ReadMe

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Contents

1 Top-level directory structure

The top-level directory structure is shown in Table 1.

File or folder	Content
./adf04_ecs/	Effective collision strength data in the adf04 format
./adf04_ocs/	Ordinary collision strength data in the adf04 format
./adf04_str/	AS-REL structure data in the adf04 format
./data/	Atomic data for selected ions
./inputs/	Data files for H- and He-like ions
./pynb/	Python notebooks to reproduce figures in the paper
./ref/	Atomic data for selected ions in reference papers
./requirements.txt	List of python3 libraries required

Table 1: Top-level directory structure

2 Input files for H- and He-like ions

Structure and collision calculation input files (./inputs/) for each H-like ion. XX = isoelectronic sequence number (e.g., 01 for H-like and 02 for He-like), YY = atomic number (e.g. 08 for O and 26 for Fe), ZZ =roman number (e.g. 02 for II and 14 for XIV). Thus, H-like O VIII is 010808.

The structure calculation is performed with the AUTOSTRUCTURE code available here. The collision calculation is performed with the R-matrix ICFT code available here.

For the outer region exchange calculations using a fine energy mesh, we duplicate the calculations four times with the same sampling points (MXE) and shift the starting point by 1/4 times the grid size (EINCR). Only one of the input files is given without duplication.

3 Effective collision strength data in the adf04 format

The file name convention in this folder (./adf04_ecs) follows the one of OPEN-ADAS.

4 Ordinary collision strength data in the adf04 format

Optimal interval-averaged ordinary collision strength data are provided (./adf04_ocs). These files are created via the adasexj code available here.

Note: The number of energy bins varies (optimally) for each transition.

File	Content
./inputs/XXYYZZ/asc_si	Input file for the AUTOSTRUCTURE run
./inputs/XXYYZZ/rmc_in/	Input files for the R-matrix inner-region calculation
./inputs/XXYYZZ/rmc_in/ex	Exchange calculation
./inputs/XXYYZZ/rmc_in/nex	Non-exchange calculation
./inputs/XXYYZZ/rmc_in/tcc	Term coupling calculation
./inputs/XXYYZZ/rmc_in/dip	Dipole calculation
./inputs/XXYYZZ/rmc_out/	Input files for the R-matrix outer-region calculation
./inputs/XXYYZZ/rmc_out/bsc	Bound-state calculation
./inputs/XXYYZZ/rmc_out/fex	Exchange calculation with a fine energy mesh
./inputs/XXYYZZ/rmc_out/cex	Exchange calculation with a coarse energy mesh
./inputs/XXYYZZ/rmc_out/nex	Non-exchange calculation
./inputs/XXYYZZ/adas/	Input files for binned Ω and Maxwellian-averaged Υ data

Table 2: Input files for H- and He-like ions.

File	Content
./adf04_ocs/XXYYZZ/adf04_om	Optimal interval-averaged ordinary collision strength data

Table 3: Optimal interval-averaged ordinary collision strength data.

5 AS-REL structure data in the adf04 format

The AS-REL energy levels and transition rates (Tables $4-7$ in the paper) are provided here (./adf04_str). The input files (das) for AUTUSTRUCTURE (v29 or later) are also provided.

6 Other general atomic data for selected ions

Selected ions include H- and He-like C, N, O, Ne, Mg, Si, S, Ar, Ca, Fe, and Ni. Data files are available at ./data/XXYYZZ following the aforementioned naming convention.

For data used in AtomDB v3.0.9, CHIANTI v10.0.1, and SPEX v3.06.01, they are named as $code = adb309, cdb1001, spex306, respectively. For data calcualted in the present work, they are named as $code = mao22fe and mao22qe for H-like and He-like ions, respectively. In addition, $code = mao22nd is for He-like Fe XXV without radiation damping (used in Figure 3).

Column-by-column description of each type of the files:

- Ionization balance data files (./data/XXYYZZ/csd_$code.dat): the 1st column is tem-

perature in K, the 2nd column the temperature in eV, and the 3rd column the (normalized) ionic fraction.

- Energy level data files (./data/XXYYZZ/lev_$code.lis): the 1st column is level index, the 2nd column the configuration, the 3rd column the spin and orbital angular momentum, the 4th column the total angular momentum, the 5th column the energy in Rydberg, the 6th column the energy in cm^{-1}.

- Transition data files (./data/XXYYZZ/tran_$code.lis): the 1st column is level index of the lower energy level, the 2nd column the level index of the upper energy level, the 3rd column the wavelength in $\mathring{A}$, the 4th column the A-value in s^{-1}, the 5th column is $\log gf$, where g is the statistical weight of the upper level and f the oscillator strength.

- Temperature grid files (./data/XXYYZZ/tk_$code.lis): The list of temperature (in K) grid. Both $code = $mao22fe (H-like) and mao22qe He-like follow the standard OPEN-ADAS temperature grid. For $code = $aggKK (KK= $09-13$), they are temperature grids used by Aggarwal et al. For $code = $si17, it is the temperature grid used by Si et al. 2017.

- Effective collision strength data files (./data/XXYYZZ/ecs_$code.lis, code = mao22fe, mao22qe, mao22ag, mao22si): The 1st column is the level index of the lower energy level, the 2nd column the level index of the upper energy level, the 3rd column the A-value in s^{-1}, the rest columns are effective collision strength at each temperature value according to the temperature grid file with the same naming code.

