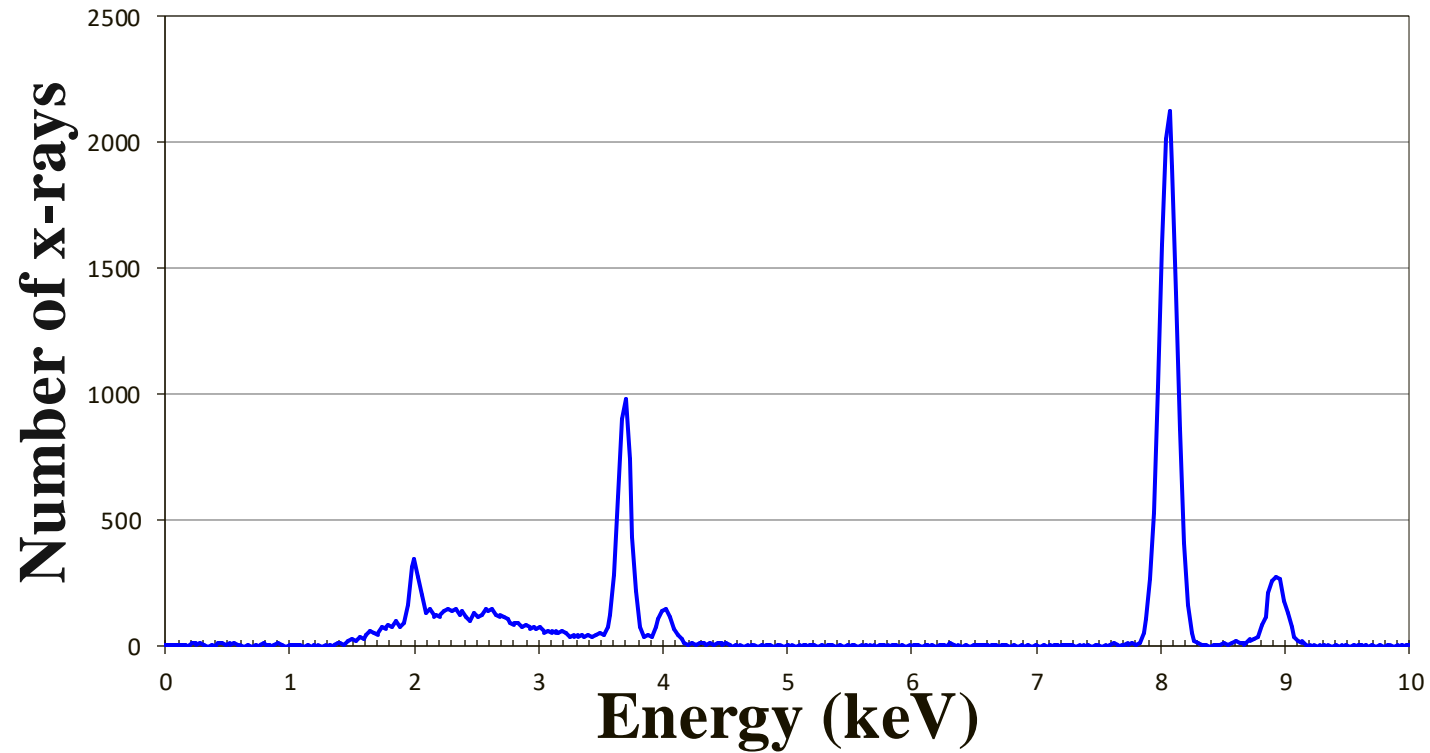


# *Determining the Elemental Target Make-up From The PIXE Spectrum*



# 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:

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

$$E_n = -\frac{Z^2 m e^4}{2(4\pi\epsilon_0)^2 n^2 \hbar^2} = -\left(\frac{m e^4}{2(4\pi\epsilon_0)^2 \hbar^2}\right) \frac{Z^2}{n^2}$$

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

$$= -(13.57 \text{ eV}) \frac{Z^2}{n^2}$$

# 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,  $K_{\alpha}$ :

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

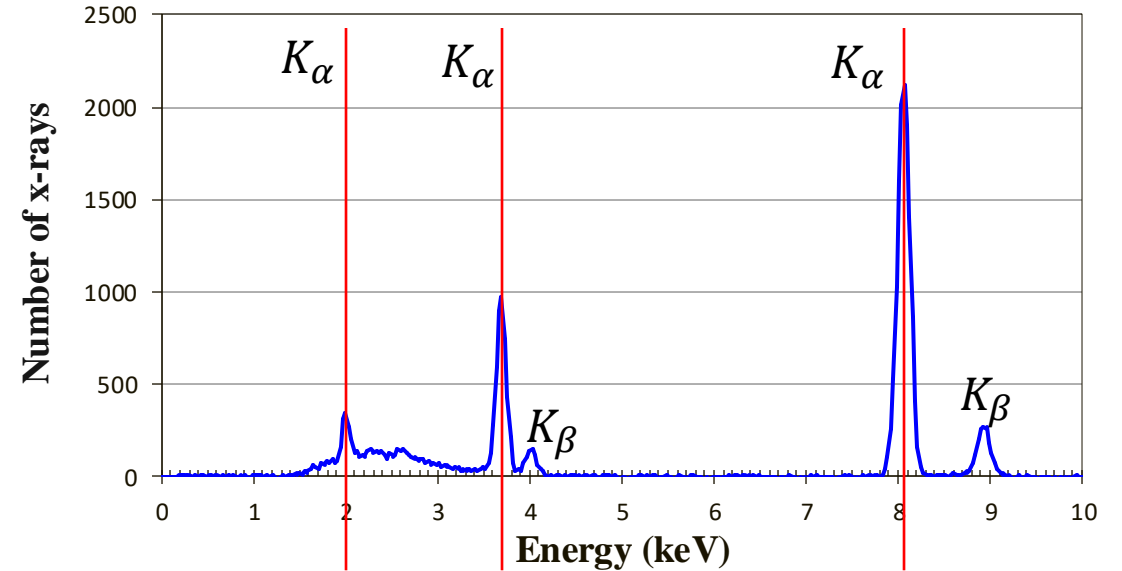
The main metal on the standard:

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

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 <sup>1</sup>	1s <sup>1</sup>																														
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										
[He]	[He]															[He]	[He]	[He]	[He]	[He]	[He]										
11	12															13	14	15	16	17	18										
Na	Mg															Al	Si	P	S	Cl	Ar										
Sodium	Magnesium															Aluminum	Silicon	Phosphorus	Sulfur	Chlorine	Argon										
[Ne]	[Ne]															[Ne]	[Ne]	[Ne]	[Ne]	[Ne]	[Ne]										
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														
[Ar]	[Ar]	[Ar]	[Ar]	[Ar]	[Ar]	[Ar]	[Ar]	[Ar]	[Ar]	[Ar]	[Ar]	[Ar]	[Ar]	[Ar]	[Ar]	[Ar]	[Ar]														
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														
[Kr]	[Kr]	[Kr]	[Kr]	[Kr]	[Kr]	[Kr]	[Kr]	[Kr]	[Kr]	[Kr]	[Kr]	[Kr]	[Kr]	[Kr]	[Kr]	[Kr]	[Kr]														
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	
[Xe]	[Xe]															[Xe]	[Xe]	[Xe]	[Xe]	[Xe]	[Xe]	[Xe]	[Xe]	[Xe]	[Xe]	[Xe]	[Xe]	[Xe]	[Xe]	[Xe]	
87	88															104	105	106	107	108	109	110	111	112	113	114	115	116	117	118	119
Ra																Rf	Db	Sg	Hs	Mt	Ds	Rg	Cn	Nh	Fl	Mc	Lv	Ts	Og		
Radium																Rutherfordium	Dubnium	Seaborgium	Hassium	Moscovium	Darmstadtium	Roentgenium	Copernicium	Nihonium	Flerovium	Moscovium	Livermorium	Tennessine	Oganesson		
[Rn]	[Rn]															[Rn]	[Rn]	[Rn]	[Rn]	[Rn]	[Rn]	[Rn]	[Rn]	[Rn]	[Rn]	[Rn]	[Rn]	[Rn]	[Rn]	[Rn]	
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																	
[Xe]	[Xe]	[Xe]	[Xe]	[Xe]	[Xe]	[Xe]	[Xe]	[Xe]	[Xe]	[Xe]	[Xe]	[Xe]	[Xe]	[Xe]																	
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																	
[Rn]	[Rn]	[Rn]	[Rn]	[Rn]	[Rn]	[Rn]	[Rn]	[Rn]	[Rn]	[Rn]	[Rn]	[Rn]	[Rn]	[Rn]																	

<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,  $K_\beta$ :

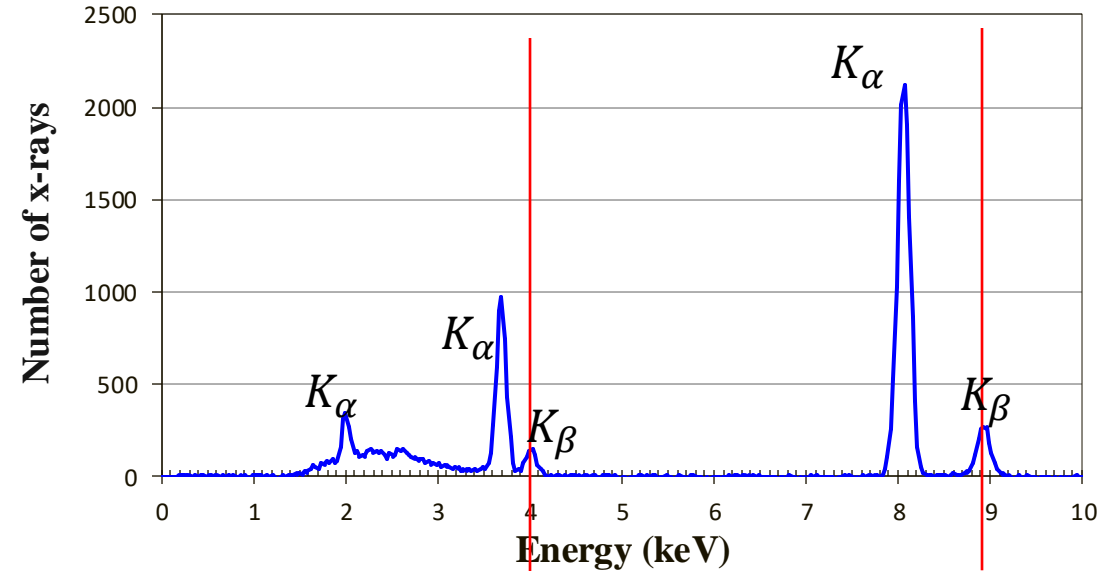
$$n_{upper} = 3; \quad n_{lower} = 1$$

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:

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

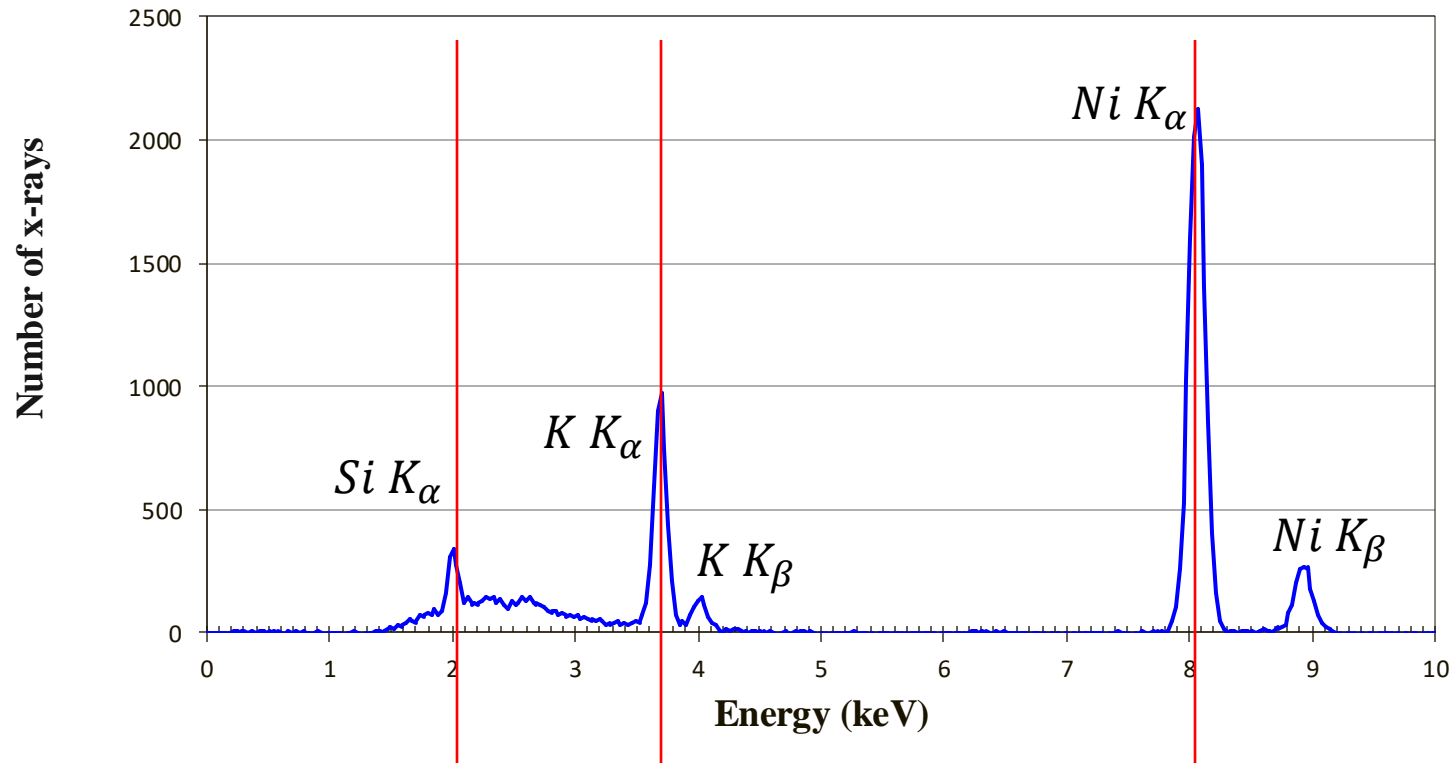


## PERIODIC TABLE OF ELEMENTS

PubChem																															
1	1																2														
H	H																He														
Hydrogen	Hydrogen																Helium														
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H	Symbol																He														
Hydrogen	Name																Helium														
1s <sup>1</sup>	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	
Fr	Ra															Rf	Db	Sg	Hs	Mt	Ds	Rg	Cn	Nh	Fl	Mc	Lv	Ts	Og		
Francium	Radium															Rutherfordium	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
																		La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb
																		Lanthanum	Cerium	Praseodymium	Neodymium	Promethium	Samarium	Europium	Gadolinium	Terbium	Dysprosium	Holmium	Erbium	Thulium	Ytterbium
																		89	90	91	92	93	94	95	96	97	98	99	100	101	102
																		Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No
																		Actinium	Thorium	Protactinium	Uranium	Neptunium	Plutonium	Americium	Curium	Berkelium	Californium	Einsteinium	Fermium	Mendelevium	Nobelium

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

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.
- $\Delta E$  is what  $\Delta E$  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,  $K_\alpha$ :

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

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

The image shows a standard periodic table of elements from PubChem. The table is color-coded by groups and includes element symbols, atomic numbers, and names. A callout box for Hydrogen (H) is shown, detailing its atomic number (1), symbol (H), name (Hydrogen), and electron configuration (1s<sup>1</sup>).

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



# The Characteristic X-ray Energies & Elemental Identification

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

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

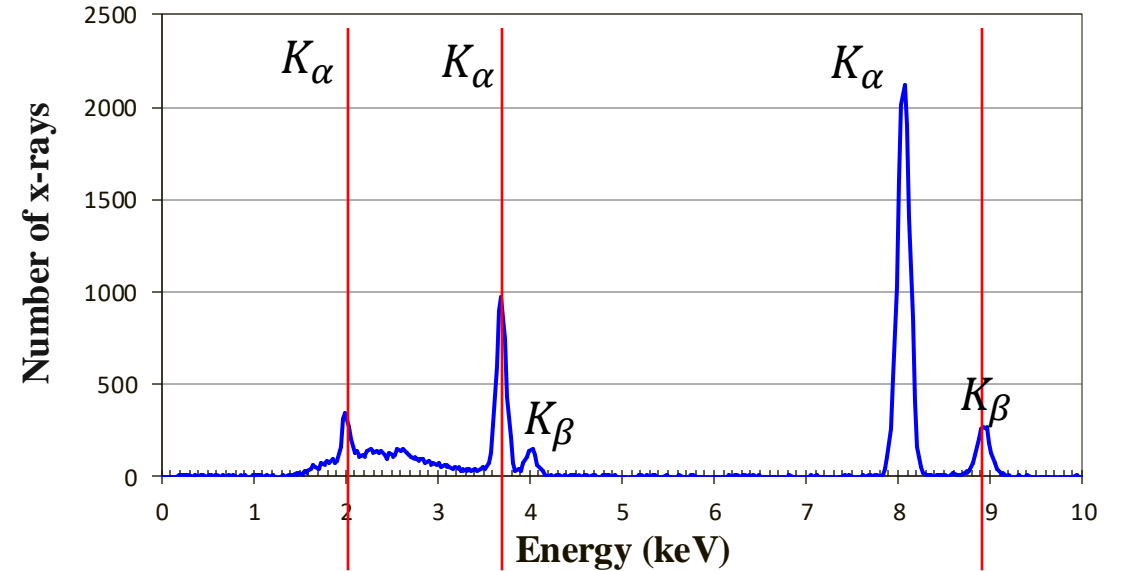
The higher energy/lower probability transition,  $K_{\beta}$ :

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

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  $K_{\beta}$  transitions should also be corrected. It's not as simple to do as the  $K_{\alpha}$  transitions.

