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Title: New Photon Library from ENDF Data

Author(s): Robert C. Little

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Los Alamos
NATIONAL LABORATORY

Date : 2/26/82

To: Buck Thompson (X-6)
From - Bob Little (X-6)
Subject: New Photon Library From ENDF Data

A new library of photon cross sections based on ENDF data has been produced and compared with the present MCPLIB library.

Cross sections for coherent scattering, incoherent scattering, photoelectric effect, and pair production come directly from ENDF via the file /ENDF/4/A/T/GAM23. Coherent form factors and incoherent form factors come directly from ENDF via the file /ENDF/4/A/T/GAM27.

There is no fluorescence information given by ENDF. As a result, the fluorescence data in the new library are taken exactly "as is" from the MCPLIB library.

Integrated coherent form factors and photon heating numbers are calculated quantities based on the previously described data. These calculations were greatly facilitated by referring to Bob Schrandt and Bill Taylor's PXSEC code.

The MCPLIB library has data for all elements from Z=1 through Z=94. The ENDF-based library has no data for Z=84,85, 87,88,89, and 93.

Two versions of the ENDF-based library exist and are ready for your use. They are stored under the /090895/PHOTON node as MERGE and MERG3. In the file MERG3, the heating numbers are produced in a manner consistent with MCNP Version 2C - in other words, secondary fluorescence is three times more probable in the heating calculations for MERG3 than in the heating calculations for the file MERGE. Otherwise, the two files are identical.

To use the new photon library in MCNP simply include the statement MCPLIB = MERG3 in the execution line.

The codes and procedures used in forming the ENDF photon library are described in detail in Appendix A.

Appendix B documents the result of some comparisons between the present MCPLIB library and the new MERG3 (ENDF) library.

In closing, it seems that a large part of the mechanics of photon transport in MCNP is not well documented. The whole procedure should be reviewed, partially with the aim of documentation and partially with the aim of possible improvements.

XC: Pat Soran
Bob Schrandt
Joe Devaney
Bob Seamon
X-6 Files

References

1. MCNP manual (Version 2B) pages 452-455, April 1981.

2. Monte Carlo Photon Codes: MCG and MCP, LA-5157-MS, March 1973.

3. MCP Code Fluorescence-Routine Revision, LA-5240-MS, May 1973.

4. Approximation for the Inverse of the Klein-Nishina Probability Distribution, LA-4448, June 1970.

5. A new method of sampling the Klein-Nishina Probability Distribution for all Incident Photon Energies Above 1 keV, LA-4663, May 1971.

6. "Comparison of Photon Cross Sections in MCPLIB with those on DLC-7E for H and O," memo to Buck Thompson from Bob Seamon and Bob Little, December 1980.

7. "Comparison of Photon Cross Sections in MCPLIB with those on DLC-7E for Fe, Pb, and Pu," memo to Buck Thompson from Bob Little and Bob Seamon, November 1981.

8. "Proposed Changes to the Fluorescence Part of MCNP (detailed photon physics - MCP)," memo to X-6 from Joe Devaney, January 1982.

9. "Everett's Comment on Fluorescence," memo to X-6 from Buck Thompson, February 1982.

Appendix A: Sequence of Codes used to Produce ENDF Photon Library

(1) PHXS

The code PHXS reads the ENDF photon cross section file (/ENDF/4/A/T/GAM23) and produces a binary file of cross sections. The format of the output file is as follows:

$$(Z_i, NE_i, E(j)_i\ j=1,NE_i, INCO(E_j)_i\ j=1,NE_i, CO(E_j)_i\ j=1,NE_i, PH(E_j)_i\ j=1,NE_i, PP(E_j)_i\ j=1,NE_i)_{i=1,87}$$

where Z is the atomic number, NE is the number of energies, INCO, CO, PH, and PP are the incoherent, coherent, photoelectric, and pair production cross sections.

The cross sections are put on a unified energy grid (actually the grid given by ENDF for the total cross section). This requires interpolation, which is always done on a log-log basis.

We read the following MT's from the ENDF file:

MT 504 incoherent cross section
MT 502 coherent cross section
MT 602 photoelectric cross section
MT 516 pair production cross section

To run PHXS, we need tape 1 to be the GAM23 file. The output file is TAPE2; which is stored as XS.

② PHFF

The code PHFF reads the ENDF photon form factor file (/ENDF/4/A/T/GAM27) and produces a binary file of form factors. The format of the output file is as follows.

$$\left(Z_i, \{INFF(v_j)\}_i \; j=1,21, \; \{COFF(v_k)\}_i \; k=1,55 \right)_{i=1,87}$$

where Z is the atomic number, INFF are the incoherent form factors, and COFF are the coherent form factors.

MCNP requires the form factors for all elements to be given on a unified grid. We need incoherent form factor at the following 21 values of v : 0., .005, .01, .05, .1, .15, .2, .3, .4, .5, .6, .7, .8, .9, 1.0, 1.5, 2.0, 3.0, 4.0, 5.0, and 8.0 . We need coherent form factors at the following 55 values of v : 0., .01, .02, .03, .04, .05, .06, .08, .10, .12, .15, .18, .20, .25, .30, .35, .40, .45, .50, .55, .60, .70, .80, .90, 1.0, 1.1, 1.2, 1.3, 1.4, 1.5, 1.6, 1.7, 1.8, 1.9, 2.0, 2.2, 2.4, 2.6, 2.8, 3.0, 3.2, 3.4, 3.6, 3.8, 4.0, 4.2, 4.4, 4.6, 4.8, 5.0, 5.2, 5.4, 5.6, 5.8, and 6.0 .

