Instructions for the "xls2ens" python program

1. Running requirements:

python 2.7.6 (not working with python 3.0.x), xlrd package (version 0.9.4)

2. The input excel file:

This file must at least have two sheets named "Header" and "Data".

"Header" sheet:

contains header information to be put in an output file such as nuclide name, reaction name, general comments, and so on. It must have two columns and at least six rows, as shown below. The names of the first column must be the same as shown below. Order and case don't matter. The content in the second column is for example.

column1	column2	
Nuclide	178Hf	
Reaction	174YB(12B,xng)	
NSR	2011Ko16	
Reference	F.G. Kondev et al., Phys. Lett. B492 (2011) 112-124	
Comment	2011Ko16: This was obtained using data	
Compiler	Compiled by W. Murray (DePaul U/ANL) and F.G. Kondev (ANL): November 13,	
	2011	
CL (or CG,CA,)	E,J\$From Adopted Levels	
Command	NEWLINE	
LCD1 (or LCD2,)	G{-0}{+2}/ G{- g}	
GCD1(or GCD2,)	anisotropy	
LCD1_KEYNUMBER	1994Pa27 (Note: keynumber to be put at the end of each LCD1 data)	
GCD1_KEYNUMBER	1994Pa27 (Note: keynumber to be put at the end of each GCD1 data)	
LUDD1_KEYNUMBER	1994Pa27 (Note: keynumber to be put at the end of each LUDD1 data)	
RI_MULTIPLY,	1.34(2)	
DRI_FORMAT	REAL	

Explanations (for names in column1 in table above):

• Nuclide:

Nuclide name to be put in col1-5 each line in output file.

• Reaction:

Reacion name to be put as dataset DSID in col10-39 of the first line in output file.

• *NSR*:

NSR keynumber.

• Reference:

Reference of the paper being compiled.

• Compiler:

Information of compiler

• Comment:

General comments of the dataset to be put before data table. Multiple "Comment" headers can be used.

• CL (or CG,CB,CA,...):

General comments for specified type of records, eg, "CL" for level record, "CG" for gamma records. Multiple headers can be used.

• Command:

For controlling display of data-as-comment in output. Multiple "command" headers can be used. Available commands are:

"NEWLINE":

put each data-as-comment (LCD1, LCD2, ..., GCD1, GCD2, ..., DCD1,..., PCD1,..., see instructions for data sheet for descriptions) in a new line. By default they are put in the same line.

"UPPERCASE":

put comments in uppercase "C". It is in lowercase by default.

"LIMIT=25":

Set uncertainty round-off limit to 25. It is set to be 99 by default.

LCD1 (or LCD2,..., GCD1, GCD2,..., DCD1,..., PCD1,...):

value in column2 is the replacement of the column name (see notes for "data sheet") in the output. This is useful for putting data-as-comment values in comment, like "E(p)(lab)=1204 {I5}". To use it, put data in a column called "LCD1" in data sheet and rename "LCD1" to "E(p)(lab)" in the "Header" sheet, like the example "Header" sheet above.

LCD1 KEYNUMBER (or GCD1 KEYNUMBER, LUDD1 KEYNUMBER, GUDD1 KEYNUMBER):

keynumber to be put at the end of each data-as-comment.

(Note: LUDD---user-defined-data for level, alternative to LCD but can have units to be put in a LUDU column in data sheet, same for GUDD)

RI_MULTIPLY:

Multiply all values in "RI" column in data sheet with a constant value in column2.

Also apply to all data fields that can have uncertainty.

Format of the keyword in column1: Field name+" "+operaton name

Available operation_name: ADD, MULTIPLY, SUBTRACT

Multiple operations on the same filed is allowed, but note that order of operation is their order in the header sheet.

• DRI_FORMAT:

Indicates the format of the values in the separate "DRI" uncertainty column in data sheet. If "REAL" is given, the values in "DRI" column will be processed as real values. By default, all numerical uncertainties in separate columns in data sheets are in ENSDF format.

