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**GAMIDENT: a program to aid
in the identification of
unknown materials by
gamma-ray spectroscopy**

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GAMIDENT: A PROGRAM TO AID IN THE IDENTIFICATION OF UNKNOWN MATERIALS BY GAMMA-RAY SPECTROSCOPY

ABSTRACT

We have written a computer code, called GAMIDENT, to help identify isotopes by their gamma-ray emissions and thus to assist in the non-destructive assay of unknown materials. The program searches a file (called GAMIN) of gamma-ray spectra, from both radioactive decays and neutron captures, for matches with observed photon energies. This report describes the search procedure used, outlines the use of the code, and gives examples.

The code is designed for operation at the Lawrence Livermore Laboratory (LLL) on a CDC-7600 computer. It is written in standard Fortran (ANSI) as much as possible, but it contains some LRLTRAN instructions required to make use of the Livermore Time-Sharing System (LTSS). The code uses about 30 000 words of SCM and about 550 000 words of LCM. Typical problems run in less than 30 seconds. The source program and the data file are available on request.

INTRODUCTION

The gamma rays emitted by an isotope undergoing radioactive decay or neutron capture have energies and intensities characteristic of that isotope. Such a set of gamma rays is often referred to as the signature of the isotope. A useful method for the non-destructive assay of unknown materials is based on the identification of such signatures in their gamma emissions.

There are thousands of known gamma rays, however, so an automated search procedure is desirable. We have created a disk file, called

GAMIN, of observed gamma ray spectra, and a computer code, called GAMIDENT, to search this file for matches with observed gamma energies. GAMIDENT lists these matching isotopes. It then applies a simple criterion that eliminates isotopes that are unlikely to have been the source of the observed photons, and lists the isotopes that are left—the likely candidates. The user must make any further analysis required to identify the actual source isotopes.

SEARCH PROCEDURE USED IN GAMIDENT

In outline the search procedure used in GAMIDENT is as follows:

1. Given a set of observed photon energies, search the tabulated data for photons with the same energies, within experimental uncertainty. Isotopes that emit such photons form the initial list of possible sources of the observed photons.

2. Examine the tabulated spectrum of each of these isotopes for gammas with higher probability of emission (per reaction) than that of the observed

gamma; any such gammas should presumably have been observed as well.

3. Examine energies of the other observed photons to see if these higher-probability gammas, if any, were in fact observed.

4. If the matched isotope's spectrum contains a higher-probability gamma, and it was not observed, remove this isotope from the list of possible sources. Isotopes that survive this test constitute the final list of possible sources.

LIMITING THE SEARCH

The search just described can be made faster, and other improbable isotopes eliminated from the final list, if other information available to the user is included in the search procedure. These additional constraints on the search are described below.

1. Ignore tabulated photons below a chosen minimum energy. There are several reasons why this may be desirable: (a) The commonly used lithium-drifted germanium (Ge-Li) detectors are usually biased in such a way that photons below some minimum energy are not recorded. (b) There may be other unknown materials between the source and the detector—containers or shielding, for example. Such materials will alter the photon spectrum of the source, especially at lower energies (since photon-interaction cross sections rise rapidly with decreasing energy). (c) There may be a very large number of observed photons, and the user may want to limit the volume of output from the program. He can do this by choosing an energy cutoff that leaves a reasonable number of higher-energy photons as inputs. If there are interposed materials, higher-energy photons are most likely to represent the spectrum of the unknown source, so this is a sensible way to limit the inputs.

2. Ignore isotopes outside some chosen range. The user may know that the source does not contain isotopes outside some range of atomic number Z and mass number A , or he may simply be uninterested in isotopes outside of some such range. The user combines the Z and A of these limiting isotopes into numbers equal to $1000Z + A$, and enters these to indicate the limits chosen.

3. Search only prompt gammas, or only those from radioactive decays, or both. If the source

could not be emitting prompt gammas, or those from decays with very short half-lives, the user can specify a minimum half-life he wants searched. He can set this value to zero if he wants to search both prompt and decay gammas. (In GAMIN prompt gammas are assigned a half-life of 10^{-14} s.)