We read the following MT's from the ENDF file:

MT 504 incoherent form factors

MT 502 coherent form factors

Interpolation of the ENDF values is done on a log-log basis.

To run PHFF, we need TAPE1 to be the GAM27 file. The output file is TAPE2; which is stored as FF.

(3) PHINTFF

The code PHINTFF reads the FF file produced in (2) and forms values of integrated coherent form factors. The format of the output file is as follows:

$$(Z_i,\ \mathrm{INTFF}(v_k)_i\ \ k=1,55)_{i=1,87}$$

where INTFF is the integrated coherent form factor. The integrated coherent form factor is described on page 8 of LA-5157-MS as

$$A(Z,V^2) = \int_0^{V^2} C^2(Z,V^2) \cdot Z^{-2}\, dV^2$$

where $A(Z,V^2)$ is the integrated coherent form factor, $C(Z,V^2)$ is the coherent form factor, and Z is the atomic number. Therefore the integrated form factor at v_i^2 is

$$A(Z,v_i^2) = A(Z,v_{i-1}^2) + \int_{V_{i-1}^2}^{V_i^2} C^2(Z,V^2)\, Z^{-2}\, dV^2$$

from whence it is assumed (perhaps incorrectly) that

C^2 is a linear function of V^2, which gives

$$A(Z, v_i^2) = A(Z, v_{i-1}^2) + \frac{(V_i^2 - V_{i-1}^2)(C^2(Z, V_{i+1}^2) + C^2(Z, V_i^2))}{2Z^2}$$

(Note: I think that in the original equation from LA-5157-MS and in the subsequent equations; the notation should be $C^2(Z, V_i)$ and not $C^2(Z, V_i^2)$)
(Second Note: I believe that the code MCNP interpolates linearly-linearly on form factors as a function of v. Since this is not the way they are given in the original data, perhaps we could change this to log-log)

To run PHINTFF, we need TAPE1 to be the FF file from (2). The output file is TAPE2; which is stored as INTFF.

(4) PHFLOR

PHFLOR is a simple code which extracts the fluorescent data from the current MCPLIB and writes is to a binary file. The format of the output file is as follows:

$$(Z_i, N_i, F(j)_i \quad j = 1, 4*N_i)_{i=12,87}$$

where Z is the atomic number, N is the number of sets of fluorescence constant for isotope i, and $F(j)$ are the fluorescence constant. For elements with $Z<12$ there are no fluorescence data given by MCPLIB.

The reason we read from the MCPLIB library is that there are no fluorescence data given by ENDF. So until better data are found, we will keep the data from MCPLIB.

To run PHFLOR, we need TAPE1 to be the MCPLIB library.

The output file, TAPE2, is stored as FLOR.

(5) PHEINCO

The code PHEINCO calculates the average photon energy deposited as a result of incoherent scattering. This is a necessary parameter in the final photon heating calculation. The format of the output file is as follows:

$(Z_i,\ EINCO(E_j)_i\ \ j=1,NE_i)_{i=1,87}$ where EINCO is the average energy deposited when undergoing incoherent scattering at E_j.

The code PHEINCO has largely been stolen from Bob Schrandt's PXSEC code (available in the LIX file /X6CODE/PHOTON/RGSPPR). The average energy deposited is calculated by selecting 1000 "random numbers" equally spaced from 0 to 1. Then the Klein-Nishina distribution is sampled, and finally the rejection technique involving the incoherent form factors is used to effectively modify the Klein-Nishina distribution. The coding for all of this is supposedly comparable to what is in MCNP.

(Note: There is one line of coding which diverges. The PXSEC code has

$$\begin{cases} t_3 = 137.0393 * t_1 \\ t_7 = 1.-1./(1.+t_3**2)**4 \end{cases}$$

while MCNP has

$$t_8 = 1.-1./(1.+137.0393*t_1^2)**4 \qquad [CP.91]$$

The t_7 of PXSEC should be equivalent to the t_8 of MCNP. Notice that the 137.0393 is not squared in MCNP; it is in PXSEC. This is probably a minor point - it only happens in the special calculation of the incoherent form factor of Hydrogen, and would only be signifigant at low energy; ie when t_1 was small. It is not clear at this time which of the two equations is correct.)

To execute the code we need TAPE1 to be the XS file from (1), and we need TAPE2 to be the FF file from (2). The output file is

(Note: Is the sampling of the K-N distribution (in MCNP) done with the latest sampling scheme - if not shouldn't we put it in?)

TAPE3, which is stored as EINCO.

⑥ PHEFLOR

The code PHEFLOR calculates the average photon energy deposited as a result of the photoelectric effect. This is a necessary parameter in the final photon heating calculation. The energy deposited from the photoelectric effect is equal to the incident photon energy minus any emitted fluorescence. The format of the output file is as follows:

$$(Z_i, EFLOR(E_j)_i \; j=1,NE_i)_{i=1,87}$$

where $EFLOR(E_j)$ is the average energy deposited when undergoing the photoelectric effect at energy E_j.