- H-like effective collision strength data files (./data/01YYZZ/ecs_$code.dat, code = adb309, cdb1001, spex306): The 1st column is the temperature grid in K, the 2nd column the temeprature grid in eV, the 3rd and 4th columns are the effective collision strength of Lyα, the 5th and 6th columns are the effective collision strength of Lyβ, the 7th and 8th columns are the effective collision strength of Lyγ, the 9th and 10th columns are the effective collision strength of Lyδ.

- He-like effective collision strength data files (./data/02YYZZ/ecs_$code.dat, code = adb309, cdb1001, spex306): The 1st column is the temperature grid in K, the 2nd column the temeprature grid in eV, the 3rd column is the effective collision strength of Heα-w, the 4th column is the effective collision strength of Heα-x, the 5th column is the effective collision strength of Heα-y, the 6th column is the effective collision strength of Heα-z, the 7th column is the effective collision strength of Heβ-w, the 8th column is the effective collision strength of Heγ-w, the 9th column is the effective collision strength of Heδ-w.

For data presented in reference publications (but not in the three atomic databases), they are available in ./ref/agg09to13/ (a series of paper lead by K. Aggarwal) and ./ref/si17 (Si et al. 2017). The column-by-column descriptions are similar to those of H- and He-like effective collision strength data files (./data/XXYYZZ/ecs_$code.dat, code = adb309, cdb1001, spex306).

7 Python 3 jupyter notebooks to reproduce figures in the paper

7.1 Figure 1

./pynb/run_plot_cfcsd.py

- Subroutine:
  - ./pynb/gps.py
  - ./pynb/gps_gridspec.py
  - ./pynb/fuuc.py
- Input:
  - ./data/XXYYZZ/csd_$db.dat
- Output:
  - ./pynb/fig/plot_cfcsd.pdf

7.2 Figure 2

./pynb/run_plot_cflpop.py

- Subroutine:
  - ./pynb/gps.py
  - ./pynb/gps_gridspec.py
  - ./pynb/fuuc.py
  - ./pynb/ptbl.py
  - ./pynb/obj_ioa.py
- Input:
  - ./pynb/dat/lpop_011414_1kev.asc
- Output:
  - ./pynb/fig/plot_cflpop.pdf

7.3 Figure 3

./pynb/run_plot_ecs_z26.py

- Subroutine:
  - ./pynb/gps.py
  - ./pynb/gps_gridspec.py
  - ./pynb/fuuc.py
  - ./pynb/plot_util.py
- Input:
  - data files in ./data/012626/
  - data files in ./data/022625/
  - ./ref/agg09to13/ecs_022625_agg13.dat
  - ./ref/si17/ecs_022625_si17.dat
- Output:
  - ./pynb/fig/plot_cfecs_z26.pdf

7.4 Figure 4

./pynb/run_plot_ecs_z20.py

- Subroutine:
  - ./pynb/gps.py
  - ./pynb/gps_gridspec.py
  - ./pynb/fuuc.py
  - ./pynb/plot_util.py
- Input:
  - data files in ./data/012020/
  - data files in ./data/022019/
  - ./ref/agg09to13/ecs_022019_agg12.dat
  - ./ref/si17/ecs_022019_si17.dat
- Output:
  - ./pynb/fig/plot_cfecs_z20.pdf

7.5 Figure 5

./pynb/run_plot_ecs_z14.py

- Subroutine:
  - ./pynb/gps.py
  - ./pynb/gps_gridspec.py
  - ./pynb/fuuc.py
  - ./pynb/plot_util.py
- Input:
  - data files in ./data/011414/
  - data files in ./data/021413/
  - ./ref/agg09to13/ecs_011414_agg10.dat
  - ./ref/agg09to13/ecs_021413_agg10.dat
- Output:
  - ./pynb/fig/plot_cfecs_z14.pdf

7.6 Figure 6

./pynb/run_plot_ecs_z08.py

- Subroutine:
  - ./pynb/gps.py
  - ./pynb/gps_gridspec.py
  - ./pynb/fuuc.py
  - ./pynb/plot_util.py
- Input:
  - data files in ./data/010808/
  - data files in ./data/020807/
  - ./ref/agg09to13/ecs_010808_agg12.dat
- Output:
  - ./pynb/fig/plot_cfecs_z08.pdf

7.7 Figure 7

./pynb/run_plot_dnma_inst.py

- Subroutine:
  - ./pynb/gps.py
  - ./pynb/gps_gridspec.py
  - ./pynb/spex_qdp.py
- Input:
  - ./qdp/qdp_simu_hubs_dfsc_220514a.qdp
  - ./qdp/qdp_simu_hubs_pwsc_220514a.qdp
  - ./qdp/qdp_simu_arcus_dfsc_220514a.qdp
  - ./qdp/qdp_simu_arcus_pwsc_220514a.qdp
- Output:
  - ./pynb/fig/plot_cf_dnma_inst.pdf

8 User guide for Anaconda3

It might be possible that users fail to reproduce the exact results due to conflict environment settings or software packages updates. In this case, to reproduce the results using python, it is recommended to build a Docker container, starting with the Anaconda3 (continuumio/anaconda3:5.3.0) basic image.