

Supporting Information

Wide band gap design of new chalcogenide compounds: KSrPS₄ and CsBaAsS₄

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X-ray fluorescence measurement

For K₂SrPS₄, the mixture K₂S, SrS, P₂S₅ was ground for 30 minutes with the element ratio of 1:1:1:4 for K, Sr, P and S. For CsBaAsS₄ the mixture Cs₂S₃, BaS, As₂S₃ was ground for 30 minutes with the element ratio of 1:1:1:4 for Cs, Ba, As and S. The samples were placed into the computer-controlled furnace. Then the sample was ground for 30 minutes again so as to be well-distributed. The results were calibrated with the obtained sample.

The X-ray fluorescence test was performed 5 times for each compound. For K₂SrPS₄, the average of each percentage of atom K, Sr, P, S are 15.1866, 14.3462, 14.9720 and 55.4954, respectively. The relative standard deviations are 1.05798%, 1.70838%, 0.655713% and 0.258994%, respectively. For CsBaAsS₄, the average of each percentage of atom Cs, Ba, As, S are 13.8774, 14.3812, 14.1068 and 57.6344, respectively. The relative standard deviations are 0.541469%, 0.399189%, 0.499279% and 0.175297%, respectively.

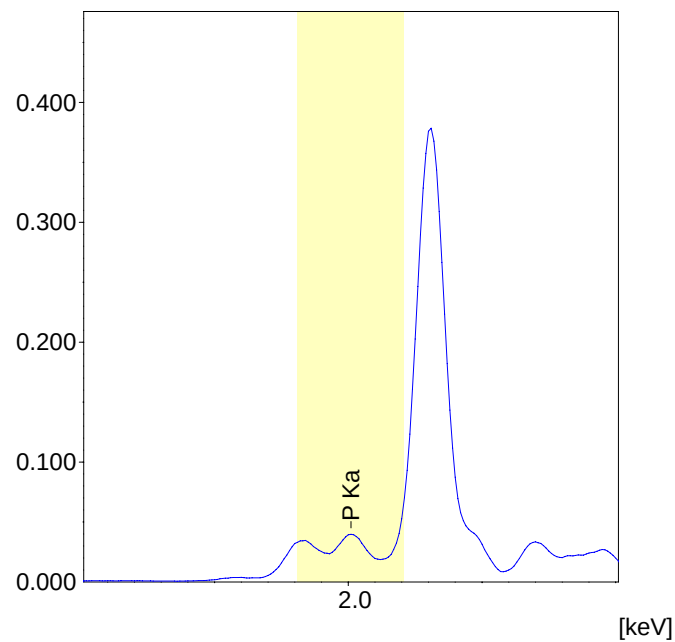
The analysis of the compounds with Shimadzu EDX-720 Energy Dispersive X-ray Fluorescence spectrometer manifested the presence of K, Sr, P, S and Ca, Ba, As, S in the approximate molar ratio of 1:1:1:4 and 1:1:1:4, respectively. The raw X-ray fluorescence spectra number 2-5 and 7-10 are shown in the following figures.

Sample : 2
Operator:

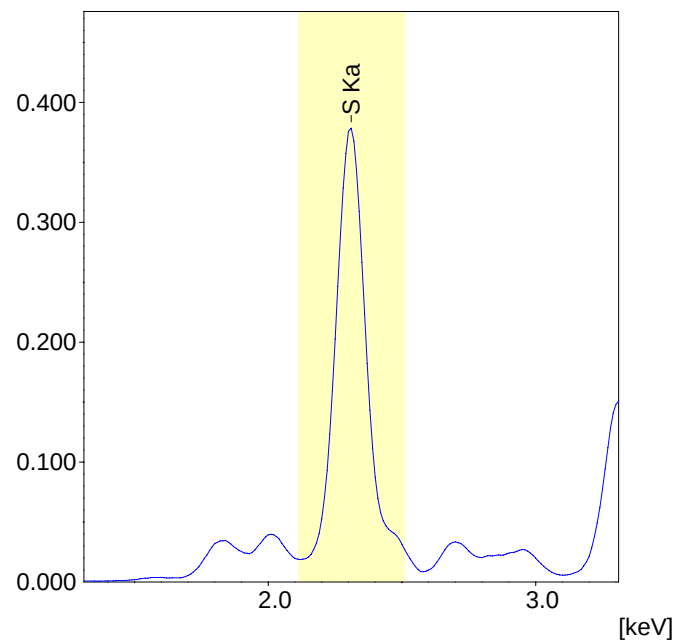
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Date : 2017-06-06 17:56:05
01/01

