

Spectral Lineshape Implementation in SFIT4

SFIT4 Dev Team

May 2020

Abstract

Initial Draft Document

This document describes the spectral lineshape options that are user optional encoded within SFIT4. The current state of auxiliary data parameters are limited to a few molecules. The user switches, data files necessary and their compatibility are described here

Contents

1	Introduction	2
2	Implementation	2
2.1	SFIT4 Lineshape Options	2
3	Data Files Required	3
4	Examples	4
4.1	Line Mixing: CO ₂	4
4.2	Galatry: HCl, HF	4
4.3	SDV: CO	4
5	Appendix	4

1 Introduction

Lineshapes are cool.

2 Implementation

Talk about codes for Voigt, Tran. [?] [?] [?].

For instance the original Voigt uses a function from Drayson, when using Boone for linemixing it uses its own based on Humlicek, as does Galatry.

2.1 SFIT4 Lineshape Options

Talk about switches and how they work together.

A brief introduction to the switches used in the *sfit4.ctl* file is given in the *sfit4_init.pdf* tables. To implement a lineshape model use the forward model flag *fw.lshapemodel* = and set to one of the switches described in Table 1:

Flag	Functionality
0	The lineshape used for a given gas is not forced. It depends on the spectroscopic values given supplied to SFIT4 from the hbin file, and on the specific switches for linemixing and SDV below
1	Force using the default Voigt lineshape model regardless of parameters supplied in the hbin file,
2	Use the Galatry if BETA_T is given, if not use Voigt,
3	Line Mixing calculation using the Voigt profile as implemented by [?],
4	Use the pCqSDHC lineshape model [?],

Table 1: *Lineshape flags to control how SFIT4 implements different lineshapes for different species.*

To specifically force the speed dependent Voigt model set

fw.lshapemodel = 4

fw.lshapemodel.sdv = .TRUE.

then this will invoke the SDV approximation in the pCqSDHC algorithm.

To implement line mixing set

fw.lshapemodel = 3, 4

fw.linemixing = .TRUE.

then, if T and line mixing parameters found, linemixing is calculated. Note that currently 1st order proximation is used [?].

As always check the detail file *sfit4.dtl* to see what was actually implemented in the retrieval. You will see something like this e.g.

GALATRY FLAG & LINES WITH GALATRY PARAMETERS FOUND : T 6

which means the Galatry flag is set and 6 lines with Galatry parameters are found, or this

LINEMIXING FLAG & LINES WITH LINEMIXING PARAMETERS FOUND : F 0

which means no linemixing used.

One can create an hbin file with the extra parameters hem switch on or off via the sfit4.ctl switches outlined above. Caution needs to be used to be sure appropriate extra parameters are used with appropriate base parameters.

does Geoff supply further parameters? For the atm files there are files for extra parameters. I would not mix them, unless you know which hitran version the atm database you use is based on.

3 Data Files Required

Talk about what is needed, where they are from, compatibility with other line lists ...

If extra line parameters are to be used, the matching spectroscopy files are listed in table 2. The spectroscopic files for the gases belong to each other, because the matching of the line parameters is done via the quantum numbers. As the line parameters may not be independent from each other and may change from one HITRAN release to another, it is important to only use them together. The SFIT4 release contains a hbin.ctl, which contains a complete spectroscopy for the current release. It is recommended to stick to this spectroscopic database unless there are strong reasons to deviate from it. Detailed knowledge about the spectroscopy is also required to do so.

Gas	Data file	Origin	Usage
CO ₂	o2_hito8_f53.par	[?]	main linelist based on HITRAN o8, 1 st order Rosenkranz linemixing parameters corresponding to the linelist above ,
	o2_hito8_f53_LM1ST.par	[?]	
CO	o5_hit16.par	HITRAN 2016	HITRAN parameters for CO, extra speed-dependent-Voigt parameters lines for CO,
	o5_hit16_SDV.txt	HITRAN 2016	
HF	14_hit16.par	HITRAN 2016	HITRAN parameters for HF, extra parameters necessary for Galatry model,
	14_hit16_Galatry.txt	HITRAN 2016	
HCl	15_hit16.par	HITRAN 2016	HITRAN parameters for HCL extra parameters necessary for Galatry model,
	15_hit16_Galatry.txt	HITRAN 2016	

Table 2: Current data parameter files useful in SFIT4.

4 Examples

4.1 Line Mixing: CO₂

CCL₄

4.2 Galatry: HCl, HF

4.3 SDV: CO

5 Appendix

List of Figures

List of Tables

1	Lineshape flags to control how SFIT4 implements different lineshapes for different species.	2
2	Current data parameter files useful in SFIT4.	4