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NXGAMEL, A Code to Calculate Continuum Photon and Electron ^{Production}~~Production~~
Cross Sections and Spectra From Neutron Induced Reactions

S. T. Perkins

February 15, 1975

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Prepared for U.S. Atomic Energy Commission under contract no. W-7405-Eng-48

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NXGAMEL, A Code to Calculate Continuum Photon and Electron Production
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ABSTRACT

NXGAMEL is a code that calculates continuum photon (gamma-rays from nuclear transitions and x-rays following internal conversion) and internal conversion electron production cross sections and spectra from neutron-induced reactions.

The input, output, and recent additions to the theory, are described.

MASTER

Introduction

NXGAMEL is a code that calculates continuum photon (gamma-rays from nuclear transitions and x-rays following internal conversion) and internal conversion electron production cross sections and spectra from neutron-induced reactions. The main body of the theory has been published previously.⁽¹⁾ In this report, the input to the code and output results are described. Furthermore, an extension to the theory which takes into account the energy not available to the continuum because of discrete transitions is described and is available on option in the code. This report supercedes all previous reports of the code.

General Comments

Some general comments are as follows:

- 1) The code is setup to operate on the LLL CDC 7600 computers.
- 2) Both fissile and non-fissile isotopes can be calculated.
- 3) Electron and x-ray production are based on K, L, and M internal conversion coefficients (summed over subshells), see e.g., ref. 2. A single set of conversion coefficients is used, regardless of the reaction and an average multipolarity mixture is assumed.
- 4) There are three energy parameters which are required for the operation of the code. EGMIN is the lowest energy in the gamma-ray spectra, i.e., the minimum allowed transition energy within a given gamma-ray cascade. It is set internally by the code at 0.01 MeV. UMIN is the minimum excitation energy in a given residual nucleus below which no contribution is made to continuum gamma-ray

production. For heavy nuclei with unknown level structure, it is generally set at 0.1 MeV. The final energy parameter is UCUT. If the excitation energy in the residual nucleus at all incident neutron energies is less than UCUT, the reaction is not considered. This parameter is used to remove all (or part of) the discrete (n,n') excitations from the analysis, as per the theory of ref. 1. In this case, both UMIN and UCUT $\geq$ EGMIN. However, if UCUT $\equiv$ 0., then the energy from all discrete transitions (e.g., n,n' discrete photons, and electrons) is not considered available to the continuum calculation, as described in a later section. If UCUT $\equiv$ 0., then UMIN $\geq$ 0.

- 5) Two disc files, INPUT and ENDL, are required for input to NXGAMEL. All input units are barns and MeV. The file INPUT contains the parameter cards for the run and its format is described in the next section. The file ENDL contains evaluated data for the isotopes of interest in the ENDL⁽³⁾ input (BCD card image) format, ordered as is done by a retrieval from the library. A retrieval using the code UPDATE orders the file by ascending ZA number (1000Z+A), by ascending CIS values and by ascending energy-parameter pairs. The file INPUT must also be ordered by these conventions.
- 6) The code only uses integrated cross sections (I = 0) and energy deposits (I = 10 and 11) from the ENDL file. If UCUT > 0. (see General Comment 4), reactions considered are $1 \leq C \leq 15$, and $20 \leq C \leq 49$. If UCUT $\equiv$ 0., then C = 55 and 57, S = 3 results

are also included. All other data, including existing continuum photon ($C = 55$, $S = 0$) and electron ($C = 57$, $S = 0$) production cross sections, are ignored. (Of course, any such data must be deleted before the output of the code is entered into the library.) A limitation of 10,000 energy-parameter pairs per given I and C is imposed.

- 7) Linear-linear interpolation is used with the ENDL file; log-log interpolation is used for the internal conversion coefficients.
- 8) Values for the parameter in a given energy-parameter table are assumed zero outside the energy domain of the table.
- 9) Tables of the R -parameter for both nonfission and fission reactions are built into the code for user convenience (may be overridden on input). Fission can also be represented by an analytic representation of the prompt gamma-ray spectrum from the thermal fission of ^{235}U , this latter approach being recommended. The justification for choosing these built-in values is described in Ref. 1.

Parameter Input

The input description for the disc file, INPUT, is described in Table I below.