Once again, the code PHEFLOR has largely been stolen from the PXSEC code. Again, the strategy is to break up the interval from 0 to 1 into 1000 equally-spaced "random numbers" and follow the procedure of the code (MCNP) to see whether the result will be no fluorescence, single fluorescence, or double fluorescence. (Note - it seems like this calculation could be done analytically - but maybe I'm wrong). It appears that the methods of PXSEC (and hence, PHEFLOR) check those in MCNP.

Devaney contends (memo of 1/18/82) that the secondary fluorescence should be tripled. This would affect line CP.181 in the coding, changing it from T1=3*(1.-XSP(I))
to T1= (1.-XSP(I))

I originally ran PHEFLOR the way Schardt had it - with the factor of three. This formed the output file saved as EFLOR. I then decided to take out the factor of 3. A new code PHEFLO3 was made. When executed, the output file was saved as EFLO3.

To run this code we need as input TAPE1 the XS file from ① and as TAPE2 the FLOR file from ④

(Note: the flourescence in MCNP is very much hard-wired. No flourescence is allowed for $Z < 12$, and double flourescence is allowed only for $Z > 30$. This is perhaps an area where we should look for the possibility of new data).

(Note: the biggest difference arising from Devaney's factor of 3 appears to be 7.7% – and this is in the heating from photoelectric, not the overall heating}. This 7.7% difference is found for $Z = 86$, at $E_\gamma = .098416$ MeV. Thus, from a heating standpoint, the question of including or excluding the 3 is a relatively minor point.)

⑦ PHHEAT

PHHEAT calculates the final values of the photon heating numbers. The format of the output file is as follows:

$$(Z_i, HEAT(E_j)_i \; j = 1, NE_i)_{i=1,87}$$

where HEAT(E_j) is the average energy deposited at energy E_j.

We calculate HEAT as follows:

$$HEAT(E) = \frac{\sigma_{INCO}(E) * E_{INCO}(E) + \sigma_{PE}(E) * E_{PE}(E) + \sigma_{PP}(E) * (E - 1.022016)}{\sigma_{total}(E)}$$

where σ_{INCO}, σ_{PE}, σ_{PP}, and σ_{total} are the incoherent, photoelectric, pair production, and total cross sections. (From ①)
E_{INCO} is the energy deposited from incoherent scattering (From ⑤)
E_{PE} is the energy deposited from photoelectric (From ⑥)
The units of HEAT are MeV/collision.

We need as input TAPE1 which is XS from ①, TAPE2 which is EINCO from ⑤, and TAPE3 which is EFLOR from ⑥. Again, the calculation has been made with and without Devaney's factor of 3. The output files are stored as HEAT and HEA3 (the latter with secondary fluorescence enhanced by a factor of 3½ using TAPE3 = EEL03). The biggest difference in overall heating is again about 7.6%, again for Z=86, and again at E_γ=.098417.

⑧ PHMERGE

The PHMERGE gathers together all the information gained above and writes it to one file. The format of the output file is identical to MCPLIB. The output file is ready to be used in MCNP.

The input files needed are:

TAPE1 = XS from ①
TAPE2 = FF from ②
TAPE3 = INTFF from ③
TAPE4 = HEAT from ⑦
TAPE5 = FLOR from ④

The output file, TAPE6, is stored as MERGE
(if Devaney's factor of 3 is used, TAPE4 = HEA3, and the output file is stored as MERG3)

⑨ ROGER

The code ROGER is taken from Seamon who stole it from Schandt's PXSEC code. It reads a binary photon library in MCPLIB format and prints out a BCD file.

The input file is TAPE2, the output file is tape10.

⑩ PHCOMP

The code PHCOMP compares two photon libraries and prints out a BCD file. The code checks the individual cross sections and form factors. All instances when differences of more than 10% are found are printed out. The results of the comparison between MCPLIB and ENDF5 are discussed in detail in appendix B.

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Note: All Files Referred to Above are Stored Under the /090895/PHOTON node

```
mass
? default dir=/090895/photon
? list -

    node name: photon
    descendants:
        phxs
        xs
        phff
        ff
        phintff
        intff
        phflor
        flor
        rgsppr
        pheinco
        einco
        pheflor
        eflor
        phheat
        heat
        phmerge
        roger
        merge
        phef lo3
        ef lo3
        hea3
        merg3
        phcomp
? end

 all done
```

2/25/82

Summary of Appendix B

This summary of the differences I found when comparing MERG3 (from ENDF) with MCPLIB was written after I re-read the memo and decided that nobody else would ever read the next 13 pages. Therefore I summarize here the major differences between the two files and refer the reader to the full appendix B for discussions about specific elements.

First of all, note that for energies greater than 15 MeV, the cross sections on the two files should be, and in fact are, the same. This is because the MCPLIB cross sections above 15 MeV came directly from ENDF.

Only difference of 10% or more are reported here and listed in Appendix B. The differences were calculated as

$$\left| \frac{(MERG3 - MCPLIB)}{(MCPLIB)} \right| \times 100 \quad (\%)$$

Once again, data are given for the following elements only on MCPLIB, not on MERG3: Z=84, Z=85, Z=87, Z=88, Z=89, Z=91, and Z=93.

Incoherent Cross Sections:

The only cases of difference greater than 10% are for Z=4, Z=5, and Z=6. The differences are below 3 keV and can be as great as 30%.

Coherent Cross Sections:

For Z=1 through Z=49 there are energies at which ENDF gives small values of the coherent cross sections while MCPLIB gives zeros. The energies at which this occurs gradually change from .08-15 MeV for Z=1, to 15 MeV only for Z=49. I should repeat that the non-zero cross sections given by ENDF are very small.

