Supplementary Materials

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Table of content

File or folder	Content
./ReadMe.md	This document
./inputs/08YYZZ/	Structure and collision calculation input files for each ion. YY = atomic number (e.g. 08 for O and 26 for Fe), ZZ = roman number (e.g. 02 for II and 14 for XIV), see descriptions below for more details
./open-adas/	Effective collision strength in the format of Atomic Data and Analysis Structure (ADAS) data class adf04
./dat/	Data files used for the plots, see descriptions below for more details
./notebooks/	Python 3 Jupyter notebooks to reproduce Figures in the paper
./eps/	EPS files of Figures
./docker_init.sh	Initialization when the Docker container is launched
./requirements.txt	List of python3 libraries required

Input files for the structure and collision calculations

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 each ion, we have the following directories | File or folder | Content | | ---|:---:| | ./inputs/08YYZZ/asc_si | Input file for the AUTOSTRUCTURE run (the last line lists the scaling parameters) | | ./inputs/08YYZZ/rmc_in/ex | Input files for the inner region exchange calculation | | ./inputs/08YYZZ/rmc_in/tcc | Input files for the inner region term coupling coefficient calculation | | ./inputs/08YYZZ/rmc_in/nex | Input files for the inner region non-exchange calculation | | ./inputs/08YYZZ/rmc_out/fex | Input files for the outer region exchange calculation with a fine energy mesh | | ./inputs/08YYZZ/rmc_out/cex | Input files for the outer region exchange calculation with a coarse energy mesh | | ./inputs/08YYZZ/rmc_out/nex | Input files for the outer region non-exchange calculation with a coarse energy mesh |

Additional data for selected ions

For Ne III (081003), Mg V (081205), Si VII (081407), S IX (081609), Ar XI (081811), Ca XIII (082013), and Fe XIX (082619), we include machine-readable energy levels, transition data, effective collision strength from previous works and the present work.

Column-by-column description for the tables

File	Content
./dat/Readme.lev	Description for the energy level tables
./dat/Readme.lev_map	Description for the energy level mapping
./dat/Readme.tran	Description for the transition data tables
./dat/Readme.tran_map	Description for the transition data mapping
./dat/Readme.tk	Description for the temperature grid of the effective collision strength
./dat/Readme.ecs	Description for the effective collision strength tables
./dat/Readme.ecs_map	Description for the effective collision strength mapping

Tabular data for each selected ion

File	Content
./dat/08YYZZ/lev_${code}.lis	Energy levels from NIST, previous works, and the present work
./dat/08YYZZ/lev_${code0}_${code1}.map	Mapping of the energy levels between two data sets.
./dat/08YYZZ/tran_${code}.lis	Transition datas from NIST, previous works, and the present work
./dat/08YYZZ/tran_${code0}_${code1}.map	Mapping of the transition data between two data sets
./dat/08YYZZ/tk_${code}.lis	Temperature grid of the effective collision strength
./dat/08YYZZ/ecs_${code}.lis	effective collision strength
./dat/08YYZZ/ecs_${code0}_${code1}_X.map	Mapping of the effective collision strength between two data sets at a low (X = l)/medium (m)/high(h)/very high(vh) temperature. The first line (as a comment) indicates the temperature values in both data sets (if not equal the closet match is used).

Python 3 jupyter notebooks to reproduce Figures in the paper

Figure 1

- ./notebooks/plot_fig1.ipynb
  - Subroutine:
    - ./ipynb/gps.py
    - ./ipynb/gps_subplot.py

    - Input:
        - ./dat/082619/lev_mao20_but08.map (Fe XIX)
        - ./dat/081811/lev_mao19_lud10.map (Ar XI)
        - ./dat/081609/lev_mao19_nist.map (S IX)
        - ./dat/081609/lev_mao19_lia11.map (S IX)
        - ./dat/081407/lev_mao19_nist.map (Si VII)
        - ./dat/081407/lev_mao19_sos14.map (Si VII)
        - ./dat/081205/lev_mao19_nist.map (Mg V)
        - ./dat/081205/lev_mao19_tay15.map (Mg V)
        - ./dat/081205/lev_mao19_wan17.map (Mg V)
        - ./dat/081003/lev_mao19_nist.map (Ne III)
        - ./dat/081003/lev_mao19_mcl11.map (Ne III)
    - Output:
        - on-screen

Figure 2

- ./notebooks/plot_fig2.ipynb
    - Subroutine:
        - ./ipynb/gps.py
        - ./ipynb/gps_subplot.py
    - Input:
    - ./dat/082619/tran_mao20_but08.map (Fe XIX)
    - ./dat/081811/tran_mao19_lud10.map (Ar XI)
    - ./dat/081609/tran_mao19_nist.map (S IX)
    - ./dat/081609/tran_mao19_lia11.map (S IX)
    - ./dat/081407/tran_mao19_nist.map (Si VII)
    - ./dat/081407/tran_mao19_sos14.map (Si VII)
    - ./dat/081205/tran_mao19_nist.map (Mg V)
    - ./dat/081205/tran_mao19_tay15.map (Mg V)
    - ./dat/081205/tran_mao19_wan17.map (Mg V)
    - ./dat/081003/tran_mao19_nist.map (Ne III)
    - ./dat/081003/tran_mao19_mcl11.map (Ne III)
    - Output:
        - on-screen

Figure 3

- ./notebooks/plot_fig3.ipynb
    - Subroutine:
        - ./ipynb/gps.py
        - ./ipynb/gps_subplot.py
    - Input:
        - ../dat/082619/ecs_mao20.lis
        - ../dat/082619/ecs_but08.lis
        - ../dat/082619/ecs_cdbv10.lis
    - Output:
        - on-screen

