

Concept Paper

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Concept Paper

XRF Escape-peaks from Natural Elements for Nuclear Medicine Imaging and Gamma-Ray Spectrometry

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Abstract

A catalog of K-XRF escape-peak energy from natural elements and for several energies of gamma-rays incident on a single-element detector is presented. The parameters of a power-model are listed In Table I for predicting the energy of such peaks. In Table II predicted peaks are arranged in order of increasing atomic number (ranging from 4 to 92) of the detector component and for the K α 2 XRF main emission. This catalog is conceived for nuclear medicine and gamma-ray spectrometry where such peak need to be recognized and known as underlying area in order to gain advantage of quantitative analysis, but, also for detector-developers as well as for spectroscopists that should be interested in the issue.

Keywords: XRF; escape

Introduction

This catalog is conceived for nuclear medicine and gamma-ray spectrometry where the escape-peak need to be recognized and known as underlying area in order to perform quantitative analysis, but, also for detector-developers as well as for spectroscopists that should be interested in the issue.

The literature energy-emissions vs atomic number Z have been fitted to a power-model, whose parameters (listed In Table I) are used for predicting the energy of such peaks.

The quite-perfect agreement between the literature data and the power-model allows to calculate the wanted escape-peak energy without requiring specific software development.

The predicted values of XRF K-escape gamma-ray energy are presented in Table II per a dozen of incident mono-energetic photons-energies and per Z -values of single-natural element.

Each row shows, from left to right: (a) the values of Z ; (b) the symbol of element; (c) the gap Kedge-K α 2 energies (where the rest of orbital emissions, i.e. K β 2, K β 1, K β 3, and K α 1 are grouped); and (d) a dozen of numbers representing the escape-peak energy predicted for incident photons.

The L and M XRF emissions are ignored in this evaluation since their energy is negligible with respect to the K-ones, so also the respective fluorescence yields are equally negligible.

The physical process of the escape of the XRF of the materials constituting a detector has been held in a certain consideration to improve its performance, with particular regard to the ability to perform quantitative analyzes. This has been recently remarked in [SR25].

In fact, since XRF photons are characterized in energy, distinctive of the element of which the detector is made, the escape-process can also change, even significantly, the response function of the detector itself with the result of relocating events from the full-energy peak towards an additional peak, sometimes completely separate from the photopeak, located at lower energy. For this reason, evaluations based on the value of the integral of the counts underlying the full-energy peak are systematically underestimated if escape photons are not taken into account.

In particular cases (like thin and/or discretized detectors with identification of multiple interactions) the number of events whose energy falls under the escape peak may even equal or even exceed that of photons under the full-energy peak making necessary corrections [AP54].

It can be said that this is due to inevitable edge-effect since a real detector has limited dimensions and fluorescence photons undergo to non-zero probability to escape from its sensitive volume, not being revealed. Only the ideal case of a detector with infinite dimensions is free from this effect, how it is theorized in Ref.[BJ54].

Policies

Literature Coverage

Fundamentals of radiation detection including the concepts herein exposed are deeply and clearly given in Ref.[KG00]. The basic X-rays data are from Kaye & Laby, UK National Physical Laboratory, Ref.[KL13], whose completeness and accuracy fulfill the requirements of these Tables.

Data Selected

Data for this catalog are taken from Ref.[KL13], limited to those of XRF energy in the columns $K\alpha_2$ and Kedge (for $4 \leq Z \leq 92$) that are used for power-function best fit performing and for evaluating the energy-gap, respectively.

Incident Gamma-Rays

Listed is in Table II a header specifying the dozen of values of mono-energetic incident gamma-rays considered for the calculations of escape-peaks of different elements.

Incident Gamma-Ray Energy

The considered values are: 100, 125, 150, 175, 200, 250, 300, 350, 400, 500, 600 and 700 keV. The range includes the energies from all the radio-isotopes used for tracing pharmaceutical administered in SPECT and PET protocols. The last interval is extended up to 700 keV for considering also the 662 keV photons from Cs-137 sources, widely used for reference.