The keyword in column1: uncertainty Field name+" FORMAT"

Available format: REAL, ENSDF (default if not set)

DELAY_TYPE:

"P" for delayed proton, "N" for delayed neutron, "A" for delayed alpha. It is optional. One can also specify the type in the data column name in data sheet, like, "EDP" for delayed-proton energy, "EDA" for delayed-alpha energy.

Other available optional settings:

For parent record in decay dataset:

PID	parent nuclide name	
EP,DEP	parent level energy and uncertainty	
JPA	parent spin-parity	
TP,DTP,TPU	parent half-life,uncertainty,unit	
QP,DQP	Parent Q-value and uncertainty	
СР	Parent comments	
PDOC	Parent document comments. (NOTE: "DP" in delay-particle)	

For N record:

NR, DNR, NT, DNT, BR, DBR, NB, DNB, NP, DNP (refer to ENSDF manual for these names)

CN: comments

NDOC: document comments (NOTE: "DN" reserved for delayed neutron)

For PN record:

NRBR, DNRBR, NTBR, DNTBR, NBBR, DNBBR, NP, DNP (refer to ENSDF manual)

PNCOM: PN COM in col77 **PNOPT**: PN option in col78

CPN: PN comments

PNDOC: PN document comments

For Q record in Adopted dataset:

Q, DQ, SN, DSN, SP, DSP, QA, DQA

QREF: keynumber

CQ: Q record comments

QDOC: Q record document comments

"Data" sheet:

- ✓ Column names have to be selected from the list below. Values can be given as "value(uncertainty)" in one column , or 'value' and 'uncertainty' in two separate columns.
- ✓ Uncertainty must be in ENSDF format. For example, level energy 274.2(4) can be put in one column "EL" as "274.2(4)" or in two separate columns "EL" and "DEL" as "274.2" and "4", respectively. Other examples, "<=1" in "RI" column or "1" and "<=" in "RI" and "DRI" columns, respectively. Similar for "~1".</p>

- ✓ Records of a gamma from a level must be put in the same row as the level record.
- ✓ Records of a decay from a level must be put in the same row as the level record.
- ✓ If there are more than one gamma records, the records for these gammas can be put in new rows with the fields for the level blank except the level energy, which tells the program which level these gammas are from.
- ✓ If the level energy field in a row for gamma record is blank, this gamma is treated as from the level in the previous row.
- ✓ Multiple flags are allowed in 'LFLAG', 'GFLAG', 'DFLAG' and 'PFLAG' fields. If this is the case, the first flag will be put in column 77 and the rest will be put in continuation record following 'FLAG='. If there is a band flag, it will be put in column 77 and all 'LFALG' will be put in continuation record.

For Level record:

Column name	description	Column name	description
'EL','DEL'	Level energy	'BAND','LFLAG'	Band flag, and level flags
'JPI'	Spin-parity	'CL'	Level comment
'T','DT'	Half-live	'LQUE'	Question mark for level
'TU'	Half-live unit	'LCD1','DLCD1'	Data1 to be put in level comment
L'	Angular mom.	'LCD2','DLCD2'	Data2 to be put in level comment
'S','DS'	C2S factor	'LCD3','DLCD3'	Data3 to be put in level comment
'ISPIN'	isospin	'BE1UP','DBE1UP','BE1WUP',	Transition prob., up to E5 and M5
'XREF'	XREF	LUDN	Name of user-defined data in comm.
'DL'	Level document	LUDU,LUDD,DLUDD	unit, data value, uncertainty
'GF','DGF'	g-factor	MOMM1,MOMM2,	Nuclear moment
'MS'	Metastable mark	'SL'	Calculated data

Explanation:

- For 'CL', the ENSDF convention should be followed. For example, "E\$...." is for level energy comment, "\$..." is for general level comment, and so on. Multiple 'CL' columns are allowed.
- Columns 'LCD1' and 'DLCD1' is for data of value and uncertainty to be put in the level comment
 with the name='LCD1", for example, the output will look like "178HF CL \$LCD1=value uncertainty".
 Right now, maximum of three such data are allowed to be put this way. It is useful to put data like
 level widths in the comment. One can rename "LCD1" in "Header" sheet. See explanation for
 "Header" sheet for details.
- Columns 'LUDN', 'LUDU', 'LUDD': similar to 'LCD1' for putting values of non-standard records in comments. The difference is that, 'LUDN', which stands for user-defined data name in level record, allows users to set a name for each value. Also the 'LUDU' column can be used to set a unit for each value. This is useful for column mixed with different type of values, like T1/2 and width.