Table I. NXGAMEL Parameter Format (Disc File INPUT)

Card Type	Column	(Format)	Parameter	Description
<u>Run description</u>	1-2	(i2)	ITOT	No. of isotopes in run.
	3-4	(i2)	NUME	No. of incident neutron energies (<50).

Card Type	Column	(Format)	Parameter	Description
	5-10	(i6)	IDATE	Date (MMDDYY).
	11	(il)	IDOTT	= 0. No electron or x-ray production in the run. = 1. Electron and x-ray production in the run.
<u>Neutron energies</u>	1-66	(6E11.4)	EN	Table of incident neutron energies (NUME values).
<u>Isotope parameters</u>	1-6	(i6)	IZA	Isotope ZA number (1000Z+A).
	7-17	(E11.4)	UCUT	See General Comment 4. If available energy at all incident neutron energy is less than UCUT, reaction not considered. (Used to remove discrete (n,n') excitations which are considered separate from this calculation.)
	18-28	(E11.4)	UMIN	See General Comment 4. Excitation energy below which no contribution is made to gamma ray production for reactions which are considered. (Usually set at 0.1 MeV when UCUT > 0.).
	29-39	(E11.4)	EGR	Photon energy above which supplemental photon production to be calculated (used for comparison to experimental data). If 0. or blank, calculation not performed.

Card Type	Column	(Format)	Parameter	Description
	40	(i1)	IROPT	= 0 if built in table of R(U) versus U used. = 1 if R(U) versus U input.
	41-43	(i3)	NUMR	Only input if IROPT = 1. Number of R(U) versus U pairs (<50).
	44	(i1)	IFISS	= 0 if no fission present. = 1 if fission present and built in constant value of R_f to be used. = 2 if fission present and $R_f(U)$ versus U input. = 3 if fission present and analytical fit for gammas from ^{235}U thermal fission used at all energies.
	45-47	(i3)	NUMRF	Only input if IFISS = 2. Number of $R_f(U)$ versus U pairs (<50).
	48	(i1)	IEOPT	= 0 if no conversion electrons or x-rays present. = 1 if conversion electrons and x-rays to be calculated.
	49-50	(A2)	MULT	Only input if IEOPT = 1. Assumed photon multipolarity e.g., E2 (only used on HSP output).
	51-53	(i3)	NKMAX(1)	Only input if IEOPT = 1. Number of $E_\gamma - \alpha_K$ pairs of K shell conversion coefficients (<100 pairs).

Card Type	Column	(Format)	Parameter	Description
	54-56	(i3)	NKMAX(2)	Only input if IEOPT = 1. Number of E_γ - α_L pairs of L shell conversion coef- ficients (≤ 100 pairs).
	57-59	(i3)	NKMAX(3)	Only input if IEOPT = 1. Number of E_γ - α_M pairs of M shell conversion coef- ficients (≤ 100 pairs).
	60	(i1)	IOUT	Only input if IEOPT = 1. = 1 prints out x-ray and gamma results.
	61-62	(i2)	IPOPT	Only input if UCUT = 0. Number of discrete photon reactions (C=55, S=3) on ENDL file ($0 \leq \text{IPOPT} \leq 50$).
	63-64	(i2)	IBOPT	Only input if UCUT = 0. Number of discrete electron reactions (C=57, S=3) on ENDL file ($0 \leq \text{IBOPT} \leq 50$).
<u>R parameter</u> (only input if IROPT = 1)	1-66	(6E11.4)	EU R	U-R pairs (NUMR pairs).
<u>R_f parameter</u> (only input if IFISS = 2)	1-66	(6E11.4)	EUF RF	U-R _f (U) pairs (NUMRF pairs).
<u>K conversion</u> <u>coefficients</u> (only input if IEOPT = 1)	1-66	(6E11.4)	EGK(1) (ALPK(1))	E_γ - α_K pairs (NKMAX(1) pairs).

