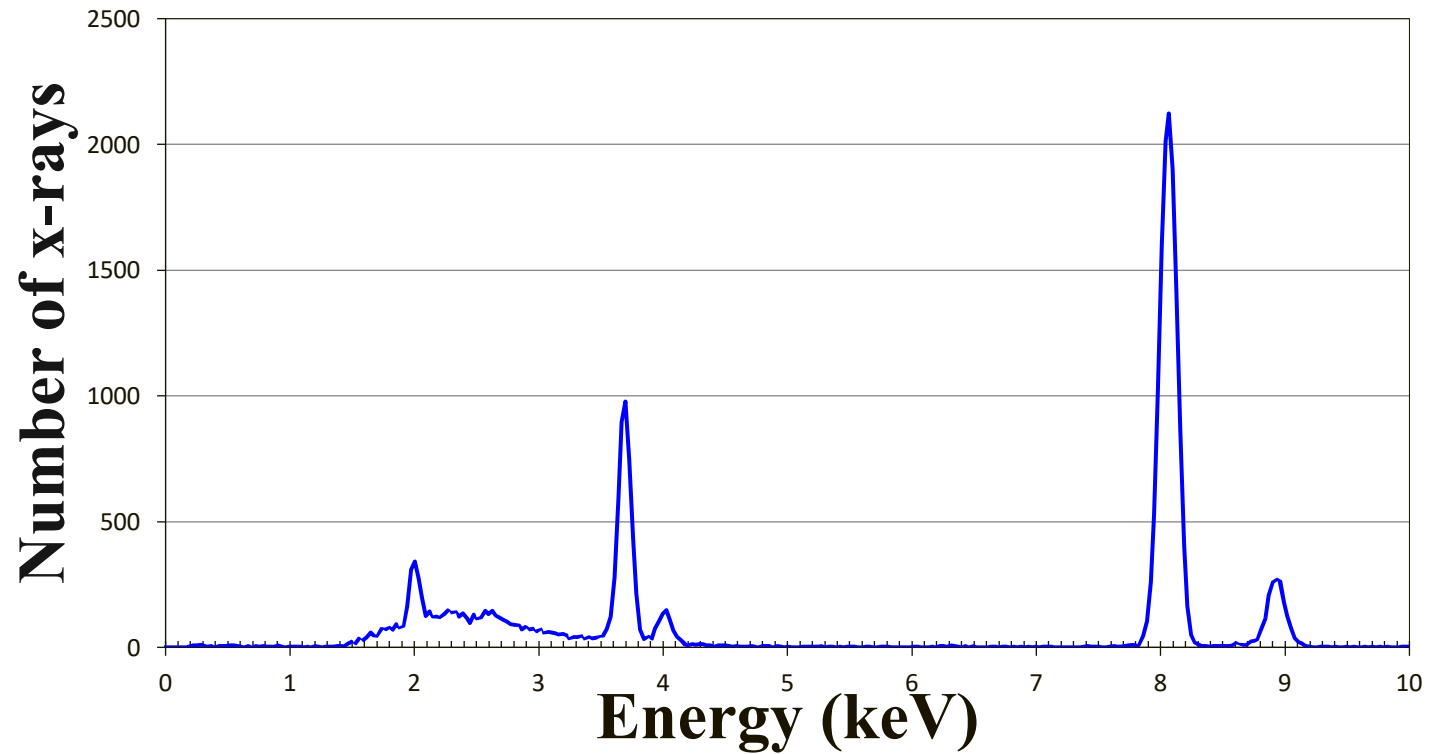


Determining the Elemental Target Make-up From The PIXE Spectrum



The Characteristic X-ray Energies & Elemental Identification

- Electronic transitions within inner shells of atoms are accompanied by large energy transfers. Therefore, we need the high energy proton beam to eject these bound electrons.
- First let's do a small calculation to simplify our lives when we calculate the energies of the orbits.

The energy of an electron in any state (orbital) is given by the sum of the electron's kinetic ($K = \frac{1}{2}mv^2$) and electric potential energies ($U = \frac{1}{4\pi\epsilon_0} \frac{Q_1Q_2}{r}$). $\longrightarrow E_n = K + U = \frac{1}{2}mv_n^2 + \frac{1}{4\pi\epsilon_0} \frac{(Ze)(-e)}{r_n}$

The speed (v) of the electron in an orbital and its distance (r) from the nucleus are quantized, meaning that they have only certain allowed energies given by:

$$v_n = \frac{Ze^2}{4\pi\epsilon_0 n\hbar} \quad r_n = \frac{4\pi\epsilon_0 n^2 \hbar^2}{mZe^2}$$

$$\begin{aligned} E_n &= -\frac{Z^2 me^4}{2(4\pi\epsilon_0)^2 n^2 \hbar^2} = -\left(\frac{me^4}{2(4\pi\epsilon_0)^2 \hbar^2}\right) \frac{Z^2}{n^2} \\ &= -\left[\frac{(9.11 \times 10^{-31} \text{ kg})(1.6 \times 10^{-19} \text{ C})^4}{32\pi^2 (8.85 \times 10^{-12} \frac{\text{C}^2}{\text{Nm}^2})^2 \left(\frac{6.63 \times 10^{-34} \text{ Js}}{2\pi}\right)^2} \times \frac{1 \text{ eV}}{1.6 \times 10^{-19} \text{ J}} \right] \frac{Z^2}{n^2} \\ &= -(13.57 \text{ eV}) \frac{Z^2}{n^2} \end{aligned}$$

The Characteristic X-ray Energies & Elemental Identification

$$\Delta E = E_{upper} - E_{lower}$$

$$\Delta E = -(13.6eV)Z^2 \left(\frac{1}{n_{upper}^2} - \frac{1}{n_{lower}^2} \right)$$

The lowest energy/highest probability transition, K_{α} :

$$n_{upper} = 2; \quad n_{lower} = 1$$

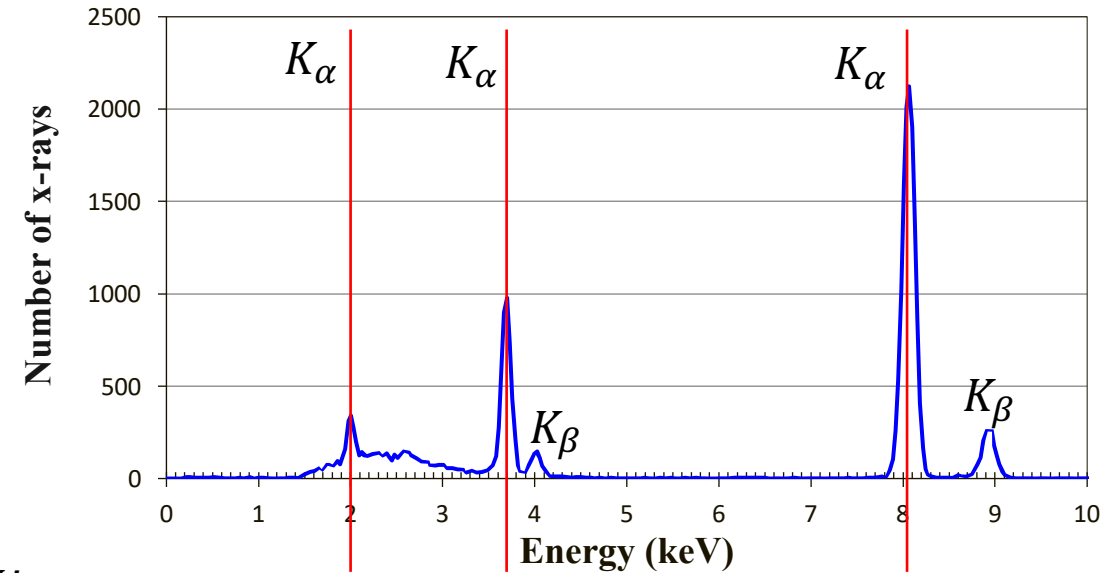
The main metal on the standard:

$$\Delta E = 8050eV = -(13.6eV)Z^2 \left(\frac{1}{2^2} - \frac{1}{1} \right) \rightarrow Z = 28 \rightarrow Ni$$

The impurities:

$$\Delta E = 2000eV = -(13.6eV)Z^2 \left(\frac{1}{2^2} - \frac{1}{1} \right) \rightarrow Z = 14 \rightarrow Si$$

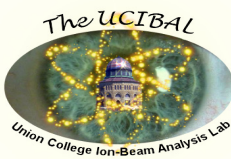
$$\Delta E = 3700eV = -(13.6eV)Z^2 \left(\frac{1}{2^2} - \frac{1}{1} \right) \rightarrow Z = 19 \rightarrow K$$



