OCO (Orbiting Carbon Observatory) -2

ABSCO User Guide

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Revision History

Revision Date	Changes	Author
3 December 2013	Initial Release of “Spectroscopic Needs for OCO-2”	V. Payne
4 March 2016	Updated for ABSCO v5.0, now named “ABSCO User Guide”	V. Payne
14 March 2017	Updated CO2 scaling recommendation for SCO2 and updated references	V. Payne
24 July 2017	Updated to indicate that ABSCO v5.0 utilized in version 8 Level 2 algorithm	V. Payne
25 February 2022	Updated for ABSCO v5.2, utilized in version 11 Level 2 algorithm. Include information on ABSCO v5.1, utilized in version 10 Level 2 algorithm.	F. Oyafuso

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Table of Contents

1 Introduction

1.1 Scope and Background

This document is intended to provide an overview of the v5.2 ACOS/OCO-2/OCO-3 absorption coefficient (ABSCO) tables, key features and issues and potential directions for future research.

The ACOS/OCO-2/OCO-3 ABSCO tables are "lookup tables" that supply cross section values for absorbing gases in the Level 2 algorithm (L2) retrieval process. They record molecular absorption cross-sections over the range of relevant wavelengths, temperatures, and pressures in units of cm^2/mol for the gases O_2, H_2O, and CO_2. During the L2 generation process the retrieval algorithm computes atmospheric absorption at each relevant temperature, pressure, and wavelength using linear interpolation. Successive versions have refined these tables by incorporating new laboratory results and theoretical models for increasingly accurate absorption coefficients. ABSCO tables are released together with each major build of the OCO-2 Level 2 algorithm. At the date of preparation of this document, publicly available Level 2 products for the duration of the OCO-2 and OCO-3 missions are derived using the version 10 algorithm, which employs ABSCO v5.1. Starting in March 2022, OCO-2 forward data processing will switch over to version 11, which uses ABSCO v5.2 tables. The OCO-2 Level 2 record will eventually all be reprocessed using version 11 (ABSCO v5.2). Version 11 reprocessing for OCO-3 is also planned as part of the end of life mission activities after that instrument leaves the International Space Station. We recommend usage of these most recent tables.

The tables can be computed at a spectral resolution of 0.002 cm^{-1} (required for validation of the tables using high resolution laboratory spectra) but the current L2 retrieval code uses a spectral resolution of 0.01 cm^{-1}.

1.2 Document Overview

Section 2 describes the absorption cross-section computation, while Section 3 describes the format of the ABSCO HDF files.

1.3 Data Usage Policy

The OCO-2 ABSCO tables are provided freely to the public, on request. We request that when publishing using the tables, please acknowledge NASA and the ACOS/OCO-2/OCO-3 projects.

- Include OCO-2 and/or OCO-3 as a keyword to facilitate subsequent searches of bibliographic databases if it is a significant part of the publication
- Include a bibliographic citation for the tables. The most relevant citations are Payne et al. (2021) for the O2 A-band and Devi et al. (2016) for the 1.6 μm weak CO2 band. There is currently no documentation for the 5.2 version of the ABSCO table for the 2.06 μm (strong) CO2 band. For the time being we recommend citation of the previous 5.0 and 5.1 versions of this table (Benner et al. (2016)).
- We recommend sending courtesy copies of publications to the OCO-2 Project Scientist, Vivienne.H.Payne@jpl.nasa.gov.

2 Absorption cross section computation

This section describes the studies providing line parameters for each of the main absorbing gases. Due to the modular nature of the ABSCO calculation, different bands rely on different codebases to compute the absorption cross sections. The LABFIT codebase from Benner (2011) provides cross sections for the primary absorbers of interest for the OCO-2/3 missions (CO_2 and O_2). For ABSCO v5.2, we implement databases from Payne et al. (2021) and Devi et al. (2016) for the O_2 A-band and the 1.6 μm CO_2 band, respectively. For the 2.06 μm CO_2 band the database previously used in ABSCO v5.0 and v5.1 (Benner et al. (2016)) has been updated by a new LABFIT parameterization employing a different line mixing formulation. The procedure and modeling assumptions for the ABSCO calculation are detailed at greater length in Thompson et al. (2012). The only molecular interferent within the spectral windows measured by OCO-2 is water. For H_2O cross sections, a simple Voigt profile is used using the ATM18 (v2020-05-12) linelist created by Toon (https://mark4sun.jpl.nasa.gov/toon/atm18/atm18.html) along with the MT_CKD v3.2 continuum model.