For Gamma record:

Column	description	Column name	description
name			
'EG','DEG'	gamma energy	'GFLAG'	gamma flags
'RI','DRI'	Gamma intensity	'CG'	Gamma comment
'EF','JF'	For final level	'DG'	Gamma document comments
'MUL'	Multi-polarity	'GQUE'	Question mark for gamma
'MR','DMR'	Mixing ratio	'GCD1','DGCD1'	Data1 to be put in gamma comment
'CC','DCC'	Conversion coeff.	'GCD2','GLCD2'	Data2 to be put in gamma comment
'TI','DTI'	Total intensity	'GCD3','GLCD3'	Data3 to be put in gamma comment
'DCO','DDCO'	DCO ratio	'BE1','DBE1','BE1W',	Transition prob., up to E5 and M5
'POL','DPOL'	polarization	'A2','DA2',	Angular distribution coeff. (up to A6)
'ECC','DECC'	Exp. total CC	'EKC','DEKC','ELC',	Sub-shell exp. CC (up to M shell)
'GCOIN'	Coincidence mark	GUDN,GUDU,GUDD,DGUDD	User-defined data-as-comment
'SG'	Calculated data		

The usage of 'CG', 'GCD1', 'GUDN', ... is the same as 'CL', 'LCD1', 'LUDN', ... for the level record.

For Decay record:

Column name	description	Column name	description
'EB','DEB'	Beta energy	'EA','DEA'	Alpha decay energy
'IB','DIB'	Beta branch (B-)	'IA','DIA'	Alpha decay branch
'IBE','DIBE'	Beta branch (B+)	'HF','DHF'	Alpha decay HF factor
'IE','DIE'	EC branch	'DQUE'	Question mark for decay record
'LOGFT','DLOGFT'	Logft value	'CA'	Comment for alpha decay record
'DFLAG'	Decay flags (B+/-,EC)	'DFLAG'	also used for coin. mark if given as "C"
'CB','CE'	Comments for B-,B+/EC	'UN'	Forbiddenness, e.g., "1U", "2U"
'DCD1','DDCD1',	Data-as-comment	'DB','DE','DA'	Document comments
'SB','SE','SA'	Calculated data		

For Delay record:

Column name	description	Column name	description
'EDP','DEDP'	Delayed-proton energy	'EDN','DEDN'	Delayed-neutron energy
'IP','DIP'	Particle intensity	'EDA','DEDA'	Delayed-alpha energy
'ED'	Intermediate level energy	'LP'	Transfer angular-momentum
'WIDTH','DWIDTH'	Transition width (keV)	'PFLAG'	Delayed-particle flags
'PCOIN'	Coincidence mark	'PQUE'	Question mark
'CDP','CDA','CDN'	comments	'PCD1',	Data-as-comment
'DDP','DDA','DDN'	Document comments		

3. Use of this program

type in a terminal,

"python xls2ens"

and then you will be asked for the name of the excel file (with or without .xls extension are both ok). The output file is "outfile.ens"

Other function: you can print out all conversion data into a file that can be used as the input for the BrlccMixing program by typing "PRINT_CC" after the excel file name, for example,

"2014ThAA PRINT_CC LEVEL"

You can order the output by "LEVEL" or "GAMMA" energy, just by specifying "LEVEL" or "GAMMA" following "PRINT_CC". The output file is "PRINT_CC.out".

4. The output file is "outfile.ens"

Jun Chen July 6, 2017