PERIODIC TABLE OF ELEMENTS

PubChem																														
1	1																2													
H	H																He													
Hydrogen	Hydrogen																Helium													
1s ¹	1s ¹																													
Atomic Number																														
Symbol																														
Name																														
Electron Configuration																														
3	4															5	6	7	8	9	10									
Li	Be															B	C	N	O	F	Ne									
Lithium	Beryllium															Boron	Carbon	Nitrogen	Oxygen	Fluorine	Neon									
11	12															13	14	15	16	17	18									
Na	Mg															Al	Si	P	S	Cl	Ar									
Sodium	Magnesium															Aluminum	Silicon	Phosphorus	Sulfur	Chlorine	Argon									
19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36													
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr													
Potassium	Calcium	Scandium	Titanium	Vanadium	Chromium	Manganese	Iron	Cobalt	Nickel	Copper	Zinc	Gallium	Germanium	Arsenic	Selenium	Bromine	Krypton													
37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54													
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe													
Rubidium	Strontium	Yttrium	Zirconium	Niobium	Molybdenum	Technetium	Ruthenium	Rhodium	Palladium	Silver	Cadmium	Indium	Tin	Antimony	Tellurium	Iodine	Xenon													
55	56															72	73	74	75	76	77	78	79	80	81	82	83	84	85	86
Cs	Ba															Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Cesium	Barium															Hafnium	Tantalum	Tungsten	Rhenium	Osmium	Iridium	Platinum	Gold	Mercury	Thallium	Lead	Bismuth	Polonium	Astatine	Radon
87	88															104	105	106	107	108	109	110	111	112	113	114	115	116	117	118
Rf	Ra															Db	Sg	Hs	Mt	Ds	Rg	Cn	Nh	Fl	Mc	Lv	Ts	Og		
Rutherfordium	Radium															Dubnium	Seaborgium	Hassium	Moscovium	Darmstadtium	Roentgenium	Copernicium	Nihonium	Flerovium	Moscovium	Livermorium	Tennessine	Oganesson		
57	58	59	60	61	62	63	64	65	66	67	68	69	70	71																
La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu																
Lanthanum	Cerium	Praseodymium	Neodymium	Promethium	Samarium	Europium	Gadolinium	Terbium	Dysprosium	Holmium	Erbium	Thulium	Ytterbium	Lutetium																
89	90	91	92	93	94	95	96	97	98	99	100	101	102	103																
Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr																
Actinium	Thorium	Protactinium	Uranium	Neptunium	Plutonium	Americium	Curium	Berkelium	Californium	Einsteinium	Fermium	Mendelevium	Nobelium	Lanthanum																

<https://pubchem.ncbi.nlm.nih.gov/periodic-table/>



The Characteristic X-ray Energies & Elemental Identification

$$\Delta E = E_{upper} - E_{lower}$$

$$\Delta E = -(13.6eV)Z^2 \left(\frac{1}{n_{upper}^2} - \frac{1}{n_{lower}^2} \right)$$

The higher energy/lower probability transition, K_β :

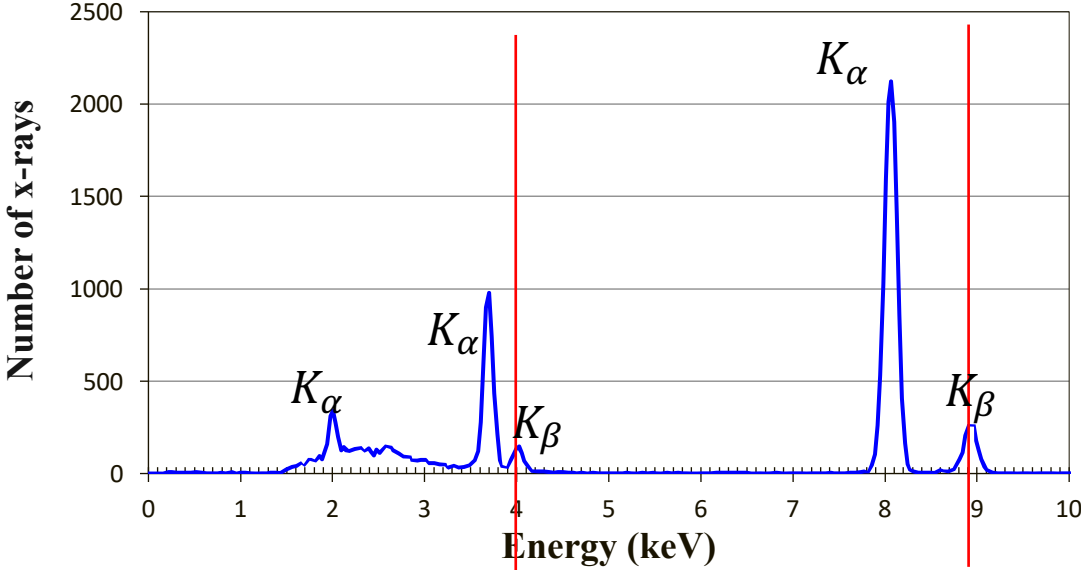
$$n_{upper} = 3; \quad n_{lower} = 1$$

The main metal on the standard:

$$\Delta E = 8950eV = -(13.6eV)Z^2 \left(\frac{1}{3^2} - \frac{1}{1} \right) \rightarrow Z = 27.2 \rightarrow Ni/Co$$

The impurities:

$$\Delta E = 4000eV = -(13.6eV)Z^2 \left(\frac{1}{3^2} - \frac{1}{1} \right) \rightarrow Z = 18.2 \rightarrow K/Ar$$



