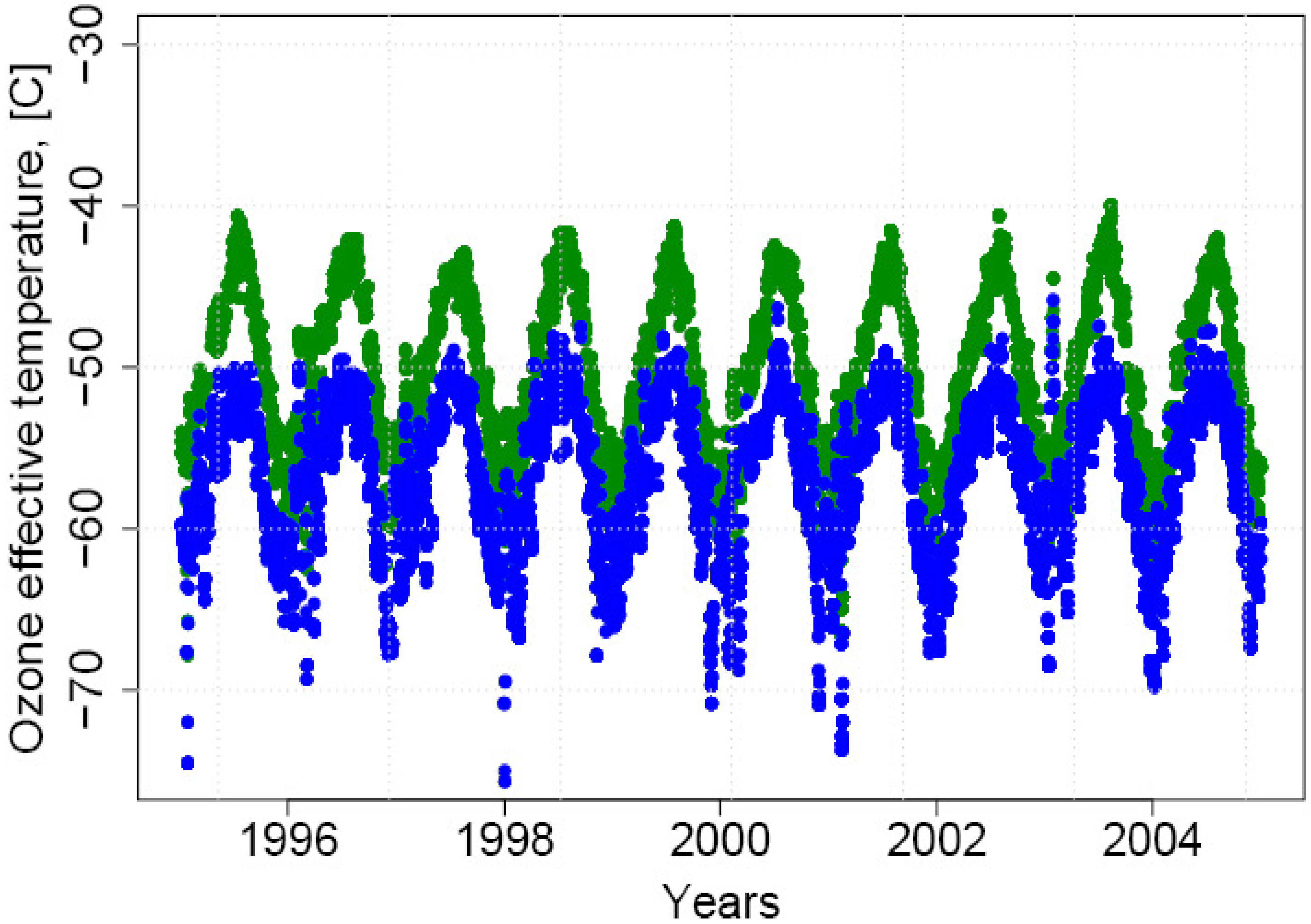
Fitting of temperature dependence of spectra:

$$\Delta\sigma_{O_3,eff}(\lambda, \Delta T) = c_0(\lambda) + c_1(\lambda)\,\Delta T + c_2(\lambda)\,\Delta T^2$$

Seasonal variation of averaged ozone concentration and temperature from ozone sondes of Payerne (1995-2004) and effective ozone temperature T_{eff} and $T_{eff}ST$



Ozone effective temperature (green) and stratospheric ozone effective temperature (blue) (from ozone sondes of Payerne (Switzerland))



b. Weighting optical slit width

Dobson: 2 slits:

- shorter wavelength: triangular shape, with around 1.8 nm
- longer wavelength: trapezoid shape: with around: 5.8 nm

