

Use of different lineshape models within LINEFIT ver 14.6

This version of LINEFIT supports several extensions over the standard Voigt lineshape model. Such extensions require provision of additional lineshape and / or line mixing parameters by the user. This document gives a short introduction describing how the linelist needs to be modified for using these extended lineshape options.

LINEFIT expects line lists formatted in the manner used in HITRAN, either the format used in HITRAN versions 1986 - 2001 or 2004 – 2012. The format is tested for each line, so in mixed-format line lists can be handled by LINEFIT (although I would not recommend creating such kind of lists, as the danger of misinterpretation by other users is considerable when such lists are circulated). Further details concerning the HITRAN line list format are provided on the HITRAN webpage:

<http://www.cfa.harvard.edu/hitran/> (follow link to database format)

Additional parameters are provided by adding auxiliary rows into the line list. Note that the parameters provided in an auxiliary row are interpreted by LINEFIT in such a manner that they are assigned to the next real HITRAN row (“real” indicates a row which provides the basis parameters: wave number, linestrength, pressure broadening parameters, etc for a spectral line) follows in the list (from now on, I will call this the parent row). Before, the auxiliary lines in the list were formatted in the same manner as a HITRAN04 entry, their nature as auxiliary line was clarified by using a species identifier which does not occur in HITRAN. In this version of LINEFIT, I have abandoned the formal similarity of an aux row with a parent row, because the pCqSDHC lineshape has so many additional parameters that it becomes inconvenient to hide these in a HIT04 formatted line. Therefore, the aux lines now have a different format, but the interpretation still is done via the imaginary species identifier and the wavenumber entry, too, is maintained for guidance of the eye in support of a visual inspection of a linelist section (note, however, that the wavenumber entry is not used. The idea is that the inserted value equals the value in the parent row, but this is not required and not checked by LINEFIT).

Supported dummy species identifiers:

(line format: 803 format(I3,F12.6,E10.3,E10.3,E10.3,E10.3,E10.3,E10.3,E10.3,E10.3))

A single or several aux lines can be associated with a single parent line entry. For a given parent line, the user has to decide for a certain line shape model (either Voigt, or Galatry, or Tran-Hartmann (TH)). Without aux lines LINEFIT will assume Voigt, and LINEFIT will generate an error message if a line is flagged both Galatry and TH. Line mixing 2nd order requires the presence of Rosenkranz line mixing parameters. LINEFIT in general requests different parameters for self- and foreign collisions.

994: line mixing second order

dumint,dumdbble,LMI0f,LMI1f,LMI0s,LMI1s,LMD0f,LMD1f,LMD0s,LMD1s

Line mixing 2nd order introduces changes in line position and the amplitude of the real part of the line shape function, both are assumed proportional to pressure squared.

! modify line intensity (acts on real part only)

twert = (Tgaskel - 296.0)

LMI = 1.0d0 + 9.74498d-7 * pbar_tot * ((pbar_tot - pbar_part) &

* (lines%LMI0f(j) + twert * lines%LMI1f(j)) &

+ pbar_part * (lines%LMI0s(j) + twert * lines%LMI1s(j)))

! modify line position

twert = (Tgaskel - 296.0)

delta0 = delta0 + 9.74498d-7 * pbar_tot * &

((pbar_tot - pbar_part) * (lines%LMD0f(j) + twert * lines%LMD1f(j)) + &

pbar_part * (lines%LMD0s(j) + twert * lines%LMD1s(j))))

995: line mixing Rosenkranz

read (zeile,803) dumint,dumdbble,LMY0f,LMY1f,LMY2f,LMY0s,LMY1s,LMY2s

twert = 0.01666666 * (Tgaskel - 260.0)

! LM 1st order

YLM = 9.87167d-4 * ((pbar_tot - pbar_part) &

* (lines%LMY0f(j) + twert * (lines%LMY1f(j) + twert * lines%LMY2f(j))) &

+ pbar_part * (lines%LMY0s(j) + twert * (lines%LMY1s(j) + twert * lines%LMY2s(j))))

996: Tran-Hartmann (/ pCqSDHC) line shape model

read (zeile,803) dumint,dumdbble,gam2f,delta2f,etaf,nueVCf,gam2s,delta2s,etas,nueVCs

gam2 = 9.87167d-4 * (pbar_part * lines%gam2s(j) + (pbar_tot - pbar_part) * lines%gam2f(j)) &

* (296.0d0 / Tgaskel)**lines%lortdepend(j)

delta2 = 9.87167d-4 * (pbar_part * lines%delta2s(j) + (pbar_tot - pbar_part) * lines%delta2f(j))

& * (296.0d0 / Tgaskel)**lines%lortdepend(j)

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eta = (pmbar_part * lines%lorwidths(j) * lines%etas(j) + (pmbar_tot - pmbar_part) &
* lines%lorwidthf(j) * lines%etaf(j)) / (pmbar_part * lines%lorwidths(j) &
+ (pmbar_tot - pmbar_part) * lines%lorwidthf(j))

nueVC = 9.87167d-4 * (pmbar_part * lines%nueVCs(j) + (pmbar_tot - pmbar_part) * lines%nueVCf(j))
& * (296.0d0 / Tgaskel) ! Annahme: prop 1/T

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The naming convention of the line shape parameters follows the original publications (Tran et al., JQSRT, 2013; Ngo et al., JQSRT, 2013). The sign of the imag part is corrected (Tran et al, Erratum, JQSRT, 2013). The original suggestion of the authors of calculating the effective parameters by superimposing the contributions by each individual type of collision partner currently seems impracticable (concerning the treatment of gas mixtures see Lisak et al. JQSRT, 2015.)

997: Galatry soft collision line shape model

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read (zeile,803) dumint,dumdbble,gam2f,delta2f,etaf,nueVCf,gam2s,delta2s,etas,nueVCs

beta = 9.87167d-4 * (pmbar_part * lines%gam2s(j) + (pmbar_tot - pmbar_part) * lines%gam2f(j)) &
* (296.0d0 / Tgaskel)**lines%lortdepend(j)

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998: Extension of line shift parameterization

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read (zeile,803) dumint,dumdbble,pshif,dpshifdT,pshis,dpshisdT

twert = (Tgaskel - 296.0)

delta0 = 9.87167d-4 * ((pmbar_tot - pmbar_part) * (lines%pshif(j) +
& twert * lines%dpshifdT(j)) + pmbar_part * (lines%pshis(j) + twert * lines%dpshisdT(j))

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