In v5.2, the table format is a four-dimensional array to accommodate an additional "foreign broadener gas" dimension. This allows cross sections to be parameterized by temperature, pressure, and the volume mixing ratio of one other atmospheric gas. All tables are provided in this 4D format, though the calculations only incorporate broadening by H_2O of O_2 and CO_2. CH_4 tables using the HITRAN line list are now also available; they are computed over both CO_2 spectral windows. The temperature range has 17 levels, centered about a different nominal temperature at each pressure level, and is intended to cover extremely low (terrestrial) temperatures. Table 1 below gives more detailed information on several key parameter sources.

2.1 Scaling of absorption cross-sections

The ABSCO v5.2 tables are used in the version 11 OCO-2 Level 2 algorithm. The scaling information provided here is based on recommendations from the ABSCO team.

The O2 table used in ABSCO v5.2 is identical to that used in v5.1. It is described in Payne (2021) and was generated using the methodology described in Drouin et al (2017). No scaling factors were applied in the generation of this table. However, retrieved surface pressures using both ground-based FTS spectra and OCO-2 data both find small positive biases on the order of several hPa. Consequently, in both the versions 10 and 11 of the OCO-2 Level 2 algorithm a *post hoc* scaling factor of 1.0048 is applied to the published O2 table.

The cross sections for the 1.6 μm (weak) CO2 band have remained unchanged since ABSCO v5.0. They were determined from the Devi et al. (2016) database, then subsequently scaled by a constant factor of 1.014. This number represents a ratio between line intensities in the Devi et al. (2016) database and reference intensity measurements from our NIST ABSCO team members, described in Polyansky et al. (2015). In tests using single-band XCO2 retrievals from ground-

based FTS spectra, we find that application of this constant scaling results in improved agreement between our single-band retrievals and the XCO2 values reported by the Total Column Carbon Observing Network (TCCON). For the 1.6 μm band, this scaling factor is already factored into the ABSCO v5.2 tables.

The previous version of the 2.06 μm (strong) CO_2 band cross sections used in ABSCO versions 5.0 and 5.1 were generated from the Benner et al. (2016) database. Based on reference intensity measurements made by Zak et al. (2016) and single band retrievals from both ground-based FTS spectra and OCO-2 measurements, an approximate scaling of the published ABSCO table by a factor of 1.004 was recommended for that table. The most recent version of ABSCO (v5.2) for the strong band has been determined from a new fit of the same spectra that were used in the previous iteration of ABSCO. However, instead of a nearest neighbor formulation ABSCO 5.2 utilizes a full relaxation matrix characterization of the line mixing for the strong band based on work by Lamouroux (2014). This new fit also incorporates an estimate of reference intensities based on preliminary results that were subsequently reported in Fleurbaey (2020). In that work, new measurements were fit to a scaling of the ab initio intensities reported in Zak (2016). The ab initio intensities described in Fleurbaey (2020) have since been found to be 0.05%-0.10% lower than those used in ABSCO 5.2. However, single band retrievals performed with ground-based TCCON spectra showed XCO2 values more than 0.1% lower (0.2-0.6%, depending on airmass) than those obtained from single band retrievals using the weak CO_2 band. These results point the need for an additional, user-specified reduction in these cross sections.

Based on additional testing using OCO-2 satellite observations, a decision was made to apply scalings of 0.994 and 0.9875 to the weak and strong bands respectively to the ABSCO v5.2 tables used in the version 11 algorithm. The choice of factors applied within the Level 2 algorithm, was made to (1) mitigate an overall persistent bias in the retrieved XCO2 and (2) aim for consistency between single-band estimates of XCO2. (For version 10, the scaling factors applied within the Level 2 algorithm to ABSCO v5.1 tables were 1.000 and 1.004 for the weak and strong bands, respectively. However, for that version, no effort was made to account for the overall persistent bias of retrieved XCO2 through spectroscopic adjustments.)