(Of course the capture process may result in the formation of a radioactive product, which will decay with its own characteristic spectrum and half-life. The user may need to consider this in deciding whether to search prompt gammas only.)

4. Do not consider gammas with low probability of emission. Clearly low-probability photons, even if present in the unknown spectrum, may not be detected. (The tabulated probabilities, also called multiplicities, are actually probabilities of emission per decay or per neutron capture.)

The user will also have to estimate the uncertainty to be associated with each observed photon energy. The Ge-Li detector has an accuracy of plus or minus a few keV for photon energies in the range from 100 keV to 10 MeV. This uncertainty arises mainly from the nonlinearity of the relationship between photon energy and detector output. (A Ge-Li detector operated at liquid-nitrogen temperature has a precision of about 0.1 keV for photons in this energy range.) Unknown energies are determined by interpolation or extrapolation from detector outputs due to known photons; typically only a few such calibration photons are used. To take account of asymmetry in the calibration the program permits the user to specify different values for the uncertainties above and below the observed energies.

PROGRAM OUTPUTS

The code provides four kinds of output information:

1. The input data (search constraints and photon energies).

2. A list of each match of an observed photon, giving the identity of the matching isotope and a list of all the photons in the spectrum of that isotope that satisfy the search constraints.

3. A list of those isotopes that had no unobserved higher-probability photons. These isotopes remain active candidates.

4. A list of the eliminated isotopes, with the multiplicity and energy of both the observed and the unobserved, higher-multiplicity photon.

GAMMA SPECTRA IN THE DATA FILE (GAMIN)

There are 18 588 entries in GAMIN, taken from two compilations^{1,2} of gamma ray spectra. The compilation of radioactive-decay gammas¹ includes the half-life for each isotope and the energy and probability of emission per decay for each gamma emitted by that isotope. We have included in GAMIN all photons from Ref. 1 for which multiplicities are tabulated. The compilation of gammas

induced by neutron capture² gives the energy and probability per capture for each photon accompanying the formation of the product nucleus. We have included all photons from Ref. 2 that have energies greater than 1 MeV and probabilities greater than 0.01. The structure of GAMIN is described in Appendix A

USING GAMIDENT

This section deals only with aspects of the use of GAMIDENTS that are independent of where the program is being run. Details on the use of this program at LLL are given in Appendix B.

The user is likely to want to enter the search constraints from his console, so that he can alter these constraints after seeing the program output. On the other hand there may be many observed photon energies, so that the ability to enter the energies from a user-created disk file would be helpful. GAMIDENTS allows the user to enter his data as just described, or to enter it all from the console, or all from his disk file. The disk file, called GAMDATA, is set up using a card-image format described in Appendix C. The data file GAMIN must always be present.

The program prompts the user as follows:

ENTER INPUT MODE, DISK OR TTY

If DISK is chosen, all user input (search constraints and observed energies) will be read from GAMDATA. If TTY is chosen, the user will enter the search constraints from the console; he will still have the option of entering his observed energies from the disk.

ENTER DETECTOR SHIFTS (MEV). LOWER THEN UPPER IN 2F7.3

Note that these uncertainties, while of the order of a few keV, are entered in MeV. The user may either use the format 2F7.3 or a field-free floating-point format, delimiting the two variables with a comma.

ENTER LOWER ENERGY LIMIT (MEV) FOR GAMMAS IN F7.3

This suppresses search of energies less than the value entered.

ENTER LOWER AND UPPER LIMITS OF ISOTOPES IN 216

These two numbers, equal to $1000Z + A$, limit the range of isotopes searched.

ENTER LOWER BOUND OF HALF-LIFE IN SEC., (F10.3)

This suppresses search of unreasonably short half-lives. Enter zero if all isotopes are to be searched, and any value (or none) if only prompt gammas are to be searched.

PROMPT GAMMAS ONLY? ENTER YES OR NO

A "YES" causes the program to ignore the previous entry. The format is A4.