Card Type	Column	(Format)	Parameter	Description
<u>L conversion coefficients</u> (only input if IEOPT = 1)	1-66	(6E11.4)	EGK(2) ALPK(2)	$E_{\gamma}-\alpha_L$ pairs (NKMAX(2) pairs).
<u>M conversion coefficients</u> (only input if IEOPT = 1)	1-66	(6E11.4)	EGK(3) ALPK(3)	$E_{\gamma}-\alpha_M$ pairs (NKMAX(3) pairs).
<u>Discrete photon reaction designators</u> (IPOPT cards)	1-2	(i2)	ICP	The ENDL file neutron induced reaction from which the discrete photon contribution is to be subtracted (e.g., C=11 corresponds to n,n').
	3-13	(E11.4)	XP1	Energy of the discrete photon. Corresponds to the X1 field (C=55, S=3) in ENDL file and is in same order.
<u>Discrete electron reaction designators</u> (IBOPT cards)	1-2	(i2)	ICB	The ENDL file neutron induced reaction C number from which the discrete electron contribution is to be subtracted (e.g., C=11 corresponds to n,n').
	3-13	(E11.4)	XB1	Energy of the discrete electron. Corresponds to the X1 field (C=57, S=3) in ENDL file, and is in same order.

Repeat card types Isotope parameters through Discrete electron reaction designators for second isotope (isotopes must be in ascending ZA order).

Repeat for all ITOT isotopes.

Code Output

Output from the code are one or two disc files (OUTPUTP and OUTPUTE), depending on whether conversion electrons are present, and HSP. The HSP output is in an abbreviated people readable form and for each isotope, the following types of information are presented:

- 1) General input description.
- 2) Tables of $R(U)$ versus U and $R_f(U)$ versus U , if input.
- 3) Tables of gamma energies versus K , L , and M internal conversion coefficients, if input.
- 4) Interpolated values (at each incident neutron energy) of input data for each reaction. These include neutron cross sections, excitation energy, and the R parameter. Values are not given for any reaction for which all excitation energies are $\leq UCUT$. If interpolated values at any given neutron energy are all zeroes, it signifies that the specific excitation energy $\leq UMIN$. If $UCUT = 0$, interpolated values (cross section only) are also given for $C = 55$ and 57 , $S = 3$ reactions.
- 5) If $UCUT = 0$., average unavailable energies per reaction.
- 6) Output results per reaction, excluding spectra ($I = 4$ data). This includes average energy, multiplicity, production cross section, and integral of the spectra for photons; also electrons, if calculated. On option when electrons are calculated ($IOUT = 1$),

corresponding results may be output for K, L, and M x-rays as well as for the gammas.

- 7) Output results summed over all reactions. Similar to output results per reaction, including the additional printout option (IOUT = 1).
- 8) Average total available energies.
- 9) Supplemental calculation - photon production cross sections above a photon energy equal to EGN. These results are useful for comparison to experiment.

The abbreviations used in the HSP tables are given in Table II.

A disc file, OUTPUTP, is always made for any run. The first data in this file are the photon spectra (C = 55, I = 4 data) at each incident neutron energy. This is in the ENDL input format and includes appropriate header and end cards. Following this for a given isotope are the photon production cross sections (C = 55, I = 0), again with appropriate header and end cards. If electrons are calculated, a disc file, OUTPUTE, is made. This file contains the corresponding electron production data (C = 57) in the ENDL input format. All output spectra are thinned by THINER; the thinning criterion is set within the code at 1%.

Unavailable Energy Due to Discrete Transitions

If there are discrete photon (C = 55, S = 3) and/or electron (C = 57, S = 3) transitions within the ENDL file, they arise from either discrete or

Table II. Abbreviations Used in HSP Tables

N	Neutron
P	Photon (gammas + x-rays)
E	Electron
(K), (L), or (M)	K, L, or M x-ray. An X() is used to identify the x-ray cross section
G	Gamma
EN	Neutron energy
U	Excitation energy (or average total available energy)
R	R parameter
EBAR	Average energy. An E() is used for x-ray energies
M	Multiplicity
C/S	Cross section
INT or INTEGRAL	Integral of the spectra
N-P or N-E	Number of points in spectra
FRACT	Fraction of spectra above EGN
4PI	4π
W	Level energy
TOT	-W+P+E, referring to total weighted average unavailable energy

continuum neutron induced reactions. The energy accounted for in these reactions is not available for production of continuum photons ($C = 55$, $S = 0$) and/or electrons ($C = 57$, $S = 0$). This energy can be taken into account if the type of neutron induced reaction (e.g., n, n') which produces the discrete components is known. It will be assumed in the following discussion that this is the situation.