Finally, the H_2O tables derive from the 2020-05-12 version of the ATM18 linelist provided by Geoff Toon (https://mark4sun.jpl.nasa.gov/toon/atm18/atm18.html). Based on both ground-based and satellite measurements, it was found that while single band retrievals of water column using the weak and strong bands are consistent, the total column water vapor had a systematic low bias of ~2%. Thus, the ABSCO 5.2 water vapor tables based on ATM18 incorporate a scaling of 0.981, applied in the generation of the tables. No additional adjustment of these tables is recommended.

Table 1: ABSCO v5.2 (Level 2 v11)Parameter Sources

	0.76μm O_2	1.61μm CO_2	2.06μm CO_2	H_2O
Spectral range	12745-13245 cm^{-1}	4700-6500cm^{-1}	4700-6500cm^{-1}	12745-13245cm^{-1} 4700-6500cm^{-1}
Spectral resolution	0.01cm^{-1} or 0.002cm^{-1}	0.01 cm^{-1} or 0.002cm^{-1}	0.01 cm^{-1} or 0.002cm^{-1}	0.01 cm^{-1} or 0.002cm^{-1}
Line parameters	Payne (2021)	Devi (2016b)	Drouin (not yet published)	Toon (2018)
ABSCO scaling	1.0048 applied within OCO-2 v11 algorithm	1.014 included in generation of tables; additionally, 0.994 is applied within OCO-2 v11 algorithm	0.9875 applied within OCO-2 v11 algorithm	0.981 included in generation of tables
Continuum	Payne (2021)	-	Thompson et al. (2012)	MT_CKD v3.2

Table 2: ABSCO v5.1 (Level 2 v10) Parameter Sources

	0.76μm O_2	1.61μm CO_2	2.06μm CO_2	H_2O
Spectral range	12745-13245 cm^{-1}	4700-6500cm^{-1}	4700-6500cm^{-1}	12745-13245cm^{-1} 4700-6500cm^{-1}
Spectral resolution	0.01cm^{-1} or 0.002cm^{-1}	0.01 cm^{-1} or 0.002cm^{-1}	0.01 cm^{-1} or 0.002cm^{-1}	0.01 cm^{-1} or 0.002cm^{-1}
Line parameters	Payne (2021)	Devi (2016b)	Benner et al. (2016)	HITRAN 2012
ABSCO scaling	1.0048 applied within OCO-2 v10 algorithm	1.014 included in generation of tables, Based on Polyansky (2015)	1.004 applied within OCO-2 v10 algorithm	None
Continuum	Payne (2021)	-	Thompson et al. (2012)	MT_CKD v3.2

0.76um O_2 Detail

Spectral line parameters, line mixing and collision-induced absorption for O2 are described in Payne et al. (2021).

Parameters for broadening of O_2 by H_2O come from the study by Drouin et al. (2014).

1.6μm and 2μm CO_2 Detail

In the previous iteration of ABSCO (v5.1) used in algorithm build 10, the CO_2 bands used line parameters and mixing models derived from studies by Devi et al. (2016) and Benner et al. (2016). The computation incorporated a speed dependent line profile with tridiagonal line mixing, and their parameters were derived from fits to laboratory spectra at multiple temperatures.

However, this line mixing model proved to be insufficient for the 2.06 μm band, as deficit of absorption between the band's P and R branch was noticed, particularly in atmospheric retrievals. To account for this missing absorption an *ad hoc* continuum term was added in the form of two Gaussian distributions centered at 4853.5 and 4789 cm^{-1}. A reanalysis of the same spectra using a full relaxation matrix model by Lamouroux (2014) obviated the need for this additional *ad hoc* term. The resulting cross sections now form the basis for the current 5.2 version of ABSCO.

Parameters for foreign broadening of CO_2 by H_2O come from studies by Sung et al (2009). This study treated the 4.3μm band only. However, it is likely that these can be safely extrapolated to the other bands as well, and we favor this approach until additional direct laboratory data is available.

H_2O Detail

We incorporate H_2O line parameters from a modified version (2020-05-12) of ATM18, provided by Geoff Toon (https://mark4sun.jpl.nasa.gov/toon/atm18/atm18.html) and compute the H_2O continuum using version 3.2 of the AER MT_CKD codes (Mlawer et al., 2012). The line parameters had already been scaled by Toon in an attempt to yield consistent water columns in retrievals over several windows within a wide spectral range. However, tests with both ground-based and satellite measurement pointed to a need for an additional slight reduction in the cross sections. The ABSCO v5.2 tables used by OCO-2, therefore, already include a 0.981 scaling of the water cross sections and are not additionally modified in the generation of the version 11 Level 2 product.