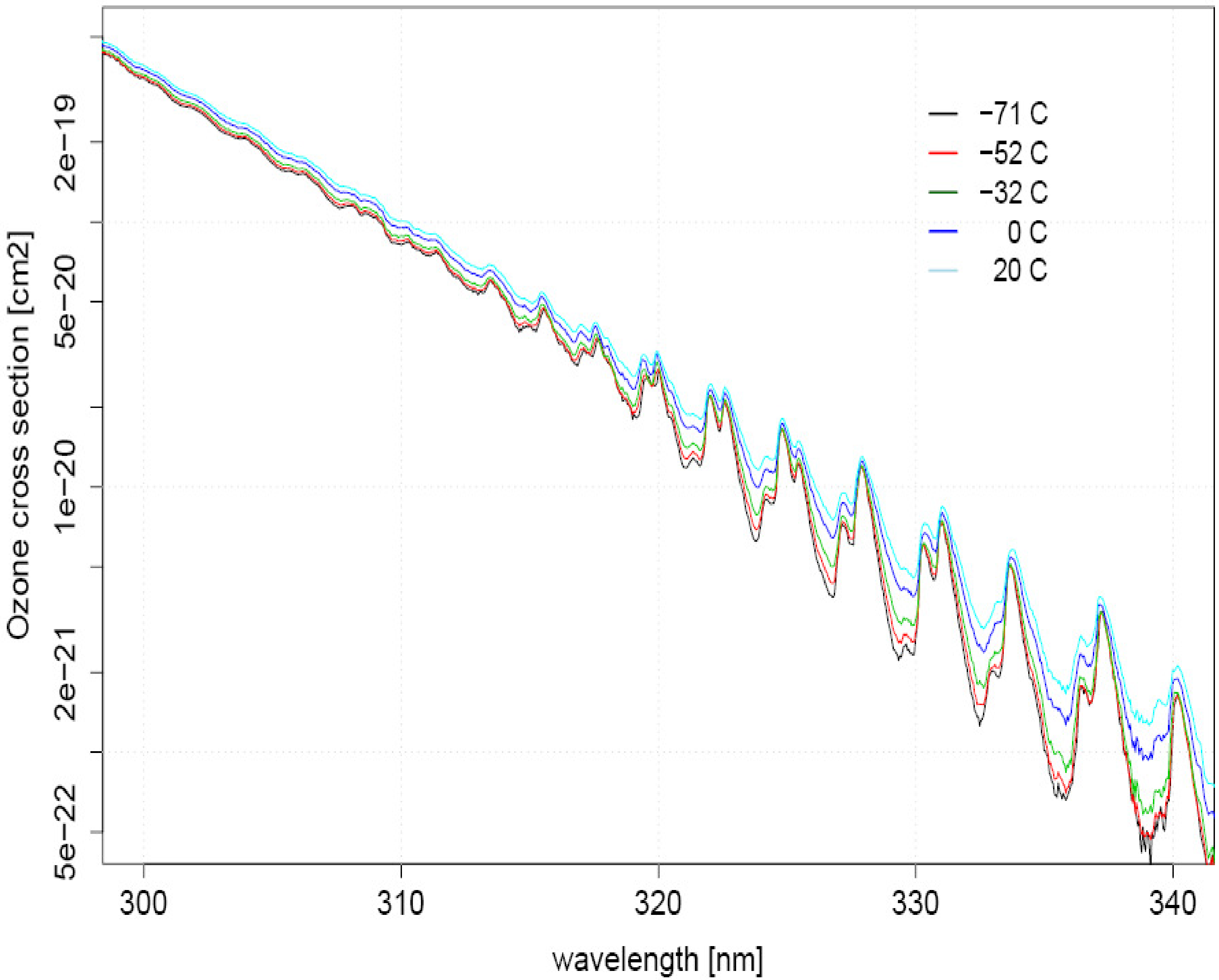
  (Information only available from World Primary Standard Instrument (D83))

Brewer: 6 slits:

- Slit width around 1.2 nm (nearly triangular)

  (Information for individual instruments available from tests)

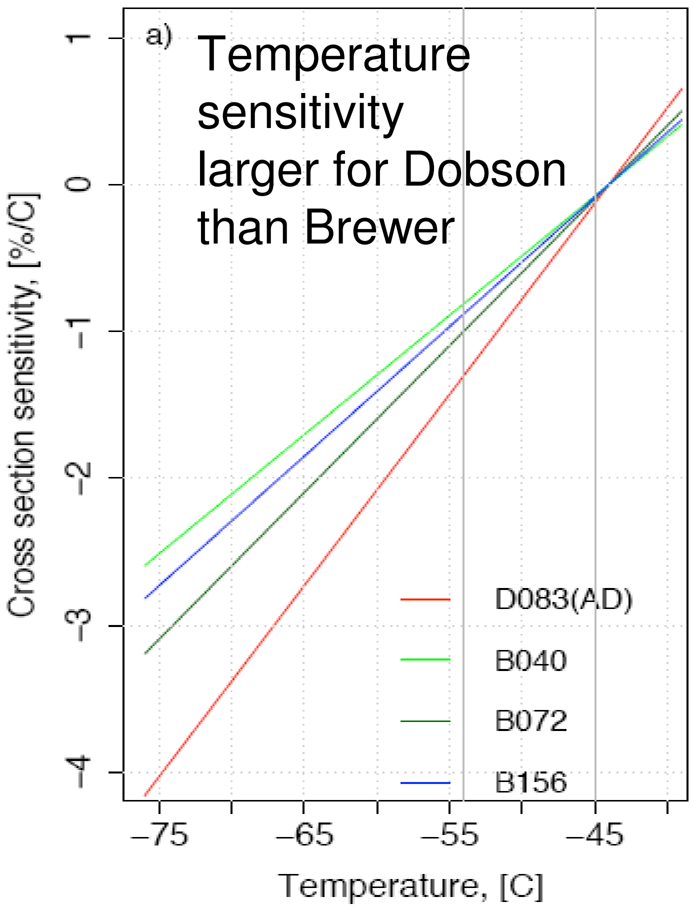
Temperature dependence of ozone cross sections according to Bass and Paur (1985)

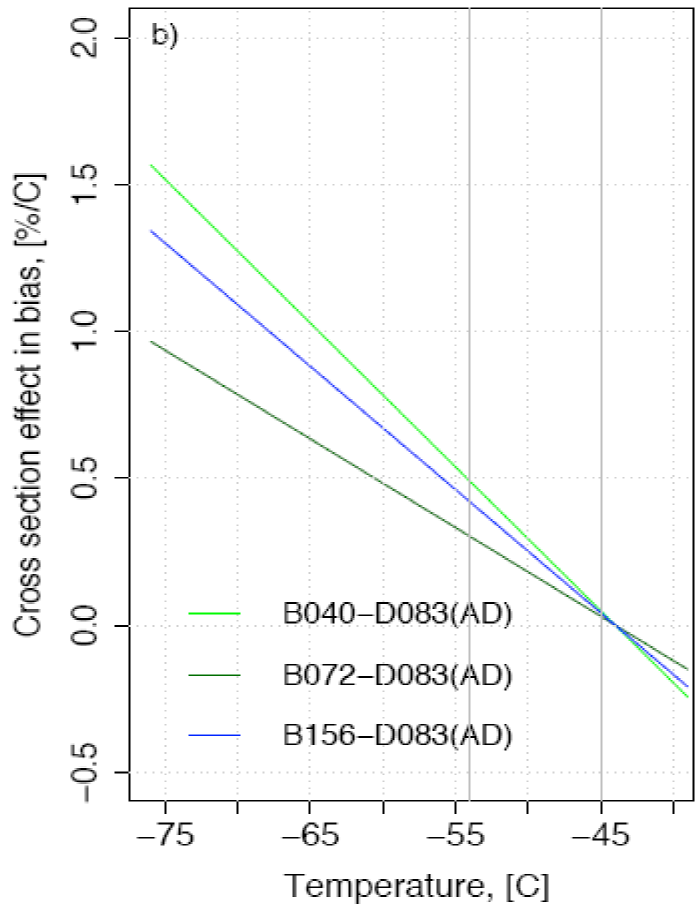


Temperature dependence of absorption coefficients for individual Brewer instruments of Arosa based on Bass and Paur (1985) and using different wavelength weightings

