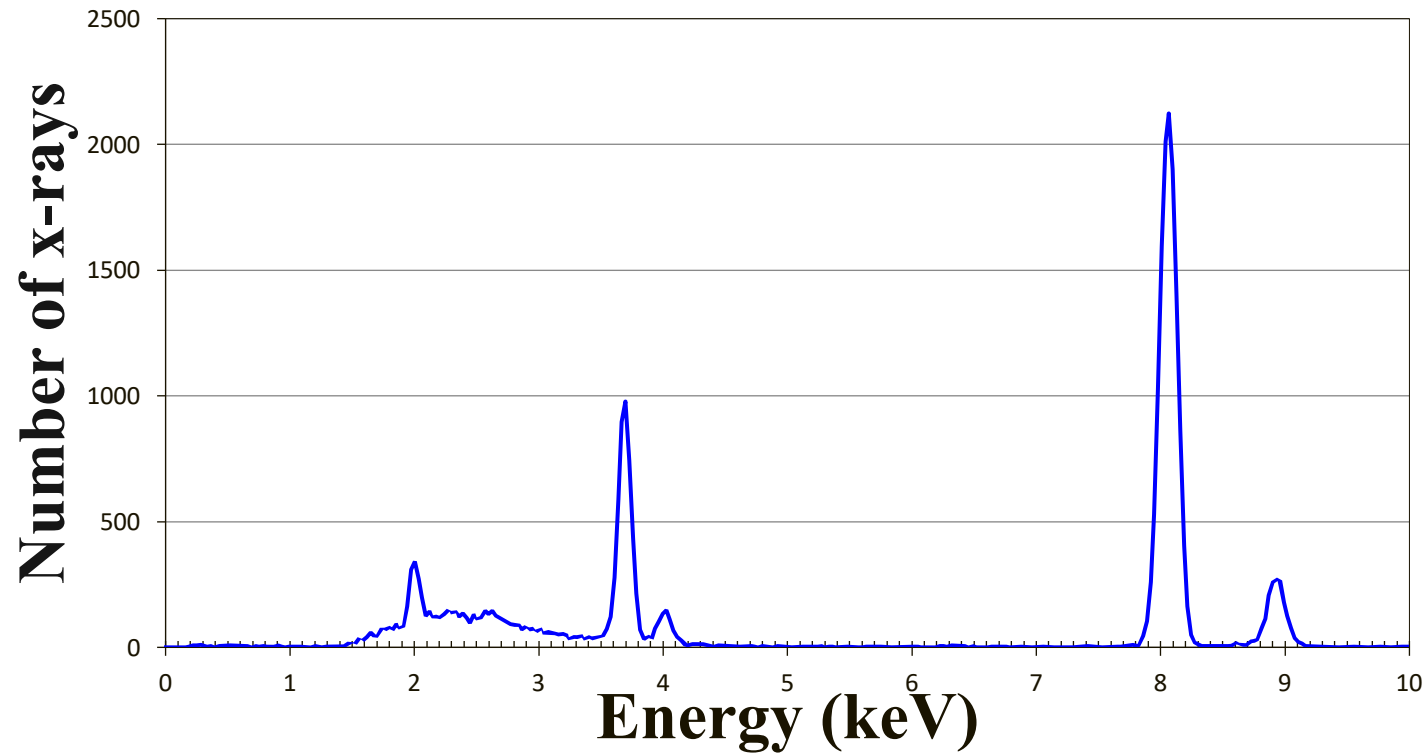


Determining the Elemental Target Make-up From The PIXE Spectrum



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} :

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

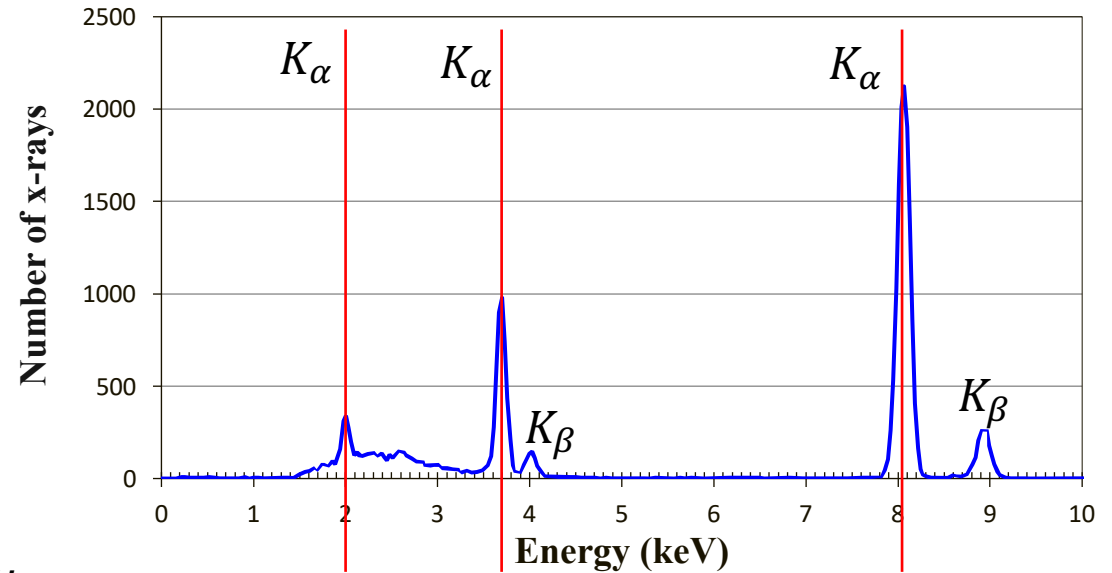
The main metal on the standard:

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

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

1

H

Hydrogen

3

Li

Lithium

4

Be

Beryllium

11

Na

Sodium

12

Mg

Magnesium

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

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

72

Hf

Hafnium

73

Ta

Tantalum

74

W

Tungsten

75

Re

Rhenium

76

Os

Osmium

77

Ir

Iridium

78

Pt

Platinum

79

Au

Gold

80

Hg

Mercury

81

Tl

Thallium

82

Pb

Lead

83

Bi

Bismuth

84

Po

Polonium

85

At

Astatine

86

Rn

Radon

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

104

Rf

Rutherfordium

105

Db

Dubnium

106

Sg

Seaborgium

107

Bh

Bohrium

108

Hs

Hassium

109

Mt

Meitnerium

110

Ds

Darmstadtium

111

Rg

Roentgenium

112

Cn

Copernicium

113

Nh

Nihonium

114

Fl

Flerovium

115

Mc

Moscovium

116

Lv

Livermorium

117

Ts

Tennessine

118

Og

Oganesson

1

H

Hydrogen

2

He

Helium

PubChem

Atomic Number

Symbol

Name

Electron Configuration

5

B

Boron

6

C

Carbon

7

N

Nitrogen

8

O

Oxygen

9

F

Fluorine

10

Ne

Neon

13

Al

Aluminum

14

Si

Silicon

15

P

Phosphorus

16

S

Sulfur

17

Cl

Chlorine

18

Ar

Argon

31

Ga

Gallium

32

Ge

Germanium

33

As

Arsenic

34

Se

Selenium

35

Br

Bromine

36

Kr

Krypton

49

In

Indium

50

Sn

Tin

51

Sb

Antimony

52

Te

Tellurium

53

I

Iodine

54

Xe

Xenon

81

Tl

Thallium

82

Pb

Lead

83

Bi

Bismuth

84

Po

Polonium

85

At

Astatine

86

Rn

Radon

113

Nh

Nihonium

114

Fl

Flerovium

115

Mc

Moscovium

116

Lv

Livermorium

117

Ts

Tennessine

118

Og

Oganesson

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

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

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



Union College Ion-Beam Analysis Lab

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 :

