WR_F_TO_S

Program for creating/modifying the XzV_F_TO_S files which describe the linking between the atomic levels (FL) and super levels (SL) for species XzV. There is no simple prescription for the optimal SL assignments. Further, the best SL assignments will depend on their use --- atmospheric structure or abundance studies. For the later, finer SL assignments might be more useful. NB: The use of model atoms with no SL assignments (i.e., No. of SL = No. of FL) might not be optimal due to inadequacies in the collisional atomic data.

Options are ordered under subject. Associated with each option are requested inputs. Some inputs are not prompted for, and can only be changed from their default values by specifying them in the call, e.g.,

ELS(CHK_P=F)

Such inputs are placed in [ ].

There are three types of options:

(1) Options, such as WR, which provide output.
(2) Options, such as RD_LNK, which read in existing data files.
(3) Options, such as ELS, which modify the SL assignments.

SVE file:

A text file containing options (transparent and hidden) used in the execution of a command
Default is to write a file 'command.sve' (e.g., rd_mod.sve) containing the options used when a command is executed.
Case is important for the sve file but not for the option.
Append sve=filename to write a new .sve file (no brackets).
To execute a previous command, enter .command (e.g., .rd_mod). Options can be changed by supplying the in () after the sve file name., e.g.,

.rd_mod(over=t)

NB: rd_obs, RD_OBS and RD_OBS1 (etc) are treated as the same option in PLT_SPEC, but write different sve files with distinct names.

BOX file:

A text file containing an ordered sequence of commands as specfied by .sve files, e.g.,

.rd_mod

.cnvlv
.norm
Type box=filename to write a .box file containing several .sve files
Type #filename to read .box file.
Particulalry useful for reading in multiple data sets etc.

Required Files:
XzV_F_OSCDAT
Additionally, files containing previous SL assignments, and level departure coefficients, can be useful.

Input:

RD_DC	Reads in departure coefficients (from an CMFGEN XzVOUT file) for a model computed with current atomic model. If model was run with N_S=N_F the DC can be output with the levels names in order to assist in deciding super level assignments. The departure coefficients at 3 distinct depths (d=1, $N_D/3+1$, $2N_D/3+1$) are read in.
RD_LNK	Read in a previously existing link file. If this file has been edited, and the links numbering is all mixed up, the CL option should be issued. Note: It is possible to edit an F_TO_S link file by hand to change SL assignments. The SL assignments in this temporary file need not be ordered or continuous. Use the RD_LNK and CL option with WR_F_TO_S to put in a form that can be used by CMFGEN.
RD_SM_LNK	This option allows links for with non-split terms to be read in. These links can then be used for a model atom with split terms. Split terms are grouped into the same SUPER level. The number of terms in both files must be identical.

Output options

AVE	Outputs to unit 31 the average energy of each SL.
SEP	Outputs the maximum energy separation between levels in EACH super level.
SL_WR	Levels belonging to a single SUPER level are output together as a group.

	Useful for diagnostic purposes only. Output filename is requested. [DC]: Output departure coefficients for each SL.
TY	Output SL assignments to terminal.
WR	Outputs Super-Level links in a format suitable for CMFGEN. [DC]: Output departure coefficients for each SL. [HEAD]: Read header information from a separate ascii file (HEAD_INFO is default).
WR_DC	Outputs Super-Level links in a format suitable for CMFGEN. [DC]: Output departure coefficients for each SL.
WR_NOJ	Outputs SLs for LS level.

Super-level assignment options

CL	Option to re-label the links between super-levels and the full levels The only requirement in the raw link is that they are unique, and +ve. They do not need to be in ordered. Very useful for splitting SLs or refining SL assignments using an existing CMFGEN assignment file. Simply copy the file to a temporary file, and edit SL assignments directly, without regard to ordering.
LS	Combines states with the same term into a common SL. Overwrites any existing SL assignments.
ELS E%LS	Group all terms belonging to the same LS multiplet. Additional grouping is done by combining terms that are within DEL_E in energy of the lowest term of the SUPER level (ELS) or which have a maximum percentage difference in their excitation energy (E%LS). The defaults is to group together only terms that have the same parity and spin, although this can be changed using HIDDEN options. DEL_E - Maximum energy difference for SL in cm^{-1}. [CHK_P] - Check parity (logical). [CHK_S] - Check spin (logical). %E - Percentage diference in excitation energy
SP	Similar to ELS except that all terms belonging to the same multiplet will not necessarily belong to the same SL.
SPLIT	Allows a coarse SUPER level assignment to be refined according to the energy

	separation of levels, and the difference in departure coefficients (e.g., as computed using FULL LS coupling). This option should be followed by the CL option. ACC: If the departure coefficients differ by more than ACC %, they will be grouped into a new super level. DEL_E: If the energy separation is > DEL_E (cm^{-1}), a new super level is created.