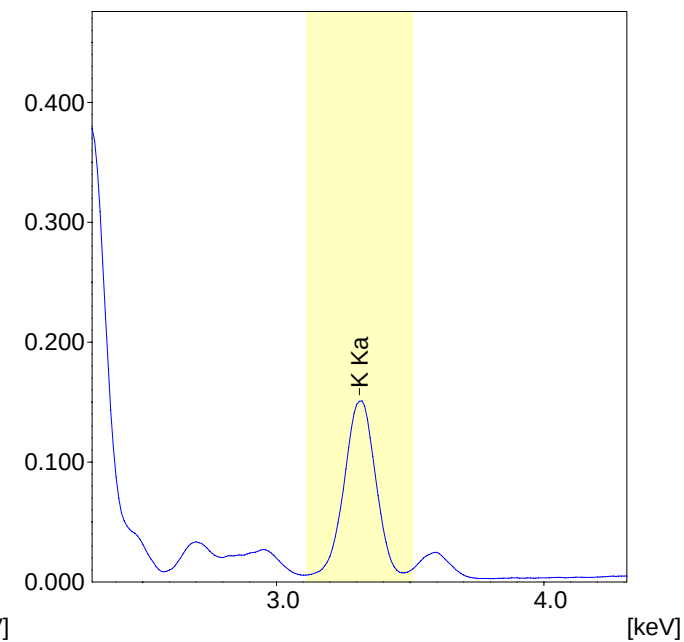
[cps/uA] P



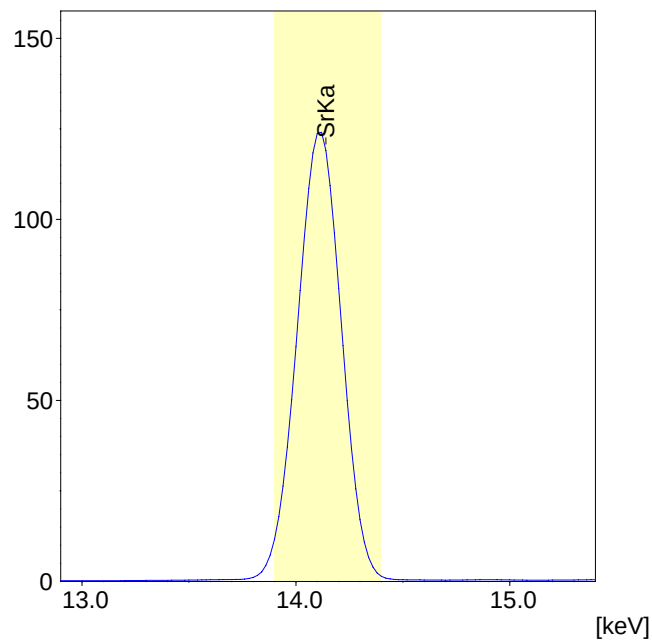
[cps/uA] S



[cps/uA] K



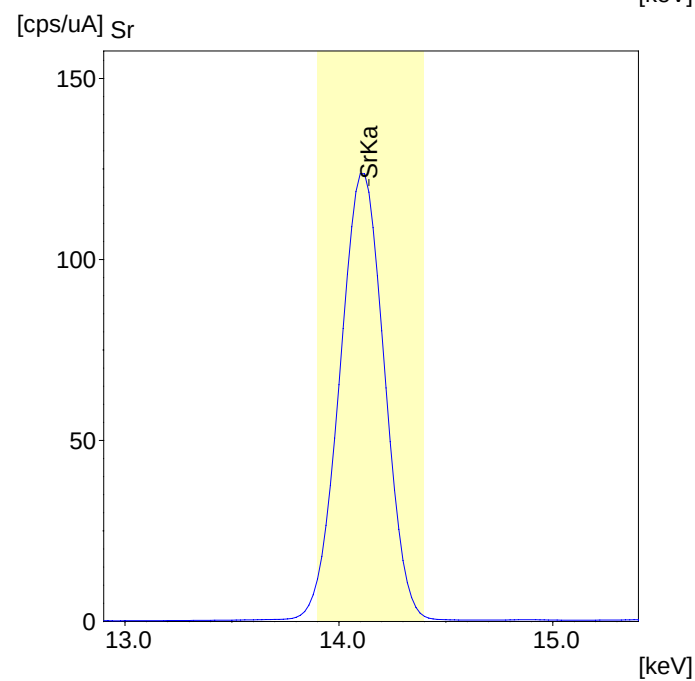
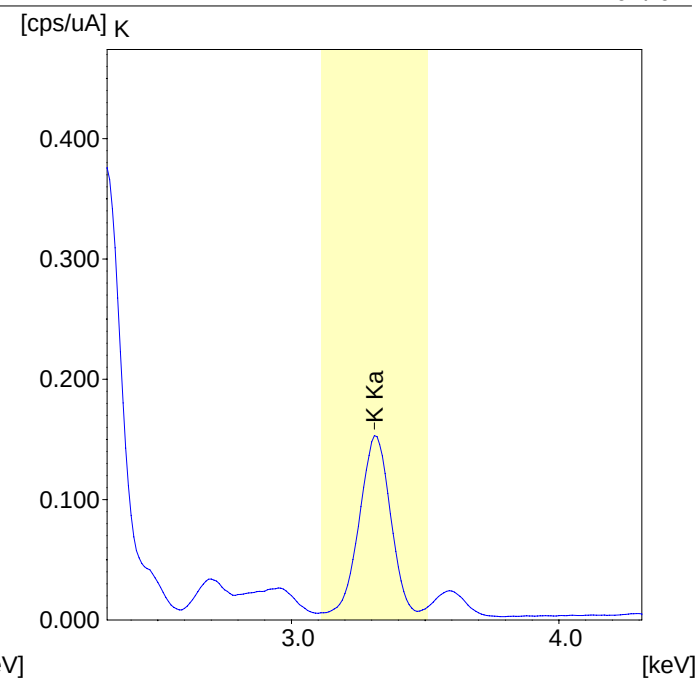
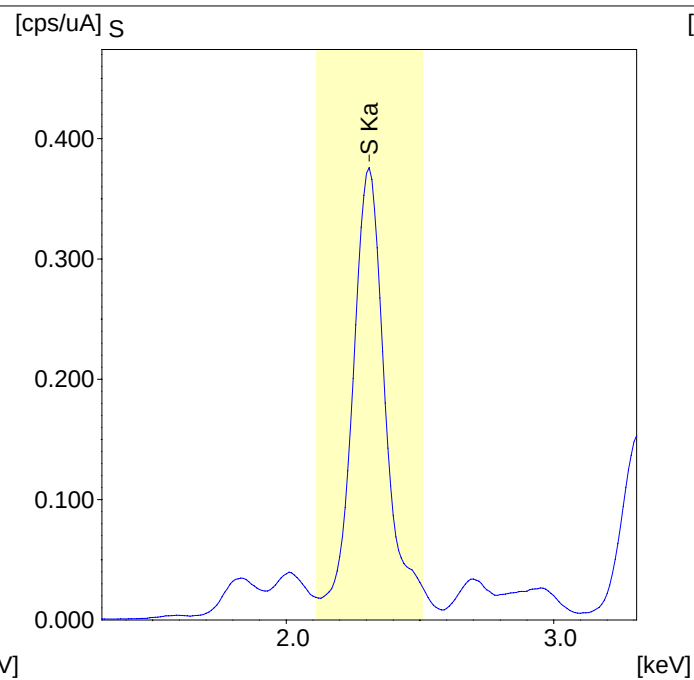
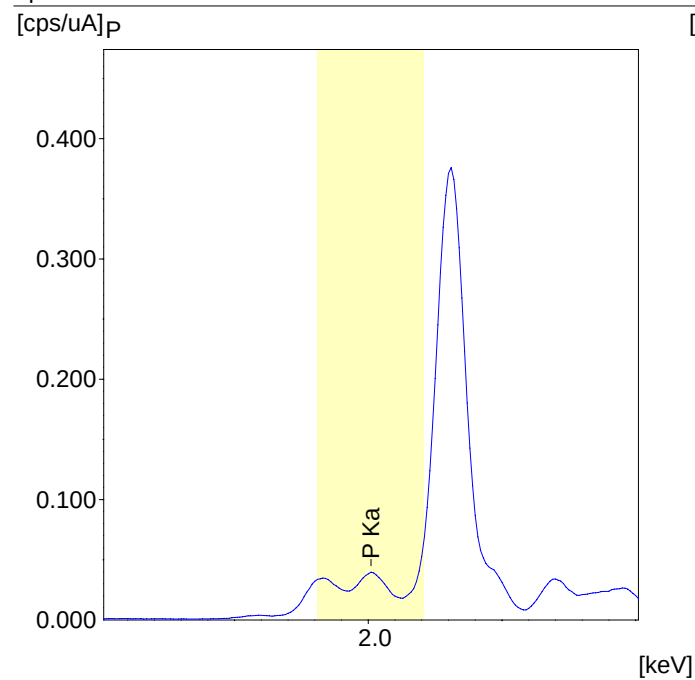
[cps/uA] Sr