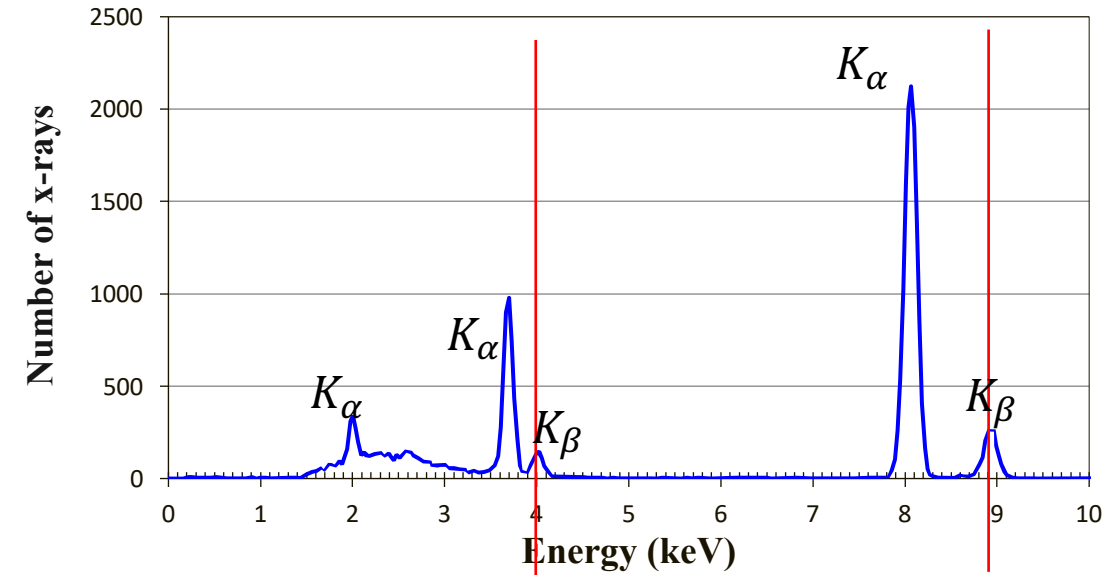
$$n_{upper} = 3; \quad n_{lower} = 1$$

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

1

H

Hydrogen

1s¹

2

He

Helium

1s²

3

Li

Lithium

[He] 2s¹

4

Be

Beryllium

[He] 2s²

5

B

Boron

[He] 2s² 2p¹

6

C

Carbon

[He] 2s² 2p²

7

N

Nitrogen

[He] 2s² 2p³

8

O

Oxygen

[He] 2s² 2p⁴

9

F

Fluorine

[He] 2s² 2p⁵

10

Ne

Neon

[He] 2s² 2p⁶

11

Na

Sodium

[Ne] 3s¹

12

Mg

Magnesium

[Ne] 3s²

13

Al

Aluminum

[Ne] 3s² 3p¹

14

Si

Silicon

[Ne] 3s² 3p²

15

P

Phosphorus

[Ne] 3s² 3p³

16

S

Sulfur

[Ne] 3s² 3p⁴

17

Cl

Chlorine

[Ne] 3s² 3p⁵

18

Ar

Argon

[Ne] 3s² 3p⁶

19

K

Potassium

[Ar] 4s¹

20

Ca

Calcium

[Ar] 4s²

21

Sc

Scandium

[Ar] 3d¹ 4s²

22

Ti

Titanium

[Ar] 3d² 4s²

23

V

Vanadium

[Ar] 3d³ 4s²

24

Cr

Chromium

[Ar] 3d⁵ 4s¹

25

Mn

Manganese

[Ar] 3d⁵ 4s²

26

Fe

Iron

[Ar] 3d⁶ 4s²

27

Co

Cobalt

[Ar] 3d⁷ 4s²

28

Ni

Nickel

[Ar] 3d⁸ 4s²

29

Cu

Copper

[Ar] 3d¹⁰ 4s¹

30

Zn

Zinc

[Ar] 3d¹⁰ 4s²

31

Ga

Gallium

[Ar] 3d¹⁰ 4s² 4p¹

32

Ge

Germanium

[Ar] 3d¹⁰ 4s² 4p²

33

As

Arsenic

[Ar] 3d¹⁰ 4s² 4p³

34

Se

Selenium

[Ar] 3d¹⁰ 4s² 4p⁴

35

Br

Bromine

[Ar] 3d¹⁰ 4s² 4p⁵

36

Kr

Krypton

[Ar] 3d¹⁰ 4s² 4p⁶

37

Rb

Rubidium

[Kr] 5s¹

38

Sr

Strontium

[Kr] 5s²

39

Y

Yttrium

[Kr] 4d¹ 5s²

40

Zr

Zirconium

[Kr] 4d² 5s²

41

Nb

Niobium

[Kr] 4d⁴ 5s¹

42

Mo

Molybdenum

[Kr] 4d⁵ 5s¹

43

Tc

Technetium

[Kr] 4d⁵ 5s²

44

Ru

Ruthenium

[Kr] 4d⁷ 5s¹

45

Rh

Rhodium

[Kr] 4d⁸ 5s¹

46

Pd

Palladium

[Kr] 4d¹⁰

47

Ag

Silver

[Kr] 4d¹⁰ 5s¹

48

Cd

Cadmium

[Kr] 4d¹⁰ 5s²

49

In

Indium

[Kr] 4d¹⁰ 5s² 5p¹

50

Sn

Tin

[Kr] 4d¹⁰ 5s² 5p²

51

Sb

Antimony

[Kr] 4d¹⁰ 5s² 5p³

52

Te

Tellurium

[Kr] 4d¹⁰ 5s² 5p⁴

53

I

Iodine

[Kr] 4d¹⁰ 5s² 5p⁵

54

Xe

Xenon

[Kr] 4d¹⁰ 5s² 5p⁶

55

Cs

Cesium

[Xe] 6s¹

56

Ba

Barium

[Xe] 6s²

57

La

Lanthanum

[Xe] 5d¹ 6s²

58

Ce

Cerium

[Xe] 4f¹ 5d¹ 6s²

59

Pr

Praseodymium

[Xe] 4f³ 6s²

60

Nd

Neodymium

[Xe] 4f⁴ 6s²

61

Pm

Promethium

[Xe] 4f⁵ 6s²

62

Sm

Samarium

[Xe] 4f⁶ 6s²

63

Eu

Europium

[Xe] 4f⁷ 6s²

64

Gd

Gadolinium

[Xe] 4f⁷ 5d¹ 6s²

65

Tb

Terbium

[Xe] 4f⁹ 6s²

66

Dy

Dysprosium

[Xe] 4f¹⁰ 6s²

67

Ho

Holmium

[Xe] 4f¹¹ 6s²

68

Er

Erbium

[Xe] 4f¹² 6s²

69

Tm

Thulium

[Xe] 4f¹³ 6s²

70

Yb

Ytterbium

[Xe] 4f¹⁴ 6s²

71

Lu

Lutetium

[Xe] 4f¹⁴ 5d¹ 6s²

72

Hf

Hafnium

[Xe] 4f¹⁴ 5d² 6s²

73

Ta

Tantalum

[Xe] 4f¹⁴ 5d³ 6s²

74

W

Tungsten

