Contents

spectr — a hodge-podge library used in the scientific work of Alan Heays

1 Install

1.1 Python dependencies

This modules has been tested and works with python 3.9 and 3.10, and will not work with version <3.9. It might be necessary to install and use it in a virtual environment (venv) on linux distributions with python version <3.9.

Many non-standard python libraries are used and are available from linux distributions or via pip, with the following package names:

- bidict
- cycler
- hitran-api
- brukeropusreader
- dill
- h5py
- matplotlib

- numpy
- openpyxl
- periodictable
- py3nj
- scipy
- sympy
- xmltodict

Matplotlib will require a graphics binding package, perhaps pyqt5.

1.2 Build fortran components

Run "make" in the root directory to create .so extensions.
The options in Makefile are for the gfortran compiler and use the lapack and openmp libraries.

1.2.1 Linux packages that might be needed to build

1. Debian/Ubuntu
    - gfortran
    - python-dev or python3-dev
    - liblapack-dev
    - libomp-dev
2. Arch Linux
    - gcc-gfortran
    - lapack

2 Usage

To import all submodules and many common functions directly into working namespace:

```
from spectr.env import *
```

Some example code is included in `./examples`.

3 Submodules

3.1 env.py

Conveniently import all submodules.

3.2 dataset.py

Storage, manipulation, and plotting of tabular data. Allows for the recursive calculation of derived quantities

3.3 tools.py

Functions for performing common mathematical and scripting tasks.

3.4 plotting.py

Functions for plotting built on matplotlib.

3.5 convert.py

Unit conversion and various conversion formulae.

3.6 optimise.py

General class for conveniently and hierarchically building numerical models with optimisable parameters.

3.7 atmosphere.py

3.8 lines.py

Dataset subclasses for storing atomic and molecular quantum-mechanical stationary-state line data.

3.9 levels.py

Dataset subclasses for storing atomic and molecular quantum-mechanical stationary-stat level data.

3.10 bruker.py

Interact with output files of Bruker OPUS spectroscopic acquisition and analysis software.

3.11 cross$_{\text{section.py}}$

CrossSection object — stub. Probably overshadowed by spectrum.Spectrum.

3.12 database.py

Interface to internal spectroscopic and chemistry database.

3.13 electronic$_{\text{states.py}}$

Calculation of diatomic level energies from potential-energy curves.

3.14 exceptions.py

Exception used to internally communicate failure conditions.

3.15 hitran.py

Access HITRAN spectroscopic data with hapy.

3.16 lineshapes.py

Simulate individual and groups of spectra lines of various shapes.

3.17 quantum$_{\text{numbers.py}}$

Functions for manipulating atomic and molecular quantum numbers.

3.18 spectrum.py

Classes for manipulating and modelling of experimental spectroscopic datea.

3.19 thermochemistry.py

Functions for computing thermochemical equilibrium with ggchem.

3.20 viblevel.py

Classes for simulating diatomic levels and lines defined by effective Hamiltonians.

3.21 fortran$_{\text{tools.f90}}$

Various fortran functions and subroutines.

4 Bugs / improvements

4.1 optimise.py

4.1.1 inhibit `add_input_function` in `input_function_method`?

4.2 viblevel.py

4.2.1 Implement general Λ-doubling formula of brown1979

Currently the o/p/q Λ-doubling is handled with effective (S,Λ)-dependent forumulae. Instead implement the last three terms of Eq. 18 of brown1979 into $\_\text{get}_{\text{linear H}}()$.