There are other differences in coherent cross sections for Z=32 through Z=94. The percent differences and energy ranges involved vary, with the following being typical values: Z=40 (10-11% differences from .4-2 MeV), Z=60 (10-17% difference from .4-4 MeV), and Z=80 (10-21% differences from .3-15 MeV). It is seen that both the magnitude of the differences, as well as the energy range affected, increase with increasing Z.

Photoelectric Cross Section

For Z=1 through Z=27 there are energies at which ENDF gives small values of the photoelectric cross section while MCPLIB gives zeros. The energies at which this occurs gradually change from .02-15 MeV for Z=1, to 15 MeV only for Z=27. Again, the non-zero cross sections given by ENDF are very small.

Most elements with Z ≤ 35 also have photoelectric cross section differences of as much as 20%. Differences show up at and near 1 keV as well as anywhere from 10 keV to 8 MeV. Check Appendix B for any elements of specific interest.

Finally, for Z ≥ 44 there are photoelectric differences at low energies. Differences may be as large as 35% and cover the energy range from 1-5 keV. There are differences in cross section values at edges in this energy range.

Pair Production Cross Section

The only cases of differences greater than 10% are for Z ≤ 5. Differences are greatest for Hydrogen (20-60% from 4-15 MeV) and decrease with increasing Z to only 11% from 10-15 MeV for Z=5.

Integrated Coherent Form Factors

No differences of greater than 10% are found.

Coherent Form Factors

Differences of 10% or more are found only for $Z \le 8$. For $Z \in (1,5)$ coherent form factors are given as 0 by MCPLIB while ENDF gives small non-zero values for large values of v. For Z=7 and Z=8 there are 10-12% differences when $v=3$ and $v=4$.

Incoherent Form Factors:

Differences of 10% or more are found only for $Z \le 6$. The differences occur at small values of v ($\le .2$) and can be as great as a factor of 2 for Z=2.

Heating:

Heating differs by 10-15% from 10-90 keV for Z=2 through Z=5. For higher values of Z there are differences in heating (not listed in Appendix B) at edge energies where fluorescence becomes possible. One problem is that the edge energies may differ in the 4th or 5th decimal place between the two files. That might be enough to make fluorescence possible, for example, at the ENDF edge energy; and impossible at the MCPLIB edge energy. The result can be radical differences in heating numbers at these edge energies.

There are always 2 energy points given at edges. The correct thing to do, I believe, (in terms of heating calculations) would be to make the fluorescence cut-in energy in the middle of the 2 energies given at the edge. This is not the way things have been handled in MCPLIB; the 2 edge energies are either both less than, both equal to, or both greater than the fluorescent threshold energy. This leads to incorrect heating numbers on one "side" of the edge.

The situation is no better on the ENDF file. I have left the edge energies exactly as given by ENDF and have left the fluorescence thresholds exactly as taken from MCPLIB. I believe that the situation warrants changing only after we are convinced we have the best fluorescence data available in the code. (Note - in neither case will there be problems with the photon transport; only in the calculation of heating numbers near fluorescence thresholds.)

To summarize this summary it is my feeling that the sensitivity of most problems will be very small with regards to the photon library used.

Appendix B: Comparison of MCPLIB Photon Library With ENDF (MERG3) Photon Library

(Differences of 10% or more between MCPLIB and MERG3 are given)

Z=1: ENDF gives very small (but non-zero) values of coherent cross sections from .08 to 15 MeV and of photoelectric cross sections from .02 to 15 MeV; MCPLIB gives zeros. Pair production differs by 20-60% from 4-15 MeV (rather small cross sections). Incoherent form factors are always given as 0 in MCPLIB; I have included the numbers given by ENDF in the new library. It really makes no difference - the incoherent form factors for Hydrogen are calculated rather than read from the file. The coherent form factor differ for $v \geq 1.2$, although the numbers are negligibly small.

Z=2: ENDF gives very small (but non-zero) values of coherent cross sections from .3-15 MeV and of photoelectric cross sections from .05-15 MeV, MCPLIB gives zeros. In addition, the photoelectric cross sections differ by 10-30% from .01-.04 MeV, and the pair production cross sections differ by 10-30% from 5-15 MeV. The heating differs by 10-15% from .01-.015 MeV. Incoherent form factors are up to a factor of 2 different (but small) for $v \leq .01$. Coherent form factors are given as 0 by MCPLIB for $v \geq 2.2$; ENDF gives small, non-zero values.

Z=3: ENDF gives very small (but non-zero) values of coherent cross sections from .4-15 MeV and of photoelectric cross sections from .1-15 MeV; MCPLIB gives zeros. In addition, the photoelectric cross sections differ by 12% at 1 keV and by 10-35% from .015-.08 MeV, while the pair production cross sections differ by 10-20% from 8-15 MeV. The heating differs by 12% at .02 MeV. Coherent form factors are given as 0 by MCPLIB for $v \geq 3.6$; ENDF gives small, non-zero values.

