LINEDB

To be filled

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Version 1.0

Abstract

TO BE FILLED

Contents

1 Test

2 Providing your own database

LINEDB accepts building a local database with a custom list of lines. This can be achieved through two ASCII files:

1. the line "catalog" *e.g.*

```
  29005   NNH+
93171.8800   .0400 -2.7844 2    0.0000  9 -29005 102 1 1         0 1
93173.7000   .0400 -2.5625 2    0.0000 15 -29005 102 1 2         0 1
93176.1300   .2200 -3.2614 2    0.0000  3 -29005 102 1 0         0 1
  30002   HC-13-O+
86754.2884  0.0046 -2.2835 2    0.0000  3 -30002 101 1           0
```

   This catalog must follow the JPL convention (in particular, column alignment) described in Appendix A. The lines must be gathered by species. Each group is identified by a first line providing the tag value and the species name. The latter should be limited to 32 characters because of internal limitations of the **LINEDB** databases. There can be no blank nor comment lines in this file.

2. the *partition function* file. It must be named `partfunc.cat` and must use the following format *e.g.*:

```
species      NNH+      29005
temperatures 300.   225.   150.   75.    37.5   18.75  9.375
qpart        3.0831 2.9586 2.7832 2.4842 2.1875 1.8952 1.6116

species      HC-13-O+  30002
temperatures 300.   225.   150.   75.    37.5   18.75  9.375
qpart        2.1599 2.0353 1.8598 1.5607 1.2637 0.9707 0.6859
```

   The tag and species name should match the catalog ones. The number of temperatures/qpart pairs are free. Those three lines must be consecutive in the file, with one set of lines per species. There can be a custom number of blank and comment (!) lines between each set of lines.

Given those files, importing them in **LINEDB** is as easy as:

```
SIC> use in mybase.dat
I-USE,  mybase.dat (offline) selected with /(partfunc.json|partfunc.cat) for par
SIC> select
I-SELECT,  4 lines found in the frequency range 0 to infinity MHz
SIC> list
  # Species        Freq[MHz] Err[MHz] Eup[K]  Gup  Aij[s-1]    Upper level -- Lo
  1 HC-13-O+       86754.288   0.005     4.2    3  1.21e-05             1 -- 0
  2 NNH+           93171.880   0.040     4.5    9  3.63e-05           1 1 -- 0
  3 NNH+           93173.700   0.040     4.5   15  2.18e-05           1 2 -- 0
  4 NNH+           93176.130   0.220     4.5    3  1.09e-04           1 0 -- 0
```

It is advised to save this catalog in the **LINEDB** binary format, *i.e.* after the previous steps:

```
SIC> use out mybase.db
SIC> insert
```

3 LINEDB Language Internal Help

3.1 Language

```
          LINEDB\ Command Language Summary
This language is an interface to on-line and off-line line catalogs.

USE       Define the atomic and molecular line database(s) used as input and
SELECT    Select lines in the input database(s) according to user defined fi
LIST      List lines from the current line index
INSERT    Insert lines from the current line index into the output database
REMOVE    Remove lines from the current line index from the output database
```

3.2 USE

LINEDB\USE IN|OUT|BOTH dbname1 [[dbname2] [dbname3...]] [/OVERWRITE]

Define the atomic and molecular line database(s) used as input and/or output.

Input databases can be either an existing filenames or a database available through internet. Recognized internet databases are

JPL	the JPL molecular spectroscopy database
CDMS,	the Cologne Database for Molecular Spectrocopy
VOPARIS	the Paris VO observatory interface to the CDMS database

These names can thus not be used as database filenames.

The input file is tested to determine whether it is a valid SQLITE database. If not, it is assumed to be an ASCII file following the JPL data format, see e.g.
http://spec.jpl.nasa.gov/ftp/pub/catalog/README, and
http://spec.jpl.nasa.gov/ftp/pub/catalog/catdir.html for examples.

Multiple input databases can be used together. However, only one output database can be defined at a given time. The OUT and BOTH keywords applies only to SQLITE databases. The /OVERWRITE option implies that the output database is first removed. The absence of the option implies that any subsequent call to the INSERT command will append lines to the already existing output database.

3.3 SELECT

LINEDB\SELECT [/ORIGIN Originname] [/SPECIES Name1 Name2 ...] [/FREQ Fmin Fmax] [/ENERGY Emax] [/AIJ Amax] [/SORTBY Order] [/EPSILON Eps]

Select lines available from the input database. An index containing the line information is formed and a SIC structure mapping these information is defined. The index can be sorted by increasing frequency or energy. One or more species name can be provided, wildcards '*' can be used.