Let us, as an example, consider a single neutron induced reaction (e.g., n, n' - levels plus continuum). The level scheme in the residual nucleus and neutron induced reaction cross sections would be as shown below:

Here, we define

subscript i = discrete neutron induced process

subscript c = continuum neutron induced process

subscript r = neutron induced reaction, i.e., $c + \sum_i$

E_n = incident neutron energy

σ = neutron induced cross section

U = excitation energy in the residual nucleus

By conservation of (average) energy (see Eq. (4) of ref. 1),

$$\sigma_r(E_n)U_r(E_n) = \sigma_c(E_n)U_c(E_n) + \sum_i \sigma_i(E_n)U_i(E_n) \quad , \quad (1)$$

where for either i or c induced processes,

$$U(E_n) = E_n + Q_0 - \overline{E_{\text{recoil}}(E_n)} - \overline{E_{n'}(E_n)} \quad , \quad (2)$$

$\rightarrow U_i$ for discrete levels (i.e., the level energy).

In Eq. (2), we define

$\overline{E_{\text{recoil}}(E_n)}$ = average recoil kinetic energy of the residual nucleus
and charged particles in the lab system,

$\overline{E_{n'}(E_n)}$ = average kinetic energy of all emergent neutrons in
the lab system,

Q_0 = reaction (binding energy difference) Q value.

Suppose now that the excited states (discrete as well as continuum) can decay both by gamma-ray transitions as well as internal conversion.

Three types of transitions can then be described:

cc = continuum neutron induced process yielding continuum photons or electrons

cd = continuum neutron induced process yielding discrete photons or electrons; summations are over j (photons) and ℓ (electrons)

dd = discrete neutron induced process yielding discrete photons or electrons; summations are over k (photons) and m (electrons)

Then again by energy conservation (see Eq. (5) and (28) of ref. 1),

$$\begin{aligned} \sigma_r(E_n) U_r(E_n) = & \sigma_{n, Xp_{cc}}(E_n) \overline{E_{p_{cc}}(E_n)} + \sum_j \sigma_{n, Xp_{cd_j}}(E_n) E_{p_{cd_j}} \\ & + \sum_k \sigma_{n, Xp_{dd_k}}(E_n) E_{p_{dd_k}} + \sigma_{n, X\beta_{cc}}(E_n) E_{\beta_{cc}}(E_n) \\ & + \sum_{\ell} \sigma_{n, X\beta_{cd_{\ell}}}(E_n) E_{\beta_{cd_{\ell}}} + \sum_m \sigma_{n, X\beta_{dd_m}}(E_n) E_{\beta_{dd_m}} \end{aligned} \quad (3)$$

where we define

p = photon (gamma's + x-rays following internal conversion)

β = conversion electrons

$\sigma_{n, Xy}$ = production cross section for particle y (y = p or β)

$\overline{E_y}$ = average kinetic energy of particle y (y = p or β); for both cd and dd transitions, this is just the kinetic energy of the discrete photon or electron

The next step will be to equate Eq. (1) and (3). We know by definition from the two equations that

$$\sum_i \sigma_i(E_n) U_i(E_n) \equiv \sum_k \sigma_{n,Xp_{dd_k}}(E_n) E_{p_{dd_k}} + \sum_m \sigma_{n,X\beta_{dd_m}}(E_n) E_{\beta_{dd_m}}, \quad (4)$$

and these terms in principal can be cancelled from both sides of the resultant equation. However in practice, it is usually not possible to separate the dd from the cd transitions and hence Eq. (4) cannot be utilized. Proceeding hence to directly equate Eq. (1) and (3) yields

$$\begin{aligned} & \sigma_c(E_n) U_c(E_n) + \sum_i \sigma_i(E_n) U_i(E_n) - \sum_j \sigma_{n,Xp_{cd_j}}(E_n) E_{p_{cd_j}} \\ & - \sum_k \sigma_{n,Xp_{dd_k}}(E_n) E_{p_{dd_k}} - \sum_l \sigma_{n,X\beta_{cd_l}}(E_n) E_{\beta_{cd_l}} - \sum_m \sigma_{n,X\beta_{dd_m}}(E_n) E_{\beta_{dd_m}} \\ & = \sigma_{n,Xp_{cc}}(E_n) \overline{E_{p_{cc}}(E_n)} + \sigma_{n,X\beta_{cc}}(E_n) \overline{E_{\beta_{cc}}(E_n)} \end{aligned} \quad (5)$$

