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Title: The Los Alamos CP2011 ACE Format Charged Particle Transport Library for MCNP6

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The Los Alamos CP2011 ACE Format Charged Particle Transport Library for MCNP6

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The CP2011 Library

Twenty-five ACE tables for MCNP6 are given for the various combinations of incident protons, deuterons, tritons, helions (He-3), and alphas onto targets of protons, deuterons, tritons, helions, alphas, Li-6 and Li-7. An appropriate xsdir file is also included. The usual convention has been followed that the lighter charged particle is defined to be the incident particle and the heavier is defined to be the target.

	Incident Particle	Particle id[1]	Target	ZAID[2,3]	Low E(MeV) code default	Low E (MeV)	High E (MeV)	Source
1	proton	h	proton	1001.71h	1	0.001	150	lanl
2	proton	h	deuteron	1002.71h	1	0.1	150	lanl
3	proton	h	triton	1003.71h	1	0.0001	12	lanl
4	proton	h	helion	2003.71h	1	0.001	20	lanl
5	proton	h	alpha	2004.71h	1	0.02	20	lanl
6	proton	h	Li-6	3006.71h	1	0.0001	2.5	lanl
7	proton	h	Li-7	3007.71h	1	0.0001	2.5	lanl
8	deuteron	d	deuteron	1002.70o	2	0.0001	10	lanl
9	deuteron	d	triton	1003.70o	2	0.0001	10	lanl
10	deuteron	d	helion	2003.70o	2	0.0001	1.4	lanl
11	deuteron	d	alpha	2004.70o	2	0.01	10	lanl
12	deuteron	d	Li-6	3006.70o	2	0.001	1	lanl
13	deuteron	d	Li-7	3007.70o	2	0.02	20	lanl
14	triton	t	triton	1003.70r	3	0.0001	2	lanl
15	triton	t	helion	2003.70r	3	0.0001	3	lanl
16	triton	t	alpha	2004.70r	3	0.1	14	lanl
17	triton	t	Li-6	3006.70r	3	0.02	20	lanl
18	triton	t	Li-7	3007.70r	3	1	200	tendl
19	helion	s	helion	2003.70s	3	0.0001	2	lanl
20	helion	s	alpha	2004.70s	3	0.02	11	lanl
21	helion	s	Li-6	3006.70s	3	0.02	20	lanl
22	helion	s	Li-7	3007.70s	3	1	200	tendl
23	alpha	a	alpha	2004.70a	4	0.1	20	lanl
24	alpha	a	Li-6	3006.70a	4	1	200	tendl
25	alpha	a	Li-7	3007.70a	4	1	200	tendl

Note 1: the particle id is used in the MCNP mode, imp, sdef, tally, phys, cut cards, and in the "xlib" option of the m cards – where x is the particle id.

Note 2: the zaid suffix letter is used in the MCNP xsdir and ACE files, and in the material specifications of the m cards.

Note 3: the use of "o" and "r" (instead of "d" and "t") for the deuterium and tritium zaid suffix letters is to avoid conflicts with discrete neutron data ("d") and with S(α,β) neutron scattering data ("t"). This "o" and "r" convention is consistent with the TALYS/TENDL ACE files produced since at least 2008 for these charged particles.

Energy Limits for the Cross Section Data

The default lower energy limits for CP transport set by MCNP6 can be over-ridden with a "cut" card. **However, MCNP6 has a hard lower limit of 0.001 MeV (or 1 keV) for all charged particle transport.** Note that some of the data files do have data below the hard limit. Also note the rather high lower limit for alpha-alpha (0.1 MeV). The evaluation data below 0.1 MeV caused problems in NJOY due to some presumably unphysical oscillations in the angular variation of elastic scattering. The TENDL evaluations also have a somewhat higher lower limit.

For incident particle energies below the ACE cross section table lower limits (and yet still above the problem-specific cutoff energy), MCNP has historically given a fatal error. Currently, MCNP simply extends the lowest energy table cross section. In the future, MCNP will be more physically realistic and will set the interaction cross sections to 0.0 – the interaction cross sections are generally quite small and rapidly decreasing in these low energy regimes. Of course, MCNP6 has model data for all charged particle cross sections for incident energies greater than the maximum energy given in the ACE tables.

Source of the Evaluation Data Files

With respect to the endf70prot library, the new 71h ACE files are different than the 70h ACE files for Li6 and Li7. There is also a first time new 71h ACE file for alpha. Otherwise, the 71h ACE files are identical to the 70h ACE files for protons incident onto protons, deuterons, tritons, and helions. The "70x" (x = o,r,s,a) ACE files for incident deuterons, tritons, helions, and alphas are all new.

