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Dictionary 227 (Nuclides) converted from NUBASE2020

(N. Otsuka, 2023-01-09, Memo CP-D/1067, A11)

Dictionary 227 (Nuclides and natural isotopic mixtures) was updated with the Atomic Mass Evaluation (AME) file and Nuclear Wallet Cards (NWC) file as inputs. This Dictionary has been frozen many years since I do not receive an updated NWC file more than 10 years. Consequently, we sometimes receive an unnecessary error message from ZCHEX (e.g., superheavy element nuclides still defined by `*` instead of `NH`, `MV` and `TS`).

Following Action 11 of the NRDC 2022 meeting, I have written a program to convert the NUBASE2020 (F.G. Kondev et al., Chinese Physics C 45 (2021) 030001) file (nubase_4.mas20) distributed from the Atomic Mass Data Center (AMDC https://www.anl.gov/phy/atomic-mass-data-resources/) to Dictionary 227.

A test dictionary generated with this new procedure is available as Dictionary 9927 in three formats (Trans, Archive and Backup) from the NDS open area: http://nds.iaea.org/nrdc/ndsx4/trans/dictionaries/. Note that all dictionaries other than 227 are equivalent to Dictionary 9127.

Features of dictionary converter

This converter

- adopts all ground states and metastable states with $T_{1/2} \geq 0.1$ sec
- adds the spin/parity when a measured value without ambiguity is given
- adds the half-life after conversion to sec when a definite value from other than systematics is given (Consequently, the half-life flag field is abolished.)
- adds flag S for stable nuclide, flag U for unstable nuclide and P for particle-unstable nuclide
- adds the isomeric transition probability for unstable nuclides and the natural isotopic abundance for stable nuclides.

Generation of lines for particle codes

The information of "particles" (e.g., photon, meson, exotic baryon) as well as natural isotopic mixtures must be added from an additional input file. I introduced the following change in these additional dictionary lines:

- Addition of the corresponding particle code as its "A-symbol" when it is defined in Dictionary 33 (e.g., `PI0`, `PIN` and `PIP` for neutral, negative, and positive π mesons, respectively).
- Addition of `0` at the last column of the internal numerical equivalents of natural isotopic mixtures.
- Replacement of `0` or `1` with a unique negative integer for the internal numerical equivalent of particles other than γ.
- Correction of the position of the atomic masses of the natural isotopic mixtures (They were coded as the isotopic abundances.).
- Addition of the particle masses in amu which were converted from the masses in MeV compiled in the latest version of Review of Particle Physics (P.A. Zyla et al., Prog. Theor. Exp. Phys. **2020** (2020) 083C01).

Use of -G, -M1 and -M2 in Dictionary 227

So far, all metastable states were defined with -M and the corresponding ground state was defined without -G in the Dictionary 227:

Example:

```
 TRA 201611  65-TB-156                  156TB  651560 -3.    5.35       D     155924755.181
 TRA 201611  65-TB-156-M                156TB  651561        24.4       H
 TRA 201611  65-TB-156-M                156TB  651562        5.3        H
 TRA 201611  65-TB-157                  157TB  651570 +1.5   71.        Y     156924033.028
 TRA 201611  65-TB-158                  158TB  651580 -3.    180.       Y     157925420.947
 TRA 201611  65-TB-158-M                158TB  651581 -0.    10.70      S
```

I believe it is more convenient for checking purpose to see `-G` for a ground state which has a metastable state, and `-M1` or `-M2` (instead of `-M`) when there are two metastable states.

Example:

```
 TRA 202200  65-TB-156-G                156TB  651560 -3.0   4.6224E+05U         155.92475
 TRA 202200  65-TB-156-M1               156TB  651561        1.9080E+04U         155.92485
 TRA 202200  65-TB-156-M2               156TB  651562        8.7840E+04U
 TRA 202200  65-TB-157                  157TB  651570        2.2405E+09U         156.92403
 TRA 202200  65-TB-158-G                158TB  651580 -3.0   5.6802E+09U         157.92542
 TRA 202200  65-TB-158-M                158TB  651581        1.0700E+01U         157.92554
```

However, this new flagging creates the following side effects related with ZCHEX and DAN2X4:

Problem 1: Unnecessary error messages from ZCHEX

ZCHEX does not understand nuclide codes defined with M1 and M2.