PERIODIC TABLE OF ELEMENTS

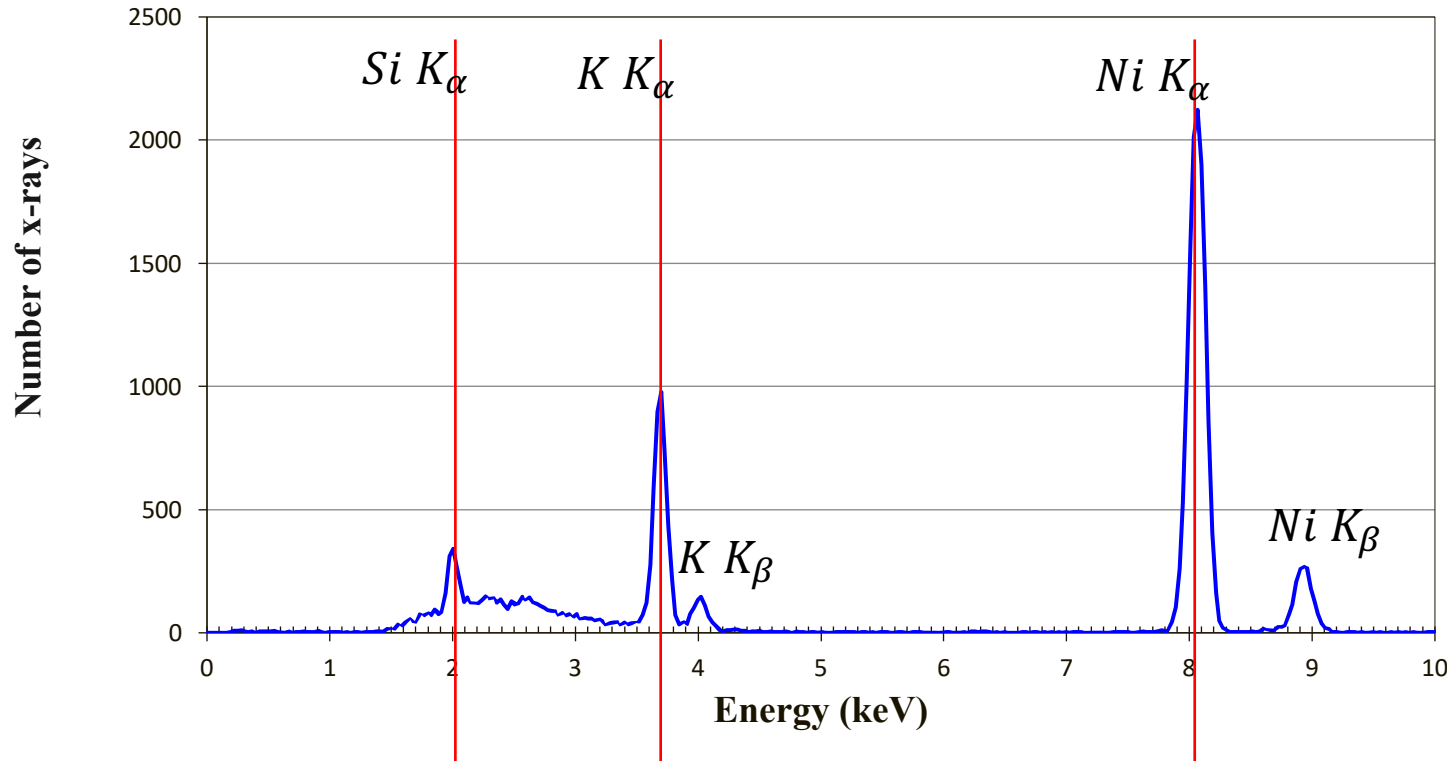
PubChem

1		1										2																							
H		Atomic Number										He																							
Hydrogen		Symbol										Helium																							
1s ¹		Name										1s ²																							
		Electron Configuration																																	
3	Li	4	Be									5	B	6	C	7	N	8	O	9	F	10	Ne												
11	Na	12	Mg									13	Al	14	Si	15	P	16	S	17	Cl	18	Ar												
19	K	20	Ca	21	Sc	22	Ti	23	V	24	Cr	25	Mn	26	Fe	27	Co	28	Ni	29	Cu	30	Zn	31	Ga	32	Ge	33	As	34	Se	35	Br	36	Kr
37	Rb	38	Sr	39	Y	40	Zr	41	Nb	42	Mo	43	Tc	44	Ru	45	Rh	46	Pd	47	Ag	48	Cd	49	In	50	Sn	51	Sb	52	Te	53	I	54	Xe
55	Cs	56	Ba			72	Hf	73	Ta	74	W	75	Re	76	Os	77	Ir	78	Pt	79	Au	80	Hg	81	Tl	82	Pb	83	Bi	84	Po	85	At	86	Rn
87	Fr	88	Ra			104	Rf	105	Db	106	Sg	107	Hs	108	Ht	109	Ds	110	Rg	111	Cn	112	Nh	113	Fl	114	Mc	115	Lv	116	Ts	117	Og		
57	La	58	Ce	59	Pr	60	Nd	61	Pm	62	Sm	63	Eu	64	Gd	65	Tb	66	Dy	67	Ho	68	Er	69	Tm	70	Yb								
89	Ac	90	Th	91	Pa	92	U	93	Np	94	Pu	95	Am	96	Cm	97	Bk	98	Cf	99	Es	100	Fm	101	Md	102	No								

<https://pubchem.ncbi.nlm.nih.gov/periodic-table/>



The Characteristic X-ray Energies & Elemental Identification



We've identified the elements present in the standard.

The problem, however, is that the main element is not nickel but copper.

Which means that the impurities probably are not correct either.

Why is that?

The Characteristic X-ray Energies & Elemental Identification

PERIODIC TABLE OF ELEMENTS

PubChem

1 H Hydrogen 1s ¹																	2 He Helium 1s ²						
3 Li Lithium [He]2s ¹	4 Be Beryllium [He]2s ²																	5 B Boron [He]2s ² 2p ¹	6 C Carbon [He]2s ² 2p ²	7 N Nitrogen [He]2s ² 2p ³	8 O Oxygen [He]2s ² 2p ⁴	9 F Fluorine [He]2s ² 2p ⁵	10 Ne Neon [He]2s ² 2p ⁶
11 Na Sodium [Ne]3s ¹	12 Mg Magnesium [Ne]3s ²																	13 Al Aluminum [Ne]3s ² 3p ¹	14 Si Silicon [Ne]3s ² 3p ²	15 P Phosphorus [Ne]3s ² 3p ³	16 S Sulfur [Ne]3s ² 3p ⁴	17 Cl Chlorine [Ne]3s ² 3p ⁵	18 Ar Argon [Ne]3s ² 3p ⁶
19 K Potassium [Ar]4s ¹	20 Ca Calcium [Ar]4s ²	21 Sc Scandium [Ar]3d ¹ 4s ²	22 Ti Titanium [Ar]3d ² 4s ²	23 V Vanadium [Ar]3d ³ 4s ²	24 Cr Chromium [Ar]3d ⁵ 4s ¹	25 Mn Manganese [Ar]3d ⁵ 4s ²	26 Fe Iron [Ar]3d ⁶ 4s ²	27 Co Cobalt [Ar]3d ⁷ 4s ²	28 Ni Nickel [Ar]3d ⁸ 4s ²	29 Cu Copper [Ar]3d ¹⁰ 4s ¹	30 Zn Zinc [Ar]3d ¹⁰ 4s ²	31 Ga Gallium [Ar]3d ¹⁰ 4s ² 4p ¹	32 Ge Germanium [Ar]3d ¹⁰ 4s ² 4p ²	33 As Arsenic [Ar]3d ¹⁰ 4s ² 4p ³	34 Se Selenium [Ar]3d ¹⁰ 4s ² 4p ⁴	35 Br Bromine [Ar]3d ¹⁰ 4s ² 4p ⁵	36 Kr Krypton [Ar]3d ¹⁰ 4s ² 4p ⁶						
37 Rb Rubidium [Kr]5s ¹	38 Sr Strontium [Kr]5s ²	39 Y Yttrium [Kr]4d ¹ 5s ²	40 Zr Zirconium [Kr]4d ² 5s ²	41 Nb Niobium [Kr]4d ⁴ 5s ¹	42 Mo Molybdenum [Kr]4d ⁵ 5s ¹	43 Tc Technetium [Kr]4d ⁵ 5s ²	44 Ru Ruthenium [Kr]4d ⁷ 5s ¹	45 Rh Rhodium [Kr]4d ⁸ 5s ¹	46 Pd Palladium [Kr]4d ¹⁰	47 Ag Silver [Kr]4d ¹⁰ 5s ¹	48 Cd Cadmium [Kr]4d ¹⁰ 5s ²	49 In Indium [Kr]4d ¹⁰ 5s ² 5p ¹	50 Sn Tin [Kr]4d ¹⁰ 5s ² 5p ²	51 Sb Antimony [Kr]4d ¹⁰ 5s ² 5p ³	52 Te Tellurium [Kr]4d ¹⁰ 5s ² 5p ⁴	53 I Iodine [Kr]4d ¹⁰ 5s ² 5p ⁵	54 Xe Xenon [Kr]4d ¹⁰ 5s ² 5p ⁶						
55 Cs Cesium [Xe]6s ¹	56 Ba Barium [Xe]6s ²	*	72 Hf Hafnium [Xe]4f ¹⁴ 5d ² 6s ²	73 Ta Tantalum [Xe]4f ¹⁴ 5d ³ 6s ²	74 W Tungsten [Xe]4f ¹⁴ 5d ⁴ 6s ²	75 Re Rhenium [Xe]4f ¹⁴ 5d ⁵ 6s ²	76 Os Osmium [Xe]4f ¹⁴ 5d ⁶ 6s ²	77 Ir Iridium [Xe]4f ¹⁴ 5d ⁷ 6s ²	78 Pt Platinum [Xe]4f ¹⁴ 5d ⁹ 6s ¹	79 Au Gold [Xe]4f ¹⁴ 5d ¹⁰ 6s ¹	80 Hg Mercury [Xe]4f ¹⁴ 5d ¹⁰ 6s ²	81 Tl Thallium [Xe]4f ¹⁴ 5d ¹⁰ 6s ² 6p ¹	82 Pb Lead [Xe]4f ¹⁴ 5d ¹⁰ 6s ² 6p ²	83 Bi Bismuth [Xe]4f ¹⁴ 5d ¹⁰ 6s ² 6p ³	84 Po Polonium [Xe]4f ¹⁴ 5d ¹⁰ 6s ² 6p ⁴	85 At Astatine [Xe]4f ¹⁴ 5d ¹⁰ 6s ² 6p ⁵	86 Rn Radon [Xe]4f ¹⁴ 5d ¹⁰ 6s ² 6p ⁶						
87 Fr Francium [Rn]7s ¹	88 Ra Radium [Rn]7s ²	**	104 Rf Rutherfordium [Rn]5f ¹⁴ 6d ² 7s ²	105 Db Dubnium [Rn]5f ¹⁴ 6d ³ 7s ²	106 Sg Seaborgium [Rn]5f ¹⁴ 6d ⁴ 7s ²	107 Bh Bohrium [Rn]5f ¹⁴ 6d ⁵ 7s ²	108 Hs Hassium [Rn]5f ¹⁴ 6d ⁶ 7s ²	109 Mt Meitnerium [Rn]5f ¹⁴ 6d ⁷ 7s ²	110 Ds Darmstadtium [Rn]5f ¹⁴ 6d ⁸ 7s ²	111 Rg Roentgenium [Rn]5f ¹⁴ 6d ⁹ 7s ²	112 Cn Copernicium [Rn]5f ¹⁴ 6d ¹⁰ 7s ²	113 Nh Nihonium [Rn]5f ¹⁴ 6d ¹⁰ 7s ² 7p ¹	114 Fl Flerovium [Rn]5f ¹⁴ 6d ¹⁰ 7s ² 7p ²	115 Mc Moscovium [Rn]5f ¹⁴ 6d ¹⁰ 7s ² 7p ³	116 Lv Livermorium [Rn]5f ¹⁴ 6d ¹⁰ 7s ² 7p ⁴	117 Ts Tennessine [Rn]5f ¹⁴ 6d ¹⁰ 7s ² 7p ⁵	118 Og Oganesson [Rn]5f ¹⁴ 6d ¹⁰ 7s ² 7p ⁶						
			57 La Lanthanum [Xe]5d ¹ 6s ²	58 Ce Cerium [Xe]4f ¹ 5d ¹ 6s ²	59 Pr Praseodymium [Xe]4f ³ 6s ²	60 Nd Neodymium [Xe]4f ⁴ 6s ²	61 Pm Promethium [Xe]4f ⁵ 6s ²	62 Sm Samarium [Xe]4f ⁶ 6s ²	63 Eu Europium [Xe]4f ⁷ 6s ²	64 Gd Gadolinium [Xe]4f ⁷ 5d ¹ 6s ²	65 Tb Terbium [Xe]4f ⁹ 6s ²	66 Dy Dysprosium [Xe]4f ¹⁰ 6s ²	67 Ho Holmium [Xe]4f ¹¹ 6s ²	68 Er Erbium [Xe]4f ¹² 6s ²	69 Tm Thulium [Xe]4f ¹³ 6s ²	70 Yb Ytterbium [Xe]4f ¹⁴ 6s ²	71 Lu Lutetium [Xe]4f ¹⁴ 5d ¹ 6s ²						
			** 89 Ac Actinium [Rn]7s ² 6d ¹	90 Th Thorium [Rn]6d ² 7s ²	91 Pa Protactinium [Rn]5f ² 6d ¹ 7s ²	92 U Uranium [Rn]5f ³ 6d ¹ 7s ²	93 Np Neptunium [Rn]5f ⁴ 6d ¹ 7s ²	94 Pu Plutonium [Rn]5f ⁶ 7s ²	95 Am Americium [Rn]5f ⁷ 7s ²	96 Cm Curium [Rn]5f ⁸ 7s ²	97 Bk Berkelium [Rn]5f ⁹ 7s ²	98 Cf Californium [Rn]5f ¹⁰ 7s ²	99 Es Einsteinium [Rn]5f ¹¹ 7s ²	100 Fm Fermium [Rn]5f ¹² 7s ²	101 Md Mendelevium [Rn]5f ¹³ 7s ²	102 No Nobelium [Rn]5f ¹⁴ 7s ²	103 Lr Lawrencium [Rn]5f ¹⁴ 6d ¹ 7s ²						