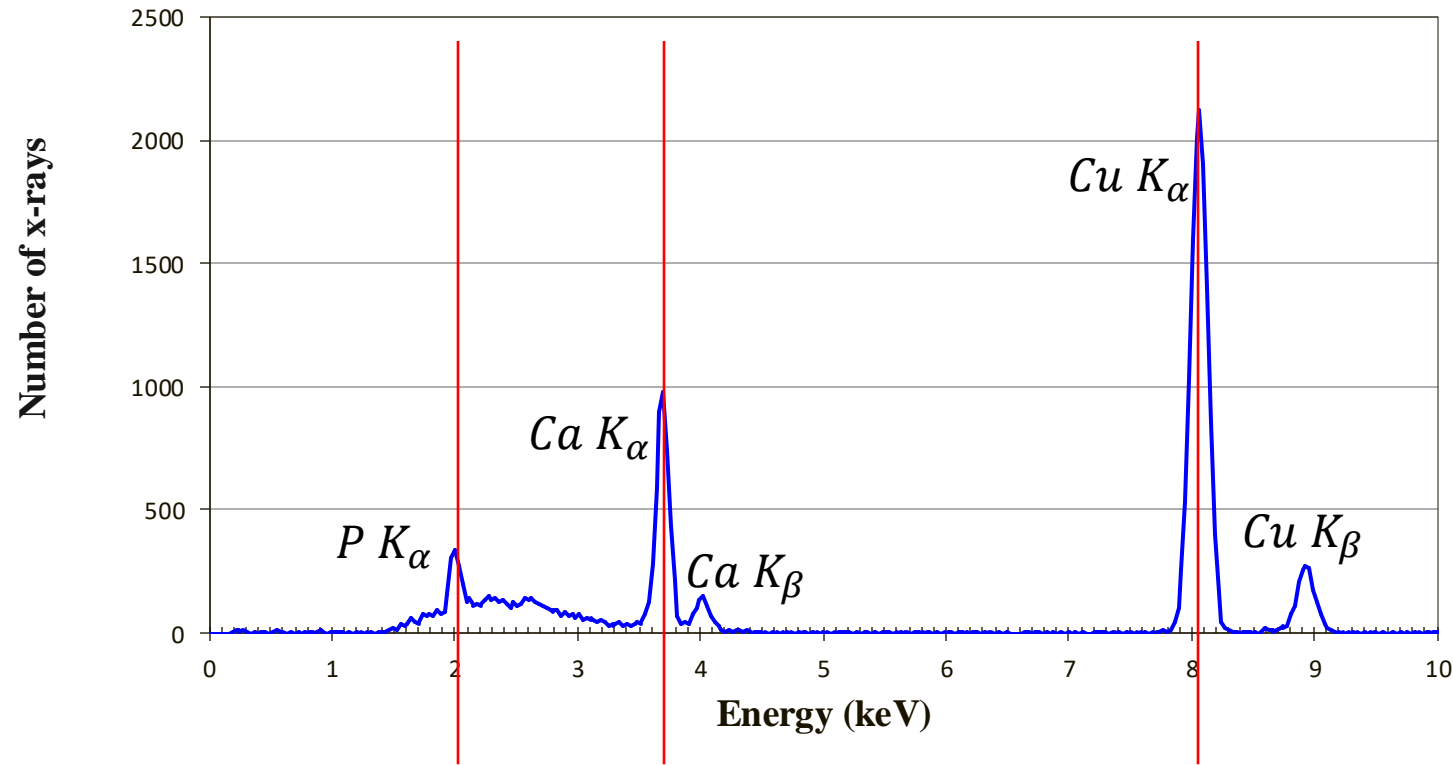


## PERIODIC TABLE OF ELEMENTS

PubChem																				
1																	2			
H Hydrogen 1s <sup>1</sup>																	He Helium			
3	4															10				
Li Lithium	Be Beryllium															Ne Neon				
11	12															18				
Na Sodium	Mg Magnesium															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															82	83	84	85	86
Cs Cesium	Ba Barium															Pb Lead	Bi Bismuth	Po Polonium	At Astatine	Rn Radon
87	88															116	117	118		
Fr Francium	Ra Radium															Lv Livermorium	Ts Tennessine	Og Oganesson		
Lanthanides																				
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									
Actinides																				
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									