4.2.2 Phase error in $^3\Pi|LS|^1\Delta$

When comparing thismodel with pgopher, everything works find except the sign of the interactions $a^3\Pi(v=12)\sim D^1\Delta(v=1)$, $a^3\Pi(v=12)\sim d^3\Delta(v=5)$, and $a^3\Pi(v=12)\sim d^3\Delta(v=6)$ needs to be reversed. There is a phase error between these interactions and others.

```
##rafals draft 2021-06-24
##
## crossing states
upper_13C18O.add_level('A¹Π(v=1)',Tv=66175.53765,Bv=1.43761743,Dv=6.11179e-06,Hv=-22.39e-12,)
upper_13C18O.add_level('D¹Δ(v=1)',Tv=66442.5076,Bv=1.12,Dv=5.79e-6,Hv=-0.22e-12,)
upper_13C18O.add_level('I¹Σ (v=2)',Tv=66595.57091,Bv=1.1146473,Dv=5.68e-6,Hv=2.25e-12,)
upper_13C18O.add_level('d³Δ(v=6)',Tv=66956.97424,Bv=1.09416857,Dv=5.31e-6,Hv=-0.60e-12,Av=-16.097,ADv=-
9.17e-5, v=0.94, v=0.76e-2,)
upper_13C18O.add_level('e³Σ (v=3)',Tv=66811.0988,Bv=1.1126549,Dv=5.55e-6,Hv=-1.50e-12, v=0.5278,)
# ## non-crossing states
upper_13C18O.add_level('d³Δ(v=5)',Tv=65949.55,Bv=1.11,Dv=5.33e-6,Hv=-0.60e-12,Av=-15.91,ADv=-9.17e-
5, v=0.85, v=0.69e-2,)
upper_13C18O.add_level('e³Σ (v=2)',Tv=65802.44,Bv=1.13,Dv=5.58e-6,Hv=-1.50e-12, v=0.54,)
upper_13C18O.add_level('I¹Σ (v=1)',Tv=65593.17,Bv=1.13,Dv=5.67e-6,Hv=2.25e-12,)
upper_13C18O.add_level('a ³Σ (v=10)',Tv=66066.95,Bv=1.07,Dv=5.17e-6,Hv=-0.30e-12,)
upper_13C18O.add_level('a ³Σ (v=11)',Tv=67037.79,Bv=1.05,Dv=5.16e-6,Hv=-0.30e-12, v=-108.84e-2, v=-0.50e-
2,)
upper_13C18O.add_level('a³Π(v=12)',Tv=66355.00,Bv=1.32,Dv=5.67e-6,Av=36.97,ADv=-20.58e-5, v=-0.49e-
2, v=0.33e-2,ov=0.64,pv=2.73e-3,qv=2.95e-5,)
# ## interactions with crossing states
upper_13C18O.add_coupling('A¹Π(v=1)','D¹Δ(v=1)', v=-6.1688e-2),
upper_13C18O.add_coupling('A¹Π(v=1)','I¹Σ (v=2)', v=7.630e-2)
upper_13C18O.add_coupling('A¹Π(v=1)','d³Δ(v=6)', v=18.0838)
upper_13C18O.add_coupling('A¹Π(v=1)','e³Σ (v=3)', v=-5.4206)# ## interactions with non-crossing states
upper_13C18O.add_coupling('A¹Π(v=1)','d³Δ(v=5)', v=15.57)
upper_13C18O.add_coupling('A¹Π(v=1)','e³Σ (v=2)', v=14.05)
upper_13C18O.add_coupling('A¹Π(v=1)','I¹Σ (v=1)', v=9.89e-2)
upper_13C18O.add_coupling('A¹Π(v=1)','a ³Σ (v=10)', v=-5.29)
upper_13C18O.add_coupling('A¹Π(v=1)','a ³Σ (v=11)', v=3.836)
## interactions not including A
upper_13C18O.add_coupling('a³Π(v=12)','I¹Σ (v=2)', v=-7.604)
# upper_13C18O.add_coupling('a³Π(v=12)','D¹Δ(v=1)', v=-7.955)
# upper_13C18O.add_coupling('a³Π(v=12)','d³Δ(v=5)', v=-38.48, v=7e-2)
# upper_13C18O.add_coupling('a³Π(v=12)','d³Δ(v=6)', v=26.31, v=5.80e-2)
upper_13C18O.add_coupling('a³Π(v=12)','D¹Δ(v=1)', v=7.955)
upper_13C18O.add_coupling('a³Π(v=12)','d³Δ(v=5)', v=38.48, v=-7e-2)
upper_13C18O.add_coupling('a³Π(v=12)','d³Δ(v=6)', v=-26.31, v=-5.80e-2)
upper_13C18O.add_coupling('a³Π(v=12)','e³Σ (v=2)', v=5.09, v=1.00e-2)
upper_13C18O.add_coupling('a³Π(v=12)','e³Σ (v=3)', v=8.24, v=1.60e-2)
```