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*Title:* SAB2002 - An S(a,b ) Library for MCNP

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## Los Alamos

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Benzene (1001, 6000, 6012)								
benz.60t	endf6.3	sab2002	09/14/99	294.	16	64	none	
benz.61t	endf6.3	sab2002	09/14/99	400.	16	64	none	
benz.62t	endf6.3	sab2002	09/14/99	600.	16	64	none	
benz.63t	endf6.3	sab2002	09/14/99	800.	16	64	none	
Beryllium Oxide (4009, 8016)								

beo.60t	endf6.3	sab2002	09/14/99	294.	16	64	coh
beo.61t	endf6.3	sab2002	09/14/99	400.	16	64	coh
beo.62t	endf6.3	sab2002	09/14/99	600.	16	64	coh
beo.63t	endf6.3	sab2002	09/14/99	800.	16	64	coh
beo.64t	endf6.3	sab2002	09/14/99	1000.	16	64	coh
beo.65t	endf6.3	sab2002	09/14/99	1200.	16	64	coh
Beryllium Metal (4009)							
be.60t	endf6.3	sab2002	09/13/99	294.	16	64	coh
be.61t	endf6.3	sab2002	09/13/99	400.	16	64	coh
be.62t	endf6.3	sab2002	09/13/99	600.	16	64	coh
be.63t	endf6.3	sab2002	09/14/99	800.	16	64	coh
be.64t	endf6.3	sab2002	09/14/99	1000.	16	64	coh
be.65t	endf6.3	sab2002	09/14/99	1200.	16	64	coh
be.69t	endf6.3	sab2002	09/17/99	77.	16	64	coh
Deuterium in Heavy Water (1002)							
hwtr.60t	endf6.3	sab2002	09/14/99	294.	16	64	none
hwtr.61t	endf6.3	sab2002	01/20/03	400.	16	64	none
hwtr.62t	endf6.3	sab2002	09/14/99	600.	16	64	none
hwtr.63t	endf6.3	sab2002	09/14/99	800.	16	64	none
hwtr.64t	endf6.3	sab2002	01/20/03	1000.	16	64	none
Graphite (6000, 6012)							
grph.60t	endf6.3	sab2002	09/14/99	294.	16	64	coh
grph.61t	endf6.3	sab2002	09/14/99	400.	16	64	coh
grph.62t	endf6.3	sab2002	09/14/99	600.	16	64	coh
grph.63t	endf6.3	sab2002	09/14/99	800.	16	64	coh
grph.64t	endf6.3	sab2002	09/14/99	1000.	16	64	coh
grph.65t	endf6.3	sab2002	09/14/99	1200.	16	64	coh
Hydrogen in Light Water (1001)							
lwtr.60t	endf6.3	sab2002	09/13/99	294.	16	64	none
lwtr.61t	endf6.3	sab2002	09/13/99	400.	16	64	none
lwtr.62t	endf6.3	sab2002	09/13/99	600.	16	64	none
lwtr.63t	endf6.3	sab2002	09/13/99	800.	16	64	none
lwtr.64t	endf6.3	sab2002	01/21/03	1000.	16	64	none
Hydrogen in Polyethylene (1001)							
poly.60t	endf6.3	sab2002	09/14/99	294.	16	64	inco
Hydrogen in Zirconium Hydride (1001)							
h/zr.60t	endf6.3	sab2002	09/14/99	294.	16	64	inco
h/zr.61t	endf6.3	sab2002	09/14/99	400.	16	64	inco
h/zr.62t	endf6.3	sab2002	09/14/99	600.	16	64	inco
h/zr.63t	endf6.3	sab2002	09/14/99	800.	16	64	inco
h/zr.64t	endf6.3	sab2002	09/14/99	1000.	16	64	inco
h/zr.65t	endf6.3	sab2002	09/14/99	1200.	16	64	inco
Hydrogen in Liquid Methane (1001)							
lmeth.60t	endf6.3	sab2002	09/17/99	100.	16	64	none
Ortho Deuterium (1002)							
dortho.60t	endf6.3	sab2002	09/16/99	19.	16	64	none
Ortho Hydrogen (1001)							
hortho.60t	endf6.3	sab2002	01/21/03	19.	16	64	none