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

# The Characteristic X-ray Energies & Elemental Identification

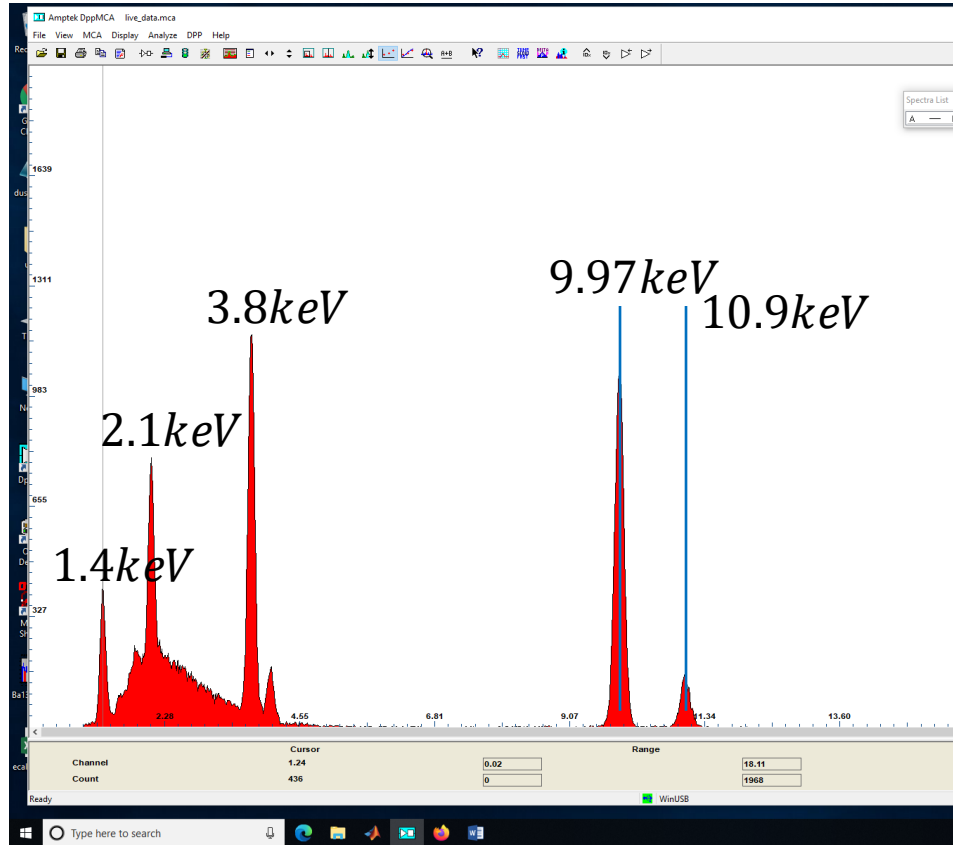


The single element standards are used to calibrate the energy scale so that we can run a real sample.

# The X-Ray Energy Table For Elemental Identification

## Characteristic X-Ray Energies

(X-ray Energies in keV)

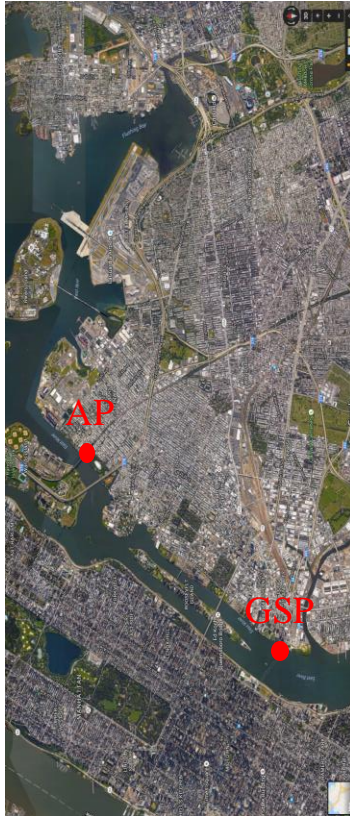


1.4keV → Al  $K_{\alpha}$   
 2.1keV → P  $K_{\alpha}$   
 3.8keV → Ca  $K_{\alpha}$

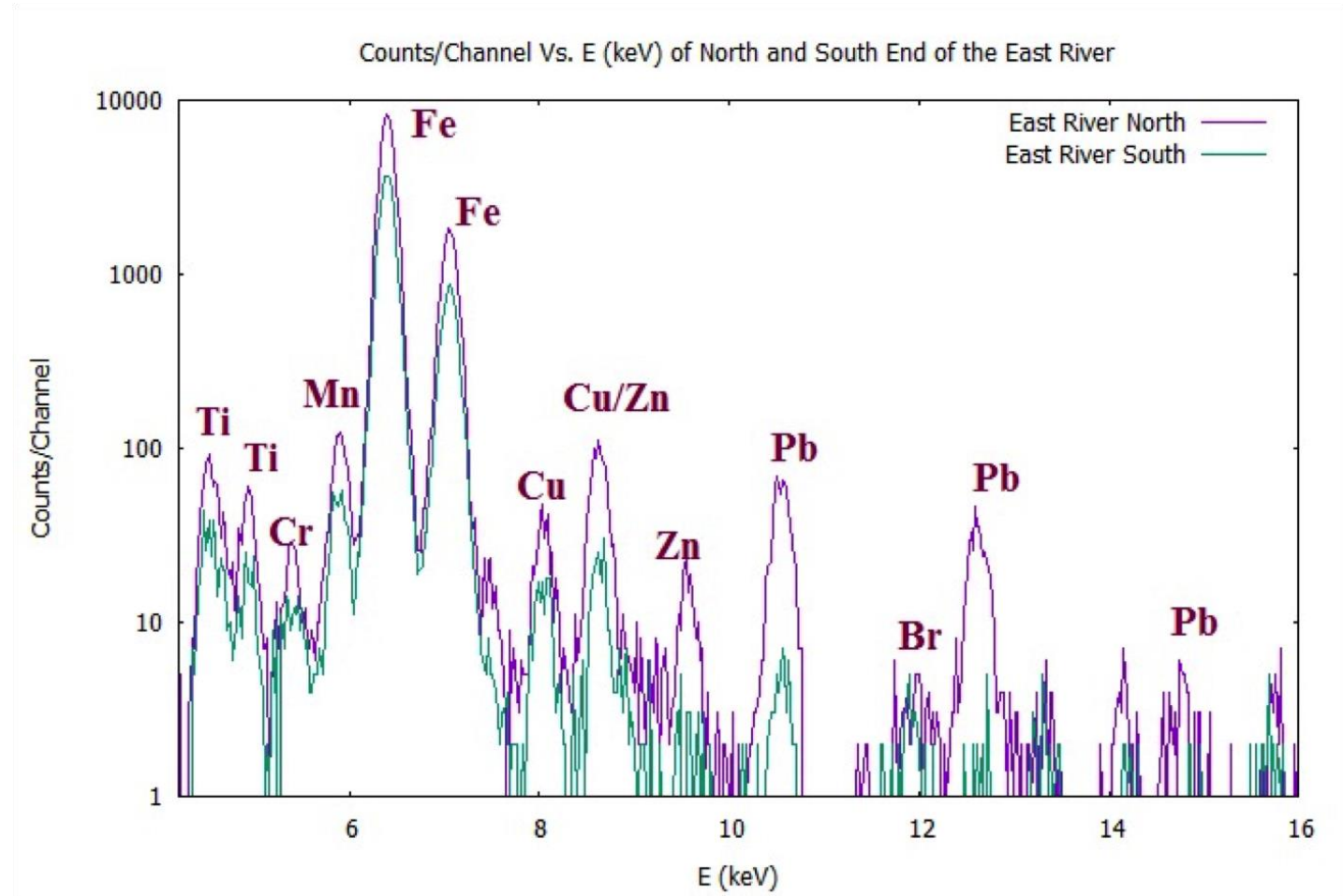
9.97keV → Ge  $K_{\alpha}$   
 10.9keV → Ge  $K_{\beta}$

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	11.9042	11.8575	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.