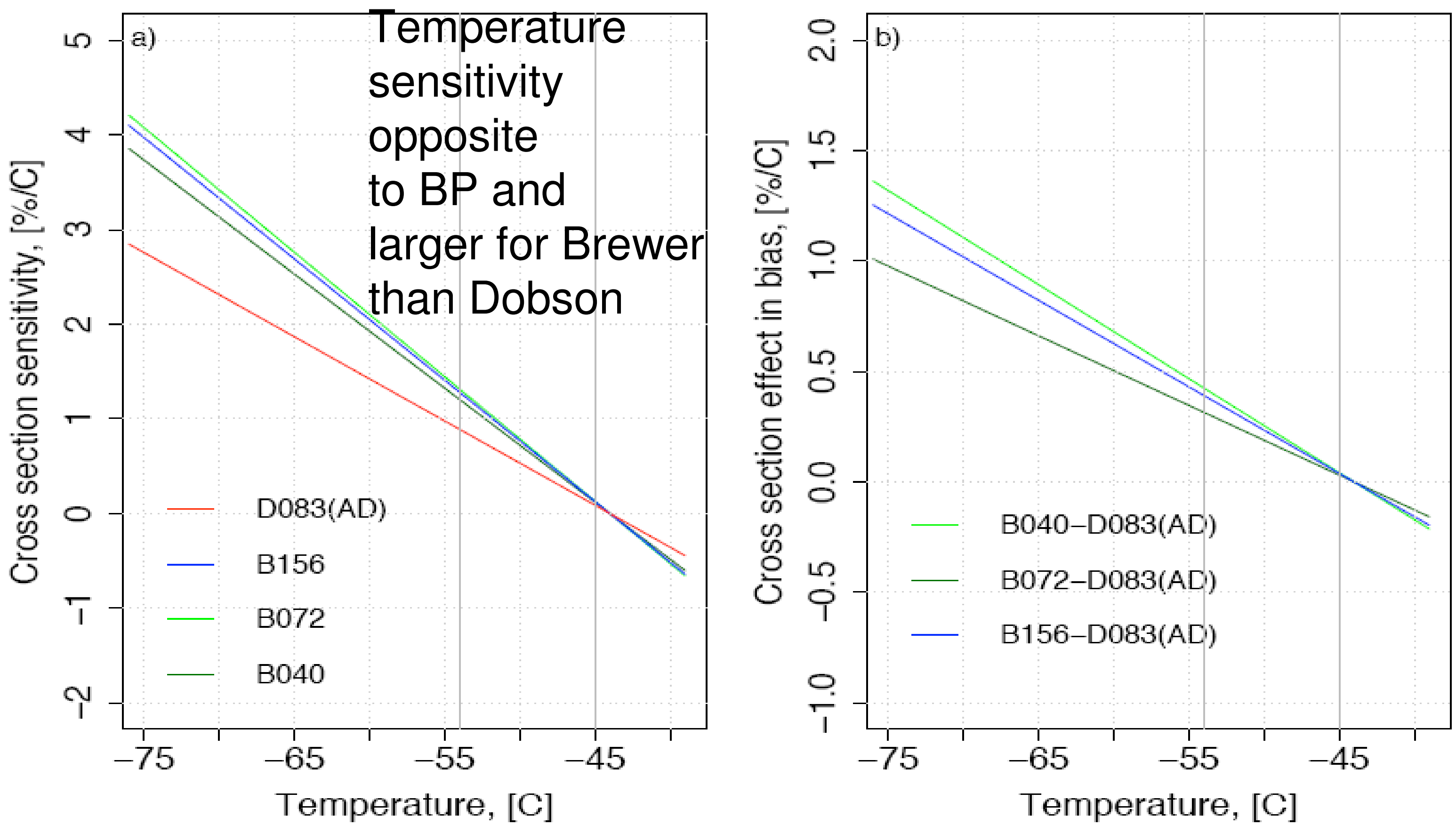
	$\Delta\alpha/\Delta T$, [%/°C]			
	This study	*Kerr et al.* [1988]	*Kerr* [2002]	This study
	All T	All T	5 lowest T	4 lowest T
	w_i, w_{i,r_i}, $w_{i,D}$			w_i, w_{i,r_i}
MKII	(B040) 0.081, 0.001, 0.256	(B014) 0.07	(B014) 0.094	0.226, 0.137
	(B072) 0.099, 0.032, 0.238	-	-	0.249, 0.182
MKIII	(B156) 0.088, 0.033, 0.245	-	-	0.114, 0.111

Left (a): temperature sensitivity of ozone absorption cross sections; right (b): Ozone absorption cross section temperature effect on difference between Dobson and Brewer for instruments operated at Arosa using temperature dependence of **Bass and Paur (1985)**