It seems like we're *one off* from nickel to get copper.

Maybe we're *one off* from the others as well.

Maybe the impurities are not *Si* and *K*, but rather *P* and *Ca*.

How do we fix this?

Note adding one, while it may work, is not really satisfying without a reason.

<https://pubchem.ncbi.nlm.nih.gov/periodic-table/>

The Characteristic X-ray Energies & Elemental Identification

- The energy formula ($\Delta E = E_{upper} - E_{lower}$) seems ok.
- ΔE is what ΔE is!! The data are what we see on the graph. So that's probably not the problem.
- What if the expression for the energy of an electron in any given state in the atom is not correct?
- The $n = 1$ state is the $1s$ -orbital. In the $1s$ orbital there are two electrons. We ejected one but there is still one left.
- The transitioning electron from say the $n = 2$ state does not simply see the full nuclear charge (Ze) but rather the one electron left in the $n = 1$ state tries to repel the transitioning electron.
- Thus, maybe the charge that the transitioning electron sees is $Z_{eff}e = Ze - e = (Z - 1)e$.

The Characteristic X-ray Energies & Elemental Identification

$$E_{old} = -\left(\frac{me^4}{2(4\pi\epsilon_0\hbar)^2}\right)\frac{Z^2}{n^2} \rightarrow E_{new} = -\left(\frac{me^4}{2(4\pi\epsilon_0\hbar)^2}\right)\frac{(Z-1)^2}{n^2} = -(13.6eV)\frac{(Z-1)^2}{n^2}$$

$$\Delta E = E_{upper} - E_{lower}$$

$$\Delta E = -(13.6eV)(Z-1)^2\left(\frac{1}{n_{upper}^2} - \frac{1}{n_{lower}^2}\right)$$

The lowest energy/highest probability transition, K_α :

$$n_{upper} = 2; \quad n_{lower} = 1$$

The main metal on the standard

$$\Delta E = 8050eV = -(13.6eV)(Z-1)^2\left(\frac{1}{2^2} - \frac{1}{1}\right) \rightarrow Z = 29 \rightarrow Cu$$

The impurities:

$$\Delta E = 2000eV = -(13.6eV)(Z-1)^2\left(\frac{1}{2^2} - \frac{1}{1}\right) \rightarrow Z = 15 \rightarrow P$$

$$\Delta E = 3700eV = -(13.6eV)(Z-1)^2\left(\frac{1}{2^2} - \frac{1}{1}\right) \rightarrow Z = 20 \rightarrow Ca$$

PERIODIC TABLE OF ELEMENTS

1 H Hydrogen																	2 He Helium
3 Li Lithium	4 Be Beryllium											5 B Boron	6 C Carbon	7 N Nitrogen	8 O Oxygen	9 F Fluorine	10 Ne Neon
11 Na Sodium	12 Mg Magnesium											13 Al Aluminum	14 Si Silicon	15 P Phosphorus	16 S Sulfur	17 Cl Chlorine	18 Ar Argon
19 K Potassium	20 Ca Calcium	21 Sc Scandium	22 Ti Titanium	23 V Vanadium	24 Cr Chromium	25 Mn Manganese	26 Fe Iron	27 Co Cobalt	28 Ni Nickel	29 Cu Copper	30 Zn Zinc	31 Ga Gallium	32 Ge Germanium	33 As Arsenic	34 Se Selenium	35 Br Bromine	36 Kr Krypton
37 Rb Rubidium	38 Sr Strontium	39 Y Yttrium	40 Zr Zirconium	41 Nb Niobium	42 Mo Molybdenum	43 Tc Technetium	44 Ru Ruthenium	45 Rh Rhodium	46 Pd Palladium	47 Ag Silver	48 Cd Cadmium	49 In Indium	50 Sn Tin	51 Sb Antimony	52 Te Tellurium	53 I Iodine	54 Xe Xenon
55 Cs Cesium	56 Ba Barium	57 La Lanthanum	58 Ce Cerium	59 Pr Praseodymium	60 Nd Neodymium	61 Pm Promethium	62 Sm Samarium	63 Eu Europium	64 Gd Gadolinium	65 Tb Terbium	66 Dy Dysprosium	67 Ho Holmium	68 Er Erbium	69 Tm Thulium	70 Yb Ytterbium	71 Lu Lutetium	
87 Fr Francium	88 Ra Radium	89 Ac Actinium	90 Th Thorium	91 Pa Protactinium	92 U Uranium	93 Np Neptunium	94 Pu Plutonium	95 Am Americium	96 Cm Curium	97 Bk Berkelium	98 Cf Californium	99 Es Einsteinium	100 Fm Fermium	101 Md Mendelevium	102 No Nobelium	103 Lr Lawrencium	

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The Characteristic X-ray Energies & Elemental Identification

$$\Delta E = E_{upper} - E_{lower}$$

$$\Delta E = -(13.6eV)(Z - 1)^2 \left(\frac{1}{n_{upper}^2} - \frac{1}{n_{lower}^2} \right)$$