[Xe] 4f¹⁴ 5d⁴ 6s²

75

Re

Rhenium

[Xe] 4f¹⁴ 5d⁵ 6s²

76

Os

Osmium

[Xe] 4f¹⁴ 5d⁶ 6s²

77

Ir

Iridium

[Xe] 4f¹⁴ 5d⁷ 6s²

78

Pt

Platinum

[Xe] 4f¹⁴ 5d⁹ 6s¹

79

Au

Gold

[Xe] 4f¹⁴ 5d¹⁰ 6s¹

80

Hg

Mercury

[Xe] 4f¹⁴ 5d¹⁰ 6s²

81

Tl

Thallium

[Xe] 4f¹⁴ 5d¹⁰ 6s² 6p¹

82

Pb

Lead

[Xe] 4f¹⁴ 5d¹⁰ 6s² 6p²

83

Bi

Bismuth

[Xe] 4f¹⁴ 5d¹⁰ 6s² 6p³

84

Po

Polonium

[Xe] 4f¹⁴ 5d¹⁰ 6s² 6p⁴

85

At

Astatine

[Xe] 4f¹⁴ 5d¹⁰ 6s² 6p⁵

86

Rn

Radon

[Xe] 4f¹⁴ 5d¹⁰ 6s² 6p⁶

87

Fr

Francium

[Rn] 7s¹

88

Ra

Radium

[Rn] 7s²

89

Ac

Actinium

[Rn] 6d¹ 7s²

90

Th

Thorium

[Rn] 6d² 7s²

91

Pa

Protactinium

[Rn] 5f² 6d¹ 7s²

92

U

Uranium

[Rn] 5f³ 6d¹ 7s²

93

Np

Neptunium

[Rn] 5f⁴ 6d¹ 7s²

94

Pu

Plutonium

[Rn] 5f⁶ 7s²

95

Am

Americium

[Rn] 5f⁷ 7s²

96

Cm

Curium

[Rn] 5f⁸ 7s²

97

Bk

Berkelium

[Rn] 5f⁹ 7s²

98

Cf

Californium

[Rn] 5f¹⁰ 7s²

99

Es

Einsteinium

[Rn] 5f¹¹ 7s²

100

Fm

Fermium

[Rn] 5f¹² 7s²

101

Md

Mendelevium

[Rn] 5f¹³ 7s²

102

No

Nobelium

[Rn] 5f¹⁴ 7s²

103

Lr

Lawrencium

[Rn] 5f¹⁴ 6d¹ 7s²

104

Rg

Roentgenium

[Rn] 5f¹⁴ 6d² 7s²

105

Nh

Nihonium

[Rn] 5f¹⁴ 6d³ 7s²

106

Fl

Flerovium

[Rn] 5f¹⁴ 6d⁴ 7s²

107

Mc

Moscovium

[Rn] 5f¹⁴ 6d⁵ 7s²

108

Lv

Livermorium

[Rn] 5f¹⁴ 6d⁶ 7s²

109

Ts

Tennessine

[Rn] 5f¹⁴ 6d⁷ 7s²

110

Og

Oganesson

[Rn] 5f¹⁴ 6d⁸ 7s²

1

H

Hydrogen

1s¹

2

He

Helium

1s²

3

Li

Lithium

[He] 2s¹

4

Be

Beryllium

[He] 2s²

5

B

Boron

[He] 2s² 2p¹

6

C

Carbon

[He] 2s² 2p²

7

N

Nitrogen

[He] 2s² 2p³

8

O

Oxygen

[He] 2s² 2p⁴

9

F

Fluorine

[He] 2s² 2p⁵

10

Ne

Neon

[He] 2s² 2p⁶

11

Na

Sodium

[Ne] 3s¹

12

Mg

Magnesium

[Ne] 3s²

13

Al

Aluminum

[Ne] 3s² 3p¹

14

Si

Silicon

[Ne] 3s² 3p²

15

P

Phosphorus

[Ne] 3s² 3p³

16

S

Sulfur

[Ne] 3s² 3p⁴

17

Cl

Chlorine

[Ne] 3s² 3p⁵

18

Ar

Argon

[Ne] 3s² 3p⁶

19

K

Potassium

[Ar] 4s¹

20

Ca

Calcium

[Ar] 4s²

21

Sc

Scandium

[Ar] 3d¹ 4s²

22

Ti

Titanium

[Ar] 3d² 4s²

23

V

Vanadium

[Ar] 3d³ 4s²

24

Cr

Chromium

[Ar] 3d⁵ 4s¹

25

Mn

Manganese

[Ar] 3d⁵ 4s²

26

Fe

Iron

[Ar] 3d⁶ 4s²

27

Co

Cobalt

[Ar] 3d⁷ 4s²

28

Ni

Nickel

[Ar] 3d⁸ 4s²

29

Cu

Copper

[Ar] 3d¹⁰ 4s¹

30

Zn

Zinc

[Ar] 3d¹⁰ 4s²

31

Ga

Gallium

[Ar] 3d¹⁰ 4s² 4p¹

32

Ge

Germanium

[Ar] 3d¹⁰ 4s² 4p²

33

As

Arsenic

[Ar] 3d¹⁰ 4s² 4p³

34

Se

Selenium

[Ar] 3d¹⁰ 4s² 4p⁴

35

Br

Bromine

[Ar] 3d¹⁰ 4s² 4p⁵

36

Kr

Krypton

[Ar] 3d¹⁰ 4s² 4p⁶

37

Rb

Rubidium

[Kr] 5s¹

38

Sr

Strontium