Figure 4

- ./notebooks/plot_fig4.ipynb

    - Subroutine:
        - ./ipynb/gps.py
        - ./ipynb/gps_subplot.py
    - Input:
        - ../dat/082013/ecs_mao20.lis
        - ../dat/082013/ecs_cdbv10.lis
    - Output:
        - on-screen

Figure 5

- ./notebooks/plot_fig5.ipynb
    - Subroutine:
        - ./ipynb/gps.py
        - ./ipynb/gps_subplot.py
    - Input:
        - ../dat/081811/ecs_mao20.lis
        - ../dat/081811/ecs_lud10.lis
        - ../dat/081811/ecs_cdbv10.lis
    - Output:
        - on-screen

Figure 7

- ./notebooks/plot_fig7.ipynb
    - Subroutine:
        - ./ipynb/gps.py
        - ./ipynb/gps_subplot.py
    - Input:
        - ../dat/081609/ecs_mao20.lis
        - ../dat/081609/ecs_lia11.lis
        - ../dat/081609/ecs_cdbv10.lis
    - Output:
        - on-screen

Figure 10

- ./notebooks/plot_fig10.ipynb
    - Subroutine:
        - ./ipynb/gps.py
        - ./ipynb/gps_subplot.py
    - Input:
        - ../dat/081407/ecs_mao20a.lis (ADAS temperature grid)
        - ../dat/081407/ecs_sos14.lis
        - ../dat/081407/ecs_cdbv10.lis
    - Output:
        - on-screen

Figure 11

- ./notebooks/plot_fig11.ipynb

    - Subroutine:
        - ./ipynb/gps.py
        - ./ipynb/gps_subplot.py
    - Input:
        - ../dat/081205/ecs_mao20a.lis (ADAS temperature grid)
        - ../dat/081205/ecs_tay15.lis
        - ../dat/081205/ecs_cdbv10.lis
    - Output:
        - on-screen

Figure 12

- ./notebooks/plot_fig12.ipynb
    - Subroutine:
        - ./ipynb/gps.py
        - ./ipynb/gps_subplot.py
    - Input:
        - ../dat/081003/ecs_mao20.lis
        - ../dat/081003/ecs_mcl11.lis
        - ../dat/081003/ecs_cdbv10.lis
    - Output:
        - on-screen

Figure A.1

- ./notebooks/plot_figA1.ipynb
    - Subroutine:
        - ./ipynb/gps.py
        - ./ipynb/gps_subplot.py
    - Input:
        - ../dat/082619/ecs_mao20_but08_l.map
        - ../dat/082619/ecs_mao20_but08_m.map
        - ../dat/082619/ecs_mao20_but08_h.map

Figure A.2

- ./notebooks/plot_figA2.ipynb
    - Subroutine:
        - ./ipynb/gps.py
        - ./ipynb/gps_subplot.py
    - Input:
        - ../dat/081811/ecs_mao20_lud10_l.map
        - ../dat/081811/ecs_mao20_lud10_m.map
        - ../dat/081811/ecs_mao20_lud10_h.map

Figure A.3

- ./notebooks/plot_figA3.ipynb
    - Subroutine:
        - ./ipynb/gps.py
        - ./ipynb/gps_subplot.py

    - Input:
        - ../dat/081609/ecs_mao20_lia11_l.map
        - ../dat/081609/ecs_mao20_lia11_m.map
        - ../dat/081609/ecs_mao20_lia11_h.map

Figure A.4

- ./notebooks/plot_figA4.ipynb
    - Subroutine:
        - ./ipynb/gps.py
        - ./ipynb/gps_subplot.py
    - Input:
        - ../dat/081407/ecs_mao20b_sos14_l.map (S14 temperature grid)
        - ../dat/081407/ecs_mao20b_sos14_m.map (S14 temperature grid)
        - ../dat/081407/ecs_mao20b_sos14_h.map (S14 temperature grid)

Figure A.5

- ./notebooks/plot_figA5.ipynb
    - Subroutine:
        - ./ipynb/gps.py
        - ./ipynb/gps_subplot.py
    - Input:
        - ../dat/081205/ecs_mao20b_tay15_l.map (T15 temperature grid)
        - ../dat/081205/ecs_mao20b_tay15_m.map (T15 temperature grid)
        - ../dat/081205/ecs_mao20b_tay15_h.map (T15 temperature grid)
        - ../dat/081205/ecs_mao20b_wan17_l.map (W17 temperature grid)
        - ../dat/081205/ecs_mao20b_wan17_m.map (W17 temperature grid)
        - ../dat/081205/ecs_mao20b_wan17_h.map (W17 temperature grid)

Figure A.6

- ./notebooks/plot_figA6.ipynb
    - Subroutine:
        - ./ipynb/gps.py
        - ./ipynb/gps_subplot.py
    - Input:
        - ../dat/081407/ecs_mao20b_mcl11_l.map
        - ../dat/081407/ecs_mao20b_mcl11_m.map
        - ../dat/081407/ecs_mao20b_mcl11_h.map

Table 3

- ./notebooks/stat_tbl3.ipynb
    - Input:
        - ../dat/082619/ecs_mao20_but08_l.map
        - ../dat/082619/ecs_mao20_but08_m.map
        - ../dat/082619/ecs_mao20_but08_h.map
    - Output:
        - on-screen Note:
        - This is an exemplary python script to print (more than) the statistics shown in Table 3 for Fe XIX. Minor changes are required

to print statistics shown in Table 3 for other ions.