hortho.61t	endf6.3	sab2002	06/14/00	20.	16	64	none
hortho.62t	endf6.3	sab2002	06/14/00	21.	16	64	none
hortho.63t	endf6.3	sab2002	06/14/00	22.	16	64	none
hortho.64t	endf6.3	sab2002	06/14/00	23.	16	64	none
hortho.65t	endf6.3	sab2002	06/14/00	24.	16	64	none
hortho.66t	endf6.3	sab2002	06/14/00	25.	16	64	none
Para Deuterium (1002)							
dpara.60t	endf6.3	sab2002	09/16/99	19.	16	64	none
Para Hydrogen (1001)							
hpara.60t	endf6.3	sab2002	06/14/00	19.	16	64	none
hpara.61t	endf6.3	sab2002	06/13/00	20.	16	64	none
hpara.62t	endf6.3	sab2002	06/14/00	21.	16	64	none
hpara.63t	endf6.3	sab2002	06/14/00	22.	16	64	none
hpara.64t	endf6.3	sab2002	06/14/00	23.	16	64	none
hpara.65t	endf6.3	sab2002	06/14/00	24.	16	64	none
hpara.66t	endf6.3	sab2002	06/14/00	25.	16	64	none
Hydrogen in Solid Methane (1001)							
smeth.60t	endf6.3	sab2002	09/17/99	22.	16	64	inco
Zirconium in Zirconium Hydride (40000, 40090, 40091, 40092, 40094, 40096)							
zr/h.60t	endf6.3	sab2002	09/14/99	294.	16	64	inco
zr/h.61t	endf6.3	sab2002	09/14/99	400.	16	64	inco
zr/h.62t	endf6.3	sab2002	09/14/99	600.	16	64	inco
zr/h.63t	endf6.3	sab2002	09/14/99	800.	16	64	inco
zr/h.64t	endf6.3	sab2002	09/14/99	1000.	16	64	inco
zr/h.65t	endf6.3	sab2002	09/14/99	1200.	16	64	inco

Given in parenthesis are the nuclides for which the  $S(\alpha,\beta)$  data are valid. For example, lwtr.60t provides scattering data only for  $^1\text{H}$ ;  $^{16}\text{O}$  would still be represented by the default free-gas treatment.

The first column of Table 1 contains the Z Aid, which is the table identification to be specified on MCNP MTn cards. The portion of the Z Aid before the decimal point provides a shorthand alphanumeric description of the material. The two digits after the decimal point differentiate among different tables for the same material. The final character in the Z Aid is a "t" which indicates thermal  $S(\alpha,\beta)$  table.

The second column of Table 1 is the evaluated source. For the SAB2002 library, all data are from ENDF/B-VI Release 3.

The third column is the library name; here, obviously, always SAB2002.

The fourth column provides the date that the data table was processed by the NJOY code.

The fifth column is the temperature of the data (in degrees Kelvin).

The sixth column contains the number of equally-likely discrete secondary cosines provided at each combination of incident and secondary energy for inelastic scattering, and for each incident energy for incoherent elastic scattering. Note that this value (16) is substantially larger than that for previous MCNP thermal data tables, leading to more resolution in the data.

The seventh column gives the number of secondary energies provided for each incident energy for inelastic scattering. Note that this value (64) is substantially larger than that for previous MCNP thermal data tables, leading to more resolution in the data.

There are three options for the elastic scattering entry in the eighth column:

none -- no elastic scattering data for this material.

coh -- coherent elastic scattering data provided for this material (Bragg scattering).

inco - incoherent elastic scattering data provided for this material.

### Verification and Validation

Only very minor changes to the tables generated by NJOY were required, generally involving updates to the list of integer nuclides for which the  $S(\alpha,\beta)$  data are valid. Cross sections for each moderator have been plotted for each temperature and each reaction. Average scattering energies and angles have been constructed and plotted. All data tables have been run in standard MCNP problems. Several data tables have been used to calculate various criticality benchmarks [6]. No problems have been identified.

### Comparison to Previous MCNP Thermal Libraries

There are two previous MCNP thermal  $S(\alpha,\beta)$  libraries. The TMCCS library contains data for 9 moderators (Be, BeO, H<sub>2</sub>O, D<sub>2</sub>O, benzene, poly, graphite, and H and Zr in ZrH) based on ENDF/B-V. Note that these evaluations had been carried over from ENDF/B-III [3]. The THERXS library contains data for 6 cold moderators based on initial work performed ~ 1989 at Los Alamos [7,8].

The cross sections for the bulk of the reactor moderator materials show only modest differences on SAB2002 compared with TMCCS. There is an improvement in the inelastic scattering cross section for H in ZrH. On the other hand, almost all of the cold moderators (with the exception of liquid methane) show substantial improvements from the data on THERXS. Finally, all data tables on SAB2002 include more detailed resolution than previous libraries in terms of secondary neutron energies and scattering angles.

### Summary

A new MCNP thermal  $S(\alpha,\beta)$  library has been created, verified, and made available to users. The library is named SAB2002 and contains a total of 64 data tables for 15 moderators based on ENDF/B-VI Release 3 evaluations. There are some substantial enhancements from previous MCNP thermal data tables that warrant the data on SAB2002 being the new default for MCNP.

### References

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