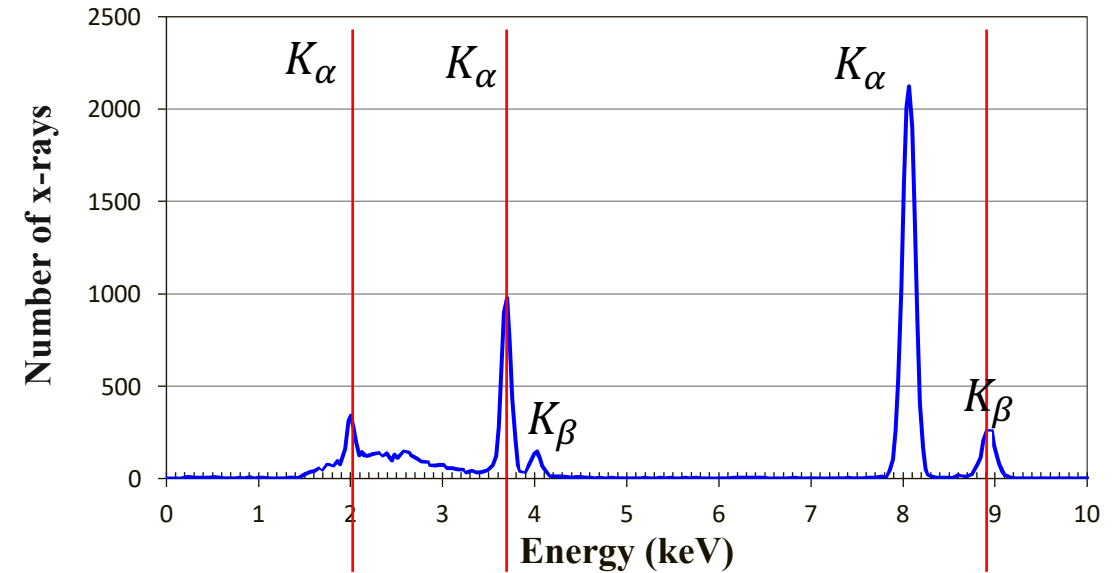
The higher energy/lower probability transition, K_{β} :

$$n_{upper} = 3; \quad n_{lower} = 1$$

The main metal on the standard:

$$\Delta E = 8950eV = -(13.6eV)(Z - 1)^2 \left(\frac{1}{3^2} - \frac{1}{1} \right) \rightarrow Z = 28.2 \rightarrow Ni/Cu$$

Notice we are still off a little. The K_{β} transitions should also be corrected. It's not as simple to do as the K_{α} transitions.



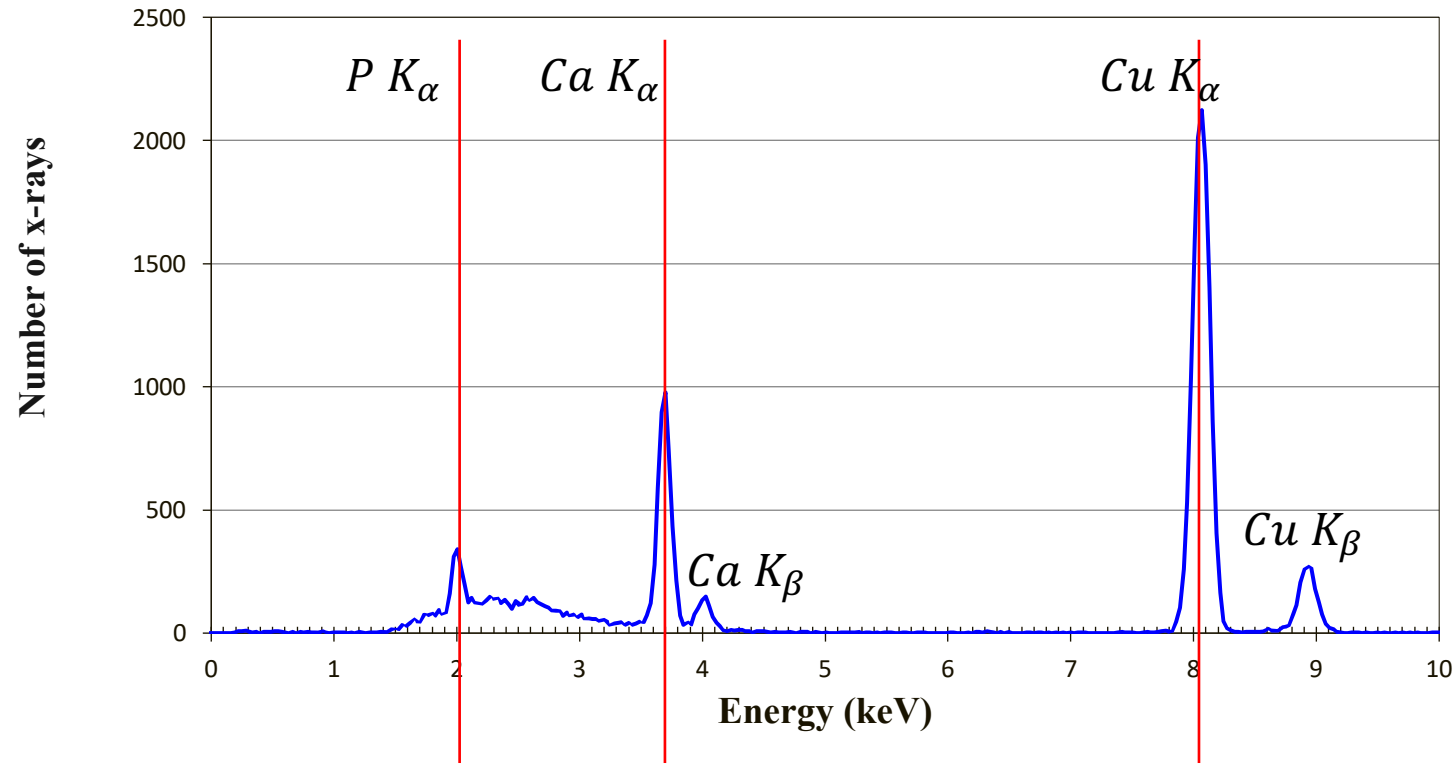
PERIODIC TABLE OF ELEMENTS

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H Hydrogen 1s ¹	Atomic Number Symbol Name Electron Configuration																He Helium																																																
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Na Sodium	Mg Magnesium															Al Aluminum	Si Silicon	P Phosphorus	S Sulfur	Cl Chlorine	Ar Argon																																												
19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36																																																
K Potassium	Ca Calcium	Sc Scandium	Ti Titanium	V Vanadium	Cr Chromium	Mn Manganese	Fe Iron	Co Cobalt	Ni Nickel	Cu Copper	Zn Zinc	Ga Gallium	Ge Germanium	As Arsenic	Se Selenium	Br Bromine	Kr Krypton																																																
37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54																																																
Rb Rubidium	Sr Strontium	Y Yttrium	Zr Zirconium	Nb Niobium	Mo Molybdenum	Tc Technetium	Ru Ruthenium	Rh Rhodium	Pd Palladium	Ag Silver	Cd Cadmium	In Indium	Sn Tin	Sb Antimony	Te Tellurium	I Iodine	Xe Xenon																																																
55	56															72	73	74	75	76	77	78	79	80	81	82	83	84	85	86																																			
Cs Cesium	Ba Barium															Hf Hafnium	Ta Tantalum	W Tungsten	Re Rhenium	Os Osmium	Ir Iridium	Pt Platinum	Au Gold	Hg Mercury	Tl Thallium	Pb Lead	Bi Bismuth	Po Polonium	At Astatine	Rn Radon																																			
87	88															104	105	106	107	108	109	110	111	112	113	114	115	116	117	118																																			
Fr Francium	Ra Radium															Rf Rutherfordium	Db Dubnium	Sg Seaborgium	Bh Bohrium	Hs Hassium	Mt Meitnerium	Ds Darmstadtium	Rg Roentgenium	Cn Copernicium	Nh Nihonium	Fl Flerovium	Mc Moscovium	Lv Livermorium	Ts Tennessine	Og Oganesson																																			
<table border="1"> <tr> <td>57</td> <td>58</td> <td>59</td> <td>60</td> <td>61</td> <td>62</td> <td>63</td> <td>64</td> <td>65</td> <td>66</td> <td>67</td> <td>68</td> </tr> <tr> <td>La Lanthanum</td> <td>Ce Cerium</td> <td>Pr Praseodymium</td> <td>Nd Neodymium</td> <td>Pm Promethium</td> <td>Sm Samarium</td> <td>Eu Europium</td> <td>Gd Gadolinium</td> <td>Tb Terbium</td> <td>Dy Dysprosium</td> <td>Ho Holmium</td> <td>Er Erbium</td> </tr> <tr> <td>89</td> <td>90</td> <td>91</td> <td>92</td> <td>93</td> <td>94</td> <td>95</td> <td>96</td> <td>97</td> <td>98</td> <td>99</td> <td>100</td> </tr> <tr> <td>Ac Actinium</td> <td>Th Thorium</td> <td>Pa Protactinium</td> <td>U Uranium</td> <td>Np Neptunium</td> <td>Pu Plutonium</td> <td>Am Americium</td> <td>Cm Curium</td> <td>Bk Berkelium</td> <td>Cf Californium</td> <td>Es Einsteinium</td> <td>Fm Fermium</td> </tr> </table>																		57	58	59	60	61	62	63	64	65	66	67	68	La Lanthanum	Ce Cerium	Pr Praseodymium	Nd Neodymium	Pm Promethium	Sm Samarium	Eu Europium	Gd Gadolinium	Tb Terbium	Dy Dysprosium	Ho Holmium	Er Erbium	89	90	91	92	93	94	95	96	97	98	99	100	Ac Actinium	Th Thorium	Pa Protactinium	U Uranium	Np Neptunium	Pu Plutonium	Am Americium	Cm Curium	Bk Berkelium	Cf Californium	Es Einsteinium	Fm Fermium
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<https://pubchem.ncbi.nlm.nih.gov/periodic-table/>