[Kr] 5s²

39

Y

Yttrium

[Kr] 4d¹ 5s²

40

Zr

Zirconium

[Kr] 4d² 5s²

41

Nb

Niobium

[Kr] 4d⁴ 5s¹

42

Mo

Molybdenum

[Kr] 4d⁵ 5s¹

43

Tc

Technetium

[Kr] 4d⁵ 5s²

44

Ru

Ruthenium

[Kr] 4d⁷ 5s¹

45

Rh

Rhodium

[Kr] 4d⁸ 5s¹

46

Pd

Palladium

[Kr] 4d¹⁰

47

Ag

Silver

[Kr] 4d¹⁰ 5s¹

48

Cd

Cadmium

[Kr] 4d¹⁰ 5s²

49

In

Indium

[Kr] 4d¹⁰ 5s² 5p¹

50

Sn

Tin

[Kr] 4d¹⁰ 5s² 5p²

51

Sb

Antimony

[Kr] 4d¹⁰ 5s² 5p³

52

Te

Tellurium

[Kr] 4d¹⁰ 5s² 5p⁴

53

I

Iodine

[Kr] 4d¹⁰ 5s² 5p⁵

54

Xe

Xenon

[Kr] 4d¹⁰ 5s² 5p⁶

55

Cs

Cesium

[Xe] 6s¹

56

Ba

Barium

[Xe] 6s²

57

La

Lanthanum

[Xe] 5d¹ 6s²

58

Ce

Cerium

[Xe] 4f¹ 5d¹ 6s²

59

Pr

Praseodymium

[Xe] 4f³ 6s²

60

Nd

Neodymium

[Xe] 4f⁴ 6s²

61

Pm

Promethium

[Xe] 4f⁵ 6s²

62

Sm

Samarium

[Xe] 4f⁶ 6s²

63

Eu

Europium

[Xe] 4f⁷ 6s²

64

Gd

Gadolinium

[Xe] 4f⁷ 5d¹ 6s²

65

Tb

Terbium

[Xe] 4f⁹ 6s²

66

Dy

Dysprosium

[Xe] 4f¹⁰ 6s²

67

Ho

Holmium

[Xe] 4f¹¹ 6s²

68

Er

Erbium

[Xe] 4f¹² 6s²

69

Tm

Thulium

[Xe] 4f¹³ 6s²

70

Yb

Ytterbium

[Xe] 4f¹⁴ 6s²

71

Lu

Lutetium

[Xe] 4f¹⁴ 5d¹ 6s²

72

Hf

Hafnium

[Xe] 4f¹⁴ 5d² 6s²

73

Ta

Tantalum

[Xe] 4f¹⁴ 5d³ 6s²

74

W

Tungsten

[Xe] 4f¹⁴ 5d⁴ 6s²

75

Re

Rhenium

[Xe] 4f¹⁴ 5d⁵ 6s²

76

Os

Osmium

[Xe] 4f¹⁴ 5d⁶ 6s²

77

Ir

Iridium

[Xe] 4f¹⁴ 5d⁷ 6s²

78

Pt

Platinum

[Xe] 4f¹⁴ 5d⁹ 6s¹

79

Au

Gold

[Xe] 4f¹⁴ 5d¹⁰ 6s¹

80

Hg

Mercury

[Xe] 4f¹⁴ 5d¹⁰ 6s²

81

Tl

Thallium

[Xe] 4f¹⁴ 5d¹⁰ 6s² 6p¹

82

Pb

Lead

[Xe] 4f¹⁴ 5d¹⁰ 6s² 6p²

83

Bi

Bismuth

[Xe] 4f¹⁴ 5d¹⁰ 6s² 6p³

84

Po

Polonium

[Xe] 4f¹⁴ 5d¹⁰ 6s² 6p⁴

85

At

Astatine

[Xe] 4f¹⁴ 5d¹⁰ 6s² 6p⁵

86

Rn

Radon

[Xe] 4f¹⁴ 5d¹⁰ 6s² 6p⁶

87

Fr

Francium

[Rn] 7s¹

88

Ra

Radium

[Rn] 7s²

89

Ac

Actinium

[Rn] 6d¹ 7s²

90

Th

Thorium

[Rn] 6d² 7s²

91

Pa

Protactinium

[Rn] 5f² 6d¹ 7s²

92

U

Uranium

[Rn] 5f³ 6d¹ 7s²

93

Np

Neptunium

[Rn] 5f⁴ 6d¹ 7s²

94

Pu

Plutonium

[Rn] 5f⁶ 7s²

95

Am

Americium

[Rn] 5f⁷ 7s²

96

Cm

Curium

[Rn] 5f⁸ 7s²

97

Bk

Berkelium

[Rn] 5f⁹ 7s²

98

Cf

Californium

[Rn] 5f¹⁰ 7s²

99

Es

Einsteinium

[Rn] 5f¹¹ 7s²

100

Fm

Fermium

[Rn] 5f¹² 7s²

101

Md

Mendelevium

[Rn] 5f¹³ 7s²

102

No

Nobelium

[Rn] 5f¹⁴ 7s²

103

Lr

Lawrencium

[Rn] 5f¹⁴ 6d¹ 7s²

104

Rg

Roentgenium

[Rn] 5f¹⁴ 6d² 7s²

105

Nh

Nihonium

[Rn] 5f¹⁴ 6d³ 7s²

106

Fl

Flerovium

[Rn] 5f¹⁴ 6d⁴ 7s²

107

Mc

Moscovium

[Rn] 5f¹⁴ 6d⁵ 7s²

108

Lv

Livermorium

[Rn] 5f¹⁴ 6d⁶ 7s²

109

Ts

Tennessine