Z=4: Incoherent cross sections differ by 15-30% from 1-2 keV. ENDF gives very small (but non-zero) values of coherent cross sections from

.6-15 MeV and of photoelectric cross sections from .15-15 MeV (MCPLIB gives zeros). In addition, photoelectric cross sections differ by 10-30% from .015-.1 MeV, and pair production cross sections differ by 15% from 10-15 MeV. Heating differs by 12% from .02-.03 MeV. Incoherent form factors are 10-30% different for $v \leq .15$. Coherent form factors are given as 0 by MCPLIB for $v \geq 4.6$; ENDF gives small, non-zero values.

Z=5: Incoherent cross sections differ by 10-20% from 1-2 keV. ENDF gives very small (but non-zero) values for coherent cross sections from .8-15 MeV and of photoelectric cross sections from .2-15 MeV; MCPLIB gives zeros. In addition, the photoelectric cross sections differs by 10-20% from .02-.15 MeV, while the pair production differs by 11% from 10-15 MeV. Heating differs by 11% from .03-.04 MeV. Incoherent form factors are 10-25% different for $v \leq .15$. Coherent form factors are given as 0 by MCPLIB for $v \geq 5.6$; ENDF gives small, non-zero values.

Z=6: Incoherent cross sections differ by 10-20% from 1-3 keV. ENDF gives very small (but non-zero) values for coherent cross sections from 1-15 MeV and for photoelectric from .3-15 MeV; MCPLIB gives zeros. In addition, the photoelectric cross sections differs by 10-15% from .02-.1 MeV. Incoherent form factors are 10-15% different for $.01 \leq v \leq .2$.

Z=7: ENDF gives very small (but non-zero) values for coherent scattering cross sections from 1.5-15 MeV, and for photoelectric from .4-15 MeV (MCPLIB gives zeros). In addition, the photoelectric cross sections differs by 11% from .04-.06 MeV. Coherent form factors are 10-12% different at $v = 3.0$ and $v = 4.0$.

Z=8: ENDF gives very small (but non-zero) values for coherent cross sections from 1.5-15 MeV, and for photoelectric from .5-15 MeV; MCPLIB gives zeros. The coherent form factors are 10% different at $v = 4.0$.

Z=9: ENDF gives very small (but non-zero) values for coherent cross sections from 2-15 MeV, and for photoelectric from .5-15 MeV; MCPLIB gives zeros.

Z=10: ENDF gives very small (but non-zero) values for coherent cross sections from 2-15 MeV, and for photoelectric from .8-15 MeV; MCPLIB gives zeros. In addition, the photoelectric cross sections differ by 10% at .5 MeV.

Z=11: ENDF gives very small (but non-zero) values for coherent cross sections from 3-15 MeV, and for photoelectric from .8-15 MeV; MCPLIB gives zeros. In addition, the photoelectric cross sections differ by 15% at 1 keV.

Z=12: ENDF gives very small (but non-zero) values for coherent cross sections from 3-15 MeV, and for photoelectric from 1-15 MeV; MCPLIB gives zeros. In addition, the photoelectric cross sections differ by 11% at 1 keV.

Z=13: ENDF gives very small (but non-zero) values for coherent cross sections from 3-15 MeV, and for photoelectric from 1.5-15 MeV; MCPLIB gives zeros. In addition, the photoelectric cross sections differ by 10-15% from .3-1 MeV.

Z=14: ENDF gives very small (but non-zero) values for coherent cross sections from 3-15 MeV, and for photoelectric from 1.5-15 MeV; MCPLIB gives zeros. In addition, the photoelectric cross sections differ by 11% at 1 MeV.

Z=15: ENDF gives very small (but non-zero) values for coherent cross sections from 4-15 MeV, and for photoelectric from 2-15 MeV; MCPLIB gives zeros. In addition, the photoelectric cross sections differ by 11% at 1 MeV.

Z=16 : ENDF gives small (but non-zero) values for coherent cross sections from 4-15 MeV, and for photoelectric from 2-15 MeV; MCPLIB gives zeros. In addition, the photoelectric cross sections differ by 10-15% from .2-.5 MeV.

Z=17: ENDF gives small values for coherent cross sections from 4-15 MeV, and for photoelectric from 3-15 MeV; MCPLIB gives zeros. In addition the photoelectric cross sections differ by 10-12% at .4 MeV and at 1 MeV.

Z=18 : ENDF gives small values for coherent cross sections from 4-15 MeV, and for photoelectric from 3-15 MeV; MCPLIB gives zeros. In addition there is a 10% difference in photoelectric cross sections at .4 MeV.

Z=19: ENDF gives small values for coherent cross sections from 5-15 MeV, and for photoelectric from 4-15 MeV; MCPLIB gives zeros.

Z=20 : ENDF gives small values for coherent cross sections from 5-15 MeV, and for photoelectric from 5-15 MeV; MCPLIB gives zeros. In addition, the photoelectric cross sections differ by 10-15% from .2-4 MeV.

Z=21 : ENDF gives small values for coherent cross sections from 5-15 MeV, and for photoelectric from 6-15 MeV; MCPLIB gives zeros. In addition, the photoelectric cross sections differ by 10% at 5 MeV. Heating numbers are 15% different near 4.5 keV.

Z=22 : ENDF gives small values for coherent cross sections from 6-15 MeV, and for photoelectric from 8-15 MeV; MCPLIB gives zeros. In addition, the photoelectric cross sections differ by 10-15% from .2-.5 MeV and from 5-6 MeV.

Z=23: ENDF gives small values for coherent cross sections from 6-15 MeV, and for photoelectric from 8-15 MeV; MCPLIB gives zeros. In addition, the photoelectric cross sections differ by 10-15% from .3-.5 MeV and from 1-6 MeV.