3 HDF5 Format Specification

The ABSCO tables are provided in an HDF5 format. The table is a 4D structure indexed in the following order:

- pressure levels 1 to N_{pres}
- temperature levels from 1 to N_{temps}
- foreign broadener vmrs from 1 to N_{vmrs}
- frequencies from 1 to N_{freqs}

In general, each table models one absorbing gas and up to one foreign broadening gas (here, always H_2O). We refer to the absorber's HITRAN gas index value with the symbol Q_{abs} and its HITRAN isotope index as R_{abs}. The foreign broadener index is $Q_{brd.}$

The HDF file is has the following format:

– **File:** The top-level file object represents a collection of one or more absorber gas cross sections that have been computed for a common spectral range and set of atmospheric conditions. The file contains top-level attributes:
    - version: a version string describing the table release
    - addl_ident: a special identifier string, if any
    - gas_name: a string such as "o2"
    - wn_begin: the starting wavenumber

    - wn_end: the ending wavenumber
    - comment: a space for notes about the table creation
- **Gas_[Q_{abs}]_Absorption** The absorption coefficients are a 4D table of size N_{pres} x N_{temps} x N_{vmrs} x N_{freqs} and are indexed in that order. The dataset attributes are:
    - addl_ident: a special identifier string, if any
    - gas_name: a string such as "o2", which should match its filename
    - comment: a space for notes
- **Gas_Index** a string containing the 2 digit HITRAN index of the principal absorbing gas, equivalent to Q_{abs} above.
- **Pressure** The pressure is a dataset of size N_{pres} representing the pressure in Pascals at each atmospheric level in the table
- **Temperature** Temperature is a 2D dataset of degrees Kelvin, of shape N_{pres} x N_{temps} It records the temperature grid point values, which might differ depending on pressure level.
- **Broadener_[Q_{brd}]_VMR** A dataset of size N_{vmrs} representing the different volume mixing ratios at which the foreign broadening gas is modeled. Q_{brd} is a HITRAN index. Now we only model H_2O broadening, so the index is always 01.
    - broadener_name: the string “h2o”
- **Broadener_Index** a string contraining the 2 digit HITRAN index of the broadening gas, equivalent to Q_{brd} above
- **Wavenumber** The Wavenumber object is a dataset of size N_{freqs} describing the frequency grid spacing.

4 References

[Benner/Devi 2011] Benner DC, Devi VM, Nugent E, Sung K, Brown LR, Miller CE. et al., Line parameters of carbon dioxide in the 4850 cm^{-1} region. In: Twenty-second Coll. on High resolution molecular spectroscopy, Dijon, Fr 2011; poster N19.

[Benner 2016] D. C. Benner, V. M. Devi, K. Sung, L. R. Brown, C. E. Miller, V. H. Payne, B. J. Drouin, S. Yu, T. J. Crawford, A. W. Mantz, M. A. H. Smith, R. R. Gamache, Line parameters including temperature dependences of air- and self-broadened line shapes of 12C16O2: 2.06 micron region, J. Mol. Spec., 2016

[Devi 2016] V. M. Devi, D. C. Benner, K. Sung, L. R. Brown, T. J. Crawford, C. E. Miller, B. J. Drouin, V. H. Payne, S. Yu, M. A. H. Smith, A. W. Mantz, R. R. Gamache, Line parameters including temperature dependences of self- and foreign-broadened line shapes of 12C16O2: 1.6 micron region, JQSRT, 2016

[Drouin 2014] B.J. Drouin, V. H. Payne, F. Oyafuso, K. Sung and E. J. Mlawer, Pressure broadening of oxygen by water, J. Quant. Spectrosc. & Radiat. Trans., 2014.

[Drouin 2017] B. J. Drouin, D. C. Benner, L. R. Brown, M. Cich, T. Crawford, V. M. Devi, A. Guillaume, J. T. Hodges, E. J. Mlawer, D. Robichaud, F. Oyafuso, V. H. Payne, K. Sung, E. Wishnow, S. Yu, Multi-spectrum analysis of the oxygen A band, JQSRT, 186, 118–138, 2017

[Fleurbaey 2020] H Fleurbaey, H Yi, EM Adkins, AJ Fleisher, JT Hodges, Cavity ring-down spectroscopy of CO2 near λ = 2.06 μm: Accurate transition intensities for the Orbiting Carbon Observatory-2 (OCO-2) “strong band”, JQSRT, 252 107104 (2020), https://doi.org/10.1016/j.jqsrt.2020.107104.