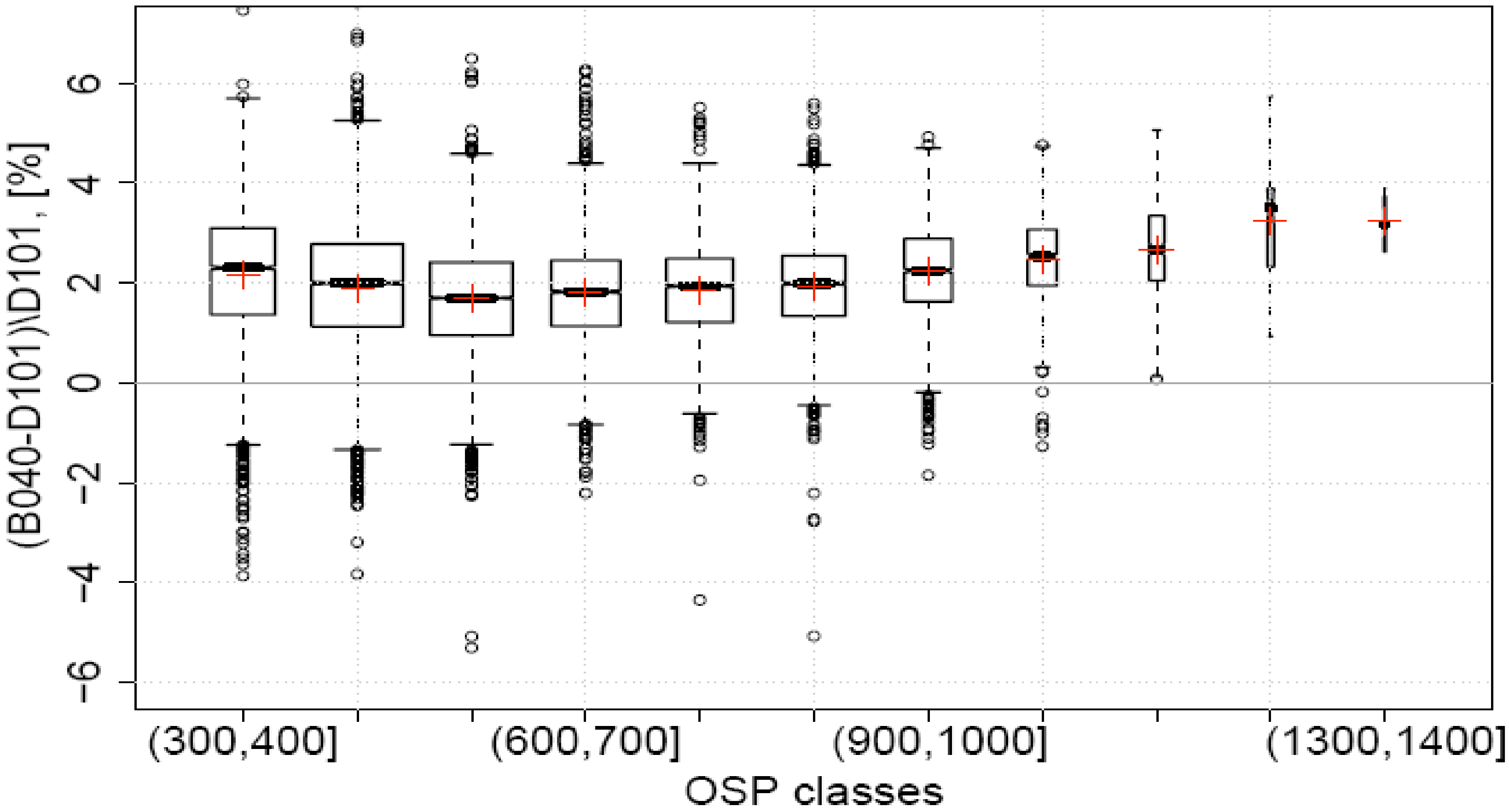




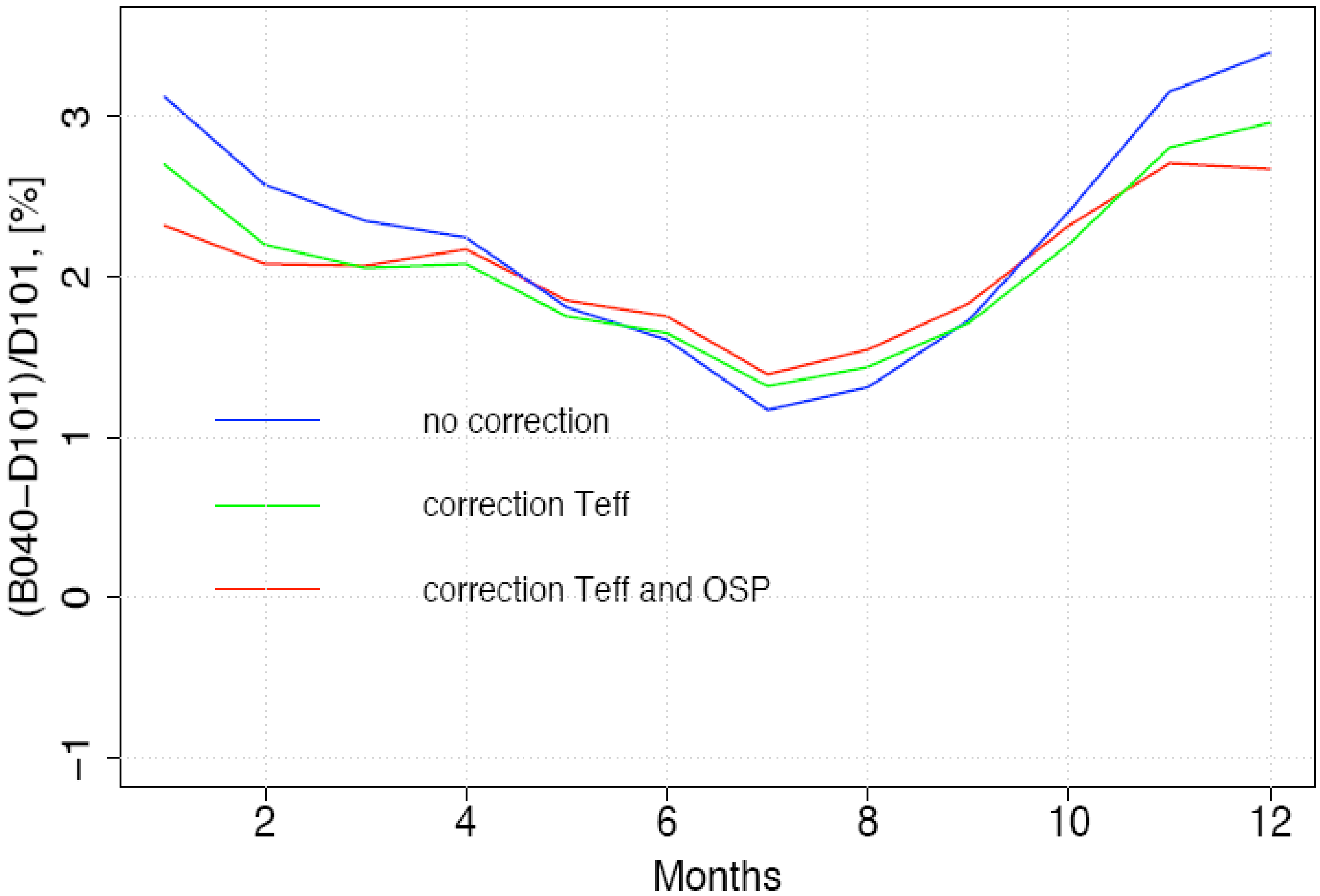
Left: temperature sensitivity of ozone absorption cross sections, right: Ozone absorption cross section temperature effect on difference between Dobson and Brewer for instruments operated at Arosa using temperature dependence of **Malicet et al., (1995)**



c. Attribution of difference of seasonal variability to stray light effects (simple approach: OSP: described by $\mu x O_3$) (grouping of quasi simultaneous measurements according ozone effective temperature)