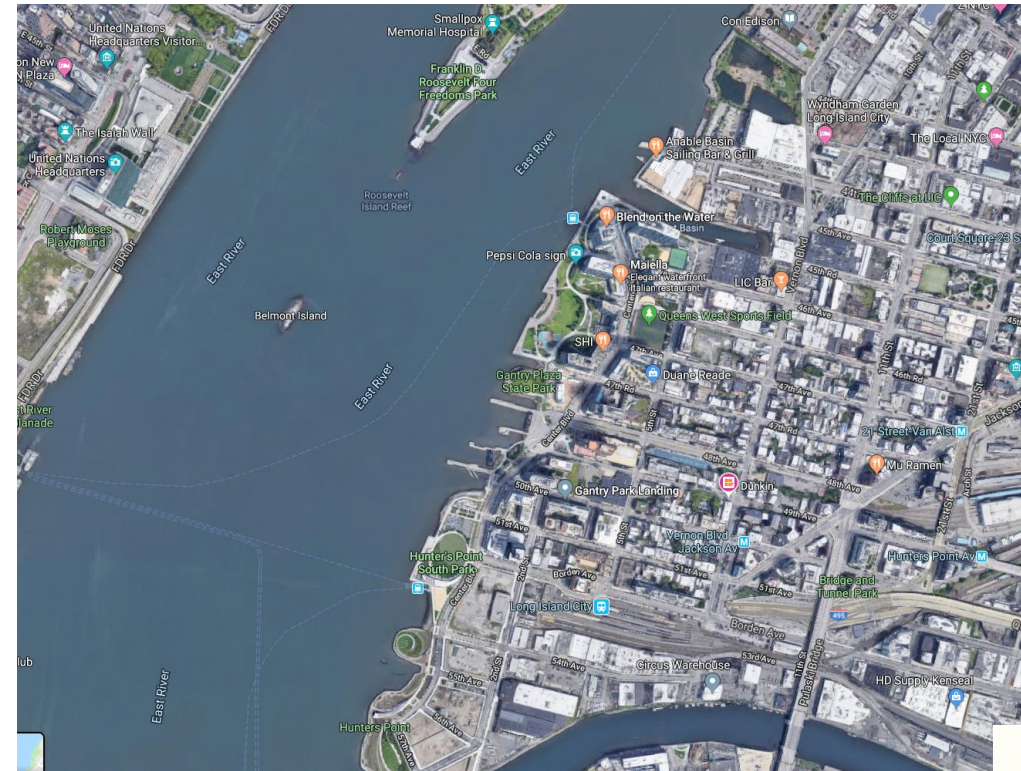


PIXE spectra on the soil samples taken from each park. What do you notice?

# 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.

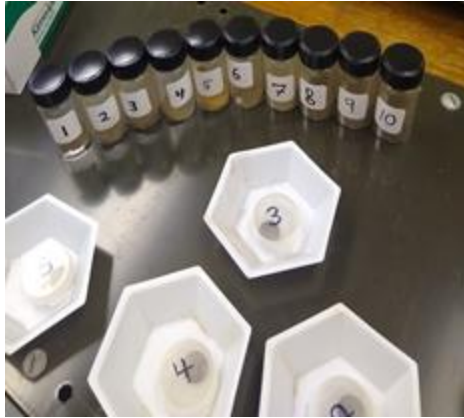
Source: <http://maps.google.com>

# Environmental Pollution Along the East River in Queens, New York

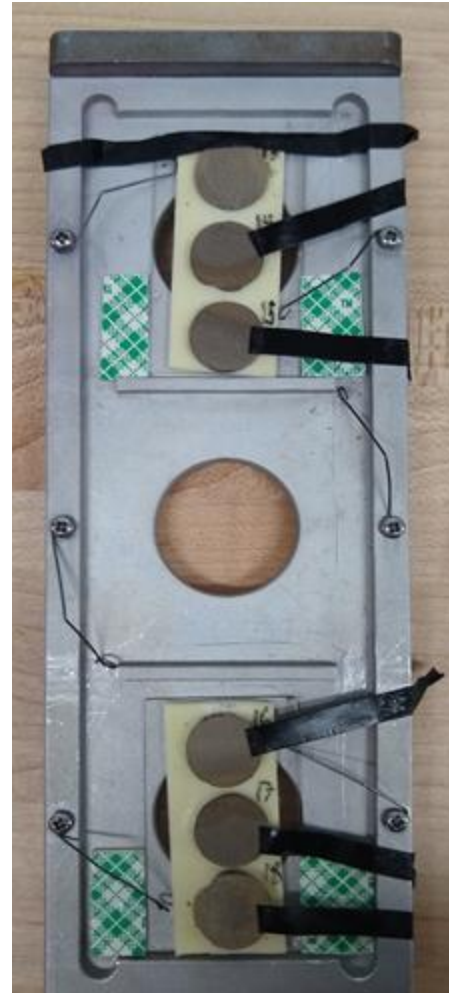


- Hell Gate Bridge is a 1000' railroad bridge built in 1916.
- Painted originally with Hell Gate Red, a lead-based paint.
- Sandblasted and repainted around 1990 with a non-lead-based paint.
- Is the bridge the source of the lead?