[Rn] 5f¹⁴ 6d⁷ 7s²

110

Og

Oganesson

[Rn] 5f¹⁴ 6d⁸ 7s²

1

H

Hydrogen

1s¹

2

He

Helium

1s²

3

Li

Lithium

[He] 2s¹

4

Be

Beryllium

[He] 2s²

5

B

Boron

[He] 2s² 2p¹

6

C

Carbon

[He] 2s² 2p²

7

N

Nitrogen

[He] 2s² 2p³

8

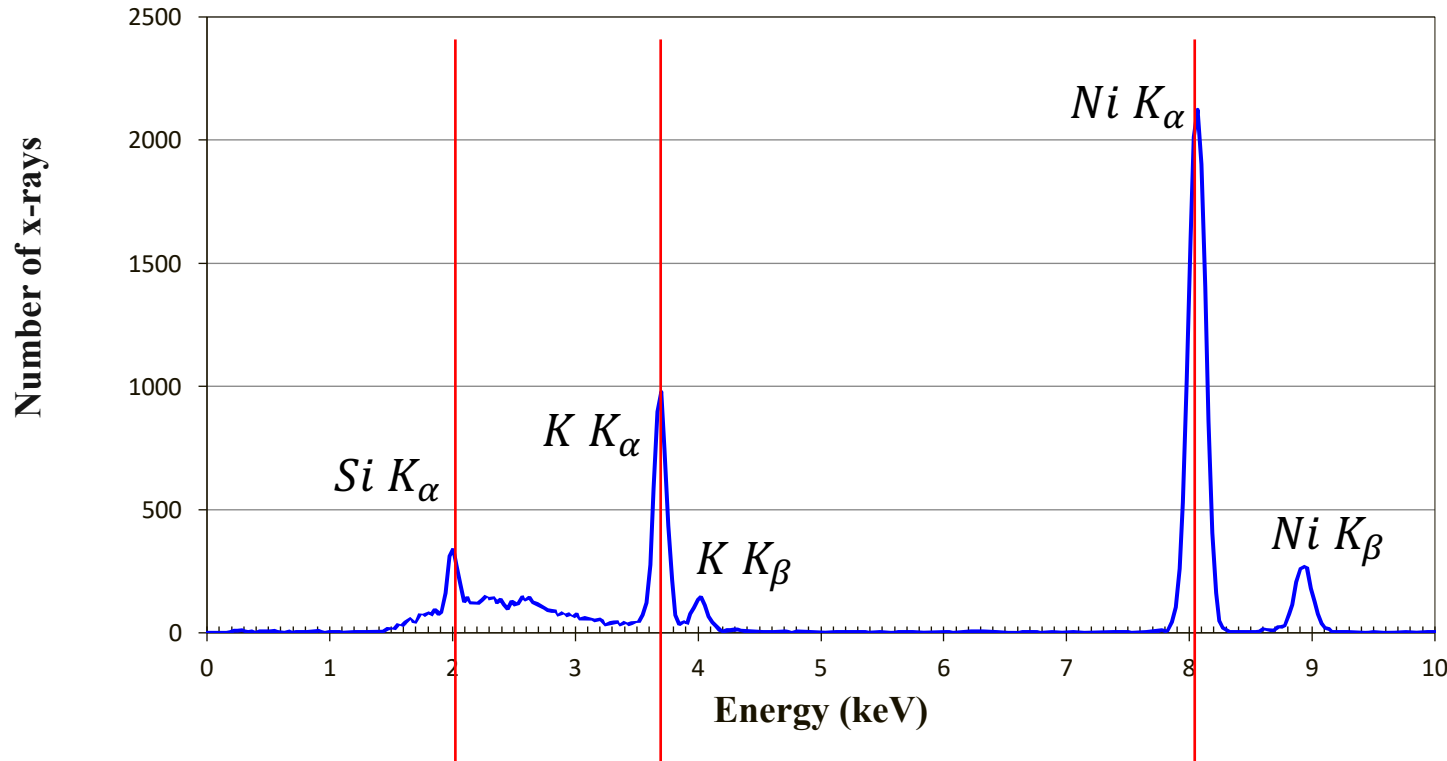
O

Oxygen

[He] 2s²

<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

<div>PubChem</div>																		2 He Helium 1s ²																	
1 H Hydrogen 1s ¹		<div>1 H Hydrogen 1s¹</div> <div>Atomic Number Symbol Name Electron Configuration</div>																																	
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]5d ¹ 6s ²	59 Pr Praseodymium [Xe]5d ¹ 6s ²	60 Nd Neodymium [Xe]5d ¹ 6s ²	61 Pm Promethium [Xe]5d ¹ 6s ²	62 Sm Samarium [Xe]5d ¹ 6s ²	63 Eu Europium [Xe]5d ¹ 6s ²	64 Gd Gadolinium [Xe]5d ¹ 6s ²	65 Tb Terbium [Xe]5d ¹ 6s ²	66 Dy Dysprosium [Xe]5d ¹ 6s ²	67 Ho Holmium [Xe]5d ¹ 6s ²	68 Er Erbium [Xe]5d ¹ 6s ²	69 Tm Thulium [Xe]5d ¹ 6s ²	70 Yb Ytterbium [Xe]5d ¹ 6s ²	71 Lu Lutetium [Xe]5d ¹ 6s ²																		
		** 89 Ac Actinium [Rn]7s ²		90 Th Thorium [Rn]7s ²	91 Pa Protactinium [Rn]7s ²	92 U Uranium [Rn]7s ²	93 Np Neptunium [Rn]7s ²	94 Pu Plutonium [Rn]7s ²	95 Am Americium [Rn]7s ²	96 Cm Curium [Rn]7s ²	97 Bk Berkelium [Rn]7s ²	98 Cf Californium [Rn]7s ²	99 Es Einsteinium [Rn]7s ²	100 Fm Fermium [Rn]7s ²	101 Md Mendelevium [Rn]7s ²	102 No Nobelium [Rn]7s ²	103 Lr Lawrencium [Rn]7s ²																		

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

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.

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

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

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

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

The lowest energy/highest probability transition, K_α :

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

The main metal on the standard

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

The impurities:

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

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

PERIODIC TABLE OF ELEMENTS

[illegible]

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

The Characteristic X-ray Energies & Elemental Identification

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

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

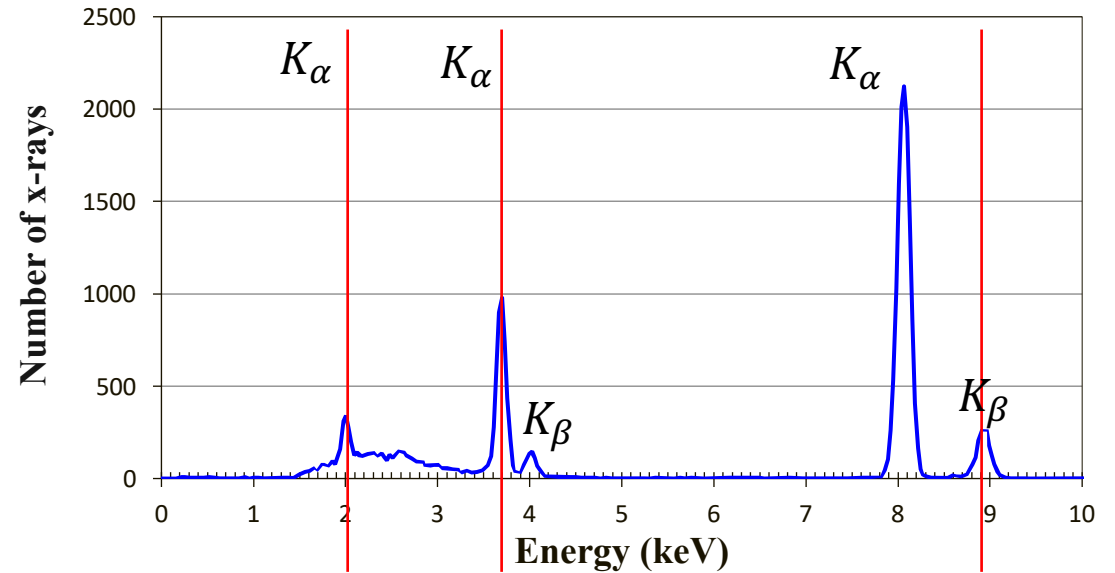
The higher energy/lower probability transition, K_β :