Example: ZCHEX input and output for EXFOR D4370.006 to 008.

```
SUBENT        D4370006   20170510                                D4370006    1
BIB                 3          5                                D4370006    2
REACTION   (65-TB-159(P,X)65-TB-158,,SIG)                       D4370006    3
DECAY-DATA (65-TB-158-G,180.YR,DG,944.189,0.439)                D4370006    4
…
SUBENT        D4370007   20170510                                D4370007    1
BIB                 3          3                                D4370007    2
REACTION   (65-TB-159(P,X)65-TB-156-M2,,SIG)                    D4370007    3
DECAY-DATA (65-TB-156-M2,5.3HR,DG,88.4,0.0115)                  D4370007    4
…
SUBENT        D4370008   20170510                                D4370008    1
BIB                 3          3                                D4370008    2
REACTION   (65-TB-159(P,X)65-TB-156-M1,,SIG)                    D4370008    3
DECAY-DATA (65-TB-156-M1,24.4HR,DG,49.63,0.741)                 D4370008    4
…

ZCHEX (Ver-2021-05-14) run on 08-Jun-2022
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 Input file: d4370.txt

…

 ENTRY D4370 20170510
  **  Illegal code in                        field  4
       REACTION   (65-TB-159(P,X)65-TB-156-M2,,SIG)                  D437000700003
                                ^^^^^^^^^^^^
  **  Illegal code in                        field  1
       DECAY-DATA (65-TB-156-M2,5.3HR,DG,88.4,0.0115)                D437000700004
                  ^^^^^^^^^^^^
  **  Missing independent variable           NUCLIDE                  D4370007

  **  Illegal code in                        field  4
       REACTION   (65-TB-159(P,X)65-TB-156-M1,,SIG)                  D437000800003
                                ^^^^^^^^^^^^
  **  Illegal code in                        field  1
       DECAY-DATA (65-TB-156-M1,24.4HR,DG,49.63,0.741)               D437000800004
                  ^^^^^^^^^^^^
  **  Missing independent variable           NUCLIDE                  D4370008
```

Problem 2: Generation of TRANS dictionary by DAN2X4 with incomplete flags
It is not possible to convert the nuclide codes defined with M1 and M2 to the TRANS dictionary.

Example: -M1 and -M2 of ^{156}Tb truncated to -M in the TRANS dictionary

```
65-TB-156-G 156TB   651560   -3.0     4.6224E+05U                30000227 2581C
65-TB-156-M 156TB   651561            1.9080E+04U                30000227 2582C
65-TB-156-M 156TB   651562            8.7840E+04U                30000227 2583C
65-TB-157   157TB   651570            2.2405E+09U                30000227 2584C
65-TB-158-G 158TB   651580   -3.0     5.6802E+09U                30000227 2585C
65-TB-158-M 158TB   651581            1.0700E+01U                30000227 2586C
```

Format of Dictionary 227 produced by the newly developed code

Line	Contents	Format	Archive	Trans	CHEX
1	Code	A12	13-24	1-12	x
	A-symbol (e.g., 197AU) or particle code (e.g., PIP)	A6	44-49	14-19	
	Internal numerical equivalent	I7	50-56	21-27	x
	Use flag Z – not to be used in REACTION SF2,3,7 as well as in DECAY-DATA, DECAY-MON, EN-SEC, HALF-LIFE, MOM-SEC, PART-DET, RAD-DET (where the appropriate particle codes are to be used)	A1	57	29	x
	Spin/parity	A6	58-63	31-36	
	State ordering flag ~~Half-life flag~~ ~~~ about~~ ~~< less than~~ * - state ordering uncertain	A1	64	38	
	Half-life (in sec)	E11	65-75	39-49	
	Decay flag ~~Half-life unit~~ S - stable U - unstable P - particle unstable	A3	76-78	50-52	x
	Isotopic abundance or isomeric transition probability	E11	79-89	54-64	
	Atomic weight (in amu, 1 amu=931.49410242 MeV)	E12	90-101	N/A	
	Explanation	A21	102-122	N/A	
2	Explanation	A21	N/A	14-34	