The original evaluation files used to produce the ACE files are the charged particle files currently available at the National Nuclear Data Center, supplemented by more recent evaluations provided by Gerry Hale of T-2 and by a few TENDL evaluations. It is anticipated that Gerry Hale's more recent evaluations will be formally adopted by CSEWG and the NNDC in the future.

Verification and Validation of the CP2011 Library

Version 99.336 of NJOY was used for most of the processing. The standard sequence of 3 ACER runs was employed – which includes quite a bit of data checking by NJOY itself and output edits for user perusal.

A sample NJOY deck for deuterons incident onto deuterium is given below. The deuterium evaluation file is copied into "tape20" and "tape21".

```
 acer
 20 21 0 31 32
 1 1 1 .70 /
 acer tape for H -  2 from endf b-vii njoy99.336
    128 0./
 /
 /
 acer
 0 31 33 34 35
  7 1 1/
 acer tape for H -  2 from endf b-vii njoy99.336
 acer
 0 34 36 37 38
  7 1 1/
 acer tape for H -  2 from endf b-vii njoy99.336
 stop
EOF
```

In the course of processing, some missing section separation cards were added to the new evaluation files. There was some concern about the evaluations (p+d and the 4 TENDL evaluations) which used the LPT=12 option for charged particle elastic scattering, but Skip Kahler resolved the concern after carefully checking the NJOY coding. There were also some inconsistent energy low and high limits in the d-alpha and the alpha-alpha files for which NJOY gave all 0.0's for the cross sections. Even after the limits were made consistent, the alpha-alpha evaluation still gave some unphysical elastic scattering results at the lowest energies. Hence, the alpha-alpha lower limit was adjusted up to 0.1 MeV (i.e., above the unphysical results).

All 25 of the ACE files have been analyzed with the nuclear data team's "CHECKACE" utility code. CHECKACE looks for the lack of cross section balance, unphysical cross sections, negative PDF's, and other indications of faulty data or faulty data processing. Two references are given below which contain a more detailed description of the modules of CHECKACE.

Each of the 25 ACE files in the CP2011 library has also been run successfully in MCNP6 to provide verification assurance. A sample MCNP6 input deck is given below for tritons incident on helions. One million triton histories are followed starting at energies distributed uniformly between the upper and lower energy cut-offs of 3 MeV and 1 keV.

```
test of t-he3 xs in 70r file
1    1  -0.30   3 -4 -1     imp:t=1
2    0           2 -3 -1     imp:t=1
3    0           4 -5 -1     imp:t=1
4    0           1:-2:5      imp:t=0

1    cz  5
2    pz  0
3    pz 25
4    pz 26
5    pz 41

m1    2003     1.0  tlib=70r
mode t
sdef  par=t erg=d1  vec=0 0 1 x=0 y=0 z=0  dir=1
si1   h  0.001 1 3
sp1   d  0 1 1
print
nps   1000000
f1:t  1 2 5
e1    1 2 3
cut:t 0 0.001
PHYS:t 3   1 -1 j  j j j
```

A set of 24 test problems devised by Grady Hughes for charged particles has also been modified to include these new ACE files (where possible) and the set has been run without errors (except for the deliberate fatal error of "inp019").

References:

Preliminary CP Memos:

D. Kent Parsons, "Release of the CP2011 Charged Particle Cross Section Library for MCNP6", Los Alamos Memo XCP-5:13-018, (2013)

Morgan C. White, "ACE Library CP2011 Charged Particles Incident on Light Isotopes", Los Alamos Memo XCP-5:MCW-12-004, (2011)

Morgan C. White, "NDI MG Library CP2011 Charged Particle Emissions from Neutrons Incident on Light Isotopes", Los Alamos Memo XCP-5:MCW-12-005, (2011)

Official Citation for TALYS/TENDL:

Arjen J. Koning and D. Rochman, "Modern Nuclear Data Evaluation with the TALYS Code System", *Nuclear Data Sheets*, Vol. 113, pp. 2814-2934, (2012)

CHECKACE Descriptions are included in these Data Library Release Memos:

Holly Trellue, Robert C. Little, and M. Beth Lee, "New ACE-Formatted Neutron and Proton Libraries Based on ENDF/B-VII.0", LA-UR-08-1999, Los Alamos National Laboratory, (2008)

Jeremy L. Conlin, D. Kent Parsons, Steven J. Gardiner, Albert C. Kahler III, M. Beth Lee, Morgan C. White, and Mark G. Gray, "Continuous Energy Neutron Cross Section Data Tables Based Upon ENDF/B-VII.1", LA-UR-13-20137, Los Alamos National Laboratory, (2013)

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