NNDC CSV Parser for Isomer Database

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Date 07/03/2025

This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Nuclear Physics and used resources of the Facility for Rare Isotope Beams (FRIB) Operations, which is a DOE Office of Science User Facility under Award Number DE-SC0023633, and by the US National Science Foundation under Grants No. PHY-20-12040 and 23-10078 “Windows on the Universe: Open Quantum Systems in Atomic Nuclei at FRIB”.

Goals

CURRENT STATE

- Upkeep of Isomer Database is done manually line-by-line, very time consuming.
- NNDC hosts large and maintained database for isomeric gamma emission.
  - File formats in CSV's available are not easily translated for LISE^{++} current Isomer Database

E(level) (keV)	XREF	J^{π}(level)	$T_{1/2}$(level)	E(γ) (keV)	I(γ)	M(γ)	Final Levels	
0	ABCDEF	9/2+	2.4 m *1* % β^- = 100					
311.37 *3*	ABCDE	1/2-	18.0 m *3* % IT = 4.4 % β^- = 95.6	311.39 *3*	100	M4	0	9/2+
604.18 *7*	AB DE	3/2-	< 1.0 ns	292.9 *1*	100	M1,E2	311.37	1/2-
654.27 *7*	AB	(3/2)+	130 ns *15*	50.2 *1* 343.0 *1*	2.1 *2* 100 *9*	[E1] E1	604.18 311.37	3/2- 1/2-
720.60 *11*	B F	(7/2+)		720.7 *2*	100		0	9/2+
788.26 *9*	AB	1/2+,3/2+	2.00 ns *15*	134.0 *1* 184.1 *1* 476.7 *3*	100 *7* 3.2 *6* 12.8 *17*	E2(+M1) [E1] [E1]	654.27 604.18 311.37	(3/2)+ 3/2- 1/2-
941.43 *8*	AB D	5/2+		153.5 *3* 287.6 *3* 337.6 *3* 941.2 *1*	2.3 *9* 14 *4* 17.4 *23* 100 *8*		788.26 654.27 604.18 0	1/2+,3/2+ (3/2)+ 3/2- 9/2+

OBJECTIVE

- Use Python and its libraries to develop a CSV parser to translate NNDC CSV files to the desired format for Isomer_DB.sqlite file
- Allows for simpler upkeep and **growth** of the LISE^{++} database saving time and resources.
- Code is adaptable for creating new tables with varying formats.

Figure 1: NNDC table for 119In isomers

Module Usage

- The NNDC_Parser.py module contains a collection of functions used to unpack the information contained in an NNDC CSV file.
- The most effective and user-friendly function contained in the package is **sqlite_entries**.
- To create new entries, call the **sqlite_entries** function with the desired NNDC CSV (form "adoptedLevels_##Symbol.csv"), user initials, the database directory **(db_dir)**, and the subtable name.
  - This will produce all gamma emissions in the NNDC file formatted for the Isomer_DB.sqlite file.
  - Optional utilities:
    - » ref_DB=Pandas.DataFrame → References existing dataframe from environment instead of .sqlite file.
    - » extra_tables=True → view how NNDC is expanded by the **expand_csv** method, check for errors.
    - » input_entries=True → use sqlite3 connection to automatically append drawn entries to the Isomer_DB.sqlite file.

```
1  nndc_parser.sqlite_entries('adoptedLevels119In.csv', 'HM', db_dir = 'Isomer_DB_TSTplaying.sqlite', subtable = 'Isomers')
✓ 0.5s
```

