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Interactive comment on “Effects of column density on I_2 spectroscopy and a determination of I_2 absorption cross section at 500 nm” *by* P. Spietz et al.

P. Spietz et al.

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The authors wish to thank the referee and the editor for their comments and suggestions. They helped to clarify the content of the manuscript and its presentation. In the following paragraphs our response to the comments of referee and editor are summarised. As there is some overlap between the two, we structure our response by content rather than by individual remark.

Formal issues:

The usage of differently normalised types of optical density, as present in the first version of the manuscript, was disadvantageous and as it contributed more to confu-

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sion than to clarity we replaced "equivalent optical density" (which was a measure for column density anyhow) by "column density". "Normalised apparent differential optical density" was replaced by "apparent differential cross section", both being quantities commonly used in the context of spectroscopy and DOAS. At the same time this avoids lengthy definitions and explanations. Likewise the usage of "spectroscopic conditions" is now clarified by an appropriate definition. The usage of this terminology is consistent throughout the manuscript. The term "coloured structures", which originates from signal processing and statistical analysis and which has its counterpart in "white noise", i.e. gaussian noise, is also clarified.

In the context of reference spectra of limited resolution the technical origin of spectra is a critical issue. Especially the discrimination between spectra obtained with a Fourier Transform Spectrum opposed to a grating spectrometer is relevant. This motivates the usage of "FTS spectrum" opposed to "grating spectrum". To be consistent with this terminology also spectra obtained with different gratings are referred to by their technical origin as e.g. a "1200 grooves/mm grating spectrum". Therefore in this point we would prefer not to follow the suggestion of the editor to specify the spectra by FWHM, as this neglects the technical origin of the spectrum.

Usage of units for concentration and cross section is changed following the comments by the editor.

The representation of numeric results requires some clarifying remark. The originally intended format for representation of numeric data (cross sections and in some instances also characterisational data of spectrometer and detector) was with the number of significant decimal places as defined by the uncertainty plus a third - reduced in size - to minimise round off errors in further use of the data. This follows a usage, which is common in a number of fields, where estimation theory and statistical analysis are applied. This format was lost in the ACPD specific formatting. For the given reason we would still prefer the originally proposed usage and add a remark to the manuscript, which clarifies this.

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Captions for tables and figures have been trimmed. Missing units (Fig. 8) have been added. Figure 1 is split into figure 1a and 1b for better readability of the inset figure.

Editorial remarks (wording, missing reference) were all taken care of. Corresponding passages were rephrased, missing references and specifications were added.

Content of the manuscript:

The referee pointed out correctly that in applications of remote sensing of I2 the uncertainties due to the unknown distribution of sources are dominant. If in comparison to that the corrections, which could be achieved by consideration of the discussed spectroscopic effects were of the order of only a few percent, it would be questionable, why one should bother about them at all. However, a systematic error of up to 13% for spectroscopic reasons is sufficiently substantial that it should be considered, wherever this could be done with reasonable efforts. Only then it is ensured that the basis for any subsequent conclusions, including those on the inhomogeneous I2 distribution itself, is reasonable and sound. A corresponding remark is added to the manuscript.

Another practical question was raised by the editor about how a suitable reference spectrum can be practically chosen if no a-priori knowledge exists about the I2 column density that is to be expected in the atmosphere. As the effect of column density was shown to be of the order of somewhat more than 10%, an approximate knowledge of the target optical density can be obtained by neglecting this effect, just as it was done for I2. In a second step the improved reference spectra at target column density can then be determined to improve the atmospheric retrieval. This is now mentioned in the discussion of spectra.

Both referee and editor stated that the manuscript is too long and needs trimming. By rephrasing different passages and e.g. by restructuring and shortening the sections on reference spectra, their comparison and discussion the length of the manuscript was reduced and its readability improved. Also the passage on correction of deposit on windows in the determination of the cross section of I2 at 500nm is rephrased, simpli-

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fied and clarified. In this context the spectral range of the spectroscopic measurement appeared to having been unclear and possibly misleading. The broad spectral coverage of 340 to 660 nm, which enables the multiple multivariate linear regression for separation of the gas phase I2 spectrum and that of the deposit (solid phase) on the windows, is explicitly pointed out in this context.

A remark to the linear regression used to determine the absorption cross section of I2: This linear regression explicitly takes into account errors in both coordinates, see Numerical recipes (Press et al. 1986: Chapt. 15.3). Therefore the error estimate obtained from this is neither error propagation (considers only error in one coordinate) nor from residual scatter. Rather it is a regression which rigorously takes into account an error in the observations and an error in the coefficients of the least squares model. The scatter of the observational data points themselves feeds into the least squares model via the residuals. The error estimate therefore contains the uncertainty of both axes of the observational data and the scatter of the individual data points with respect to the linear fit. This is clarified in the text now.

Interactive comment on Atmos. Chem. Phys. Discuss., 5, 5183, 2005.