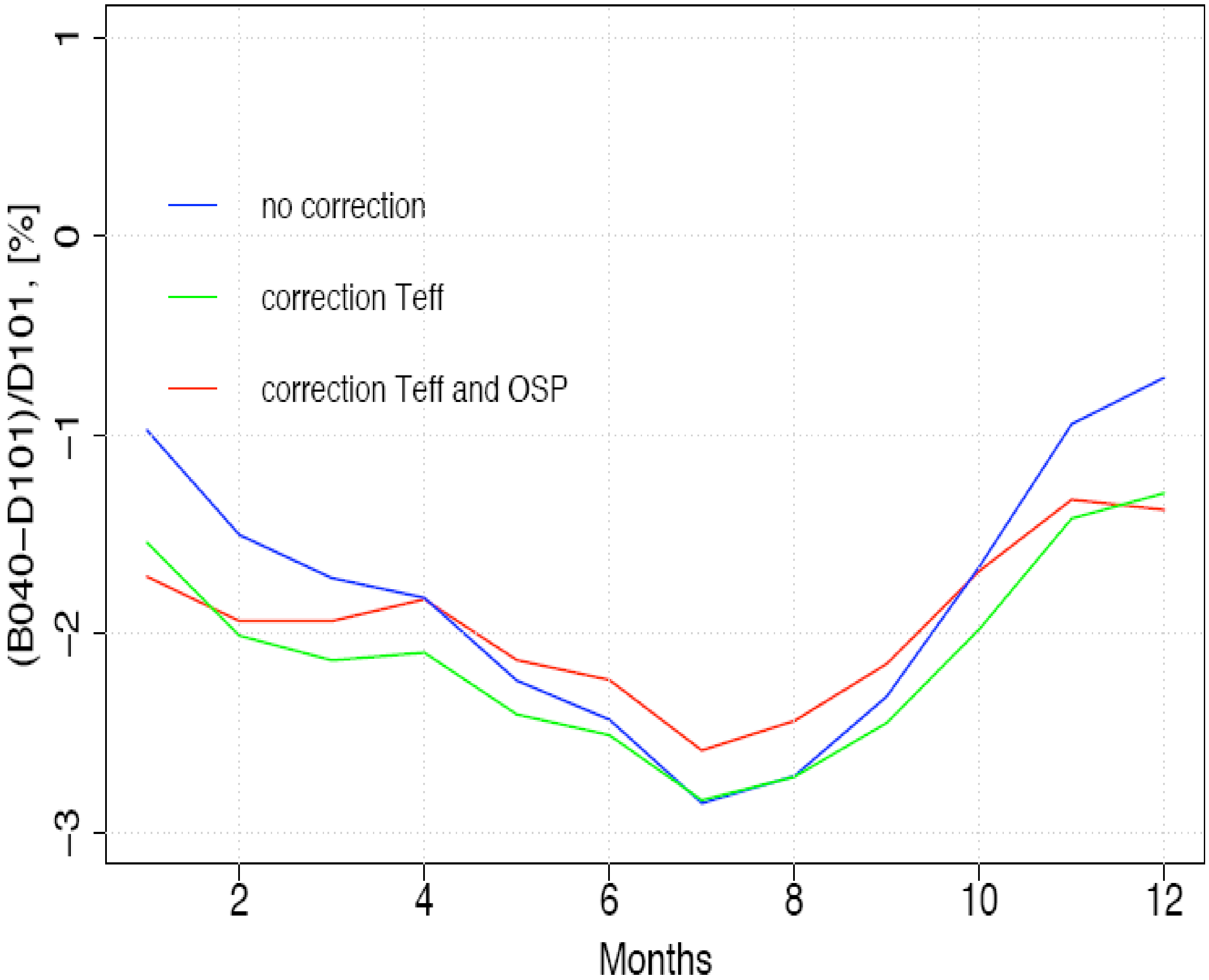


4. ATTRIBUTION SEASONAL DIFFERENCE TO SPECTRAL DATA
Bass and Paur (1985)



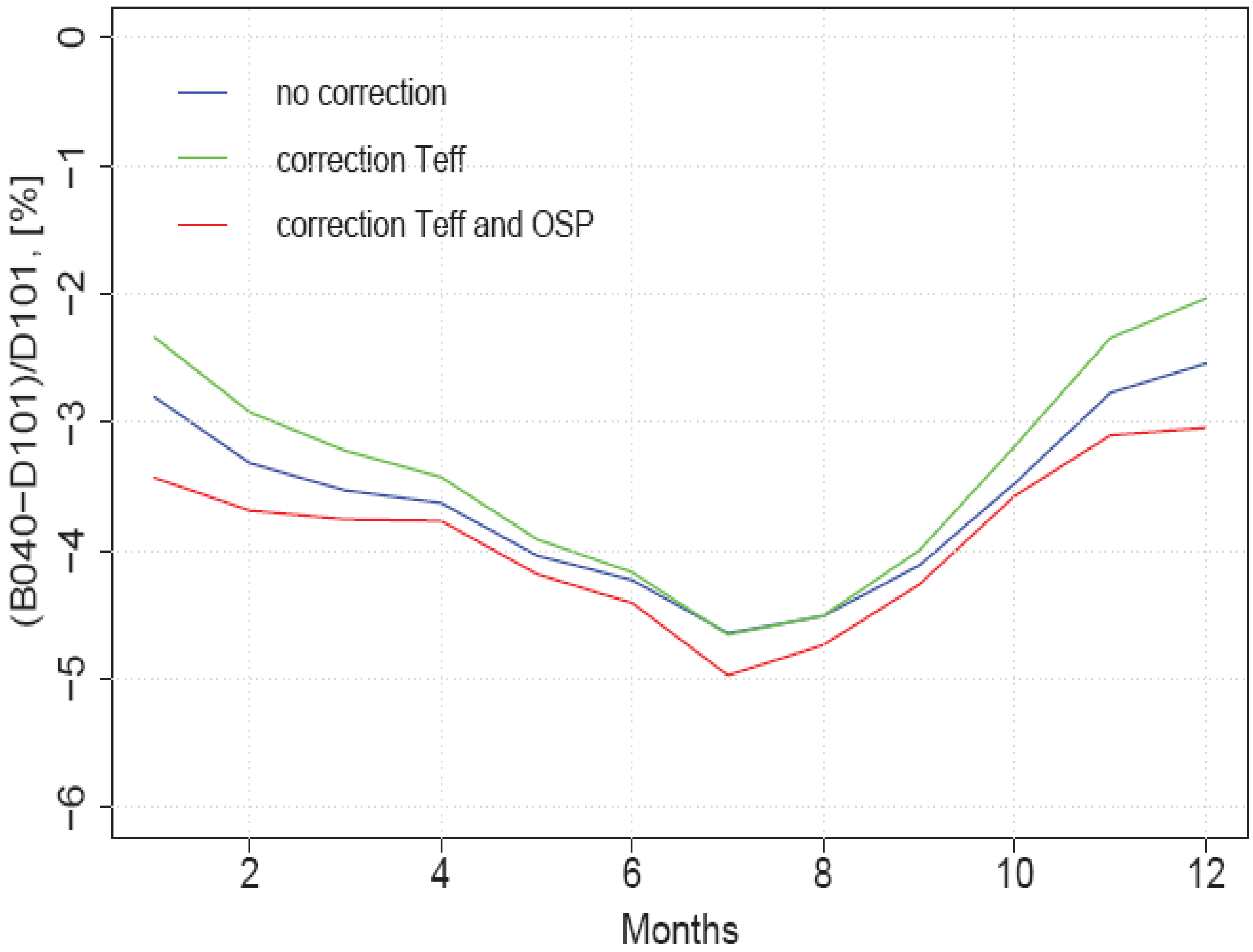
(Rel.) difference of monthly mean values B40 and D101(AD); correction by temperature effect using **Bass and Paur (1985)** plus stray light effects

Malicet et al (1995)



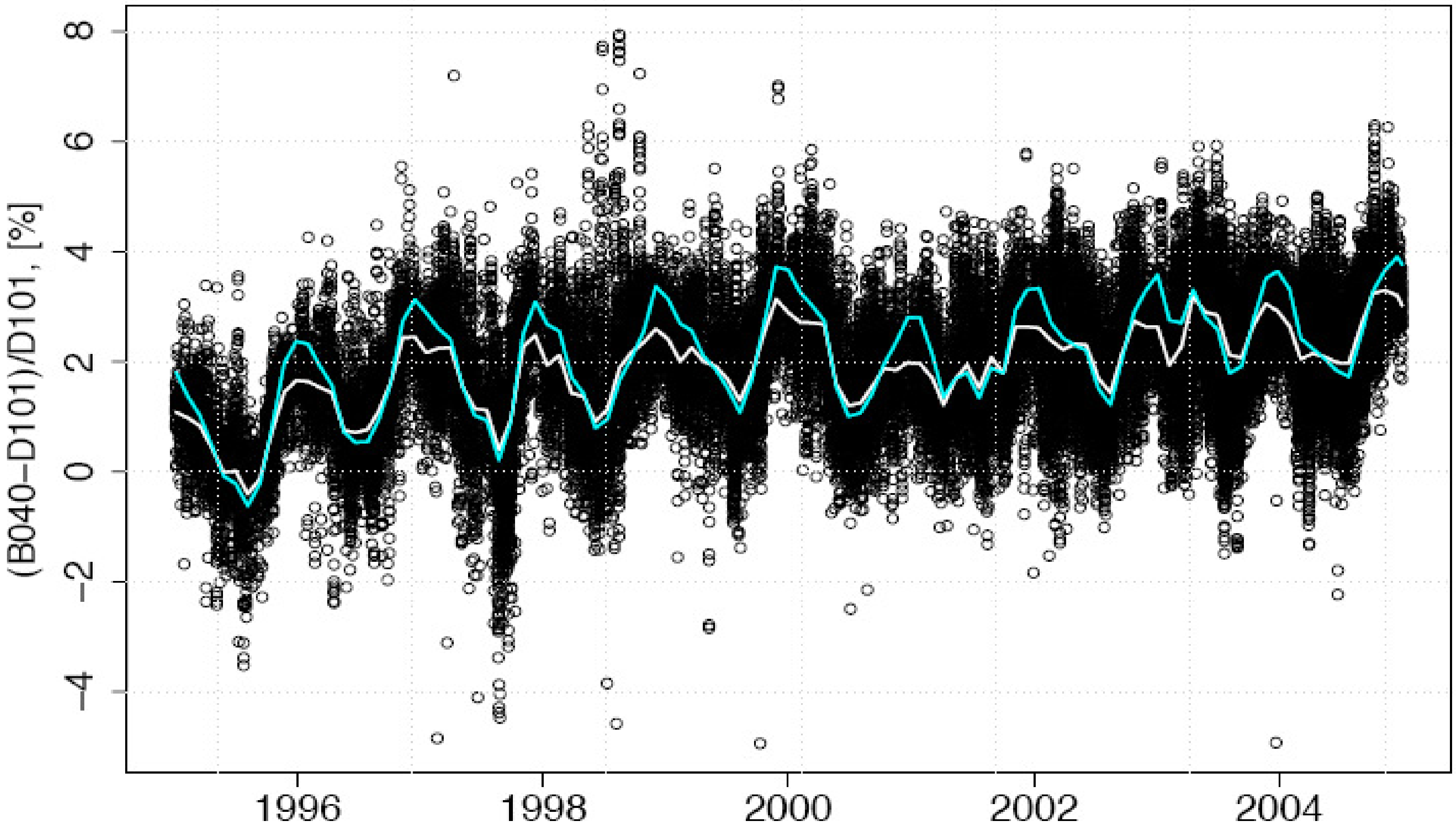
(Rel.) difference of monthly mean values of B40 and D101(AD); correction by temperature effect using **Malicet et al (1995)** plus stray light effects

Burrows et al.1999



(Rel.) difference monthly mean values of B40 and D101(AD); correction by temperature effect using **Burrows et al.1999** plus stray light effects

Part of seasonal difference can be „explained" applying empirical model using BP spectral data and Optical slant path



5. CONCLUSION

„Instrumental Precision“ of well maintained instruments: from large data set of quasi-simultaneous measurements at Arosa (performed within maximally 10 min, 1σ value):

- Dobson AD-observations: ± 0.5%
- Brewer instrument: ± 0.15%

Characteristics of seasonal variation (opertaed at Arosa) depends on instrument type (Dobson vs. Brewer (MKII and MKIII)

Ozone cross sections (including temperature dependence): limiting factor for accuracy of ground-based spectrophotometers

Absolute values unchanged in this study, focus difference in seasonal variation

CONCLUSIONS, cont.