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

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

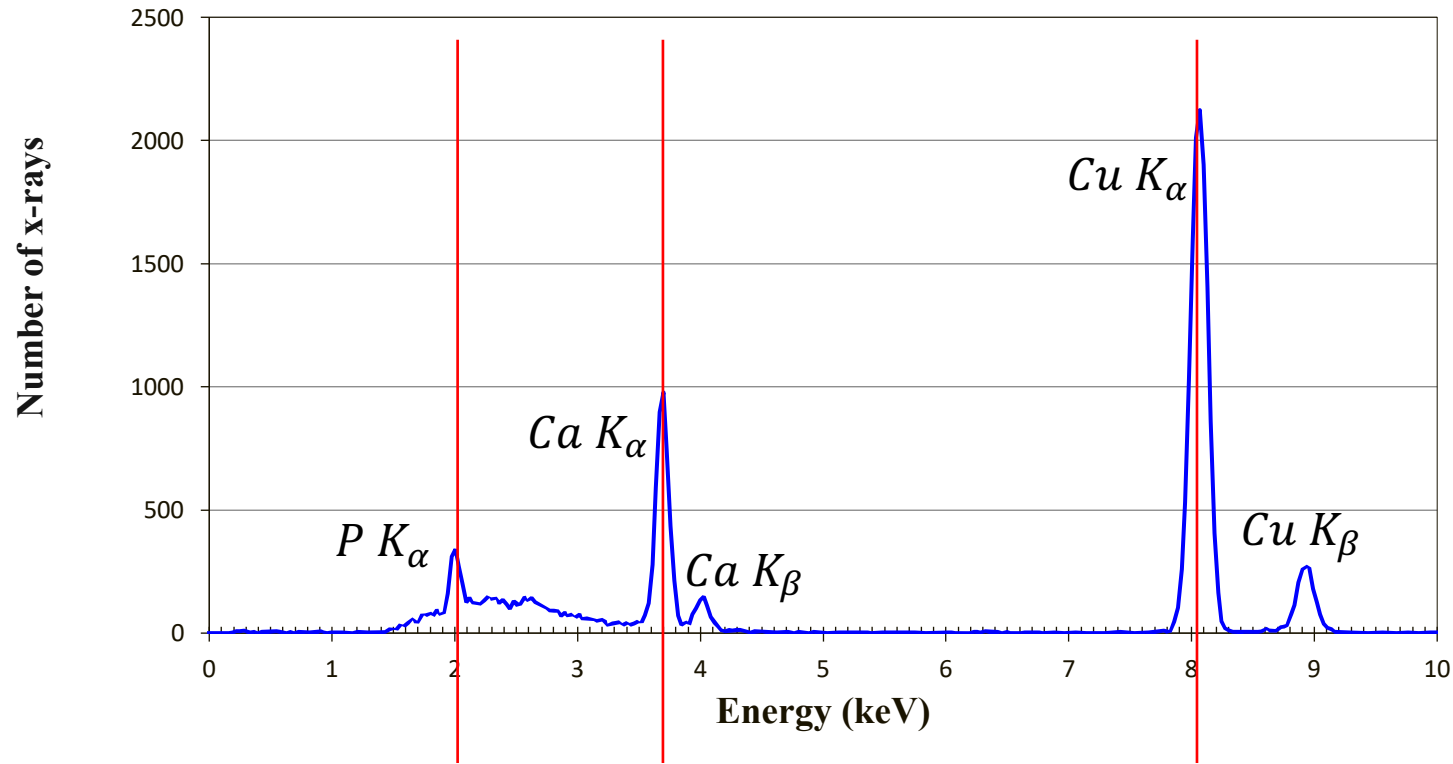
<div>PubChem</div>																		<div>2</div> <div>He</div> <div>Helium</div>																																									
<div>1</div> <div>H</div> <div>Hydrogen</div>		<div>1</div> <div>H</div> <div>Hydrogen</div> <div>1s¹</div>																		<div>Atomic Number</div> <div>Symbol</div> <div>Name</div> <div>Electron Configuration</div>																																							
<div>3</div> <div>Li</div> <div>Lithium</div>		<div>4</div> <div>Be</div> <div>Beryllium</div>		<div>11</div> <div>Na</div> <div>Sodium</div>		<div>12</div> <div>Mg</div> <div>Magnesium</div>		<div>21</div> <div>Sc</div> <div>Scandium</div>		<div>22</div> <div>Ti</div> <div>Titanium</div>		<div>23</div> <div>V</div> <div>Vanadium</div>		<div>24</div> <div>Cr</div> <div>Chromium</div>		<div>25</div> <div>Mn</div> <div>Manganese</div>		<div>26</div> <div>Fe</div> <div>Iron</div>		<div>27</div> <div>Co</div> <div>Cobalt</div>		<div>28</div> <div>Ni</div> <div>Nickel</div>		<div>29</div> <div>Cu</div> <div>Copper</div>		<div>30</div> <div>Zn</div> <div>Zinc</div>		<div>31</div> <div>Ga</div> <div>Gallium</div>		<div>32</div> <div>Ge</div> <div>Germanium</div>		<div>33</div> <div>As</div> <div>Arsenic</div>		<div>34</div> <div>Se</div> <div>Selenium</div>		<div>35</div> <div>Br</div> <div>Bromine</div>		<div>36</div> <div>Kr</div> <div>Krypton</div>																					
<div>19</div> <div>K</div> <div>Potassium</div>		<div>20</div> <div>Ca</div> <div>Calcium</div>		<div>37</div> <div>Rb</div> <div>Rubidium</div>		<div>38</div> <div>Sr</div> <div>Strontium</div>		<div>39</div> <div>Y</div> <div>Yttrium</div>		<div>40</div> <div>Zr</div> <div>Zirconium</div>		<div>41</div> <div>Nb</div> <div>Niobium</div>		<div>42</div> <div>Mo</div> <div>Molybdenum</div>		<div>43</div> <div>Tc</div> <div>Technetium</div>		<div>44</div> <div>Ru</div> <div>Ruthenium</div>		<div>45</div> <div>Rh</div> <div>Rhodium</div>		<div>46</div> <div>Pd</div> <div>Palladium</div>		<div>47</div> <div>Ag</div> <div>Silver</div>		<div>48</div> <div>Cd</div> <div>Cadmium</div>		<div>49</div> <div>In</div> <div>Indium</div>		<div>50</div> <div>Sn</div> <div>Tin</div>		<div>51</div> <div>Sb</div> <div>Antimony</div>		<div>52</div> <div>Te</div> <div>Tellurium</div>		<div>53</div> <div>I</div> <div>Iodine</div>		<div>54</div> <div>Xe</div> <div>Xenon</div>																					
<div>55</div> <div>Cs</div> <div>Cesium</div>		<div>56</div> <div>Ba</div> <div>Barium</div>		<div>87</div> <div>Fr</div> <div>Francium</div>		<div>88</div> <div>Ra</div> <div>Radium</div>		<div>101</div> <div>Db</div> <div>Dubnium</div>		<div>102</div> <div>Sg</div> <div>Seaborgium</div>		<div>103</div> <div>Bh</div> <div>Berkelium</div>		<div>104</div> <div>Hs</div> <div>Hassium</div>		<div>105</div> <div>Mt</div> <div>Moscovium</div>		<div>106</div> <div>Ds</div> <div>Darmstadtium</div>		<div>107</div> <div>Rg</div> <div>Roentgenium</div>		<div>108</div> <div>Cn</div> <div>Copernicium</div>		<div>109</div> <div>Nh</div> <div>Nihonium</div>		<div>110</div> <div>Fl</div> <div>Flerovium</div>		<div>111</div> <div>Mc</div> <div>Moscovium</div>		<div>112</div> <div>Lv</div> <div>Livermorium</div>		<div>113</div> <div>Ts</div> <div>Tennessine</div>		<div>114</div> <div>Uu</div> <div>Ununquadium</div>		<div>115</div> <div>Uut</div> <div>Ununtrium</div>		<div>116</div> <div>Uuh</div> <div>Ununhexium</div>		<div>117</div> <div>Uus</div> <div>Ununseptium</div>		<div>118</div> <div>Uuo</div> <div>Ununoctium</div>																	
<div>57</div> <div>La</div> <div>Lanthanum</div>		<div>58</div> <div>Ce</div> <div>Cerium</div>		<div>59</div> <div>Pr</div> <div>Praseodymium</div>		<div>60</div> <div>Nd</div> <div>Neodymium</div>		<div>61</div> <div>Pm</div> <div>Promethium</div>		<div>62</div> <div>Sm</div> <div>Samarium</div>		<div>63</div> <div>Eu</div> <div>Europium</div>		<div>64</div> <div>Gd</div> <div>Gadolinium</div>		<div>65</div> <div>Tb</div> <div>Terbium</div>		<div>66</div> <div>Dy</div> <div>Dysprosium</div>		<div>67</div> <div>Ho</div> <div>Holmium</div>		<div>68</div> <div>Er</div> <div>Erbium</div>		<div>69</div> <div>Tm</div> <div>Thulium</div>		<div>70</div> <div>Yb</div> <div>Ytterbium</div>		<div>71</div> <div>Lu</div> <div>Lutetium</div>		<div>72</div> <div>Hf</div> <div>Hafnium</div>		<div>73</div> <div>Ta</div> <div>Tantalum</div>		<div>74</div> <div>W</div> <div>Tungsten</div>		<div>75</div> <div>Re</div> <div>Rhenium</div>		<div>76</div> <div>Os</div> <div>Osmium</div>		<div>77</div> <div>Ir</div> <div>Iridium</div>		<div>78</div> <div>Pt</div> <div>Platinum</div>		<div>79</div> <div>Au</div> <div>Gold</div>		<div>80</div> <div>Hg</div> <div>Mercury</div>		<div>81</div> <div>Tl</div> <div>Thallium</div>		<div>82</div> <div>Pb</div> <div>Lead</div>		<div>83</div> <div>Bi</div> <div>Bismuth</div>		<div>84</div> <div>Po</div> <div>Polonium</div>		<div>85</div> <div>At</div> <div>Astatine</div>		<div>86</div> <div>Rn</div> <div>Radon</div>	
<div>89</div> <div>Ac</div> <div>Actinium</div>		<div>90</div> <div>Th</div> <div>Thorium</div>		<div>91</div> <div>Pa</div> <div>Protactinium</div>		<div>92</div> <div>U</div> <div>Uranium</div>		<div>93</div> <div>Np</div> <div>Neptunium</div>		<div>94</div> <div>Pu</div> <div>Plutonium</div>		<div>95</div> <div>Am</div> <div>Americium</div>		<div>96</div> <div>Cm</div> <div>Curium</div>		<div>97</div> <div>Bk</div> <div>Berkelium</div>		<div>98</div> <div>Cf</div> <div>Californium</div>		<div>99</div> <div>Es</div> <div>Einsteinium</div>		<div>100</div> <div>Fm</div> <div>Fermium</div>																																					