The **nuclide code** has the format *Z-S-A*(-X~~M~~)

where: *Z* = the charge number, up to 3 digits, no leading zeros;
S = the element symbol; 1 or 2 characters;
A = the mass number; up to 3 digits, no leading zeros; a single zero denotes natural isotopic composition.
X= G for the ground state when a metastable state exists
M for the metastable state if only one metastable state exists
M1 for the first metastable state
M2 for the second metastable state

The code is right adjusted on Z, *i.e.*, the Z ends in the 3rd position, and continuing with no blanks in the code. ~~All metastable states are labelled as –M.~~

The data associated with a nucleus are taken from the NUBASE Evaluation ~~Nuclear Wallet Cards and the Atomic Mass Evaluation (AME) Tables~~. All ground states and metastable states defied with half-lives longer than 0.1 sec ~~nuclides given in the Nuclear Wallet Cards~~ are included.

Comparison of the Archive Dictionary 227 generated from the old procedure and new procedure for boron isotopes

Original (generated from AME 2012 and NWC 2011)

```
----+----1----+----2----+----3----+----4----+----5----+----6----+----7----+----8----+----9----+----0----+----1----+----2---
 TRA 198202   5-B-0                          B    5000                        10.8110             Natural boron
 TRA 201611   5-B-6                         6B    50060        unbound.   47.            6050800.
 TRA 201611   5-B-7                         7B    50070        1.4        MEV            7029712.000
 TRA 201611   5-B-8                         8B    50080 +2.    770.       MS             8024607.326
 TRA 201611   5-B-9                         9B    50090 -1.5   0.54       KEV            9013329.649
 TRA 201611   5-B-10                       10B    50100 +3.    STABLE.    19.19.9       10012936.949
 TRA 201611   5-B-11                       11B    50110 -1.5                80.1       11009305.355
 TRA 201611   5-B-12                       12B    50120 +1.    20.20      MS             12014352.658
 TRA 201611   5-B-13                       13B    50130 -1.5   17.33      MS             13017780.166
 TRA 201611   5-B-14                       14B    50140 -2.    12.5       MS             14025404.012
 TRA 201611   5-B-15                       15B    50150        9.93       MS             15031087.680
 TRA 201611   5-B-16                       16B    50160 -0.   <190.       PS             16039841.663
 TRA 201611   5-B-17                       17B    50170        5.08       MS             17046989.906
 TRA 201611   5-B-18                       18B    50180       <26.        NS             18055660.189
 TRA 201611   5-B-19                       19B    50190        2.92       MS             19063100.
 TRA 201611   5-B-20                       20B    50200                                  20072070.
 TRA 201611   5-B-21                       21B    50210                                  21081290.
```

New (generated from Nubase2020)

```
----+----1----+----2----+----3----+----4----+----5----+----6----+----7----+----8----+----9----+----0----+----1----+----2---
 TRA 202200   5-B-0                        B      50000                                 10.8110    Natural boron
 TRA 202200   5-B-6                        6B     50060                  P
 TRA 202200   5-B-7                        7B     50070         5.7000E-22U              7.02971
 TRA 202200   5-B-8                        8B     50080         7.7190E-01U              8.02461
 TRA 202200   5-B-9                        9B     50090         8.0000E-19U              9.01333
 TRA 202200   5-B-10                       10B    50100 +3.0                19.65       10.01294
 TRA 202200   5-B-11                       11B    50110 -1.5                80.35       11.00931
 TRA 202200   5-B-12                       12B    50120 +1.0    2.0200E-02U              12.01435
 TRA 202200   5-B-13                       13B    50130         1.7160E-02U              13.01778
 TRA 202200   5-B-14                       14B    50140         1.2360E-02U              14.02540
 TRA 202200   5-B-15                       15B    50150         1.0180E-02U              15.03109
 TRA 202200   5-B-16                       16B    50160         0.0000E+00U              16.03984
 TRA 202200   5-B-17                       17B    50170         5.0800E-03U              17.04694
 TRA 202200   5-B-18                       18B    50180                  U               18.05560
 TRA 202200   5-B-19                       19B    50190         2.9200E-03U              19.06417
 TRA 202200   5-B-20                       20B    50200         0.0000E+00U              20.07450
 TRA 202200   5-B-21                       21B    50210         0.0000E+00U              21.08414
```