Z=24: ENDF gives small values for coherent cross sections from 6-15 MeV, and for photoelectric from 10-15 MeV; MCPLIB gives zeros. In addition, the photoelectric cross sections differ by 10-15% from .2-.5 MeV and from 1-8 MeV.

Z=25: ENDF gives small values for coherent cross sections from 8-15 MeV, and for photoelectric from 10-15 MeV; MCPLIB gives zeros. In addition, the photoelectric cross sections differ by 10% at 1 keV and by 10-13% from .3-.5 MeV and from 1-8 MeV.

Z=26: ENDF gives small values for coherent cross sections from 8-15 MeV, and for photoelectric at 15 MeV; MCPLIB gives zeros. In addition, the photoelectric cross sections differ by 10-14% from 1-10 MeV.

Z=27: ENDF gives small values for coherent cross sections from 8-15 MeV, and for photoelectric at 15 MeV; MCPLIB gives zeros. In addition, the photoelectric cross sections differ by 12% at 1 keV.

Z=28: ENDF gives small values for coherent cross sections from 8-15 MeV; MCPLIB gives zeros. The photoelectric cross sections differ by 10-11% from 2-10 MeV.

Z=29: ENDF gives small values for coherent cross sections from 8-15 MeV; MCPLIB gives zeros. The photoelectric cross sections differ by 10-20% from 1-2 keV, and by 10-13% from 1-10 MeV.

Z=30: ENDF gives small values for coherent cross sections from 8-15 MeV; MCPLIB gives zeros. In addition, the photoelectric cross sections differ by 10-20% at edges below 1.2 keV, and by 11% at 2 MeV.

Z=31: ENDF gives small values for coherent cross sections from 8-15 MeV; MCPLIB gives zeros. Photoelectric cross sections differ by 10-20% from 1-2 keV.

Z=32: ENDF gives small values for coherent cross sections from 10-15 MeV; MCPLIB gives zeros. In addition, the coherent cross sections differ by 10% at .6 and 1.5 MeV, while photoelectric differs by 10-30% from 1-2 keV.

Z=33: ENDF gives small values for coherent cross sections from 10-15 MeV; MCPLIB gives zeros. In addition, the coherent cross sections differ by 10-11% from .6-1.5 MeV, while photoelectric differs by 10-16% from 1-2 keV.

Z=34: ENDF gives small values for coherent cross sections from 10-15 MeV; MCPLIB gives zeros. In addition, the coherent cross sections differ by 10-11% from .6-1.5 MeV; while photoelectric differs by 10-12% from 1-1.5 keV. The heating varies by 20% at 0.4 MeV (this is probably due to an error on MCPLIB).

Z=35: ENDF gives small values for coherent cross sections from 10-15 MeV; MCPLIB gives zeros. In addition, the coherent cross sections differ by 10-11% from .5-1.5 MeV, while photoelectric differs by 10% near the 1.6 keV edge.

Z=36: ENDF gives small values for coherent cross sections from 10-15 MeV; MCPLIB gives zeros. In addition, the coherent cross sections differ by 10-11% from .5-1.5 MeV.

Z=37: ENDF gives a small value for coherent scattering at 15 MeV;

MCPLIB gives zero. In addition, the coherent cross sections differ by 10-11% from .5-2 MeV.

Z=38: ENDF gives a small value for coherent scattering at 15 MeV; MCPLIB gives zero. In addition, the coherent cross sections differ by 10-12% from .5-2 MeV.

Z=39: ENDF gives a small value for coherent scattering at 15 MeV; MCPLIB gives zero. In addition, the coherent cross sections differ by 10-12% from .4-2 MeV.

Z=40: ENDF gives a small value for coherent scattering at 15 MeV; MCPLIB gives zero. In addition, the coherent cross sections differ by 10-11% from .4-2 MeV, while photoelectric differs by 10% at 1 keV

Z=41: ENDF gives a small value for coherent scattering at 15 MeV; MCPLIB gives zero. In addition, the coherent cross sections differ by 10-12% from .4-2 MeV

Z=42: ENDF gives a small value for coherent scattering at 15 MeV; MCPLIB gives zero. In addition, the coherent cross sections differ by 10-12% from .4-2 MeV.

Z=43: ENDF gives a small value for coherent scattering at 15 MeV; MCPLIB gives zero. In addition, the coherent cross sections differ by 10-12% from .4-3 MeV.

Z=44: ENDF gives a small value for coherent scattering at 15 MeV; MCPLIB gives zero. In addition, the coherent cross sections differ by 10-12% from .4-3 MeV, while photoelectric differs by 12% at 1 keV.

Z=45: ENDF gives a small value for coherent scattering at 15 MeV; MCPLIB gives zero. In addition, the coherent cross sections differ by 10-13% from .4-2 MeV, while photoelectric differs by 19% at 1 keV.

Z=46: ENDF gives a small value for coherent scattering at 15 MeV; MCPLIB gives zero. In addition, the coherent cross sections differ by 10-13% from .4-2 MeV and at 8 MeV, while photoelectric differs by 21% at 1 keV.

Z=47: ENDF gives a small value for coherent scattering at 15 MeV; MCPLIB gives zero. In addition, the coherent cross sections differ by 10-13% from .4-3 MeV and at 8 MeV, while photoelectric differs by 14% at 1 keV.