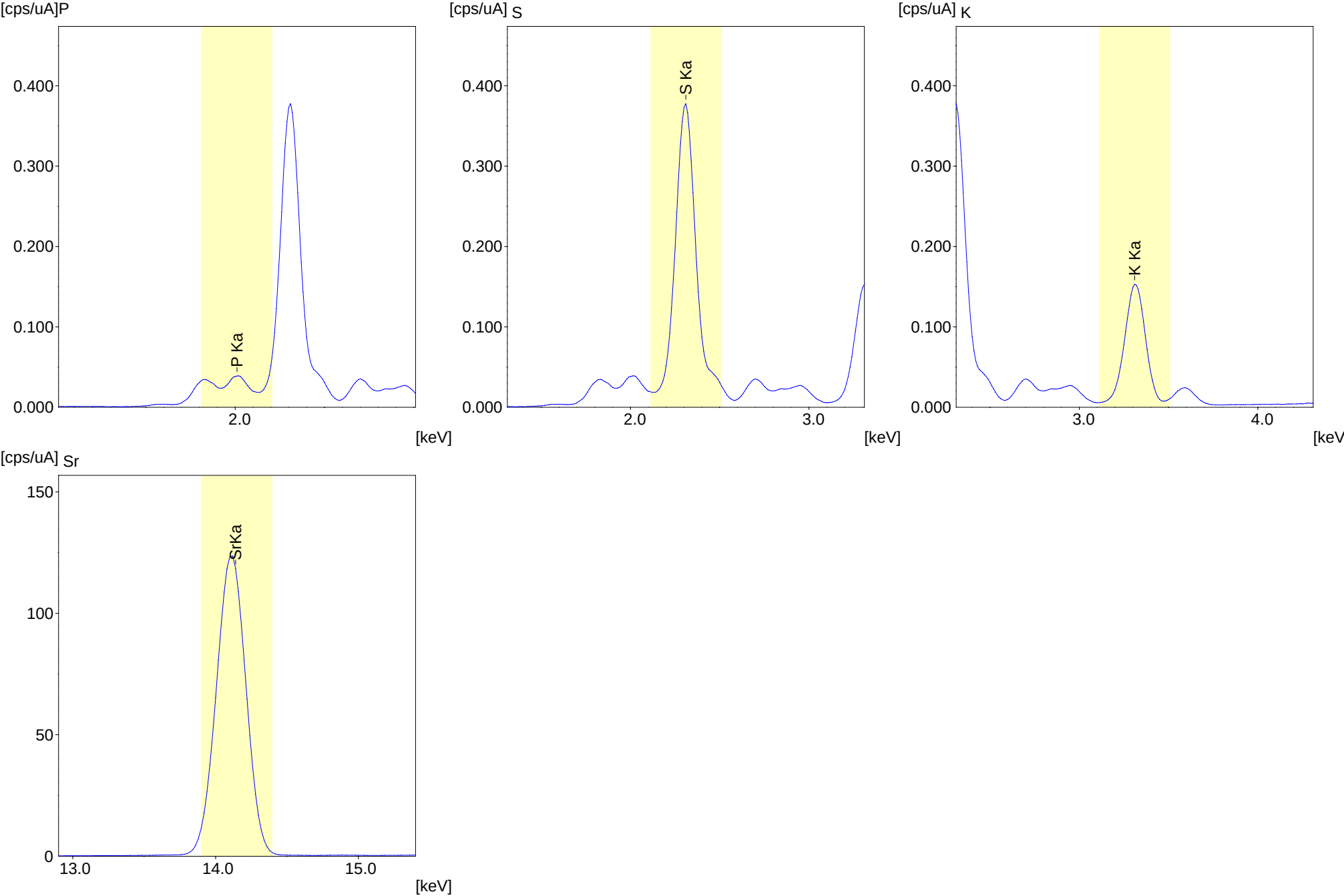


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Operator:

Group : 170606-3
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Date : 2017-06-06 18:03:54
01/01



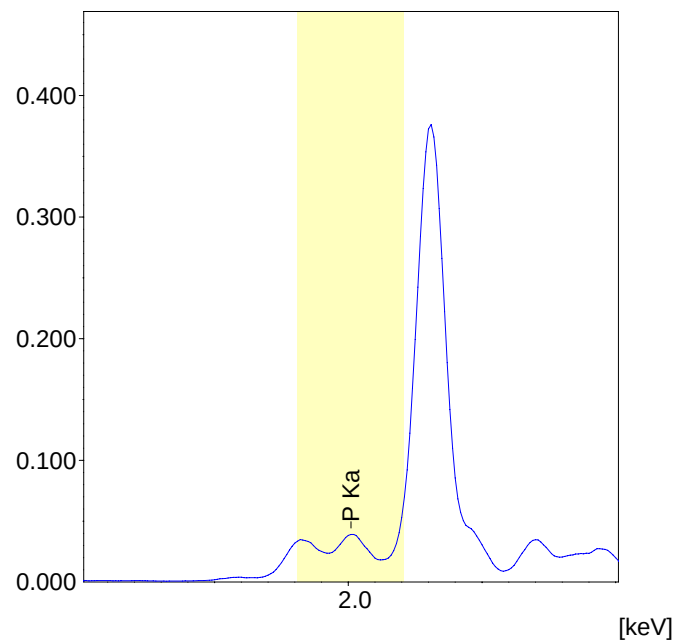


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Operator:

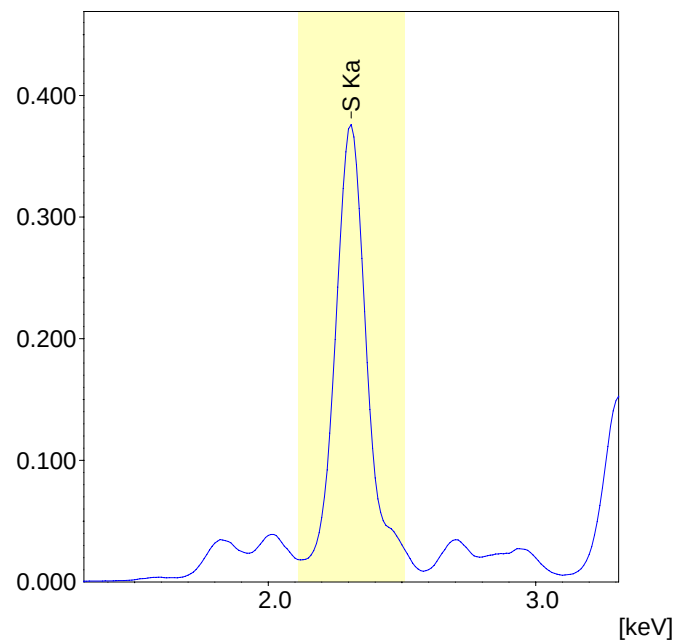
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01/01