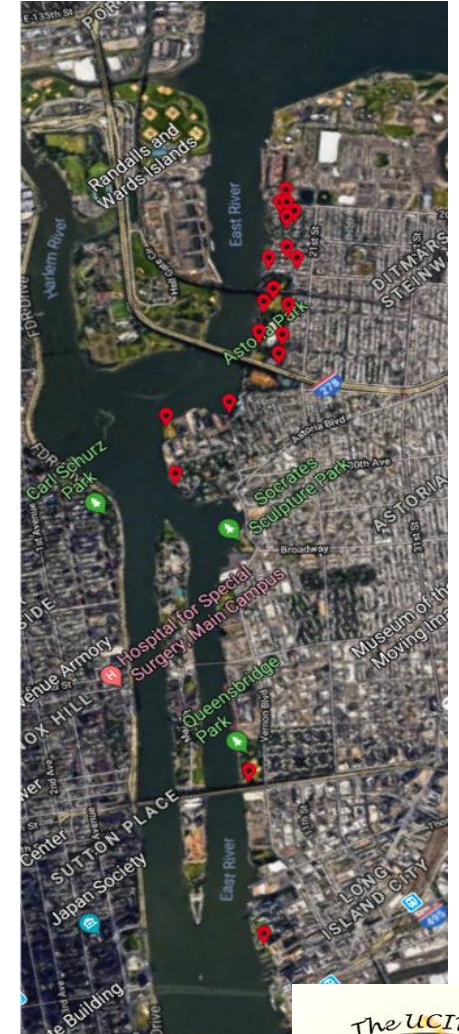
# Environmental Pollution Along the East River in Queens, New York



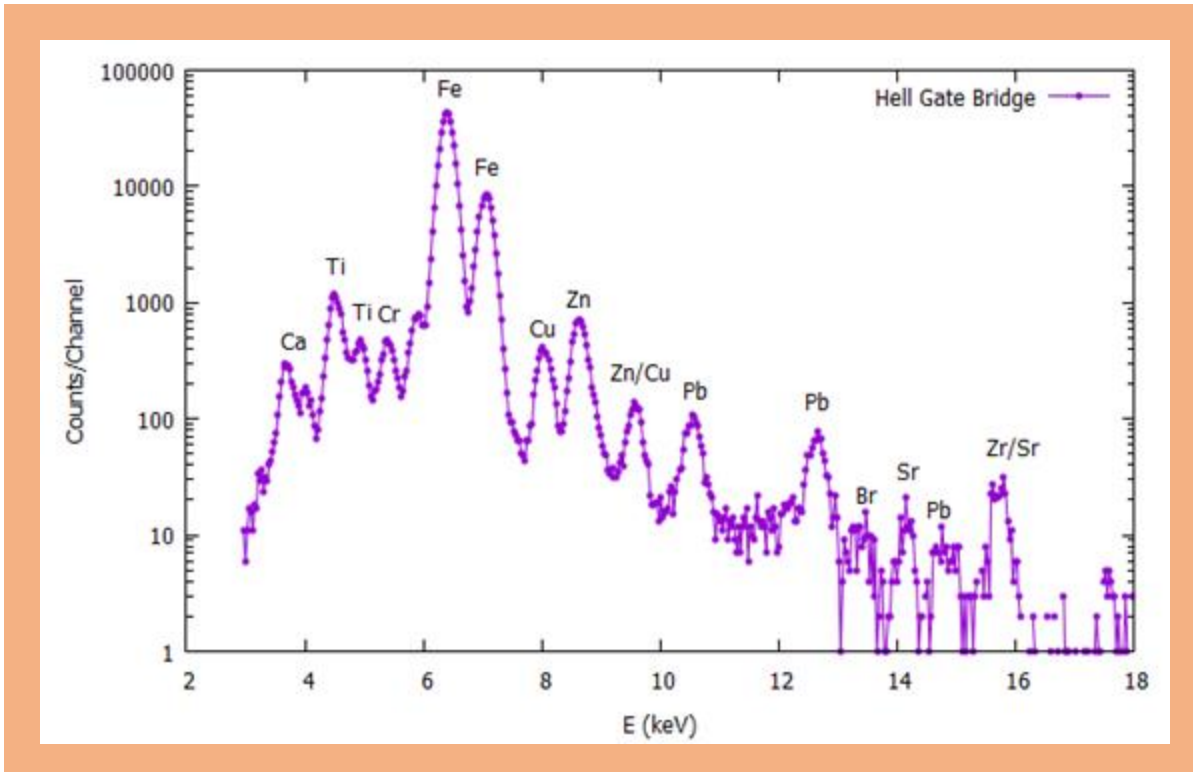
- We've taken 20 samples along the east river from Astoria to Gantry State park in 2018 – 2019.
- In the summer of 2019, we took 20 more samples surrounding the Hell Gate Bridge.
- Above are the soil samples from summer 2019 and on the right the soil pellets mounted on the target ladder.