Escape-Energy Uncertainty

The uncertainty of 0.2-0.3 keV can be assumed, despite submission to the fitting process. On the other hand the tabulated X-rays can be considered affected by uncertainties in the order of a few eV because they are listed in keV with 3 decimal places.

Escape Gamma-Ray Intensity

The intensity of escape-gamma-ray cannot be easily estimated like their energy. Appropriate Monte Carlo simulation studies of the detector-source systems must be performed aimed to predict intensity values.

Element Identification

Both the atomic number Z and the chemical symbol of the element are given Table II.

Photo-Electric Peak

The response of a detector to mono-energetic gamma-rays $E\gamma$ is mainly made, in an ideal pulse-height spectrum, of a vertical segment, representing the photo-electric interactions, whose abscissa is proportional to $E\gamma$ and whose length is proportional to the number of incident gammas. In the reality, the segment become a Gaussian curve, being the enlargement produced by the detector-energy-resolution.

Compton-Effect

Another process affecting the detector response is the Compton scattering, that produces a continuum ranging from zero to the so-called Compton-edge, arising at the end of this continuum. The energy-distance between the Compton edge and the centroid of photo-electric peak can be calculated as (see [KG00], p. 310):

$$EC = E\gamma / (1 + 2 (E\gamma / m0 c^2)) , \text{ that is } < E\gamma .$$

Detector Response-Function (DRF)

If $E\gamma < 2 m0 c^2$ the response function shows only the two items above described. Based on these values it is reasonable, in a first approximation, to localize the energy at which a valley occurs between the photoelectric-peak and the Compton-edge, as: $E_{valley} = \frac{1}{2} (E\gamma + EC)$.

Escape Peaks

Energies of gamma-ray peaks which result from escape of XRF photons from the detector are calculated, according to Ref. [KG00], as: $EE_{escape} = E\gamma - EX_{RF}$. Based on the energy of a given escape photon and on the above considerations regarding the DRF these photons can be classified according to their position on the DRF. The three following styles are used in Table II to show the predicted values of escape photon energy: (1) underline for values overlapping the Compton continuum; (2) **bold** for those falling in the valley between Compton edge and photo-electric peak; (3) *Italic* for photons overlapped to the photo-peak left-tail.

Table I. Results of power-function best fit of XRF energy vs. Z for Kα2 orbitals. See pages 2-3 for Policies and Explanation.

orbital	a	b	Rsquare
K-α2	0.00560144430106232	2.19086250995425	0.999952133940893

Input data are from Ref.[KL13]. The fitting has been limited to the elements having $4 \leq Z \leq 92$.

Table II. Predicted values of XRF escape energy $E\gamma$ -Kα2 (keV) - part 1 of 2, for Z = 4 , ... , 50. See pages 2-3 for Policies and Explanation.

Z-Sy	$E_{edge-K\alpha2}$ (keV)	incident-photon energy $E\gamma$ (keV)											
		100.0	125.0	150.0	175.0	200.0	250.0	300.0	350.0	400.0	500.0	600.0	700.0
4-Be	0.006	99.9	124.9	149.9	174.9	199.9	249.9	299.9	349.9	399.9	499.9	599.9	699.9