The initial origin of the line (e.g. JPL, CDMS or private catalog), the name of the species, a frequency range, the maximum energy of the upper level and the maximum Einstein coefficient Amax can be used as filters in the line selection process.

As an output, the LINES SIC structure will contain the content of the current index, i.e.,

```
LINES%           Global structure
LINES%N          Integer scalar       [---] Number of lines in current inde
LINES%SPECIES    Character[LINES%N]   [---] Species names
LINES%FREQUENCY  Double[LINES%N]      [MHz] Frequencies
LINES%UNCERTAINTY Real[LINES%N]       [MHz] Uncertainty of the line frequen
LINES%AIJ        Double[LINES%N]      [s-1] Einstein coefficient
LINES%EUP        Real[LINES%N]        [  K] Upper level energy
LINES%GUP        Real[LINES%N]        [---] Upper level degeneracy
LINES%QNUP       Character[LINES%N]   [---] Upper level quantum numbers
LINES%ELOW       Real[LINES%N]        [  K] Lower level energy
LINES%GLOW       Real[LINES%N]        [---] Lower level degeneracy
LINES%QNLOW      Character[LINES%N]   [---] Lower level quantum numbers
```

The lines will be sorted according to Order, which can be any combination of "frequency", "energy" and "aij", and all the subsequent permutations. Default is frequency. If sortby is ["energy", "aij"] and if epsilon is specified, aij will be used as a criterion when the difference in energy is less than epsilon.

3.4 LIST

LINEDB\LIST [/FULL] [/TOC]

List a set of columns for all lines found in the current index built

during the last SELECT command. The option /FULL lists all the columns available in the database.

The /TOC option partitions the lines by equivalence class (species name) and gives a count of each class.

3.5 INSERT

LINEDB\INSERT

Insert the entries (lines properties and partition functions) of the current line index (result of the last SELECT command) into the output database.

3.6 REMOVE

LINEDB\REMOVE

Remove the entries (lines properties and partition functions) of the current line index (result of the last SELECT command) into the output database. The partition function is erased only if no other line of the same species remains in the database.

A JPL convention

The JPL convention, as of March 24th 2014, is reproduced here. This is the expected format for ASCII local databases supported by **LINEDB**. See the online version of the document at: http://spec.jpl.nasa.gov/ftp/pub/catalog/README

```
The catalog data files are composed of 80-character card images, with one card
image per spectral line.  The format of each card image is:
  FREQ, ERR, LGINT, DR,  ELO, GUP, TAG, QNFMT,  QN',  QN"
(F13.4,F8.4, F8.4,  I2,F10.4,  I3,  I7,    I4,  6I2,  6I2)

FREQ:  Frequency of the line in MHz.
ERR:   Estimated or experimental error of FREQ in MHz.
LGINT: Base 10 logarithm of the integrated intensity in units of nm^2 MHz at
       300 K.
DR:    Degrees of freedom in the rotational partition function (0 for atoms,
       2 for linear molecules, and 3 for nonlinear molecules).
ELO:   Lower state energy in cm^{-1} relative to the ground state.
GUP:   Upper state degeneracy.
TAG:   Species tag or molecular identifier.
       A negative value flags that the line frequency has
       been measured in the laboratory.  The absolute value of TAG is then the
       species tag and ERR is the reported experimental error.  The three most
       significant digits of the species tag are coded as the mass number of
       the species.
QNFMT: Identifies the format of the quantum numbers
QN':   Quantum numbers for the upper state.
QN":   Quantum numbers for the lower state.

The on-line version of the catalog contains individual files for each
molecular species.  Line files are designated as ctttttt.cat, where tttttt
is the zero-filled catalog tag number. For example,
the H atom line list is in file c001001.cat.

A directory of the catalog is found in a file called 'catdir.cat.'
Each element of this directory is an 80-character record with the following
format:
TAG,  NAME, NLINE,  QLOG,  VER
(I6,X, A13,    I6, 7F7.4,  I2)
```

TAG: The species tag or molecular identifier.
NAME: An ASCII name for the species.
NLINE: The number of lines in the catalog.
QLOG: A seven-element vector containing the base 10 logorithm of the partition function for temperatures of 300 K, 225 K, 150 K, 75 K, 37.5 K, 18.75 K, and 9.375 K, respectively.
VER: The version of the calculation for this species in the catalog. The version number is followed by * if the entry is newer than the last edition of the catalog.