ENTER LOWER BOUND OF MULTI- PLICITIES (F7.3)

This suppresses search of low-probability photons.

This completes the entry of the search constraints. Next the program prompts for the mode of input for observed energies:

ENTER INPUT MODE FOR OBSERVED ENERGIES, DISK OR TTY

If TTY is chosen, the following prompt will appear:

**ENTER UP TO 10 GAMMA ENERGIES
(MEV) IN 10F7.3**

The format 10F7.3 may be used, or the energies may be entered in field-free format, delimited by commas. If there are 10 or fewer energies to enter they should all be put on this line. If there are more than 10 energies, exactly 10 should go on this line; the program will prompt for additional energies ("ENTER NEXT 10 GAMMA ENERGIES IN 10F7.3") until it encounters a zero or a line with fewer than 10 entries.

After output is completed the user is prompted for further problems:

**IF ANOTHER PROBLEM ENTER
GAMMA ENERGIES, IF NOT ENTER
RETURN**

The user enters another set of energies, as before, if desired; otherwise he hits RETURN, and the program ends.

EXAMPLE INPUT

- Assume observed photon energies are 0.058, 0.826, 1.173, 1.332, and 2.158 MeV.

- Consider all tabulated isotopes between $^{40}_{20}\text{Ca}$ and $^{207}_{82}\text{Pb}$ with half lives greater than 660 s (11 min).

- Consider all tabulated photons with energies greater than 0.80 MeV and probabilities greater than 10%.

- Accept as a match any photon that satisfies the criteria above and is within plus or minus 0.005 MeV (5 keV) of an observed photon.

The user would enter these data from his console as shown in the dialogue below.

ENTER INPUT MODE, DISK OR TTY
TTY

ENTER DETECTOR SHIFTS (MEV),
LOWER THEN UPPER IN 2F7.3
.005,.005

ENTER LOWER ENERGY LIMIT (MEV)
FOR GAMMAS IN F7.3
.80

ENTER LOWER AND UPPER LIMITS OF
ISOTOPES IN 2I6
20040 82207

ENTER LOWER BOUND OF HALF-LIFE
IN SEC., (F10.3)
660

PROMPT GAMMAS ONLY? ENTER YES
OR NO
NO

ENTER LOWER BOUND OF MULTIPLI-
CITIES (F7.3)
.1

ENTER INPUT MODE FOR OBSERVED
ENERGIES, DISK OR TTY
TTY

ENTER UP TO 10 GAMMA ENERGIES
(MEV) IN 10F7.3
.058, .826, 1.173, 1.332, 2.158

IF ANOTHER PROBLEM ENTER
GAMMA ENERGIES, IF NOT RETURN
(RETURN)

SAMPLE OUTPUT

A disk file of results, called HSPO, is generated when GAMIDENT is run. The user prints out these

results. The results from the example problem are listed and explained below.

1. The input variables are printed out.

```

DETECTOR SHIFTS ARE: LOWER = 0.005 UPPER = 0.005
LOWER LIMIT FOR PHOTONS IS: 0.800
LOWER AND UPPER LIMIT FOR ISOTOPES ARE: 20040 82207
LOWER LIMIT FOR HALF-LIVES IS: 6.600E+02 SECONDS
PHOTON ENERGIES OBSERVED ARE:
0.058 0.826 1.173 1.332 2.158
LOWER BOUND OF MULTIPLICITIES IS: 0.100
    
```

2. The GAMIN table is searched for isotopes that satisfy the input criteria. Each such isotope is printed out, accompanied by a list of other gamma

emissions one might expect to see from that isotope. For the example problem the list below gives the possible isotopes found in this way.

