**Analysis of the spectrum ExampleCNF**

The spectrum ExampleCNF was measured as part of a proficiency-test exercise. It was measured with a soil sample contaminated with radionuclides, which are commonly used in proficiency tests. The spectrum analysis was performed using the following parameters:

Energy calibration: *E* [keV]= 0.10 + 0.3565\**ch* + 0.5452\**ch*2

FWHM calibration *FWHM* [keV] = 0.74 + 0.0378\**E*1/2

1. **Automatic analysis**

The peak analysis was performed with the Genie2000 software.

Peak locate: Unidentified 2nd-Diff. with the following values of parameters: Start channel: 100, Stop channel: 8182 channel, Significance threshold: 3.00

Peak analysis: Sum / Non-Linear LSQ Fit: Continuum 4 Channels, Continuum function: Linear, Max. Num. FWHMs between peaks: 3, Max. Num. FWHMs for left limit: 2, Max. Num. FWHMs for right limit: 2, 95% Critical level test: no, Fit singlets: no, Reject zero peak areas: yes.

The characteristic limits were calculated with *k*1-α = *k*1-β = 1.645. *n*# was calculated using *u*rel(*w*) = 0.05. The characteristic limits were calculated assuming no peaked background, i.e., *n*B = 0 and *u*(*n*B) =0.

Table 1. Results of the peak analysis of the spectrum ExampleCNF and the characteristic limits computed with the Calculator