The Characteristic X-ray Energies & Elemental Identification

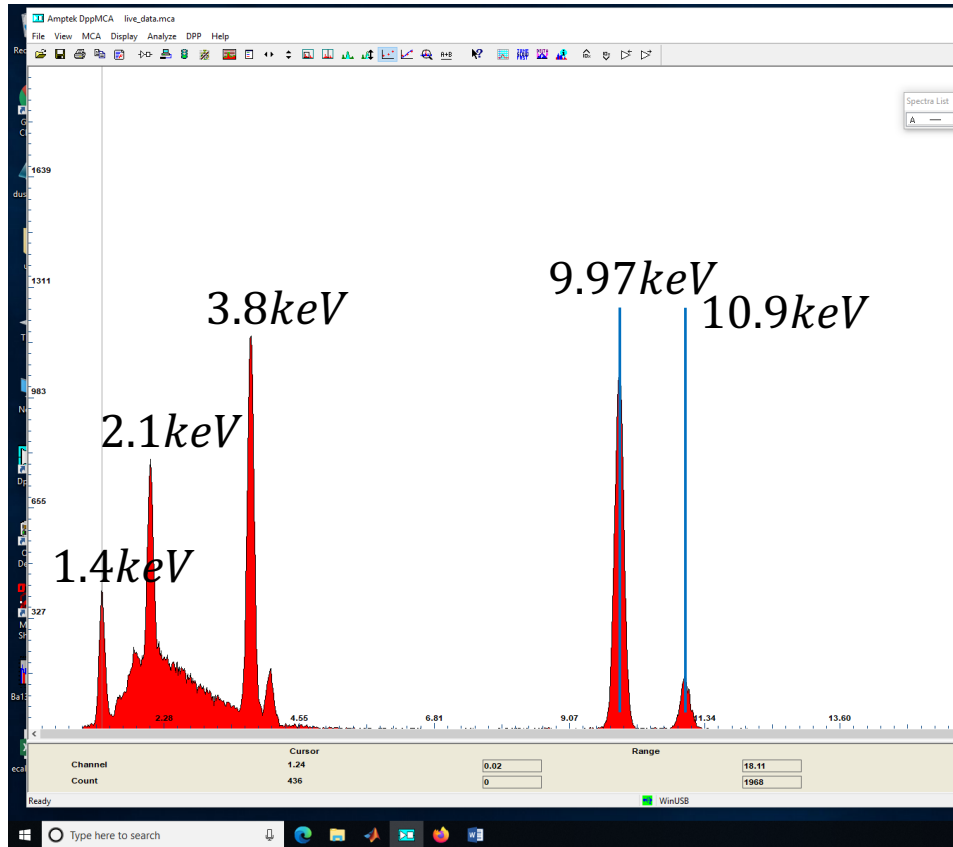


The single element standards are used to calibrate the energy scale so that we can run a real sample.

The X-Ray Energy Table For Elemental Identification

Characteristic X-Ray Energies

(X-ray Energies in keV)