Temperature dependence of BP (85) and Malicet et al. (1995) allow to explain (only) part of the seasonal difference of Dobson and Brewer total ozone measurement

Effect on seasonal variation: temperature sensitivity opposite using Malicet et al. (1995) than BP (85)

Other not well characterized instrumental differences ?

Uncertainty of calibration of station instruments ?

Seasonal (temperature dependent) variability could be included in an extended retrieval algorithm for Dobson and Brewer instruments

Concl.: Instrument related problems: Dobson AD vs. CD observations (Bhartia)

- Komhyr, Mateer, and Hudson, JGR, Vol 98, D11, pp 20,451-20,465, 1993) suggested **an empirical correction to make the Dobson AD and CD double pairs to agree**. Daumont et al. would make the biases somewhat worse. However, Daumont et al. measurements do not support the empirical 2% adjustment to the D-pair O3 absorption coefficients that was made. The key conclusion that is emerging is that there are **uncharacterized errors in either the Dobson slit function, wedge calibration, or internal straylight**. Until these errors are better understood one should assume that the Dobson total O3 accuracy is no better than ~2% and that this accuracy cannot be improved by changing from Bass & Paur to Daumont et al. X-sections.
- However, there does seem to be errors in the temperature dependence of B&P O3 cross-sections. Until these errors are resolved it is premature to correct the Dobson record for variations in atmospheric temperature, as recommended by Komhyr et al..

Instrument's related wavelength weightings of Brewer instruments significantly deviate from values used in network used and calibration

		F_3	F_4	F_5	F_6
w_i		1.00	-0.50	-2.20	1.70
w_{i,r_i}	B040	1.00	0.19	-3.55	2.36
w_{i,r_i}	B072	1.00	0.08	-3.32	2.24
w_{i,r_i}	B156	1.00	-0.06	-3.06	2.12

Large effect of wavelength weightings and used spectral data on ozone absorption coefficients (reported for retrieval temperatures) for Brewer instruments

	$\alpha_{B040}(MS9,-44)$	$\alpha_{B072}(MS9,-44)$	$\alpha_{B156}(MS9,-44)$
	cm^{-1}		
	$\mathrm{w}_i,\ \mathrm{w}_{i,r_i},\ \mathrm{w}_{i,D}$		
Bass and Paur [1985]	0.336, 0.487, 0.414	0.342, 0.473, 0.409	0.347, 0.447, 0.406
Malicet et al. [1995]	0.358, 0.526, 0.394	0.373, 0.511, 0.402	0.372, 0.475, 0.409
Burrows et al. [1999]	0.309, 0.451, 0.421	0.361, 0.497, 0.409	0.344, 0.442, 0.407

Small effect of used spectral data on ozone absorption coefficients (reported for retrieval temperatures) for Dobson instrument (slit width information not available for individual instruments)

	$\alpha_{D083}(AD, -46)$ cm^{-1}
Bass and Paur [1985]	1.421
Malicet et al. [1995]	1.451
Burrows et al. [1999]	1.456

Conclusions: Instrument related problems: Brewer

Brewer instruments very sensitive to (exact) spectral data, Dobson less sensitive (larger slit width, not available for individual instruments)

Weighting coefficients in Brewer algorithms (optimized for polluted conditions) need attention

(retrieval development ?)

Ozone Absorption Coefficients determined by Kerr, from Brewer measurements at Hawaii