1	NUCLEUS	PHOTON	MULTIPLICITY	HALF-LIFE	SOURCE
	27-CO- 60	1.173	0.999000	5.260E+00 Y	SPONT
	27-CO- 60	1.332	1.000000	5.260E+00 Y	SPONT
		1.173	0.999000	5.260E+00 Y	SPONT
		1.332	1.000000	5.260E+00 Y	SPONT
	27-CO- 62	1.173	0.980000	1.350E+01 M	SPONT
		1.163	0.690000	1.350E+01 M	SPONT
		1.173	0.980000	1.350E+01 M	SPONT
		2.004	0.190000	1.350E+01 M	SPONT
	29-CU- 60	0.826	0.217000	2.340E+01 M	SPONT
	29-CU- 60	1.332	0.880000	2.340E+01 M	SPONT
		0.826	0.217000	2.340E+01 M	SPONT
		1.332	0.880000	2.340E+01 M	SPONT
		1.792	0.454000	2.340E+01 M	SPONT
	35-BR- 82	0.828	0.243000	3.550E+01 H	SPONT
		0.828	0.243000	3.550E+01 H	SPONT
		1.044	0.278000	3.550E+01 H	SPONT
		1.317	0.274000	3.550E+01 H	SPONT
		1.475	0.166000	3.550E+01 H	SPONT
	37-RB- 82	0.828	0.250000	6.400E+00 H	SPONT
		0.828	0.260000	6.400E+00 H	SPONT
		1.044	0.310000	6.400E+00 H	SPONT
	41-NB- 98	1.169	0.180000	5.100E+01 M	SPONT
		0.833	0.100000	5.100E+01 M	SPONT
		1.169	0.180000	5.100E+01 M	SPONT
	45-RH-106	0.825	0.137000	2.180E+00 H	SPONT
		0.805	0.131000	2.180E+00 H	SPONT
		0.825	0.137000	2.180E+00 H	SPONT
		1.047	0.307000	2.180E+00 H	SPONT
		1.128	0.136000	2.180E+00 H	SPONT
		1.220	0.115000	2.180E+00 H	SPONT
		1.529	0.177000	2.180E+00 H	SPONT
	47-AG-106	0.824	0.160000	8.400E+00 D	SPONT
		0.804	0.246000	8.400E+00 D	SPONT
		0.824	0.160000	8.400E+00 D	SPONT
		1.046	0.280000	8.400E+00 D	SPONT
		1.128	0.106000	8.400E+00 D	SPONT
		1.199	0.106000	8.400E+00 D	SPONT
		1.527	0.150000	8.400E+00 D	SPONT
	47-AG-115	2.157	0.160000	2.100E+01 M	SPONT
		2.157	0.160000	2.100E+01 M	SPONT
	51-SB-120	1.172	1.000000	5.800E+00 D	SPONT
		1.023	0.933000	5.800E+00 D	SPONT
		1.172	1.000000	5.800E+00 D	SPONT
	52-TE-133	1.333	0.110000	1.250E+01 M	SPONT
		1.333	0.110000	1.250E+01 M	SPONT