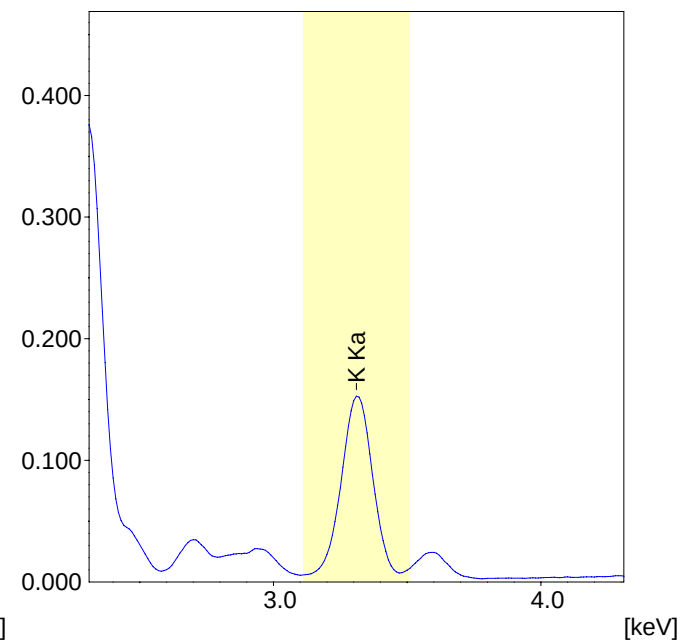
[cps/uA] P



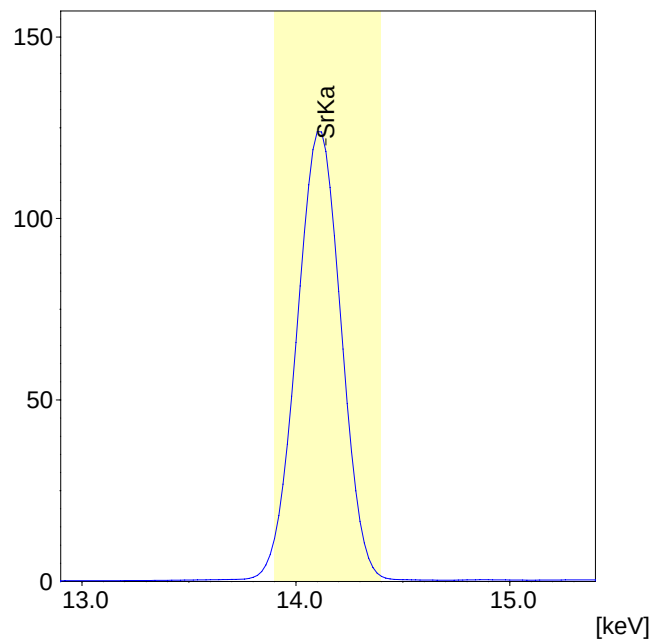
[cps/uA] S



[cps/uA] K



[cps/uA] Sr

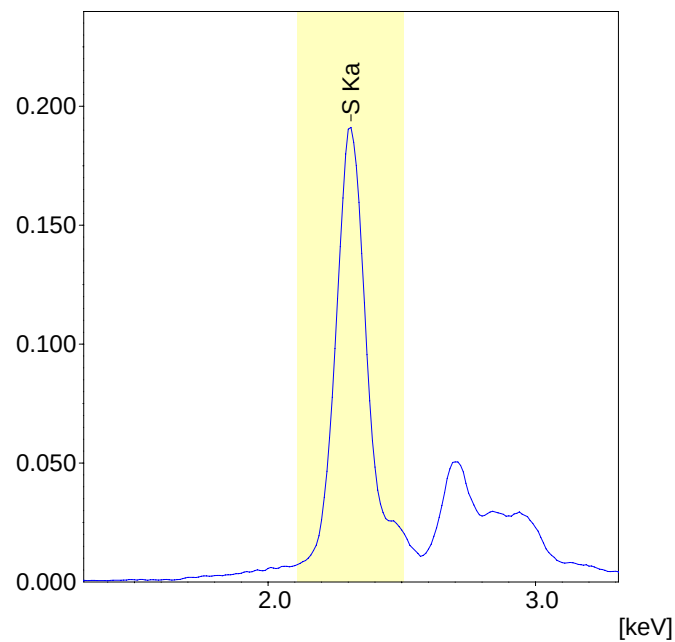


Sample : 7
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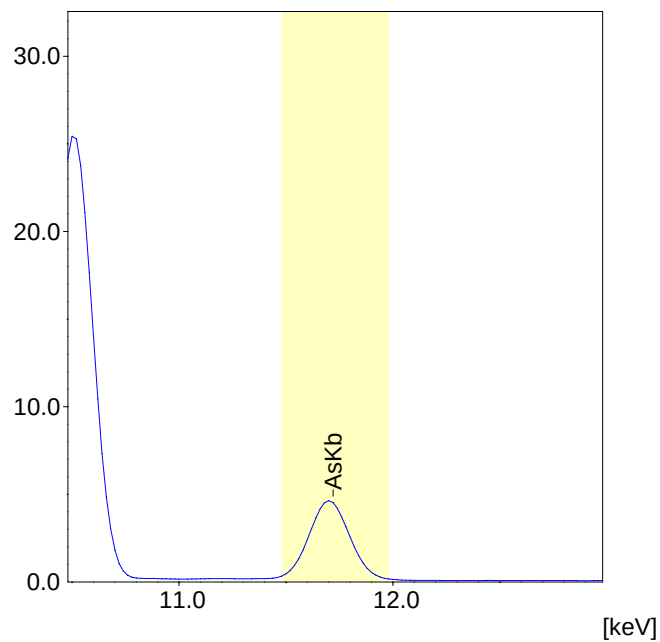
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Date : 2017-06-06 16:29:07
01/01