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

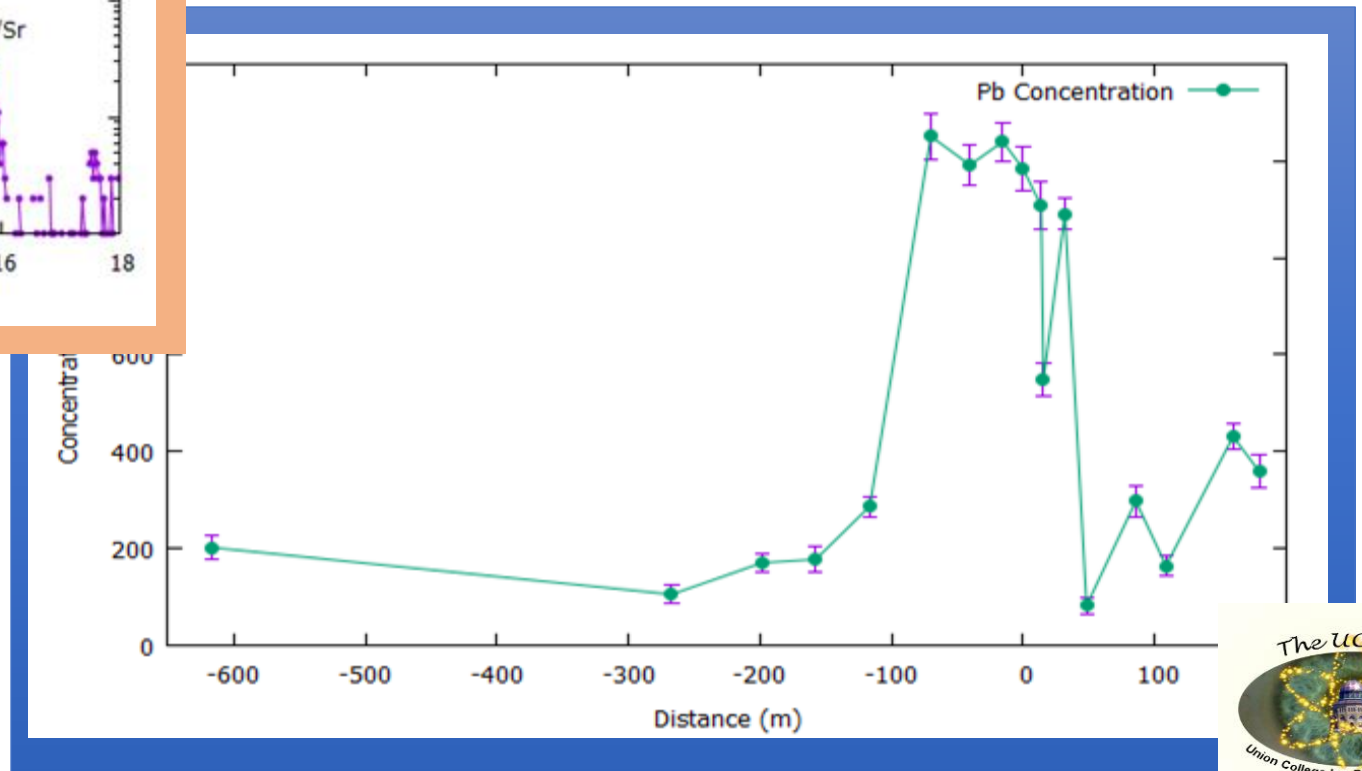


# Environmental Pollution Along the East River in Queens, New York



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

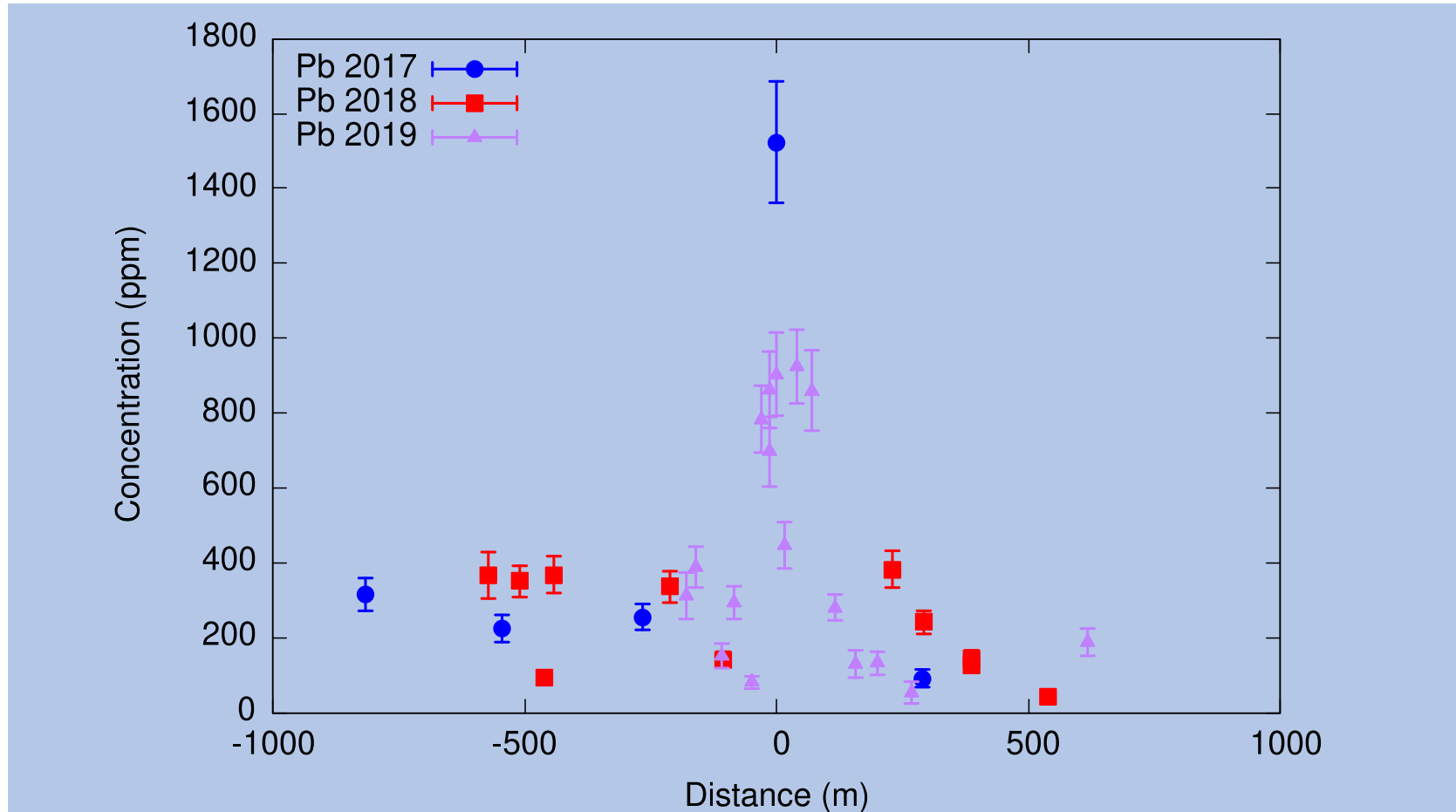
On the right, a plot of the lead concentration around the Hell Gate Bridge, in Astoria, Queens, NY.



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?