57-LA-143	1.170	0.570000	1.430E+01	M	SPONT
	1.070	0.250000	1.430E+01	M	SPONT
	1.170	0.570000	1.430E+01	M	SPONT
	1.530	0.220000	1.430E+01	M	SPONT
	1.700	0.190000	1.430E+01	M	SPONT
	1.580	0.350000	1.430E+01	M	SPONT
	2.460	0.130000	1.430E+01	M	SPONT
	2.560	0.270000	1.430E+01	M	SPONT
	2.850	0.150000	1.430E+01	M	SPONT
58-CE-135	0.827	0.230000	1.720E+01	H	SPONT
	0.827	0.250000	1.720E+01	H	SPONT
	0.870	0.160000	1.720E+01	H	SPONT
60-ND-139	0.828	0.280000	5.500E+00	H	SPONT
	0.802	0.200000	5.500E+00	H	SPONT
	0.810	0.190000	5.500E+00	H	SPONT
	0.828	0.280000	5.500E+00	H	SPONT
	0.910	0.220000	5.500E+00	H	SPONT
	0.982	0.790000	5.500E+00	H	SPONT
	2.060	0.150000	5.500E+00	H	SPONT
65-TB-160	1.178	0.148000	7.210E+01	D	SPONT
	0.879	0.300000	7.210E+01	D	SPONT
	0.962	0.102000	7.210E+01	D	SPONT
	0.966	0.247000	7.210E+01	D	SPONT
	1.178	0.148000	7.210E+01	D	SPONT
67-HO-166	0.831	0.120000	1.200E+03	Y	SPONT
	0.811	0.760000	1.200E+03	Y	SPONT
	0.831	0.120000	1.200E+03	Y	SPONT
68-EU-161	0.826	0.609000	3.240E+00	H	SPONT
	0.825	0.609000	3.240E+00	H	SPONT
69-TM-166	1.178	0.330000	7.700E+00	H	SPONT
	0.375	0.160000	7.700E+00	H	SPONT
	1.178	0.390000	7.700E+00	H	SPONT
	1.275	0.610000	7.700E+00	H	SPONT
	1.375	0.200000	7.700E+00	H	SPONT
	1.868	0.140000	7.700E+00	H	SPONT
	2.054	0.770000	7.700E+00	H	SPONT
69-TM-168	2.081	0.270000	7.700E+00	H	SPONT
	0.821	0.179000	8.700E+01	D	SPONT
	0.816	0.495000	8.700E+01	D	SPONT
	0.821	0.179000	8.700E+01	D	SPONT
70-YB-166	1.178	0.390000	5.750E+01	H	SPONT
	0.875	0.160000	5.750E+01	H	SPONT
	1.178	0.390000	5.750E+01	H	SPONT
	1.275	0.610000	5.750E+01	H	SPONT
	1.375	0.200000	5.750E+01	H	SPONT
	1.868	0.140000	5.750E+01	H	SPONT
	2.054	0.770000	5.750E+01	H	SPONT
75-RE-190	2.081	0.270000	5.750E+01	H	SPONT
	0.829	0.140000	2.800E+00	H	SPONT
76-OS-181	0.829	0.140000	2.800E+00	H	SPONT
	0.827	0.208000	1.050E+02	M	SPONT
	0.827	0.203000	1.050E+02	M	SPONT
81-TL-200	0.828	0.111000	2.610E+01	H	SPONT
	0.828	0.111000	2.610E+01	H	SPONT
	1.206	0.307000	2.610E+01	H	SPONT

3. The elimination criterion (no unobserved higher-multiplicity photon) is applied, and those isotopes that survive this test are listed.

S U M M A R Y

ISOTOPES THAT CANNOT BE ELIMINATED BECAUSE OF PHOTONS THAT SHOULD BE PRESENT AND ARE NOT

ISOTOPE	NO. OF MATCHES
27-CO-60	2 OF 2
27-CO-62	1 OF 3
41-NB-98	1 OF 2
47-AG-115	1 OF 1
51-SB-120	1 OF 2
52-TE-123	1 OF 1
57-LA-143	1 OF 8
58-CE-135	1 OF 2
62-EU-131	1 OF 1
75-RE-190	1 OF 1
76-OS-181	1 OF 1

Of these candidates $^{27}\text{Co}^{60}$ is most probable, since it has two gammas that meet the search criteria, and both were observed. The other isotopes, for which

only one of one or more possible gammas were observed, are less-probable candidates.

4. The isotopes eliminated in the preceding step are listed.

ISOTOPE	PHOTONS THAT SHOULD BE OBSERVED AND ARE NOT			MULTIPLICITY
	LEAST MULT. OBSERVED	OBSERVED PHOTON	UNOBSERVED PHOTON	
29-CU- 60	0.217	0.826		
35-BR- 82	0.243	0.828	1.792	0.454
			1.044	0.278
			1.317	0.274
37-RB- 32	0.260	0.828		
45-RH-106	0.137	0.825	1.044	0.310
			1.047	0.307
			1.529	0.177
47-AG-106	0.160	0.824		
60-ND-139	0.280	0.828	1.046	0.260
65-TB-160	0.148	1.178	0.982	0.790
			0.879	0.300
			0.966	0.247
67-HO-166	0.120	0.831		
69-TM-166	0.390	1.178	0.811	0.760
			1.275	0.610
			2.054	0.770
69-TM-168	0.119	0.821		
70-YB-166	0.390	1.178	0.816	0.495
			1.275	0.610
			2.054	0.770
81-TL-200	0.111	0.828	1.206	0.307