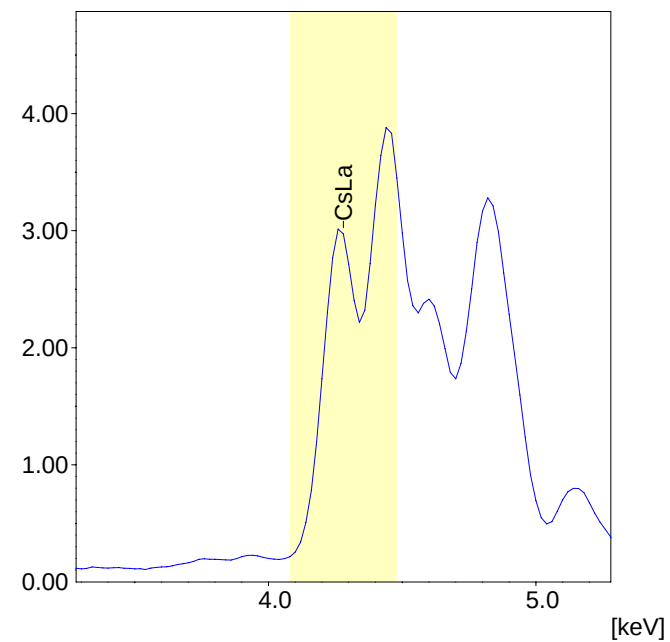
[cps/uA] S



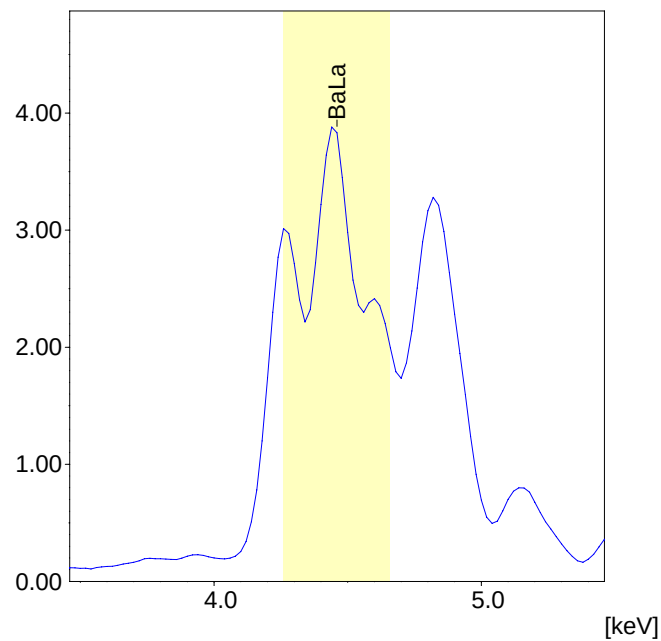
[cps/uA] As



[cps/uA] Cs



[cps/uA] Ba

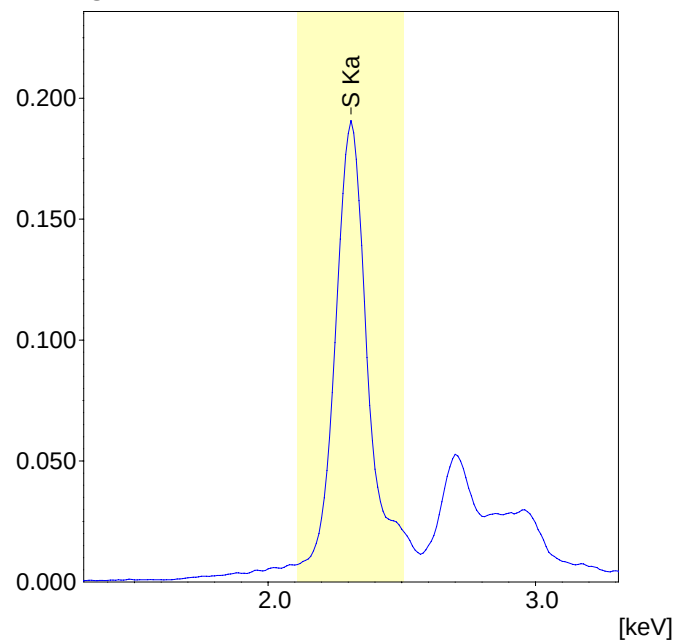


Sample : 8
Operator:

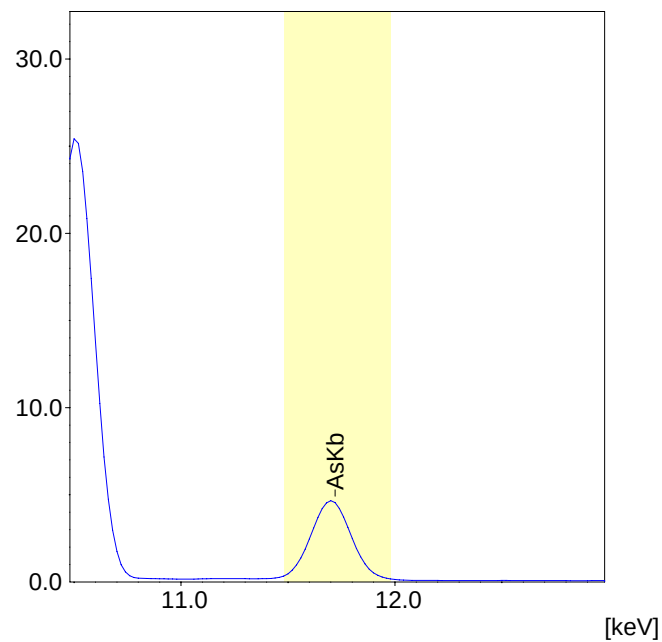
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01/01