5-B	0.005	99.8	124.8	149.8	174.8	199.8	249.8	299.8	349.8	399.8	499.8	599.8	699.8
6-C	0.005	99.7	124.7	149.7	174.7	199.7	249.7	299.7	349.7	399.7	499.7	599.7	699.7
7-N	0.004	99.6	124.6	149.6	174.6	199.6	249.6	299.6	349.6	399.6	499.6	599.6	699.6
8-O	-0.002	99.5	124.5	149.5	174.5	199.5	249.5	299.5	349.5	399.5	499.5	599.5	699.5
9-F	0.015	99.3	124.3	149.3	174.3	199.3	249.3	299.3	349.3	399.3	499.3	599.3	699.3
10-Ne	0.010	99.2	124.2	149.2	174.2	199.2	249.2	299.2	349.2	399.2	499.2	599.2	699.2
11-Na	0.039	99.0	124.0	149.0	174.0	199.0	249.0	299.0	349.0	399.0	499.0	599.0	699.0
12-Mg	0.056	98.8	123.8	148.8	173.8	198.8	248.8	298.8	348.8	398.8	498.8	598.8	698.8
13-Al	0.076	98.5	123.5	148.5	173.5	198.5	248.5	298.5	348.5	398.5	498.5	598.5	698.5
14-Si	0.101	98.3	123.3	148.3	173.3	198.3	248.3	298.3	348.3	398.3	498.3	598.3	698.3
15-P	0.130	98.0	123.0	148.0	173.0	198.0	248.0	298.0	348.0	398.0	498.0	598.0	698.0
16-S	0.164	97.7	122.7	147.7	172.7	197.7	247.7	297.7	347.7	397.7	497.7	597.7	697.7
17-Cl	0.204	97.4	122.4	147.4	172.4	197.4	247.4	297.4	347.4	397.4	497.4	597.4	697.4
18-Ar	0.247	97.1	122.1	147.1	172.1	197.1	247.1	297.1	347.1	397.1	497.1	597.1	697.1
19-K	0.296	96.7	121.7	146.7	171.7	196.7	246.7	296.7	346.7	396.7	496.7	596.7	696.7
20-Ca	0.346	96.4	121.4	146.4	171.4	196.4	246.4	296.4	346.4	396.4	496.4	596.4	696.4
21-Sc	0.400	96.0	121.0	146.0	171.0	196.0	246.0	296.0	346.0	396.0	496.0	596.0	696.0
22-Ti	0.460	95.6	120.6	145.6	170.6	195.6	245.6	295.6	345.6	395.6	495.6	595.6	695.6
23-V1	0.519	95.1	120.1	145.1	170.1	195.1	245.1	295.1	345.1	395.1	495.1	595.1	695.1
24-Cr	0.582	94.7	119.7	144.7	169.7	194.7	244.7	294.7	344.7	394.7	494.7	594.7	694.7
25-Mn	0.649	94.2	119.2	144.2	169.2	194.2	244.2	294.2	344.2	394.2	494.2	594.2	694.2
26-Fe	0.721	93.7	118.7	143.7	168.7	193.7	243.7	293.7	343.7	393.7	493.7	593.7	693.7
27-Co	0.797	93.2	118.2	143.2	168.2	193.2	243.2	293.2	343.2	393.2	493.2	593.2	693.2
28-Ni	0.878	92.6	117.6	142.6	167.6	192.6	242.6	292.6	342.6	392.6	492.6	592.6	692.6
29-Cu	0.965	92.0	117.0	142.0	167.0	192.0	242.0	292.0	342.0	392.0	492.0	592.0	692.0
30-Zn	1.057	91.4	116.4	141.4	166.4	191.4	241.4	291.4	341.4	391.4	491.4	591.4	691.4
31-Ga	1.155	90.8	115.8	140.8	165.8	190.8	240.8	290.8	340.8	390.8	490.8	590.8	690.8
32-Ge	1.259	90.2	115.2	140.2	165.2	190.2	240.2	290.2	340.2	390.2	490.2	590.2	690.2
33-As	1.368	89.5	114.5	139.5	164.5	189.5	239.5	289.5	339.5	389.5	489.5	589.5	689.5
34-Se	1.485	88.8	113.8	138.8	163.8	188.8	238.8	288.8	338.8	388.8	488.8	588.8	688.8
35-Br	1.605	88.1	113.1	138.1	163.1	188.1	238.1	288.1	338.1	388.1	488.1	588.1	688.1
36-Kr	1.732	87.4	112.4	137.4	162.4	187.4	237.4	287.4	337.4	387.4	487.4	587.4	687.4
37-Rb	1.866	86.6	111.6	136.6	161.6	186.6	236.6	286.6	336.6	386.6	486.6	586.6	686.6
38-Sr	2.008	85.9	110.9	135.9	160.9	185.9	235.9	285.9	335.9	385.9	485.9	585.9	685.9
39-Y	2.155	85.1	110.1	135.1	160.1	185.1	235.1	285.1	335.1	385.1	485.1	585.1	685.1
40-Zr	2.305	84.2	109.2	134.2	159.2	184.2	234.2	284.2	334.2	384.2	484.2	584.2	684.2
41-Nb	2.464	83.4	108.4	133.4	158.4	183.4	233.4	283.4	333.4	383.4	483.4	583.4	683.4
42-Mo	2.628	82.5	107.5	132.5	157.5	182.5	232.5	282.5	332.5	382.5	482.5	582.5	682.5
43-Tc	2.797	81.6	106.6	131.6	156.6	181.6	231.6	281.6	331.6	381.6	481.6	581.6	681.6
44-Ru	2.973	80.7	105.7	130.7	155.7	180.7	230.7	280.7	330.7	380.7	480.7	580.7	680.7
45-Rh	3.156	79.8	104.8	129.8	154.8	179.8	229.8	279.8	329.8	379.8	479.8	579.8	679.8
46-Pd	3.344	<u>78.8</u>	103.8	128.8	153.8	178.8	228.8	278.8	328.8	378.8	478.8	578.8	678.8