Z=48: ENDF gives a small value for coherent scattering at 15 MeV; MCPLIB gives zero. In addition, the coherent cross sections differ by 10-13% from .4-3 MeV and from 8-10 MeV, while photoelectric differs by 10-25% from 1-1.5 keV.

Z=49: ENDF gives a small value for coherent scattering at 15 MeV; MCPLIB gives zero. In addition, the coherent cross sections differ by 10-13% from .4-3 MeV and from 8-10 MeV, while photoelectric differs by 10-25% from 1-1.5 keV and by 10-12% near the 4 keV edges.

Z=50: The coherent cross sections differ by 10-13% from .4-3 MeV and from 8-10 MeV, while photoelectric differs by 10-35% from 1-2 keV.

Z=51: The coherent cross sections differ by 10-13% from .4-3 MeV and at 10 MeV, while photoelectric differs by 10-30% from 1-1.5 keV.

Z=52: The coherent cross sections differ by 10-14% from .4-3 MeV and at 10 MeV, while photoelectric differs by 10-35% from 1-2 keV.

Z=53: The coherent cross sections differ by 10-13% from .4-3 MeV and at 10 MeV, while photoelectric differs by 10-30% from 1-2 keV.

Z=54: The coherent cross sections differ by 10-14% from .4-4 MeV and at 10 MeV, while photoelectric differs by 15-20% near 1 keV.

Z=55: The coherent cross sections differ by 10-14% from .4-4 MeV and from 10-15 MeV, while photoelectric differs by 10-30% from 1-4 keV.

Z=56: The coherent cross sections differ by 10-14% from .4-3 MeV and from 10-15 MeV, while photoelectric differs by 10-40% from 1-3 keV.

Z=57: The coherent cross sections differ by 10-14% from .4-4 MeV and from 10-15 MeV, while photoelectric differs by 10-35% from 1-3 keV.

Z=58: The coherent cross sections differ by 10-14% from .4-4 MeV and from 10-15 MeV, while photoelectric differs by 10-35% from 1-4 keV.

Z=59: The coherent cross sections differ by 10-16% from .4-4 MeV and from 10-15 MeV, while photoelectric differs by 10-35% from 1-5 keV.

Z=60: The coherent cross sections differ by 10-17% from .4-4 MeV and from 10-15 MeV, while photoelectric differs by 10-35% from 1-5 keV.

Z=61: The coherent cross sections differ by 10-18% from .4-6

MeV and from 10-15 MeV, while photoelectric differs by 10-35 % from 1-5 keV.

Z=62: The coherent cross sections differ by 10-19 % from .4-5 MeV and from 10-15 MeV, while photoelectric differs by 10-35 % from 1-4 keV.

Z=63: The coherent cross sections differ by 10-20 % from .4-5 MeV and from 10-15 MeV, while photoelectric differs by 10-40 % from 1-5 keV.

Z=64: The coherent cross sections differ by 10-20% from .4-6 MeV and from 10-15 MeV, while photoelectric differs by 10-30% from 1-4 keV

Z=65: The coherent cross sections differ by 10-20% from .3-6 MeV and from 10-15 MeV, while photoelectric differs by 10-35% from 1-5 keV.

Z=66: The coherent cross sections differ by 10-22% from .3-15 MeV, while photoelectric differs by 10-35 % from 1-5 keV.

Z=67: The coherent cross sections differ by 10-23% from .3-15 MeV, while photoelectric differs by 10-35 % from 1-4 keV.

Z=68: The coherent cross sections differ by 10-23 % from .3-15 MeV, while photoelectric differs by 10-35 % from 1-4 keV and by 11% near 10 keV.

Z=69: The coherent cross sections differ by 10-23 % from .3-15 MeV, while photoelectric differs by 10-35 % from 1-4 keV.

Z=70: The coherent cross sections differ by 10-24 % from

.3-15 MeV, while photoelectric differs by 10-30% from 1-4 keV.

Z=71: Coherent cross sections differ by 10-23% from .3-15 MeV, while photoelectric differs by 10-30% from 1-4 keV.

Z=72: Coherent cross sections differ by 10-23% from .3-15 MeV, while photoelectric differs by 10-30% from 1-4 keV.

Z=73: Coherent cross sections differ by 10-23% from .3-15 MeV, while photoelectric differs by 10-30% from 1-4 keV.

Z=74: Coherent cross sections differ by 10-22% from .3-15 MeV, while photoelectric differs by 10-30% from 1-3 keV.

Z=75: Coherent cross sections differ by 10-21% from .3-15 MeV, while photoelectric differs by 10-30% from 1-4 keV.

Z=76: Coherent cross sections differ by 10-21% from .3-15 MeV, while photoelectric differs by 10-27% from 1-4 keV.

Z=77: Coherent cross sections differ by 10-20% from .3-15 MeV, while photoelectric differs by 10-28% from 1-4 keV.

Z=78: Coherent cross sections differ by 10-21% from .3-15 MeV, while photoelectric differs by 10-25% from 1-5 keV.

Z=79: Coherent cross sections differ by 10-21% from .3-15 MeV, while photoelectric differs by 10-24% from 1-3.5 keV.

Z=80: Coherent cross sections differ by 10-21% from .3-15 MeV, while photoelectric differs by 10-28% from 1-4 keV.

Z=81: Coherent cross sections differ by 10-21% from .3-15 MeV, while photoelectric differs by 10-24% from 1-4 keV.