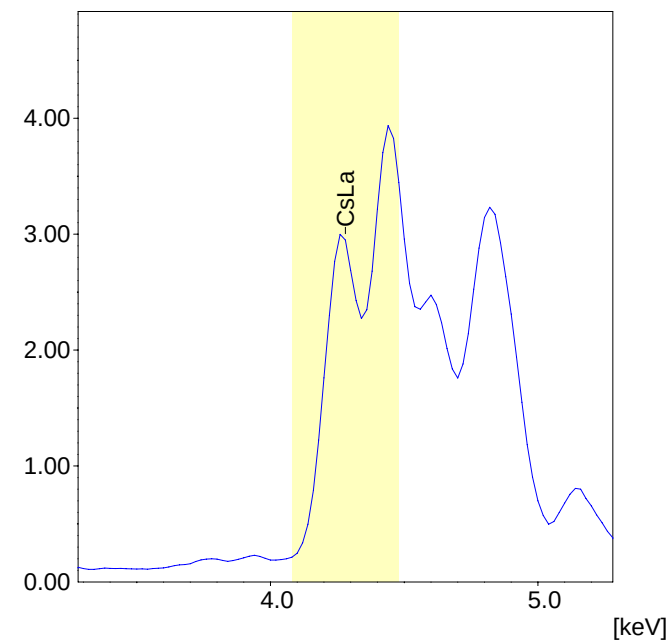
[cps/uA] S



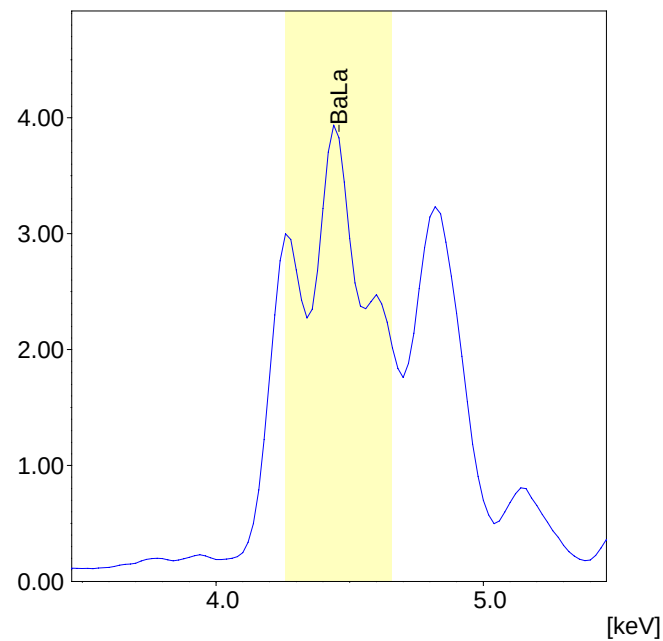
[cps/uA] As



[cps/uA] Cs



[cps/uA] Ba

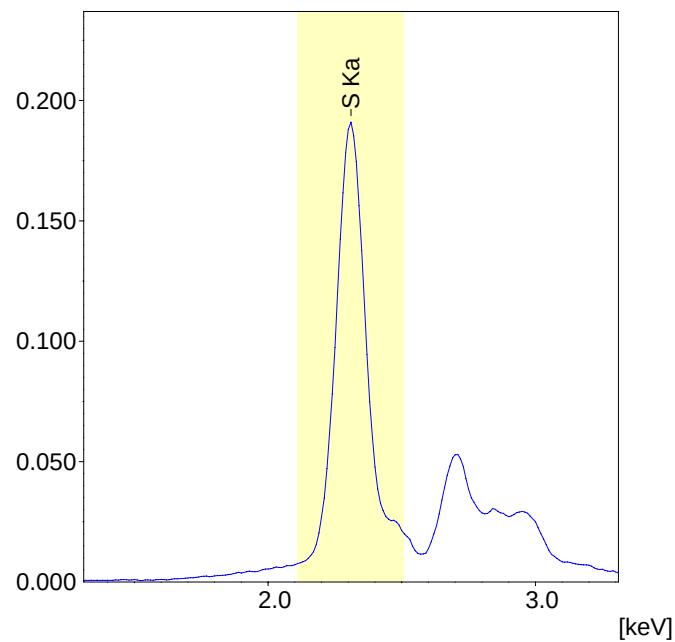


Sample : 9
Operator:

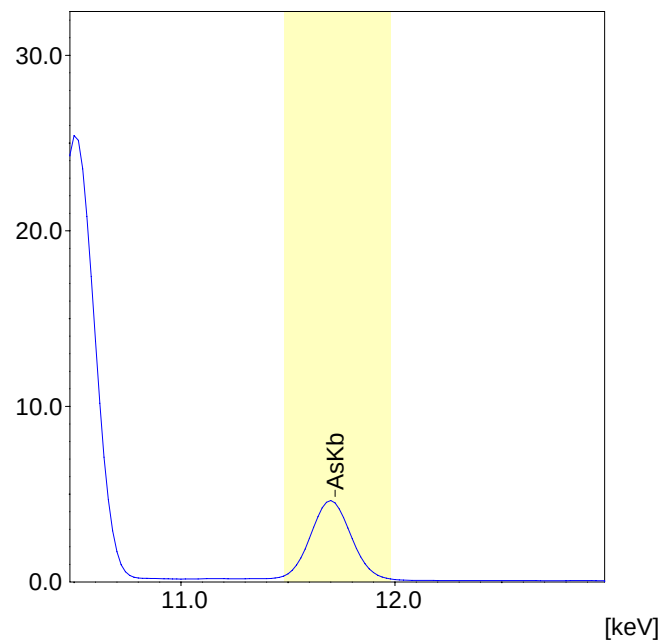
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Date : 2017-06-06 16:53:06
01/01