47-Ag	3.540	<u>77.8</u>	102.8	127.8	152.8	177.8	227.8	277.8	327.8	377.8	477.8	577.8	677.8
48-Cd	3.742	<u>76.8</u>	101.8	126.8	151.8	176.8	226.8	276.8	326.8	376.8	476.8	576.8	676.8
49-In	3.951	<u>75.8</u>	100.8	125.8	150.8	175.8	225.8	275.8	325.8	375.8	475.8	575.8	675.8
50-Sn	4.167	<u>74.7</u>	99.7	124.7	149.7	174.7	224.7	274.7	324.7	374.7	474.7	574.7	674.7
Styles for estimated escape peak position							<u>Underscore</u> : overlapped to the Compton continuum;						
in the detector response function:							Bold : in the valley between Compton edge and photo-electric peak;						
							<i>Italic</i> : overlapped to the photo-peak left-tail.						

Table III. Predicted values of XRF escape energy E γ -K α 2 (keV) - part 2 of 2, for Z = 51 , ... , 92. See pages 2-3 for Policies and Explanation.

Z-Sy	E _{edge-Kα2} (keV)	incident photon energy E γ (keV)											
		100.0	125.0	150.0	175.0	200.0	250.0	300.0	350.0	400.0	500.0	600.0	700.0
51-Sb	4.389	<u>73.6</u>	98.6	123.6	148.6	173.6	223.6	273.6	323.6	373.6	473.6	573.6	673.6
52-Te	4.616	<u>72.5</u>	97.5	122.5	147.5	172.5	222.5	272.5	322.5	372.5	472.5	572.5	672.5
53-I	4.851	<u>71.4</u>	96.4	121.4	146.4	171.4	221.4	271.4	321.4	371.4	471.4	571.4	671.4
54-Xe	5.092	<u>70.2</u>	95.2	120.2	145.2	170.2	220.2	270.2	320.2	370.2	470.2	570.2	670.2
55-Cs	5.341	<u>69.1</u>	<u>94.1</u>	119.1	144.1	169.1	219.1	269.1	319.1	369.1	469.1	569.1	669.1
56-Ba	5.597	<u>67.9</u>	<u>92.9</u>	117.9	142.9	167.9	217.9	267.9	317.9	367.9	467.9	567.9	667.9
57-La	5.860	<u>66.6</u>	<u>91.6</u>	116.6	141.6	166.6	216.6	266.6	316.6	366.6	466.6	566.6	666.6
58-Ce	6.131	<u>65.4</u>	<u>90.4</u>	115.4	140.4	165.4	215.4	265.4	315.4	365.4	465.4	565.4	665.4
59-Pr	6.408	<u>64.1</u>	<u>89.1</u>	<u>114.1</u>	139.1	164.1	214.1	264.1	314.1	364.1	464.1	564.1	664.1
60-Nd	6.691	<u>62.8</u>	<u>87.8</u>	112.8	137.8	162.8	212.8	262.8	312.8	362.8	462.8	562.8	662.8
61-Pm	6.981	<u>61.5</u>	<u>86.5</u>	111.5	136.5	161.5	211.5	261.5	311.5	361.5	461.5	561.5	661.5