Z=82: Coherent cross sections differ by 10-22% from .3-15 MeV, while photoelectric differs by 10-21% from 1-4 keV.

Z=83: Coherent cross sections differ by 10-22% from .3-15 MeV, while photoelectric differs by 10-28% from 1-4 keV.

Z=84: Cross sections given only by MCPLIB; not by ENDF.

Z=85: Cross sections given only by MCPLIB; not by ENDF.

Z=86: Coherent cross sections differ by 10-22% from .3-15 MeV, while photoelectric differs by 10-13% from 1-5 keV.

Z=87: Cross sections given only by MCPLIB; not by ENDF.

Z=88: Cross sections given only by MCPLIB; not by ENDF.

Z=89: Cross sections given only by MCPLIB; not by ENDF.

Z=90: Coherent cross sections differ by 10-23% from .3-15 MeV, while photoelectric differs by 10-23% from 3-5.2 keV.

Z=91: Cross sections given only by MCPLIB; not by ENDF.

Z=92: Coherent cross sections differ by 10-23% from .3-15 MeV, while photoelectric differs by 10-18% from 1-4.4 keV.

Z=93: Cross sections given only by MCPLIB; not by ENDF.

Z=94: Coherent cross sections differ by 10-24% from .3-15 MeV, while photoelectric differs by 10-21% from 3-6 keV.

New Photon Libraries

1090895/PHOTON/MCPLIB (7600) 127370 82/12/13 11:09:55.994

1090895/PHOTON/MCPLIBC (CRAY) 135243B 82/12/13 11:13:25.474

12/13/82

Addition to 2/26/82 memo "New Photon Library from ENDF Data"

Bob Schrandt realized that we should re-calculate the average energy loss from incoherent scattering because of the change in MCNP in sampling the Klein-Nishina distribution. The code NEWINCO was written to replace the KN sampling found in PHEINCO. This produced an output file stored as NEWEINCO. PHHEAT was rerun, producing NEWHEA3, and PHMERGE gave us NEWMERG3.

There was a problem with convergence of the heating calculation (due to the difficulty of sampling the K-N) and another code, called NEWESTI, was written. This code does analytic calculation of the pdf of the KN as a function of cosine. As before, the incoherent form factors are used to determine what fraction of times a given cosine will be accepted. This code produced NEWESTEINC and was much more well-behaved.

In the end, however, it turned out that there was an error in all of the codes. All three were replaced and re-run, giving new versions of EINCO, NEWEINCO, and NEWESTEINC. EINCO was used in PHHEAT and PHMERGE to produce a new version of MERG3 and MERG3C.

For the final library, however, we want the results using NEWESTI. PHHEAT was re-run, producing a new NEWHEA3, and PHMERGE was re-run, producing a new NEWMERG3. (Also CRAY version NEW3CRAY)

Two new codes were written:

(A) DIRECT

This code re-orders the dictionary to make the ENDF library (with no values for several Z's) compatible with MCNP which requires the Z's to appear in the Zth location in the dictionary.

(L) ADDZ

This code merges all of the data found on the ENDF library with that found on the present MCPLIB for Z's not found in ENDF. Tape1 is NEWMERG3, TAPE2 is the present MCPLIB, and the output file TAPE3 is the future MCPLIB, which is stored as MCPLIB and MCPLIBC.

Here is an updated listing of all of the files contained under the /090895/PHOTON node

```
mass list /090895/photon

     node name: photon
     descendants:
          phxs
          xs
          phff
          ff
          phintff
          intff
          phflor
          flor
          rgsppr
          pheinco
          einco
          pheflor
          eflor
          phheat
          heat
          phmerge
          roger
          merge
          pheflo3
          eflo3
          hea3
          merg3
          phcomp
          mergec
          merg3c
          newinco
          neweinco
          newhea3
          newmerg3
          newesti
          newesteinc
          direct
          new3cray
          addz
          mcplib
          mcplibc

all done
```

If I had to re-run the entire sequence of codes, this is how I would do it now.

1. PHXS

Input TAPE1 = GAM23
Output TAPE2 = XS

2. PHFF

Input TAPE1 = GAM27
Output TAPE2 = FF

3. PHINTFF

Input TAPE1 = FF
Output TAPE2 = INTFF

4. PHFLOR

Input TAPE1 = MCPLIB
Output TAPE2 = FLOR

5. NEWESTI

Input TAPE1 = XS
TAPE2 = FF
Output TAPE3 = NEWESTEINC

6. PHEFLO3

Input TAPE1 = XS
TAPE2 = FLOR
Output TAPE3 = EFLO3

7. PHHEAT

Input TAPE1=XS

TAPE2= NEWESTEINC

TAPE3 = EFLO3

Output TAPE4= NEWHEA3

8. PHMERGE

Input TAPE1=XS

TAPE2=FF

TAPE3=INTFF

TAPE4= NEWHEA3

TAPE5 = FLOR

Output TAPE6

9. DIRECT

Input TAPE1 ← (TAPE6 from "8)

Output TAPE1 = NEWMERG3

10. ADDZ

Input TAPE1 = NEWMERG3

TAPE2 = MCPLIB (present)

Output TAPE3 = MCPLIB (new)

11. ROGER

Input TAPE2 = MCPLIB

Output TAPE10

1076997/R028/ROGER 527B 81/10/26 16:46:14.7