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Peak analysis results | | | | | | | | | | Method | | Char. Limits | | |
| Peak No. | See  rem. 1 | *E*  [keV] | *n*g,  Rem. 4 | *n*p | *u*(*n*p) | FWHM  [keV] | *ΔE*  [keV] | *E*p2  [ch] | Excel  sheet | | *n*\* | | *n*# |
| 1 | S | 46.9 | 15311 | 904 | 183 |  |  |  | ROIpeak | | 297 | | 600 |
| 2 | S | 60.0 | 22035 | 3380 | 234 |  |  |  | ROIpeak | | 373 | | 754 |
| 3 | T | 73.3 | 57268 | 2310 | 110 | 1.07 | 2.0 | 217.2 | Rem. 2 | | 192 | | 384 |
| 4 | T | 75.3 | 57268 | 6250 | 137 | 1.07 |  |  | ROIpeak | | Rem. 3 | | Rem. 3 |
| 5 | T | 77.5 | 57268 | 3590 | 124 | 1.07 | 2.2 | 217.2 | Rem. 2 | | 222 | | 443 |
| 6 | S | 81.4 | 29800 | 6770 | 248 |  |  |  | ROIpeak | | 367 | | 742 |
| 7 | S | 129.4 | 25294 | 985 | 249 |  |  |  | ROIpeak | | 406 | | 821 |
| 8 | S | 161.3 | 15074 | 159 | 173 |  |  |  | ROIpeak | | 284 | | 574 |
| 9 | S | 186.4 | 28619 | 2670 | 278 |  |  |  | ROIpeak | | 449 | | 908 |
| 10 | S | 209.6 | 19962 | 1130 | 220 |  |  |  | ROIpeak | | 358 | | 723 |
| 11 | D | 239.0 | 50306 | 13900 | 162 | 1.28 | 3.1 | 678.8 | Rem. 2 | | 330 | | 660 |
| 12 | D | 242.1 | 50306 | 2860 | 106 | 1.28 | 3.1 | 670.2 | Rem. 2 | | 193 | | 385 |
| 13 | S | 270.5 | 19135 | 1520 | 233 |  |  |  | ROIpeak | | 378 | | 764 |
| 14 | S | 276.8 | 20562 | 3390 | 234 |  |  |  | ROIpeak | | 373 | | 753 |
| 15 | S | 295.6 | 20940 | 5290 | 229 |  |  |  | ROIpeak | | 357 | | 722 |
| 16 | D | 300.5 | 28471 | 853 | 84 | 1.29 | 2.7 | 850.2 | Rem. 2 | | 145 | | 289 |
| 17 | D | 303.2 | 28471 | 6730 | 125 | 1.29 | 2.7 | 842.6 | Rem. 2 | | 247 | | 492 |
| 18 | S | 328.2 | 12109 | 791 | 175 |  |  |  | ROIpeak | | 284 | | 575 |
| 19 | S | 338.7 | 15392 | 3010 | 187 |  |  |  | ROIpeak | | 294 | | 595 |
| 20 | D | 352.2 | 51982 | 8950 | 123 | 1.31 | 4.2 | 999.3 | Rem. 2 | | 255 | | 509 |
| 21 | D | 356.4 | 51982 | 20100 | 166 | 1.31 | 4.2 | 987.8 | Rem. 2 | | 369 | | 738 |
| 22 | S | 384.2 | 13351 | 3320 | 176 |  |  |  | ROIpeak | | 274 | | 554 |
| 23 | S | 409.8 | 6430 | 214 | 116 |  |  |  | ROIpeak | | 189 | | 384 |
| 24 | S | 437.4 | 8435 | 671 | 145 |  |  |  | ROIpeak | | 235 | | 475 |
| 25 | S | 463.3 | 9442 | 838 | 160 |  |  |  | ROIpeak | | 259 | | 524 |
| 26 | S | 475.6 | 7757 | 586 | 139 |  |  |  | ROIpeak | | 225 | | 456 |
| 27 | S | 511.1 | 16321 | 7299 | 195 |  |  |  | ROIpeak | | 289 | | 584 |
| 28 | S | 563.4 | 9924 | 2890 | 155 |  |  |  | ROIpeak | | 239 | | 484 |
| 29 | S | 569.4 | 12075 | 5060 | 162 |  |  |  | ROIpeak | | 241 | | 488 |
| 30 | S | 583.4 | 11578 | 5640 | 148 |  |  |  | ROIpeak | | 210 | | 425 |
| 31 | D | 604.9 | 56270 | 34400 | 198 | 1.55 | 4.6 | 1709.7 | Rem. 2 | | 487 | | 973 |
| 32 | D | 609.5 | 56270 | 9080 | 112 | 1.55 | 4.6 | 1596-8 | Rem. 2 | | 244 | | 487 |
| 33 | D | 661.8 | 32333 | 20300 | 164 | 1.61 | 3.8 | 1867.0 | Rem. 2 | | 389 | | 776 |
| 34 | D | 665.6 | 32333 | 343 | 53 | 1.61 | 3.8 | 1856.5 | Rem. 2 | | 92 | | 182 |
| 35 | S | 727.5 | 5555 | 1080 | 118 |  |  |  | ROIpeak | | 186 | | 378 |
| 36 | D | 768.5 | 8898 | 703 | 63 | 1.56 | 4.3 | 2168.0 | Rem. 2 | | 111 | | 221 |
| 37 | D | 772.8 | 8898 | 122 | 49 | 1.56 | 4.3 | 2156-0 | Rem. 2 | | 91 | | 180 |
| 38 | S | 785.9 | 5288 | 221 | 129 |  |  |  | ROIpeak | | 211 | | 427 |