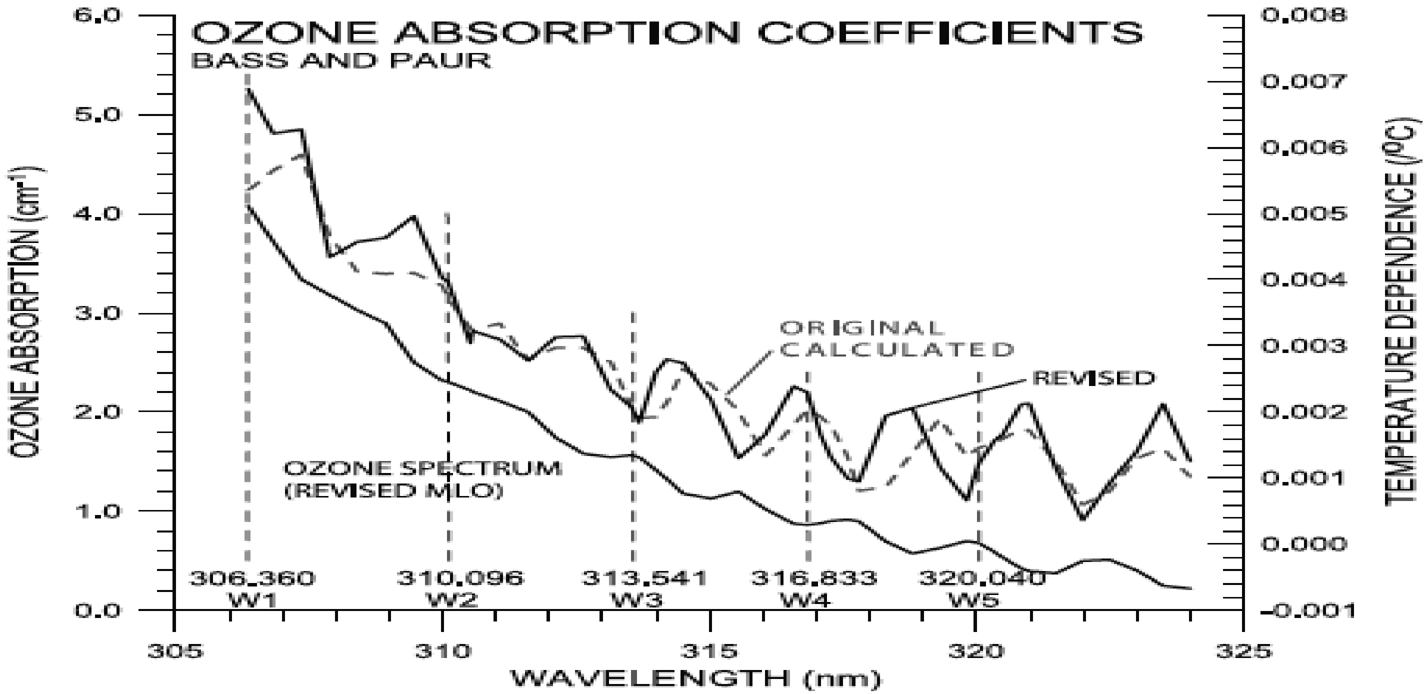
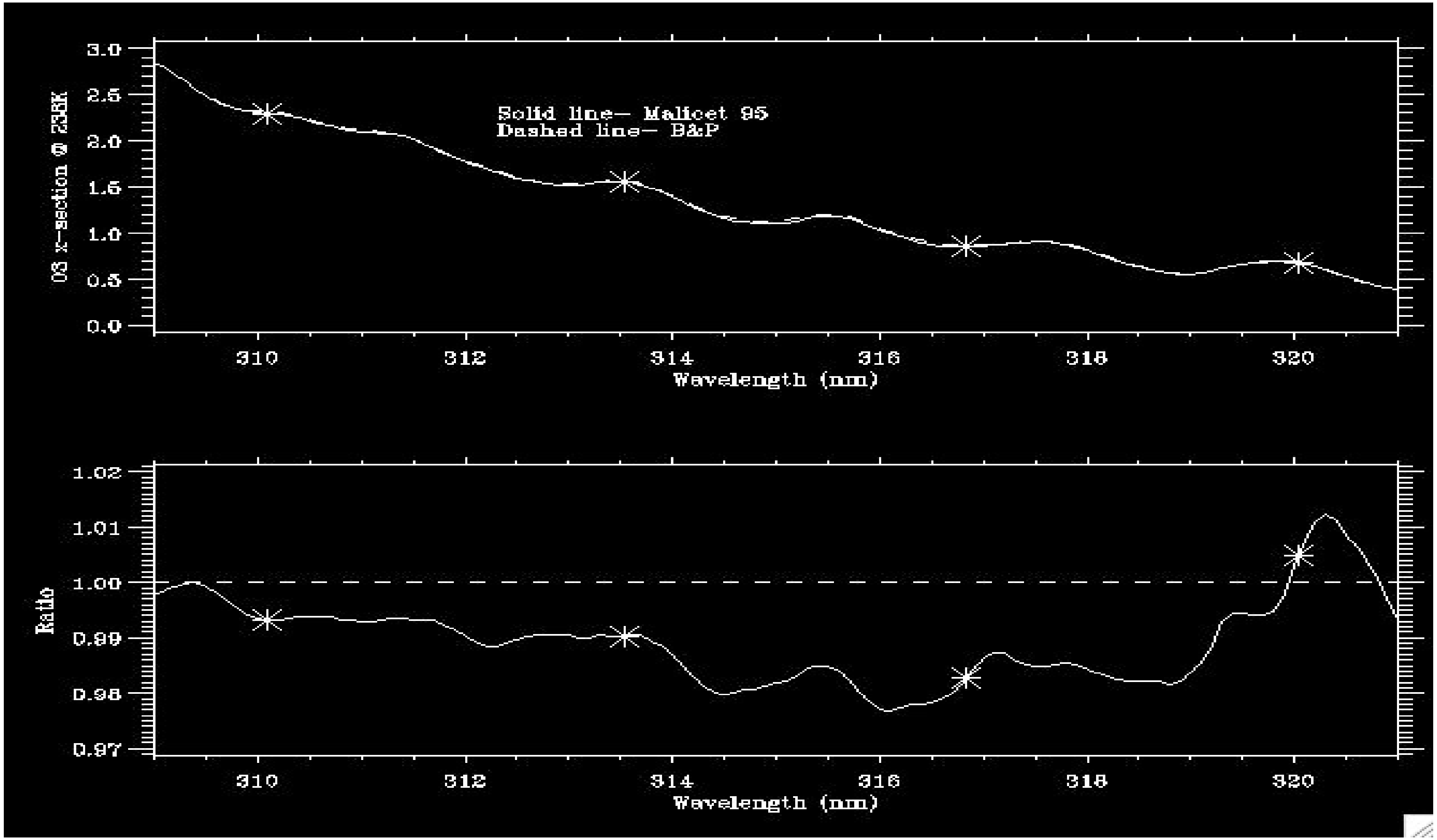


Figure 24. The revised and calculated (from Figure 8) spectra of temperature dependence values with the MLO revised ozone absorption coefficients. There are large differences between the calculated and revised results. The revised set of temperature dependence values show better alignment with the peaks and valleys of the absorption coefficients than do the original temperature dependence values. The normal operational wavelengths for the Brewer instrument are shown.

Difference between B&P and M95, with Brewer wavelengths marked with stars (Bhartia): Difference small, but much larger when propagated through Brewer mechanism (Bhartia)



Suggestions (1) PK Bhartia

(i) Compare the wavelength dependence of the temperature coefficients of ozone absorption cross-sections measured in the laboratory by different groups.

(ii) Evaluate using molecular theory and field measurements, such as Jim Kerr's Mauna Loa study, and analysis of spectral fitting residuals of satellite data.

(iii) Provide a consensus estimate of these coefficients, particularly the slope of the cross-sections with temperature around -45C.

Suggestions (2) PK Bhartia

- Compare ozone absorption cross-sections at -45C measured in the laboratory by different groups, focusing on the 310-350 nm wavelength region where high accuracy is critical for the study of tropospheric ozone and other trace gases for which ozone is an interference. Evaluate using residuals from the spectral fitting of the radiance and irradiance data collected from ground-based and satellite instruments. Provide a consensus estimate.