Molpop automated client

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Abstract

The Basecol/MOLPOP python client fetches molecular data from the central Basecol database at the Meudon Observatory and creates on the user's computer input data files for the MOLPOP-CEP radiative transfer program. This manual describes how to configure and run the tool, and the results of these runs.

Status of This Document

This is a Document-Type. The first release of this document was December 2006.

Contents

I. Introduction

This tool allows users to collect a large amount of data from the Basecol database and create on their local computer a set of data files with tabulations of the radiative and collisional properties of selected molecules in a suitable format. Currently, the format of the locally created files is geared toward MOLPOP-CEP, a program that offers an exact solution of the radiative transfer problem for any multi-level system. The data files generated by the Basecol/MOLPOP tool are directly readable by MOLPOP, allowing exact analysis of every molecular species listed in the Basecol central database.

The Basecol/MOLPOP tool is composed of two parts. The first one is a distant HTTP service, running on the Basecol server at Meudon. The second is local client software, developed in Python, that queries the HTTP service and creates local output files. As the client is open source, it is possible for the user to modify the output at will.

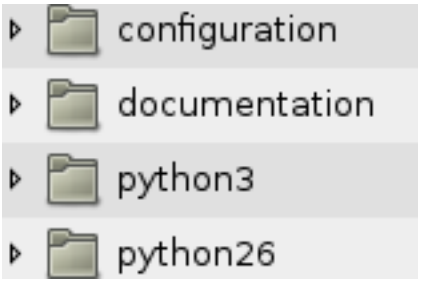
II. Quick Start

Unpack the package, preserving the directory structure. The client archive includes 2 versions. One is compatible with Python 2.6, the other with Python 3 which introduced backward incompatible modifications to the language. Select the executable directory that matches the version of Python on your machine. It should contain the two files `elements.txt` and `execute.py`. Run `execute.py`. It should produce the new sub-directory `output\S_yyyy-mm-dd`, where `yyyy-mm-dd` is the current date, containing data files for CO rotational transitions, as explained below.

III. Presentation

1. Directory Structure

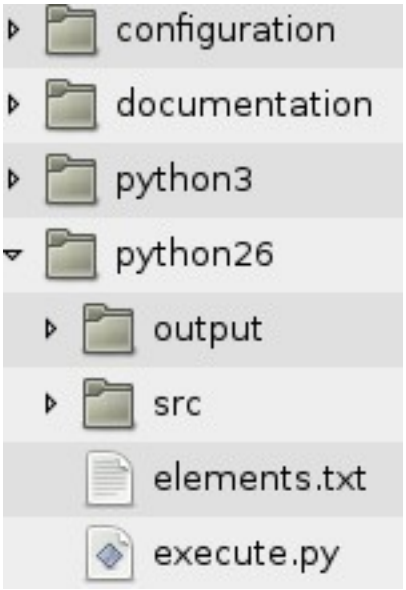
a) The root directory



- configuration: contains the configuration file
- documentation: contains this documentation
- python3: version compatible with python3
- python26: version compatible with python 2.6

b) Executable directory

The python3 and python26 directories share a similar structure.



Main files :

- execute.py: file containing the main function
- elements.txt: list of the molecular species whose data is available in the Basecol database

Directory `src`:
This directory contains source files. It also contains some classes in its `classes` subdirectory.

Directory `output`:
Contains all the data generated by the tool, ordered by date.

2. Configuration

The program uses a configuration file called `config.xml` to know where the service returning data is located. The default configuration should not be modified.

File syntax:

```
<CONFIGDOCUMENT>
	<PROGRAM_PARAMETERS>
		<CONNECTION_PARAMETERS>
			<SERVER>molpop-service.obspm.fr</SERVER>
			<!-- service returning the list of collisions-->
			<COLLISIONS_URL>/index.php</COLLISIONS_URL>
			<!-- service returning the list of elements -->
			<ELEMENTS_URL>/getElements.php</ELEMENTS_URL>
			<METHOD>GET</METHOD>
		</CONNECTION_PARAMETERS>

		<OUTPUT_PARAMETERS>
			<OUTPUT_DIRECTORY>output</OUTPUT_DIRECTORY>
			<XML_FILE_NAME>monfichier.xml</XML_FILE_NAME>
		</OUTPUT_PARAMETERS>
	</PROGRAM_PARAMETERS>
</CONFIGDOCUMENT>
```

3. Using the client

a) The elements.txt file

This file contains the list of all the molecules and associated processes available for the tool on the Basecol database. Each molecule is listed on a separate line. All text following the # character is ignored. For example, the first three entries in the supplied `elements.txt` are:

```
#c-C3H2	#processes : rotation - symmetries : ortho para
CO	#processes : rotation
#CS	#processes : rotation ro-vibration
```

Only the CO entry is processed when the tool is run without options (see below) since the other entries are de-selected. Selecting and de-selecting entries as desired, you can choose the entries needed for your calculations. The `elements.txt` file can be updated and re-generated by running the tool with the option `-e` (see below).

b) Running the script

To run the client you launch the `execute.py` file. This executable supports 4 arguments:

no option	gets all data for the selected elements
-a, --all	gets all data for all the listed elements (including those de-selected)
-c, --collision	gets only collision rates for the selected elements
-e, --element	generates a new `elements.txt` listing all available entries
-h, --help	displays help

The program execution can take several minutes, depending on the option selected. Once it is finished, all the files will be available locally in the output directory, stored as ASCII files. Since the `–c` option generates only collision rates data, it should be used only after all other data (energy levels and A-coefficients) for the relevant molecule have been generated in previous runs that used either `–a` or no option; the `–c` option is included for quick maintenance jobs (it can be combined with the `–a` option to get collisional data for all systems).

c) The -e/--element option

This option generates the file `elements.txt` in the same directory as `execute.py`. This file contains the list of molecules available in the Basecol database. If a file `elements.txt` already exists when you use this option, a new file will be created called `yyyy-mm-dd_elements.txt`. You can then manually merge the files, if you wish.