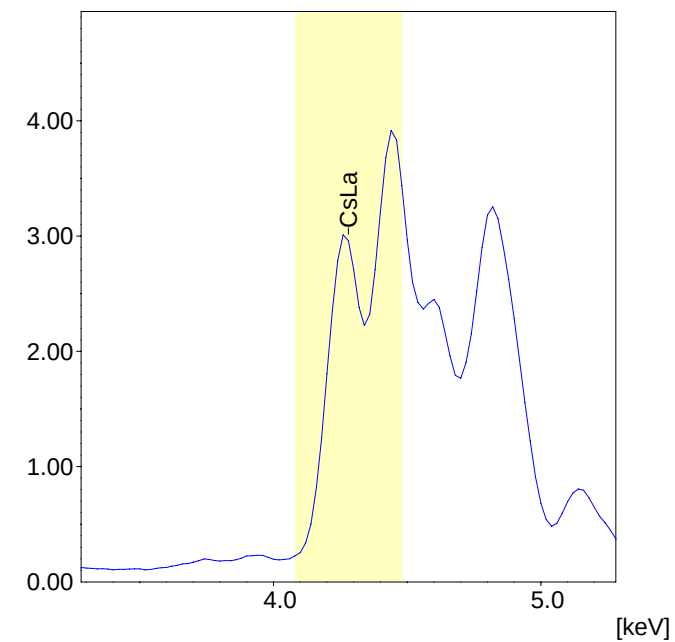
[cps/uA] S



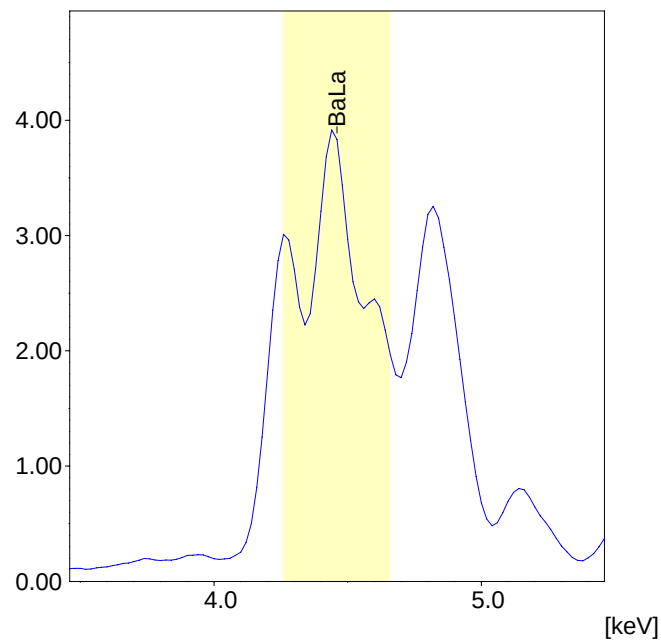
[cps/uA] As



[cps/uA] Cs



[cps/uA] Ba



Sample : 10

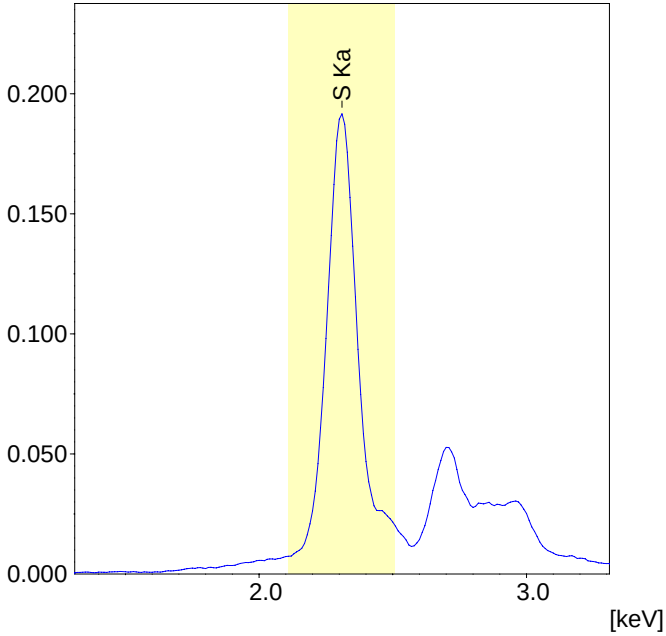
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Date : 2017-06-06 17:00:26
01/01

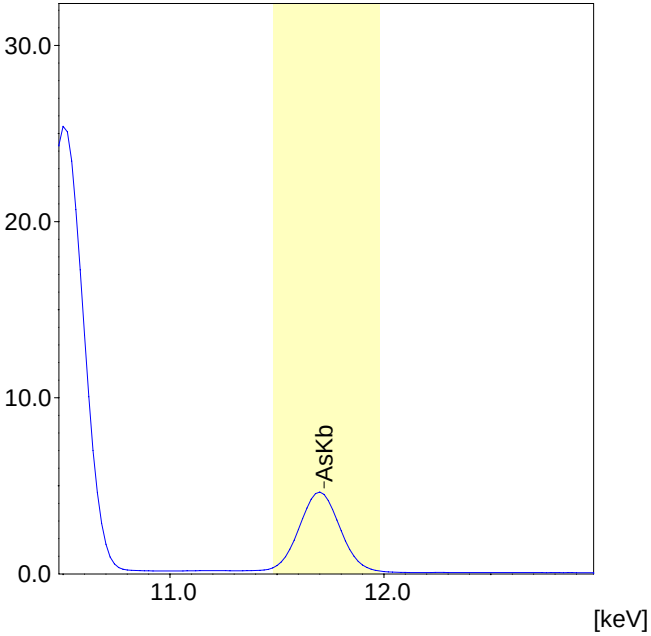
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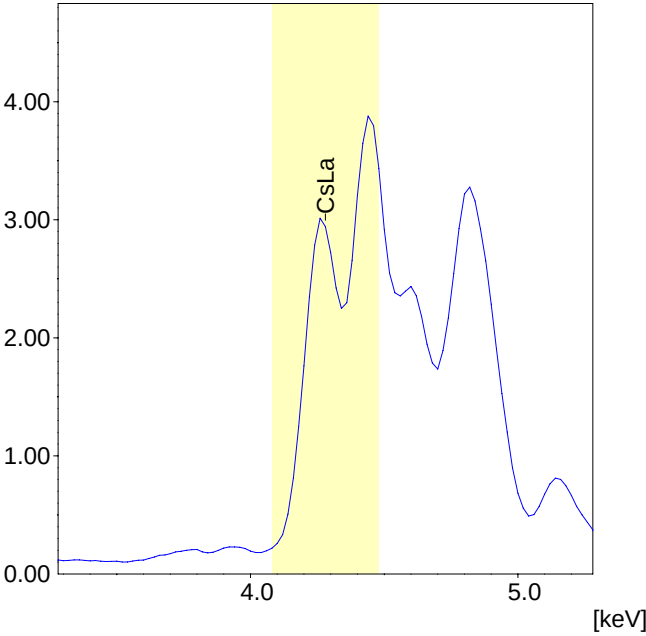
[cps/uA] S



[cps/uA] As



[cps/uA] Cs



[cps/uA] Ba