[Lamouroux 2014] J Lamouroux, L. Régalia b, X. Thomas b, J. Vander Auwera c, R.R. Gamache d, J.-M. Hartmann, “CO2 line-mixing database and software update and its tests in the 2.1 μm and 4.3 μm regions”, JQSRT, 151, 88-96 (2015), http://dx.doi.org/10.1016/j.jqsrt.2014.09.017

[Mlawer 2012] Mlawer, E.J., V.H. Payne, J.-L. Moncet, J.S. Delamere, M.J. Alvarado, D.D. Tobin, Development and recent evaluation of the MT_CKD model of continuum absorption, *Phil. Trans. Roy. Soc.A*, June 13, 2012 370 1968 2520-2556.

[Mondelain 2013] D. Mondelain, A. Aradj, S. Kassi and A. Campargue, The water vapor self continuum by CRDS at room temperature in the 1.6 μm transparency window, J. Quant. Spectrosc. Radiat. Transfer, 130, 381–391

[Payne 2021] V Payne, BJ Drouin, F Oyafuso, et al, "Absorption coefficient (ABSCO) tables for the Orbiting Carbon Observatories: Version 5.1", *Journal of Quantitative Spectroscopy and Radiative Transfer*. 255, p. 107217, https://doi.org/10.1016/J.JQSRT.2020.107217

[Polyansky 2015] Oleg L. Polyansky, Katarzyna Bielska, Mélanie Ghysels, Lorenzo Lodi, Nikolai F. Zobov, Joseph T. Hodges, and Jonathan Tennyson, High accuracy CO2 line intensities determined from theory and experiment, Phys. Rev. Lett. 114, 243001 – Published 15 June 2015

[Ptashnik 2011] Ptashnik et al. *Journal of Geophysical Research*, vol. 116, D16305, doi:10.1029/2011JD015603, 2011.

[Rothman 2009] Rothman, L. S. et al. *The HITRAN 2008 molecular spectroscopic database.* Journal of Quantitative Spectroscopy and Radiative Transfer, 110 (2009) 533–572.

[Rothman 2010] Rothman, L. S., I. E. Gordon, R. J. Barber, H. Dothe, R. R. Gamache, A. Goldman, V. I. Perevalov, S. A. Tashkun, J. Tennyson (2010). HITEMP, the high-temperature molecular spectroscopic database. *Journal of Quantitative Spectroscopy and Radiative Transfer*. 111:15, p. 2139-2150.

[Sung 2009] Keeyoon Sung; L. R. Brown, R. A. Toth, T. J. Crawford. Fourier transform infrared spectroscopy measurements of H_20-broadened half-widths of CO_2 at 4.3 um. *Canadian Journal of Physics*; May 2009, Vol. 87 Issue 5, p. 469.

[Thompson 2012] Thompson, D. R., D.. C. Benner, L. R. Brown, D. Crisp, V. Malathy Devi, Y. Jiang, V. Natraj, F. Oyafuso, K. Sung, D. Wunch, R. Castaño a, C. E. Miller Atmospheric validation of high accuracy CO_2 absorption coefficients for the OCO-2 mission. *Journal of Quantitative Spectroscopy and Radiative Transfer* (2012), http://dx.doi.org/10.1016/j.jqsrt.2012.05.021.

[Wunch 2010] Wunch, D., Toon, G. C., Wennberge, P. O. et al. Calibration of the total carbon column observing network using aircraft profile data. *Atmos Meas. Tech. Discuss.*, *3*, 2603-2632, 2010. www.atmos-meas-tech-discuss.net/3/2603/2010/ doi:10.5194/amtd-3-2603-2010

[Zak 2016] E. Zak, J. Tennyson, O. L. Polyansky, L. .Lodi, N. F. Zobov, S. A. Tashkun, V. I. Perevalov, A room temperature CO2 line list with ab initio computed intensities, JQSRT, Volume 177, July 2016, Pages 31–42