| 39 | S | 796.0 | 31191 | 25600 | 216 |  |  |  | ROIpeak | | 239 | | 483 |
| 40 | D | 802.1 | 9463 | 1870 | 72 | 1.46 | 4.4 | 2262.4 | Rem. 2 | | 138 | | 274 |
| 41 | D | 806.5 | 9463 | 902 | 45 | 1.46 | 4.4 | 2250.2 | Rem. 2 | | 75 | | 149 |
| 42 | S | 840.0 | 3336 | 138 | 90 |  |  |  | ROIpeak | | 137 | | 298 |
| 43 | S | 860.6 | 5716 | 885 | 131 |  |  |  | ROIpeak | | 210 | | 425 |
| 44 | S | 911.3 | 10571 | 5020 | 162 |  |  |  | ROIpeak | | 240 | | 485 |
| 45 | S | 934.1 | 5030 | 604 | 120 |  |  |  | ROIpeak | | 193 | | 392 |
| 46 | D | 964.8 | 11716 | 826 | 56 | 1.77 | 4.3 | 2719.0 | Rem. 2 | | 103 | | 203 |
| 47 | D | 969.1 | 11716 | 2820 | 77 | 1.77 | 4.3 | 2706.8 | Rem. 2 | | 154 | | 306 |
| 48 | S | 1001.3 | 2928 | 245 | 53 |  |  |  | ROIpeak | | 134 | | 173 |
| 49 | S | 1039.1 | 3323 | 235 | 85 |  |  |  | ROIpeak | | 154 | | 313 |
| 50 | S | 1120.4 | 6795 | 2940 | 128 |  |  |  | ROIpeak | | 191 | | 387 |
| 51 | S | 1155.6 | 3304 | 616 | 95 |  |  |  | ROIpeak | | 151 | | 306 |
| 52 | D | 1168.1 | 40520 | 663 | 47 | 2.07 | 5.2 | 3292.2 | Rem. 2 | | 88 | | 174 |
| 53 | D | 1173.3 | 40520 | 33700 | 190 | 2.07 | 5.2 | 3277.6 | Rem. 2 | | 511 | | 1017 |
| 54 | S | 1238.3 | 13778 | 1270 | 99 |  |  |  | ROIpeak | | 152 | | 309 |
| 55 | S | 1280.7 | 1985 | 261 | 77 |  |  |  | ROIpeak | | 124 | | 252 |
| 56 | S | 1332.5 | 32378 | 30400 | 195 |  |  |  | ROIpeak | | 133 | | 292 |
| 57 | S | 1365.2 | 1925 | 894 | 62 |  |  |  | ROIpeak | | 89 | | 183 |
| 58 | S | 1377.7 | 2572 | 941 | 88 |  |  |  | ROIpeak | | 136 | | 276 |
| 59 | S | 1385.3 | 1533 | 147 | 72 |  |  |  | ROIpeak | | 117 | | 238 |
| 60 | S | 1400.7 | 2628 | 1220 | 81 |  |  |  | ROIpeak | | 120 | | 245 |
| 61 | S | 1408.0 | 1952 | 495 | 77 |  |  |  | ROIpeak | | 121 | | 427 |
| 62 | S | 1440.8 | 667 | 58 | 39 |  |  |  | ROIpeak | | 63 | | 129 |
| 63 | S | 1460.8 | 23802 | 22500 | 167 |  |  |  | ROIpeak | | 121 | | 246 |
| 64 | S | 1509.2 | 1498 | 477 | 67 |  |  |  | ROIpeak | | 104 | | 213 |
| 65 | D | 1588.1 | 2390 | 468 | 33 | 2.15 | 4.8 | 4470.4 | Rem. 2 | | 65 | | 127 |
| 66 | D | 1592.9 | 2390 | 402 | 41 | 2.15 | 4.8 | 4457.1 | Rem. 2 | | 61 | | 119 |
| 67 | S | 1620.9 | 1098 | 235 | 57 |  |  |  | ROIpeak | | 90 | | 185 |
| 68 | S | 1630.8 | 715 | 216 | 40 |  |  |  | ROIpeak | | 61 | | 126 |
| 69 | S | 1661.0 | 962 | 263 | 65 |  |  |  | ROIpeak | | 86 | | 177 |
| 70 | S | 1729.4 | 1404 | 694 | 63 |  |  |  | ROIpeak | | 94 | | 192 |
| 71 | S | 1747.6 | 338 | 26 | 29 |  |  |  | ROIpeak | | 47 | | 97 |
| 72 | S | 1764.5 | 4465 | 3899 | 82 |  |  |  | ROIpeak | | 89 | | 182 |
| 73 | S | 1796.3 | 283 | 14 | 26 |  |  |  | ROIpeak | | 42 | | 88 |
| 74 | S | 1847.3 | 988 | 443 | 51 |  |  |  | ROIpeak | | 76 | | 157 |
| 75 | S | 2064.8 | 240 | 23 | 25 |  |  |  | ROIpeak | | 39 | | 81 |
| 76 | S | 2103.5 | 1231 | 610 | 58 |  |  |  | ROIpeak | | 86 | | 177 |
| 77 | S | 2118.5 | 325 | 245 | 43 |  |  |  | ROIpeak | | 66 | | 135 |
| 78 | S | 2204.0 | 1792 | 1270 | 61 |  |  |  | ROIpeak | | 81 | | 167 |
| 79 | S | 2447.5 | 652 | 332 | 41 |  |  |  | ROIpeak | | 61 | | 125 |
| 80 | S | 2505.5 | 933 | 686 | 43 |  |  |  | ROIpeak | | 56 | | 116 |
| 81 | S | 2614.4 | 6388 | 6140 | 83 |  |  |  | ROIpeak | | 45 | | 93 |
|  |  |  |  |  |  |  |  |  |  | |  | |  |
|  |  |  |  |  |  |  |  |  |  | |  | |  |