> **NOTE:** If `elements.txt` does not exist, the script will not run. You will then get a warning that "`execute.py -e`" must be launched first.

4. Output

a) The `Output` directory

This directory contains the result of all the program executions . The name of each directory is composed of three parts:

- a prefix indicating the type of the run :
  - A : all data for all elements
  - S : all data for selected elements
  - CA: collisions data for all elements
  - CS: collisions data for selected elements
- the date it was created, in the format `yyyy-mm-dd`
- a number that is incremented if several directories are created on the same date

Example:

- A_2006-12-15
- A_2006-12-15_2

Each directory further contains a subdirectory `Coll` that stores all the tabulations of collision rates and a log file that lists all the modifications that have been made compared with the previous runs. The first time the program is launched, the log file contains just the date of creation (since everything is new). Data files can be modified in either their contents or headers, and the log file indicates the part that has changed.

Each directory contains the file `mol_list.dat` that informs MOLPOP what are the species whose data have been generated locally. For example, the `mol_list.dat` file produced with the supplied package contains a single entry for the CO rotational transitions:

```
                mol_name        N_lev       mol_mass
>
             'CO_rotation'        36         27.99
```

For additional information about `mol_list.dat`, see its header and the MOLPOP manual. For each entry listed in `mol_list.dat`, the following two files are generated :

- `mol_name.lev` energy levels data
- `mol_name.aij` A-coefficients data

All the collision rate tabulations for this species, involving either different colliders or different theoretical calculations, are stored in the subdirectory `Coll`. The `Coll` directory contains the file `collision_tables.dat` that lists all the `.kij` files (see below) in this directory. Directories produced with the –`c` option (those that start with CA or CS) contain only `Coll` subdirectories; they do not contain either `mol_list.dat` or any `.lev` or `.aij` files.

The several output types of data files are described below.

b) Energy levels

Energy level tabulations are stored in files with the extension `.lev`. The levels are listed in increasing order of energy, and the tabulation includes the level statistical weight and a string describing its quantum numbers. The file name identifies the molecular species, its symmetry (when applicable) and the transition type.

Here are the first few lines from `c-C3H2_ortho_rotation.lev`:

```
levels from c-C3H2 symmetry : ortho, processus :rotation
source database : jpl
N : rotational quantum number
Ka : is the K value in the limiting case of a prolate symmetric-top
Kc : is the K value in the limiting case of an oblate symmetric-top
tau : (Ka) - (Kc), varies between -N and +N
epsilon : epsilon is the symmetry coefficient in wavefunction, can be 1 or -1
  N     g   Energy in cm^{-1}
>
  1     9        1.633200000e+00                'N = 1  Ka = 0  Kc = 1  tau = -1  epsilon = -1  '
  2     9        2.245100000e+00                 'N = 1  Ka = 1  Kc = 0  tau = 1  epsilon = 1  '
```

For more information see the MOLPOP manual.

c) Einstein A-coefficients

The file extension is `.aij`, its name is the same as the `.lev` file corresponding to the same entry in `mol_list.dat`. Here are the first few lines from `c-C3H2_ortho_rotation.lev`:

Einstein coefficients A_ij for c-C3H2 ortho
source database : jpl

I	J	A_ij (s^{-1})
>		
2	1	4.2263065752e-07
3	1	2.55334550477e-05
4	2	7.46365079557e-05

d) Collision rate coefficients

Collision rate tabulations are stored in the subdirectory `Coll` of each output directory. The file `collision_tables.dat` identifies all the collision rate files, with extension `.kij`, in `Coll`. Each entry in `collision_tables.dat` lists a collision rate file, identifies the collision process it describes and provides the reference source for the rate coefficients. Here are the first few lines from a sample `collision_tables.dat`:

List of available tables of collision rates.

>
H2O_4.kij
Rotational excitation of ortho-H$_2$O by He (Green & al., 1993) stateTostate
S.Green;S.Maluendes;A.~D.McLean,Ap. J. S.,85,181
****
CS_10.kij
Rotational excitation of CS by para-H$_2$, 20K < T < 300K, lowest 21 levels (Turner & al, 1992) stateTostate
B.~E.Turner;Kin-WingChan;S.Green;D.~A.Lubowich, Ap. J.,399,114-133
****

Each file with extension `.kij` contains the rate coefficients of a collisional process. The file name is comprised of the target molecule an an identifier. Here are the first few lines of the collision rate file `c-C3H2_46.kij`:

References : S.Chandra;W.~H.Kegel,Astron. Astrophys. Sup.,142,113--118
Rotational Excitation of ortho-cyclopropendyle by He (Chandra & al., 2000)
>
Number of temperature columns = 4

I	J	Temperature (K)			
		30	60	90	120
2	1	8.032000e-12	8.321000e-12	8.281000e-12	8.160000e-12
3	1	2.091000e-11	2.096000e-11	2.091000e-11	2.098000e-11
3	2	1.609000e-12	1.895000e-12	2.102000e-12	2.170000e-12

For more information on these tabulations and how they are handled in MOLPOP see the program manual.