	INDEX_IT	A_IT	Z_IT	E_GAMMA	D_EG	IT_RATIO	D_IT_RATIO	T12	D_T12	LEVEL	...	I_GAMMA	D_IG	M_GAMMA	M_RATIO	D_MRATIO	CONV	D_CONV	SOURCE	NAME	ROW
0	11949311	119	49	311.39	3	10	NaN	1080000000.0	1800.0	311.37	...	100	NaN	M4	NaN	NaN	NaN	NaN	NNDC	HM	3721
1	11949293	119	49	292.9	1	10	NaN	0.001	LT	604.18	...	100	NaN	M1,E2	NaN	NaN	NaN	NaN	NNDC	HM	3722
2	1194950	119	49	50.2	1	10	NaN	0.13	0.000002	654.27	...	2.1	2	[E1]	NaN	NaN	NaN	NaN	NNDC	HM	3723
3	11949343	119	49	343.0	1	10	NaN	0.13	0.000002	654.27	...	100	9	E1	NaN	NaN	NaN	NaN	NNDC	HM	3724
4	11949721	119	49	720.7	2	10	NaN	0.002	0.000002	720.60	...	100	NaN	NaN	NaN	NaN	NaN	NaN	NNDC	HM	3725
...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...
106	119491540	119	49	1539.9	3	10	NaN	0.24	0.000003	2564.64	...	55	15	NaN	NaN	NaN	NaN	NaN	NNDC	HM	3827
107	119491623	119	49	1623.0	5	10	NaN	0.24	0.000003	2564.8	...	30	13	NaN	NaN	NaN	NaN	NaN	NNDC	HM	3828
108	119491911	119	49	1911.0	10	10	NaN	0.24	0.000003	2564.8	...	31	19	NaN	NaN	NaN	NaN	NaN	NNDC	HM	3829
109	119491961	119	49	1960.7	3	10	NaN	0.24	0.000003	2564.8	...	100	19	NaN	NaN	NaN	NaN	NaN	NNDC	HM	3830
110	11949152	119	49	152		10	NaN	0.24	0.000003	2656.9	...	NaN	NaN	(E2)	NaN	NaN	NaN	NaN	NNDC	HM	3831

Figure 3: Entries drawn for 119In data from NNDC

Additional Functions

- The functions called within **sqlite_entries** are also available to the user, independent of the mapping scheme from **sqlite_entries**. Each function contains docstrings that describe the intended usage of the functions and what they produce.
- Users may utilize these internal functions to create their own tables from NNDC CSV files or append to existing databases with their own programming.
- Function summaries:
  - **sqlite_characterize_table**: Produce recent GUID value and columns.
  - **sqlite_to_pandas**: Convert .sqlite database table to Pandas DataFrame.
  - **parse_isomerID**: Creates isotope ID from CSV file name.
  - **stretch_csv**: CSV → DataFrame with rows for gamma emissions.
  - **sqlite_entries**: Maps stretch_csv result to Isomer_DB.sqlite format.
  - **input_entries**: Append information from Pandas DataFrame to .sqlite.

```
1  nndc_parser.__all__
✓ 0.0s

['sqlite_characterize_table',
 'sqlite_to_pandas',
 'parse_isomerID',
 'stretch_CSV',
 'sqlite_entries',
 'input_entries']
```

Figure 4: List of functions in NNDC_READER module

Process Insight (1)

E(level) (keV)	XREF	J^{π}(level)	$T_{1/2}$(level)	E(γ) (keV)	I(γ)	M(γ)	Final Levels	
0	ABCDEF	9/2+	2.4 m *1* % β⁻ = 100					
311.37 *3*	ABCDE	1/2-	18.0 m *3* % IT = 4.4 % β⁻ = 95.6	311.39 *3*	100	M4	0	9/2+
604.18 *7*	AB DE	3/2-	< 1.0 ns	292.9 *1*	100	M1,E2	311.37	1/2-
654.27 *7*	AB	(3/2)+	130 ns *15*	50.2 *1* 343.0 *1*	2.1 *2* 100 *9*	[E1] E1	604.18 311.37	3/2- 1/2-
720.60 *11*	B F	(7/2+)		720.7 *2*	100		0	9/2+
788.26 *9*	AB	1/2+,3/2+	2.00 ns *15*	134.0 *1* 184.1 *1* 476.7 *3*	100 *7* 3.2 *6* 12.8 *17*	E2(+M1) [E1] [E1]	654.27 604.18 311.37	(3/2)+ 3/2- 1/2-
941.43 *8*	AB D	5/2+		153.5 *3* 287.6 *3* 337.6 *3* 941.2 *1*	2.3 *9* 14 *4* 17.4 *23* 100 *8*		788.26 654.27 604.18 0	1/2+,3/2+ (3/2)+ 3/2- 9/2+