Remarks:

1. Designation for overlap among peaks: S: non-overlapping, D: two overlapping peaks, T three overlapping peaks.

2. Excel sheets used for overlapping peaks: rCorrection, correlcoef, correlcoefB, LSQnp1np2.

3. The characteristic limits cannot be calculated for the central peak. The characteristic limits for the side peaks were calculated as for two overlapping peaks, using the counts registered in the whole region of the multiplet for *n*g.

4. *n*g within an energy region is obtained from the Status Page MARKER INFO under the parameter Integral, when the markers are set to the first and last channel of the region.

If the peak analysis is performed by Sum / Non-Linear LSQ Fit with the parameter Fit singlets set to Yes, for the calculation of the characteristic limits for isolated peaks the Excel sheet LSQisolated must be used. The energies remain unchanged, as well as the analysis results for overlapping peaks. Since in the LSQ method *n*g denotes the total number of counts in the fitted region, *n*g must be obtained as the sum of the counts in the peak region and both adjacent regions used to determine the continuous background. If the Continuum parameter in the Non-Linear LSQ is set to 4, the peak width must be extended for four channels towards lover energies and for four channels towards higher energies. For some isolated peaks, the analysis yields:

Table 2. Results of the peak analysis of the spectrum ExampleCNF, obtained by fitting isolated peaks with Gaussian functions, and the characteristic limits computed with the Calculator

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Peak analysis results | | | | | | Method | Char. Limits | |
| Peak No. | Overlap | *E*  [keV] | *n*g | *n*p | *u*(*n*p) | Excel sheet | *n*\* | *n*# |
| 1 | S | 46.9 | 26837 | 837 | 103 | LSQisolated | 165 | 334 |
| 2 | S | 59,9 | 34473 | 3480 | 122 | LSQisolated | 185 | 374 |
| 80 | S | 2505.4 | 999 | 689 | 30 | LSQisolated | 26 | 56 |
| 81 | S | 2614.3 | 6334 | 6060 | 79 | LSQisolated | 26 | 57 |

In the example spectrum ExampleCNF the peak analysis recognized only overlapping peaks with a separation in excess of 2 FWHM, consequently the correlation coefficients between both peak areas, *r*(*n*p1,*n*p2), are between -0.005 and zero. Since these peaks actually do not overlap, it is appropriate to analyze them separately, using the sheet LSQisolated, by determining *n*g manually between the border of the fitted region and the position of the minimum in the spectrum between both peaks. The Table 3 presents results of this analysis, for the peaks at the energy 604.9 keV and 609.5 keV, classified by the peak analysis as overlapping.

Table 3. Results of the peak analysis of the spectrum ExampleCNF obtained by separating neighboring peaks, analyzed as overlapping peaks, although are actually well separated.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Peak analysis results | | | | | | Method | Char. Limits | |
| Peak No. | Overlap | *E*  [keV] | *n*g | *n*p | *u*(*n*p) | Excel sheet | *n*\* | *n*# |
| 31 | D | 604.9 | 41640 | 34400 | 198 | LSQisolated | 130 | 264 |
| 32 | D | 609.5 | 15029 | 9080 | 112 | LSQisolated | 109 | 223 |

2. **Manual peak analysis**

The automatic analysis did not locate peaks at the energies 85.3 keV, 87.8 keV, 90.3 keV and 93.2 keV. A manual analysis of the peaks at 85.3 keV, 87.8 keV and 90.3 keV is not possible because they overlap.

A manual analysis of the peak at 93.2keV, using the Excel sheet ROImethod:

Input: FWHM: 1.1, DeltaCh1: 0.3565, h: 2.5, Nb1: 2, Nb2: 6, nb1: 3776, nb2: 11281, ng: 18512. Characteristic limits: *n*\* = 285, *n*# = 578.

3. **Calculation of common characteristic limits for multi-gamma-ray emitters using the Excel sheet MultiGamma.**

To calculate the decision thresholds and detection limits, the conversion factors *W*, which convert the counts in the peaks to activities, activity concentrations or activity densities must be known. The following table presents the calculation of the common decision threshold and the common detection limit for Cs-134 from the analysis of the spectrum using the MultiGamma sheet. The conversion factors *W* are calculated for the measurement time, disregarding the coincidence-summing corrections. The Table 4 presents calculation of the common decision threshold and the common detection limit with the sheet MultiGamma.

Table 4. Example calculation of the common characteristic limits for the radionuclide Cs-134.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Energy | *W* | Inputs | | Results | |
| keV | Bq/kg | *y*\* / Bq/kg | *y*# / Bq/kg | *y*C\* / Bq/kg | *y*C# / Bq/kg |
| 563 | 0.0341 | 8.1 | 16.5 | 0.82 | 1.6 |
| 569 | 0.0187 | 4.5 | 9.1 |  |  |
| 605 | 0.00307 | 1.5 | 3.0 |  |  |
| 796 | 0.00427 | 1.0 | 2.1 |  |  |
| 802 | 0.0426 | 5.9 | 11.7 |  |  |
| 1365 | 0.175 | 20.1 | 41.5 |  |  |

4. **Inconsistent multiplet deconvolution data**

The Excel sheet LSQoverlapping is used for auxiliary purposes when calculating the characteristic limits for closely overlapping peaks. If the peak-analysis results do not comply with the Poisson probability distribution of channel contents, the sheet LSQnp1np2 cannot yield the characteristic limits (This can happen in the case of closely spaced peaks). Then the sheet LSQoverlapping can be used, where the properties of the overlapping peak are disregarded, except its area. In the peak analysis of the spectrum ExampleCNF, no closely spaced peaks were located. It should be noted that the peak analysis of the spectrum ExampleCNF did not recognize any closely overlapping peaks.