62-Sm	7.278	<u>60.1</u>	<u>85.1</u>	110.1	135.1	160.1	210.1	260.1	310.1	360.1	460.1	560.1	660.1
63-Eu	7.584	<u>58.8</u>	<u>83.8</u>	108.8	133.8	158.8	208.8	258.8	308.8	358.8	458.8	558.8	658.8
64-Gd	7.898	<u>57.4</u>	<u>82.4</u>	<u>107.4</u>	132.4	157.4	207.4	257.4	307.4	357.4	457.4	557.4	657.4
65-Tb	8.221	<u>55.9</u>	<u>80.9</u>	<u>105.9</u>	130.9	155.9	205.9	255.9	305.9	355.9	455.9	555.9	655.9
66-Dy	8.553	<u>54.5</u>	<u>79.5</u>	<u>104.5</u>	129.5	154.5	204.5	254.5	304.5	354.5	454.5	554.5	654.5
67-Ho	8.894	<u>53.0</u>	<u>78.0</u>	<u>103.0</u>	128.0	153.0	203.0	253.0	303.0	353.0	453.0	553.0	653.0
68-Er	9.243	<u>51.5</u>	<u>76.5</u>	<u>101.5</u>	126.5	151.5	201.5	251.5	301.5	351.5	451.5	551.5	651.5
69-Tm	9.601	<u>50.0</u>	<u>75.0</u>	<u>100.0</u>	125.0	150.0	200.0	250.0	300.0	350.0	450.0	550.0	650.0
70-Tb	9.968	<u>48.4</u>	<u>73.4</u>	<u>98.4</u>	123.4	148.4	198.4	248.4	298.4	348.4	448.4	548.4	648.4
71-Lu	10.346	<u>46.9</u>	<u>71.9</u>	<u>96.9</u>	121.9	146.9	196.9	246.9	296.9	346.9	446.9	546.9	646.9
72-Hf	10.734	<u>45.3</u>	<u>70.3</u>	<u>95.3</u>	<u>120.3</u>	145.3	195.3	245.3	295.3	345.3	445.3	545.3	645.3
73-Ta	11.128	<u>43.6</u>	<u>68.6</u>	<u>93.6</u>	<u>118.6</u>	143.6	193.6	243.6	293.6	343.6	443.6	543.6	643.6
74-W	11.535	<u>42.0</u>	<u>67.0</u>	<u>92.0</u>	<u>117.0</u>	142.0	192.0	242.0	292.0	342.0	442.0	542.0	642.0
75-Re	11.952	<u>40.3</u>	<u>65.3</u>	<u>90.3</u>	<u>115.3</u>	140.3	190.3	240.3	290.3	340.3	440.3	540.3	640.3
76-Os	12.382	<u>38.6</u>	<u>63.6</u>	<u>88.6</u>	<u>113.6</u>	138.6	188.6	238.6	288.6	338.6	438.6	538.6	638.6
77-Ir	12.824	<u>36.9</u>	<u>61.9</u>	<u>86.9</u>	<u>111.9</u>	136.9	186.9	236.9	286.9	336.9	436.9	536.9	636.9
78-Pt	13.277	<u>35.1</u>	<u>60.1</u>	<u>85.1</u>	<u>110.1</u>	135.1	185.1	235.1	285.1	335.1	435.1	535.1	635.1
79-Au	13.739	<u>33.4</u>	<u>58.4</u>	<u>83.4</u>	<u>108.4</u>	<u>133.4</u>	183.4	233.4	283.4	333.4	433.4	533.4	633.4
80-Hg	14.215	<u>31.6</u>	<u>56.6</u>	<u>81.6</u>	<u>106.6</u>	<u>131.6</u>	181.6	231.6	281.6	331.6	431.6	531.6	631.6