Figure 1: NNDC table for 119In isomers

	E(level)(keV)	XREF	Jπ(level)	T1/2(level)	E(γ)(keV)	I(γ)	M(γ)	Final Levels	Final Jπ	RATIOS	DECAY_PARENT
0	[311.37, 3]	ABCDE	1/2-	[18.0, m, 3]	[311.39, 3]	[100,]	M4	0	9/2+	[' % IT = 4.4', ' % B- = 95.6']	
1	[604.18, 7]	ABDE	3/2-	[1.0, ns, <]	[292.9, 1]	[100,]	M1,E2	311.37	1/2-		
2	[654.27, 7]	AB	(3/2)+	[130, ns, 15]	[50.2, 1]	[2.1, 2]	[E1]	604.18	3/2-		
3	[654.27, 7]	AB	(3/2)+	[130, ns, 15]	[343.0, 1]	[100, 9]	E1	311.37	1/2-		
4	[720.60, 11]	BF	(7/2+)	[2.00, ns, 15]	[720.7, 2]	[100,]	NaN	0	9/2+		788.26 9
...	...	...	...	...	...	...	...	...	...	...	...
106	[2564.64, 17]	B	(11/2-)	[240, ns, 25]	[1539.9, 3]	[55, 15]		1025.02	(11/2+)		2656.9 18
107	[2564.8, 3]	A	1/2+,3/2+,5/2+	[240, ns, 25]	[1623.0, 5]	[30, 13]		941.43	5/2+		2656.9 18
108	[2564.8, 3]	A	1/2+,3/2+,5/2+	[240, ns, 25]	[1911.0, 10]	[31, 19]		654.27	(3/2)+		2656.9 18
109	[2564.8, 3]	A	1/2+,3/2+,5/2+	[240, ns, 25]	[1960.7, 3]	[100, 19]		604.18	3/2-		2656.9 18
110	[2656.9, 18]	F	(25/2+)	[240, ns, 25]	[152,]	NaN	(E2)	2504.9	(21/2+)		2656.9 18

111 rows × 11 columns

- This example follows for isomers of 119In.
- From the NNDC data seen in Fig. 1,the downloaded CSV is expanded with **stretch_csv** to the table in Fig. 5 with rows per gamma emission
  - Half-lives are shared from multiple entries (like in 1438 keV E(level)).
  - Lists in [value, units, uncertainty] or [value, uncertainty] order if units defined.
    - » Empty uncertainty assumes great enough precision.
  - Decay parents included for transient isomers
  - Transmission ratios stored when present

Figure 5: Expanded table with **stretch_csv** for 119In

Process Insight (2)

- When using **sqlite_entries**, the data frame seen in Fig. 5 is then iterated over and mapped to a new data frame which contains values consistent with the Isomer_DB.sqlite formatting.
  - Unexpected symbols such as “<” are translated to “LT”.
  - Conversion for $T_{1/2}$ units applied to standardize entries in micro-seconds.
  - Empty entries to NaN type objects.
  - Separate lists into appropriate columns.
- The information contained in the translated entries table can then be appended to the database as mentioned in Slides 3 and 4.

	INDEX_IT	A_IT	Z_IT	E_GAMMA	D_EG	IT_RATIO	D_IT_RATIO	T12	D_T12	LEVEL	D_LEVEL	JPI	I_GAMMA	D_IG	M_GAMMA	M_RATIO	D_MRATIO	CONV	D_CONV
0	11949311	119	49	311.39	3	10	NaN	1080000000.0	1800.0	311.37	3	9/2+	100	NaN	M4	NaN	NaN	NaN	NaN
1	11949293	119	49	292.9	1	10	NaN	0.001	LT	604.18	7	1/2-	100	NaN	M1,E2	NaN	NaN	NaN	NaN
2	1194950	119	49	50.2	1	10	NaN	0.13	0.000002	654.27	7	3/2-	2.1	2	[E1]	NaN	NaN	NaN	NaN
3	11949343	119	49	343.0	1	10	NaN	0.13	0.000002	654.27	7	1/2-	100	9	E1	NaN	NaN	NaN	NaN
4	11949721	119	49	720.7	2	10	NaN	0.002	0.000002	720.60	11	9/2+	100	NaN	NaN	NaN	NaN	NaN	NaN
...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...
106	119491540	119	49	1539.9	3	10	NaN	0.24	0.000003	2564.64	17	(11/2+)	55	15	NaN	NaN	NaN	NaN	NaN
107	119491623	119	49	1623.0	5	10	NaN	0.24	0.000003	2564.8	3	5/2+	30	13	NaN	NaN	NaN	NaN	NaN
108	119491911	119	49	1911.0	10	10	NaN	0.24	0.000003	2564.8	3	(3/2)+	31	19	NaN	NaN	NaN	NaN	NaN
109	119491961	119	49	1960.7	3	10	NaN	0.24	0.000003	2564.8	3	3/2-	100	19	NaN	NaN	NaN	NaN	NaN
110	11949152	119	49	152		10	NaN	0.24	0.000003	2656.9	18	(21/2+)	NaN	NaN	(E2)	NaN	NaN	NaN	NaN

111 rows × 19 columns

Figure 6: Entries drawn from stretched table