1.4keV → Al K_{α}

2.1keV → P K_{α}

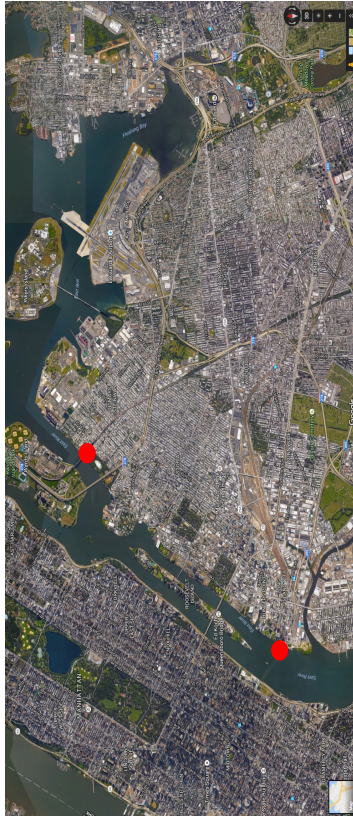
3.8keV → Ca K_{α}

9.97keV → Ge K_{α}

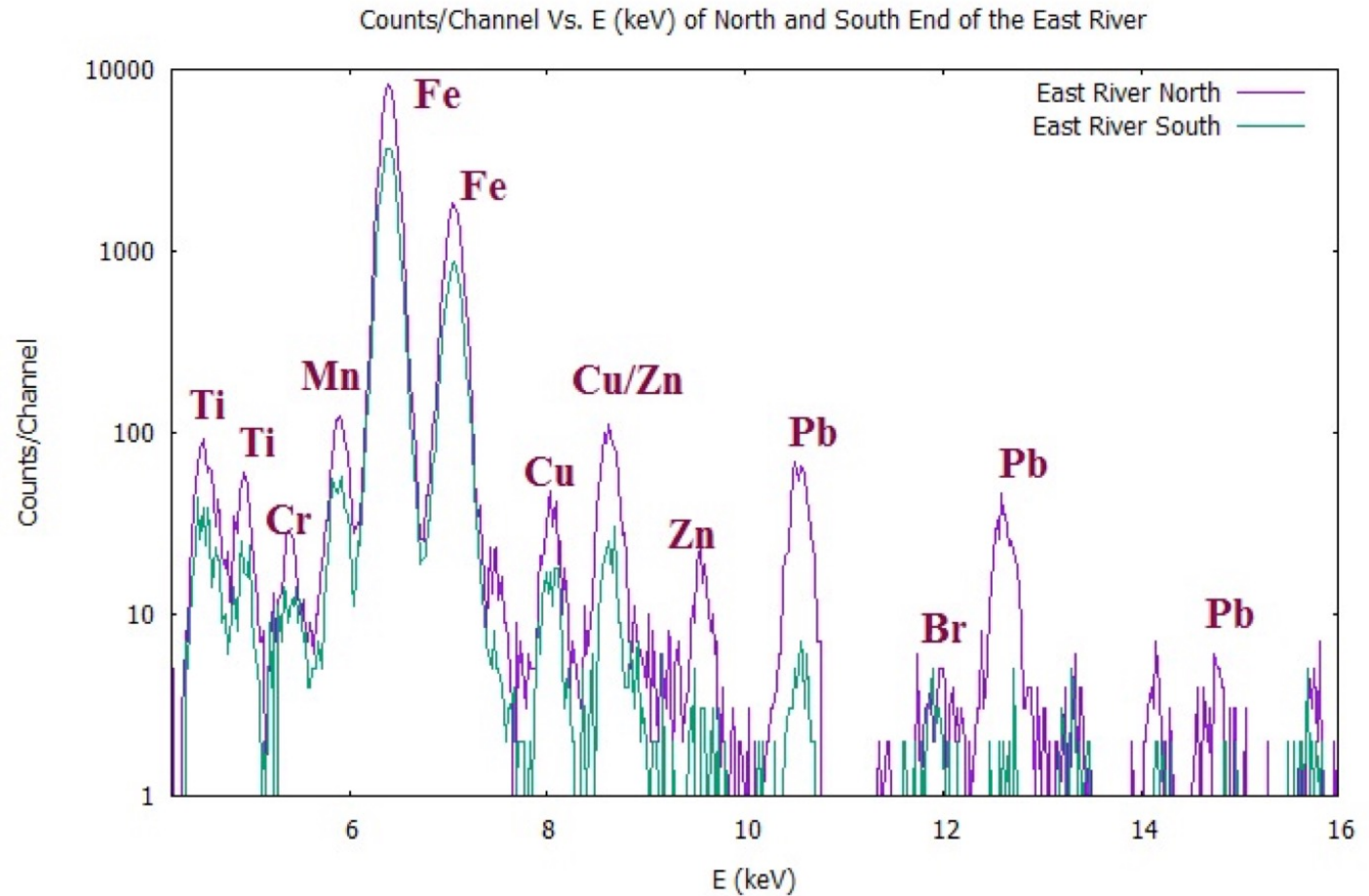
10.9keV → Ge K_{β}

Z	Element	Ka1	Ka2	Kb1	La1	La2	Lb1	Lb2	Lg1
3	Li	0.0543							
4	Be	0.1085							
5	B	0.1833							
6	C	0.277							
7	N	0.3924							
8	O	0.5249							
9	F	0.6768							
10	Ne	0.8486	0.8486						
11	Na	1.04098	1.04098	1.0711					
12	Mg	1.25360	1.25360	1.3022					
13	Al	1.48670	1.48627	1.55745					
14	Si	1.73998	1.73938	1.83594					
15	P	2.0137	2.0127	2.1391					
16	S	2.30784	2.30664	2.46404					
17	Cl	2.62239	2.62078	2.8156					
18	Ar	2.95770	2.95563	3.1905					
19	K	3.3138	3.3111	3.5896					
20	Ca	3.69168	3.68809	4.0127	0.3413	0.3413	0.3449		
21	Sc	4.0906	4.0861	4.4605	0.3954	0.3954	0.3996		
22	Ti	4.51084	4.50486	4.93181	0.4522	0.4522	0.4584		
23	V	4.95220	4.94464	5.42729	0.5113	0.5113	0.5192		
24	Cr	5.41472	5.405509	5.94671	0.5728	0.5728	0.5828		
25	Mn	5.89875	5.88765	6.49045	0.6374	0.6374	0.6488		
26	Fe	6.40384	6.39084	7.05798	0.7050	0.7050	0.7185		
27	Co	6.93032	6.91530	7.64943	0.7762	0.7762	0.7914		
28	Ni	7.47815	7.46089	8.26466	0.8515	0.8515	0.8688		
29	Cu	8.04778	8.02783	8.90529	0.9297	0.9297	0.9498		
30	Zn	8.63886	8.61578	9.5720	1.0117	1.0117	1.0347		
31	Ga	9.25174	9.22482	10.2642	1.09792	1.09792	1.1248		
32	Ge	9.88642	9.85532	10.9821	1.18800	1.18800	1.2185		
33	As	10.54372	10.50799	11.7262	1.2820	1.2820	1.3170		
34	Se	11.2224	11.1814	12.4959	1.37910	1.37910	1.41923		
35	Br	11.9242	11.8776	13.2014	1.48042	1.48042	1.52500		

Environmental Pollution Along the East River in Queens, New York



Google map showing the two locations that were originally taken; one sample was taken in Astoria Park and the other 3 miles south in Gantry State Park.



PIXE spectra on the soil samples taken from each park. What do you notice?

Environmental Pollution Along the East River in Queens, New York



On the left, Astoria State Park along the East River in North Queens.



On the right, Gantry Plaza State Park along the East River in South Queens.

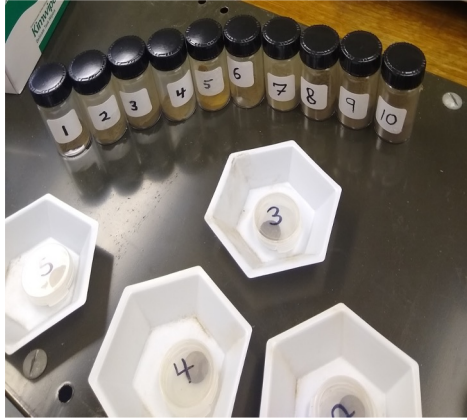
Source: <http://maps.google.com>

Environmental Pollution Along the East River in Queens, New York

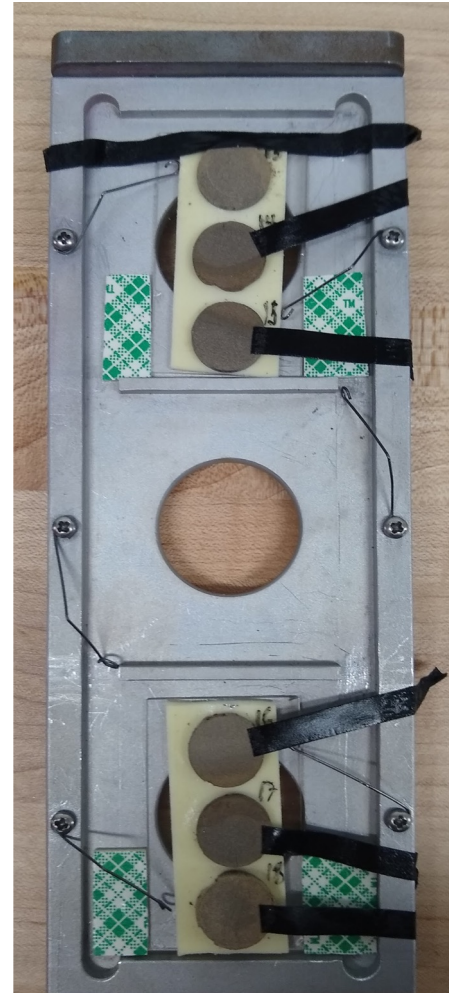


- Hell Gate Bridge is a 1000' railroad bridge built in 1916.
- Painted originally with Hell Gate Red, a lead-based paint.
- Sandblasted and repainted around 1990 with a non-lead-based paint.
- Is the bridge the source of the lead?

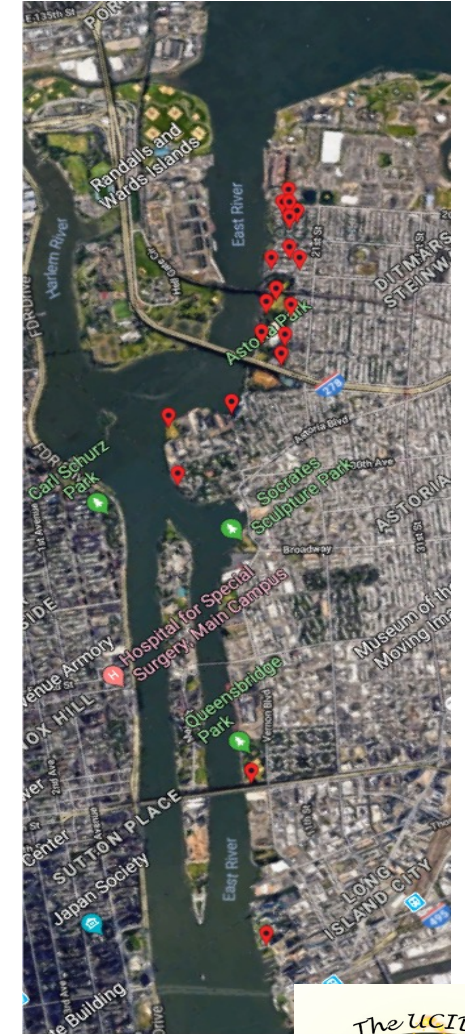
Environmental Pollution Along the East River in Queens, New York



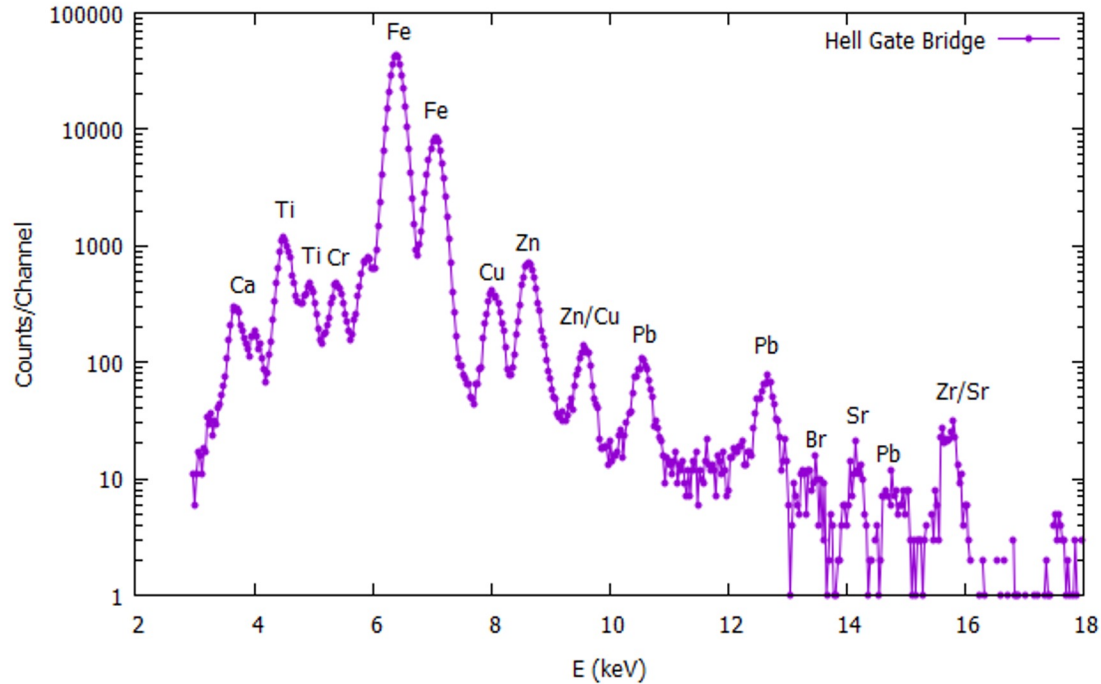
- We've taken 20 samples along the east river from Astoria to Gantry State park in 2018 – 2019.
- In the summer of 2019, we took 20 more samples surrounding the Hell Gate Bridge.
- Above are the soil samples from summer 2019 and on the right the soil pellets mounted on the target ladder.