REFERENCES

1. W. W. Bowman and K. W. MacMurdo, "Radioactive-Decay Gammas," *Atomic Data and Nuclear Data Tables* **13**, 89-292 (1974).
2. V. J. Orphen et al., *Line and Continuum Gamma-Ray Yields from Thermal-Neutron Capture in 75 Elements*, Gulf General Atomic, Inc., DASA 2570 GA-10248 (1970).

APPENDIX A: FILE STRUCTURE OF GAMIN

GAMIN must be present to run with GAMIDENT. Each photon tabulated in GAMIN takes one record in the file. The table below describes the card-image format of a single record.

Columns	Variable name	Format	Description
1	IFL	I1	EOF indicator: blank on data cards, 1 (or other digit) on last card in file, which is otherwise blank.
2-7	IZ	I6	Combined atomic number (Z) and mass number (A), in the form 1000Z + A.
8-12	blank	5X	
13-19	GAM	F7.3	Observed photon energy (in MeV).
20-24	blank	5X	
25-33	AI	F9.6	Probability (same as multiplicity) of this photon per decay or per capture.
34-38	blank	5X	
39-48	TIME	E10.3	Half-life of isotope, numerical value only (unit is next variable): equal to 1.000E-14 if this is a prompt (n-capture) photon.
49	blank	1X	
50	IUNIT	A1	Unit used for half-life: second (S), minute (M), day (D), or year (Y).
51-55	blank	5X	
55-60	SOURCE	A5	Emission mode: SPONT if spontaneous decay, N.GAM if prompt (n-capture).

APPENDIX B: RUNNING THE PROGRAM AT LLL

At LLL both a source deck (**GAMIDENTS**) and a controllee (a compiled, loaded, ready-to-execute version, called **GAMIDENT**) are available from photostore. They may be accessed by the **XPORT** command

RD .247350:GAMIDENTS [GAMIDENTS GAMIN GAMDATA GAMIDENT]

GAMIDENTS is the source deck, prefaced by **ORDER** cards that instruct the computer to compile, load, and execute the program on a CDC 7600. Execution will produce the disk file called **GAMIDENT**, described below. Since **GAMIDENT** is already available, recompilation of **GAMIDENTS** is necessary only if it is changed by the user.

To compile **GAMIDENT**, type

ORDER GAMIDENTS / T V .

where **T** and **V** are appropriate time and value numbers.

GAMIDENT is the executable controllee. To run a problem, type

GAMIDENT / T V .

The time and value numbers can be adjusted to the status of the computer. A typical problem requires less than 0.5 minutes.

Please note that disk file **GAMIN** must be present.

APPENDIX C: FILE STRUCTURE OF GAMDATA

This is an optional, user-created data file. Records 1 through 6 contain the search constraints; they need not appear in the file if the user wants to enter them from the console. Records 7, 8, etc., contain the user's observed photon energies, and must appear in the file if it is to be used at all.

Record No.	Variables	Format	Description
1	DEL, DEU	2F7.3	Lower and upper detector uncertainties (shifts) in MeV.
2	GAMLOW	F7.3	Low-energy limit of search.
3	IZL, IZU	2I6	Lower and upper limits of the isotope variable $1000Z + A$.
4	TT	F10.3	Lower limit of half lives to be searched, in seconds.
5	TU	A4	YES (if only prompt gammas to be searched) or NO.
6	ABU	F7.3	Lowest multiplicity to be searched.
7, 8,...	GR	10F7.3	User's observed energies, 10 to a card. A zero, or fewer than 10 energies on a card, indicates end of entries. Entries can also be made in free format, 10 to a card, with commas as delimiters.

Below is an example of what GAMDATA would look like if all input data were supplied to the program from the user's private disk file.

[illegible]