81-Tl	14.700	<u>29.7</u>	<u>54.7</u>	<u>79.7</u>	<u>104.7</u>	<u>129.7</u>	179.7	229.7	279.7	329.7	429.7	529.7	629.7
82-Pb	15.204	<u>27.9</u>	<u>52.9</u>	<u>77.9</u>	<u>102.9</u>	<u>127.9</u>	177.9	227.9	277.9	327.9	427.9	527.9	627.9
83-Bi	15.725	<u>26.0</u>	<u>51.0</u>	<u>76.0</u>	<u>101.0</u>	<u>126.0</u>	176.0	226.0	276.0	326.0	426.0	526.0	626.0
84-Po	16.250	<u>24.1</u>	<u>49.1</u>	<u>74.1</u>	<u>99.1</u>	<u>124.1</u>	174.1	224.1	274.1	324.1	424.1	524.1	624.1
85-At	16.787	<u>22.2</u>	<u>47.2</u>	<u>72.2</u>	<u>97.2</u>	<u>122.2</u>	172.2	222.2	272.2	322.2	422.2	522.2	622.2
86-Rn	17.337	<u>20.2</u>	<u>45.2</u>	<u>70.2</u>	<u>95.2</u>	<u>120.2</u>	170.2	220.2	270.2	320.2	420.2	520.2	620.2
87-Fr	17.900	<u>18.3</u>	<u>43.3</u>	<u>68.3</u>	<u>93.3</u>	<u>118.3</u>	168.3	218.3	268.3	318.3	418.3	518.3	618.3
(*) 88-Ra	18.475	<i>100.0</i>	<u>41.3</u>	<u>66.3</u>	<u>91.3</u>	<u>116.3</u>	166.3	216.3	266.3	316.3	416.3	516.3	616.3 (*)
(*) 89-Ac	19.063	<i>100.0</i>	<u>39.2</u>	<u>64.2</u>	<u>89.2</u>	<u>114.2</u>	164.2	214.2	264.2	314.2	414.2	514.2	614.2 (*)
(*) 90-Th	19.689	<i>100.0</i>	<u>37.2</u>	<u>62.2</u>	<u>87.2</u>	<u>112.2</u>	162.2	212.2	262.2	312.2	412.2	512.2	612.2 (*)
(*) 91-Pa	20.312	<i>100.0</i>	<u>35.1</u>	<u>60.1</u>	<u>85.1</u>	<u>110.1</u>	160.1	210.1	260.1	310.1	410.1	510.1	610.1 (*)
(*) 92-U	20.947	<i>100.0</i>	<u>33.0</u>	<u>58.0</u>	<u>83.0</u>	<u>108.0</u>	158.0	208.0	258.0	308.0	408.0	508.0	608.0 (*)

(*) For $Z \geq 88$ the value of E_γ is under the threshold of XRF K-emissions.

Styles for estimated escape peak position
in the detector response function:

Underscore: overlapped to the Compton continuum;
Bold: in the valley between Compton edge and photo-electric peak;
Italic: overlapped to the photo-peak left-tail.

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