On the right, a Google map showing the 20 sampling locations between Astoria State Park and Gantry Plaza State Park.

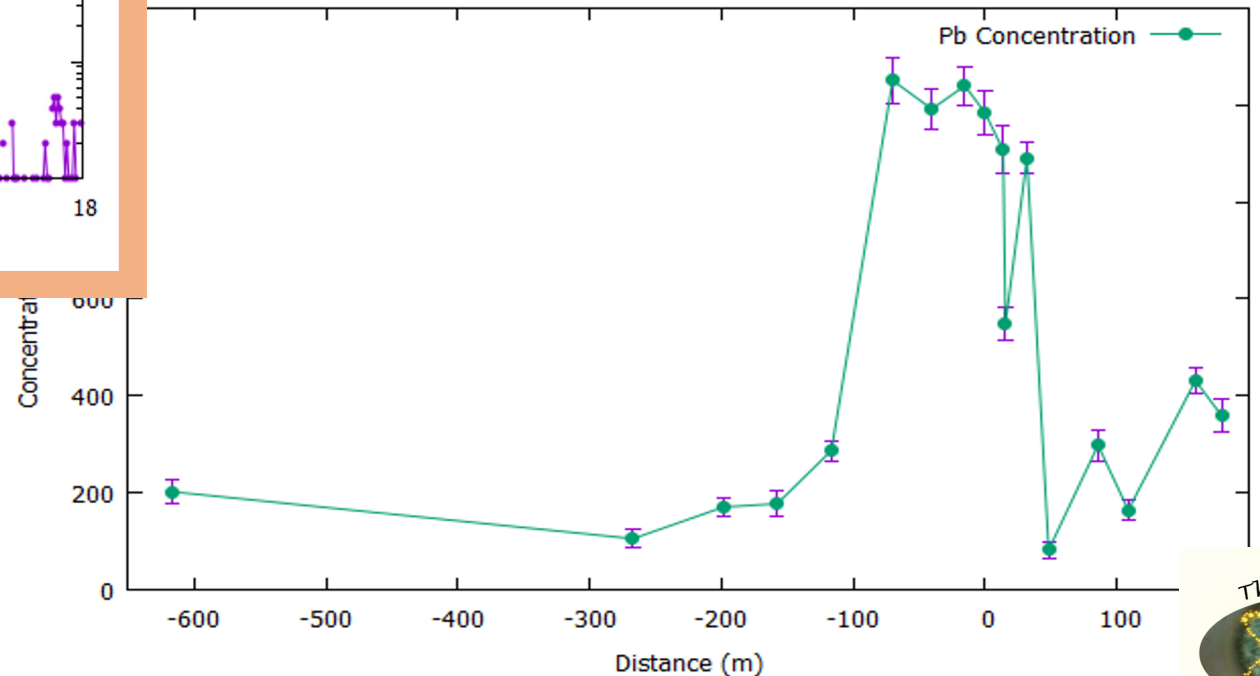


Environmental Pollution Along the East River in Queens, New York



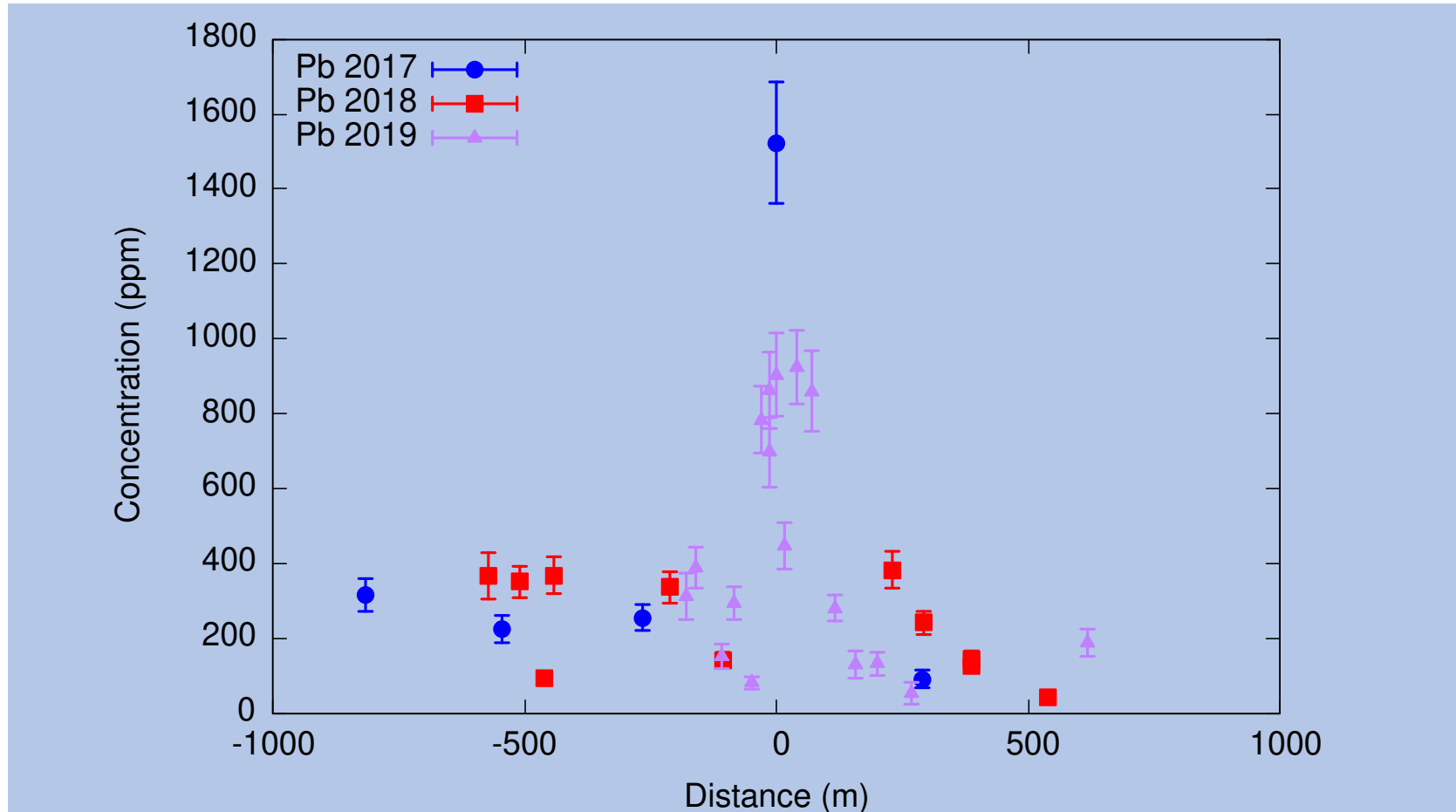
On the left, a typical PIXE spectrum for a soil sample taken near the Hell Gate Bridge, in Astoria, Queens, NY.

On the right, a plot of the lead concentration around the Hell Gate Bridge, in Astoria, Queens, NY.



Data/Graph: M. Villaneuve & S. LaBrake

Environmental Pollution Along the East River in Queens, New York



A plot of the lead concentration of samples taken around the Hell Gate Bridge as a function of distance from the bridge. The bridge is taken at zero and north of the bridge is taken as positive.

Conclusions

- So, we can calculate the x-ray transition energies to a high degree of accuracy.
- There are lots of other effects we haven't looked at, absorption of x-ray, attenuation of x-rays, failure to produce an x-ray (Auger electrons)...
- Screened Bohr model seems to work well to describe the transitions.
- X-ray energies for K-series transitions scale with $(Z - 1)^2$.
- L-series x-rays are more complicated how do we describe them?
- Further, how much of the elements are present?
- What are the environmental sources of the elements you found?
- What is the chemical identity of the elements – what are the elements bonded too?