The multiplicity for particle y, $M_y(E_n)$, is given by (Eq. (7) of Ref. 1)

$$M_y(E_n) = \frac{\sigma_{n,Xy}(E_n)}{\sigma(E_n)} \quad (6)$$

Also, the photon production cross section for cc transitions can be divided into its gamma and x-ray components (summation over r is for the x-rays),

$$\sigma_{n,Xp_{cc}}(E_n) \overline{E_{p_{cc}}(E_n)} = \sigma_{n,X\gamma_{cc}}(E_n) \overline{E_{\gamma_{cc}}(E_n)} + \sum_{r=K,L,M} \sigma_{n,Xr_{cc}}(E_n) E_{r_{cc}} \quad (7)$$

Dividing Eq. (5) by $\sigma_c(E_n)$ and using Eq. (6) and (7) leads to

$$U_c(E_n) - U_{na}(E_n) = M_{\gamma_{cc}}(E_n) \overline{E_{\gamma_{cc}}(E_n)} + M_{\beta_{cc}}(E_n) \overline{E_{\beta_{cc}}(E_n)} + \sum_{r=K,L,M} M_{r_{cc}}(E_n) E_{r_{cc}}, \quad (8)$$

where $U_{na}(E_n)$ is the energy not available to cc transitions,

$$U_{na}(E_n) = \frac{1}{\sigma_c(E_n)} \left[- \sum_i \sigma_i(E_n) U_i(E_n) + \sum_j \sigma_{n,Xp_{cdj}}(E_n) E_{p_{cdj}} + \sum_k \sigma_{n,Xp_{ddk}}(E_n) E_{p_{ddk}} + \sum_l \sigma_{n,X\beta_{cdl}}(E_n) E_{\beta_{cdl}} + \sum_m \sigma_{n,X\beta_{ddm}}(E_n) E_{\beta_{ddm}} \right]. \quad (9)$$

Equation (8) is identical to Eq. (28) of ref. 1 if we replace $U_c(E_n)$ by $U_c(E_n) - U_{na}(E_n)$. The remainder of the equations in ref. 1 also follow directly with this change. As mentioned earlier, dd and cd transitions cannot always be separated. Thus, going to ENDL nomenclature for a specific neutron induced reaction c;

$$\sigma_{c,s=0}(E_n) = \sigma_c(E_n), \quad (10)$$

$$\sum_i \sigma_i(E_n) U_i(E_n) \Big|_{\substack{c \\ s=1}} = \sum_i \sigma_i(E_n) U_i(E_n), \quad (11)$$

$$\sum_h \sigma_h(E_n) E_h \Big|_{\substack{c=55 \\ s=3}} = \sum_j \sigma_{n,Xp_{cdj}}(E_n) E_{p_{cdj}} + \sum_k \sigma_{n,Xp_{ddk}}(E_n) E_{p_{ddk}}, \quad (12)$$

$$\sum_h \sigma_h(E_n) E_h \Big|_{\substack{c=57 \\ s=3}} = \sum_\ell \sigma_{n,X\beta_{cd_\ell}}(E_n) E_{\beta_{cd_\ell}} + \sum_m \sigma_{n,X\beta_{dd_m}}(E_n) E_{\beta_{dd_m}}, \quad (13)$$

where the $c = 55$ and 57 , $s = 3$ have been specifically identified as arising from the specified neutron induced reaction. Equation (9) then becomes

$$U_{na}(E_n) = \frac{1}{\sigma_{c,s=0}(E_n)} \left[\sum_i \sigma_i(E_n) U_i(E_n) \Big|_{\substack{c \\ s=1}} + \sum_h \sigma_h(E_n) E_h \Big|_{\substack{c=55 \\ s=3}} + \sum_h \sigma_h(E_n) E_h \Big|_{\substack{c=57 \\ s=3}} \right] \quad (14)$$

This is the form of the equation that is used in the code when $UCUT = 0$.

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