Interactive comment on “High spectral resolution ozone absorption cross-sections – Part 2: Temperature dependence” by A. Serdyuchenko et al.

Anonymous Referee #2

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General comments:

This paper presents the second part of an extensive laboratory work which aimed at performing new, independent measurements of the absorption cross-section of ozone in a large spectral range, with high spectral resolution, and at an increased number of temperatures compared to already published values. It meets an important requirement expressed by users of ozone cross-sections in terms of data quality and availability of a large set of values. As ozone was produced on site and its concentration assessed by pressure measurements, the results also provide an additional independent dataset so as to progress in the current effort of selection of the most accurate ozone absorption cross-section values. This second paper focuses on the temperature dependence of the ozone absorption cross-section and provides a comprehensive analysis of these results in comparison with published datasets. It is generally well written and supported with appropriate figures of good quality but the structure could be further improved. It was certainly a difficult choice to present this extensive work in one or two papers. The authors have preferred the second choice, which has the advantage of being more structured. However, it has the drawback of leaving room for duplication. There are some in this second paper that could be avoided. In general, more strength on the temperature dependence should appear in this paper, both during the presentations of results and during the comparison with other data. I recommend the publication of this paper in AMT after consideration of the specific comments detailed below.

Specific comments:

(S1) A long discussion on absolute/relative measurements in the literature takes place in the introduction of this paper, while it misses in the first paper. As this part 2 is devoted to the temperature dependence, the introduction should focus much more on this aspect. I suggest moving part of relative/absolute discussion to part 1, while giving more details on the approach chosen by the authors to deal with the temperature dependence in this introduction. The sentence in bracket page 6616 (“details will be given below”) is too short compared to what was done in the paper. Having performed measurements at eleven different temperatures in an extended temperature range while keeping a large spectral range is certainly the strong point of this work and this should be much more highlighted within this introduction. The introduction should also finish on a more detailed description of the sections within the paper.

(S2) Temperature dependence treatment: it is not very clear why the polynomial parameterization was only applied in part of the spectrum, here the Huggins band. Was it considered inappropriate in other bands? In the Hartley band, an alternative model is proposed with the Gaussian profile shifted with temperature. The absence of models...
for other parts of the spectrum should be clarified and some justification provided.

(S3) Terminology: accuracy is normally a concept not expressed with numbers. Consider using "relative uncertainty" or "standard uncertainty" when it relates to a measurement result. Same with the word "error", to be replaced with "uncertainty".

Specific comments on specific parts (page, line):

(6616, 13) The introductory sentence gives the impression that only absolute measurements are accurate. This might not be true, if for example a strong bias on the ozone purity was not detected or any other experimental issue. Consider rephrasing, for example highlighting the good quality of BMD data, the low uncertainty they reached or using another argument.

(6616, 25) Here it is written that absolute measurements were performed in the Hartley band. I am confused as table 1 in paper 1 indicates "relative measurements" in this band. This should be clarified.

(6617, 13-20) the explanation on the pre-cooling of ozone-oxygen mixtures would be better situated in part 1 paper. The use of copper is surprising and more supporting information should be provided to demonstrate that no ozone was destroyed.

(6617, 21-24) calibration is normally performed using a reference. Why "several alcohol thermometers" can be considered as a reference? “the calibration was verified” means that no correction was applied. In the opposite case, the internal sensors were calibrated. What about the Pt-sensors?

(6617, 27) Homogeneity of the cell temperature: would be expected to be dependent on the cell length. Was it the case or so similar that 1% was representative of all cells?

(6620, 2) why the comment that only BMD and Burrows data were measured absolutely?

(6621) Polynomial parameterization: Orphal 2003 proposed three different models and finally recommended a second order polynomial. However this was based on sets of five temperatures. Here eleven temperatures were used, and this provides a stronger test of the different models. Were the two other models tested? Some discussion on the model would be valuable, with some statistical criteria such as the goodness of fit or the residuals standard deviation. This would strengthen the choice of a polynomial.

(6621, 21) clarify the units of all terms in equation 1.

(6623, 2-4) The rationale for limiting the comparison exercise to the spectral range 325 nm to 340 nm should be better stated. I suggest inserting just one sentence and moving the reference to part-1 paper earlier in the section, as more explanation is provided there. Then some duplication with part-1 paper (see next comment) could be avoided and this section could only focus on the temperature dependence.

(6623,10-12) this sentence already appears as such in part-1 paper. Reference to this paper would be sufficient.

(6624) As in part-1 paper, the comparison between new values and BP and BMD data recorded at a different temperature brings some confusion and the value of doing that is not very clear. Once the parameterization of the temperature dependence is demonstrated, comparisons at the same temperature using extrapolation appears meaningful.

(6625) This section starts with the region of minimum absorption (lines 2-11). This should be titled as such, to follow the structure of part-1 paper. In addition part-1 paper goes further in the conclusion, as the new dataset is successfully compared with BDM and Axson data. A consistent conclusion with further comments on the temperature dependency is suggested here.

(6625, 13) An additional title would be helpful, like in part-1 paper :“visible region 450-700 nm”

(6626, 11) Same suggestion to introduce a subtitle “NIR region 700-1100 nm”

(6626, 21) Again, the fact that some published data were scaled to other data is not
a strong argument. It means that those measurements are correlated and have at least the uncertainty of the first published data, but it does not prevent them from being accurate, provided the reference was accurate.

(6626, 25) The comment on a reduced ozone decomposition at low temperatures is interesting. It should also be reflected in the uncertainty budget presented in table 2.

Table 2: contains some inconsistencies with part 1 paper table 2: oxygen purity/oxygen impurity, ozone initial pressure/ozone decay. Why is there a line “temperature measurements” that does not appear in part 1 paper? As for part 1 table, the uncertainties are not constant and this should be dealt with. Compared to part 1, the temperature introduces an additional dependency. The uncertainty could be fitted or the table divided into temperature ranges of the same uncertainty.

Table 3: this table contains a lot of values that are not easy to analyse. Consider replacing with graphs unless the values are meant to be used further by some users.

Figure 4.b) This graph is too busy. What is the goal? If this is to show that a second order polynomial was appropriate, then statistical tools can be used, such as residuals standard deviations. If the authors want to provide the ranges of residuals for each wavelength in the graph, then a table might be more appropriate.

Figure 6: I suggest removing from the figure the data for temperatures that were not reached in this work. Displayed as such, it is confusing: if no extrapolation was done, then there are in fact two temperatures involved (for example 213 K – this work and 218 K-BMD). In addition there are two values for the same dataset (BMD) and the reason is not given.

Editorial/technical corrections:

(6616, 10) consider rephrasing the sentence to avoid the structure “none...fulfils”
(6622, 10) suggestion “The deviations... fits at the wavelengths described above”.