The UC

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

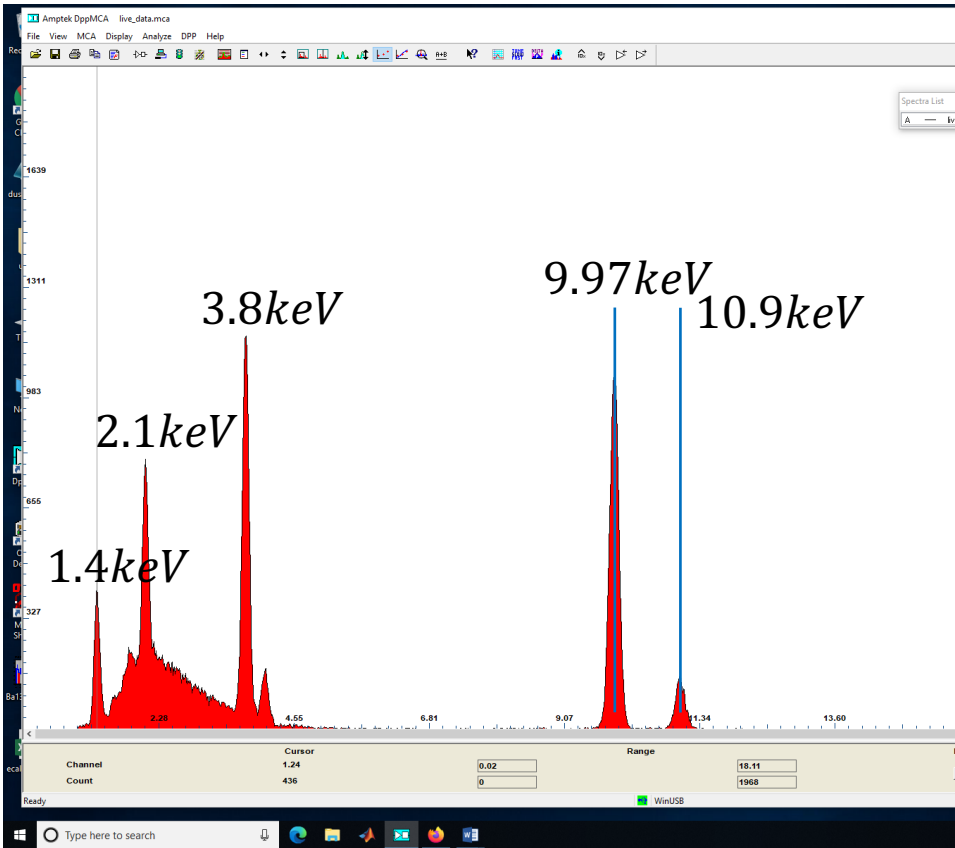


The Characteristic X-ray Energies & Elemental Identification



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

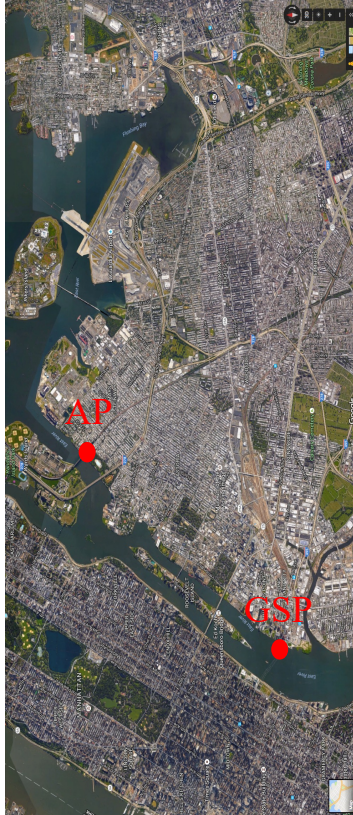


1.4keV → Al K_{α}
2.1keV → P K_{α}
3.8keV → Ca K_{α}
9.97keV → Ge K_{α}
10.9keV → Ge K_{β}

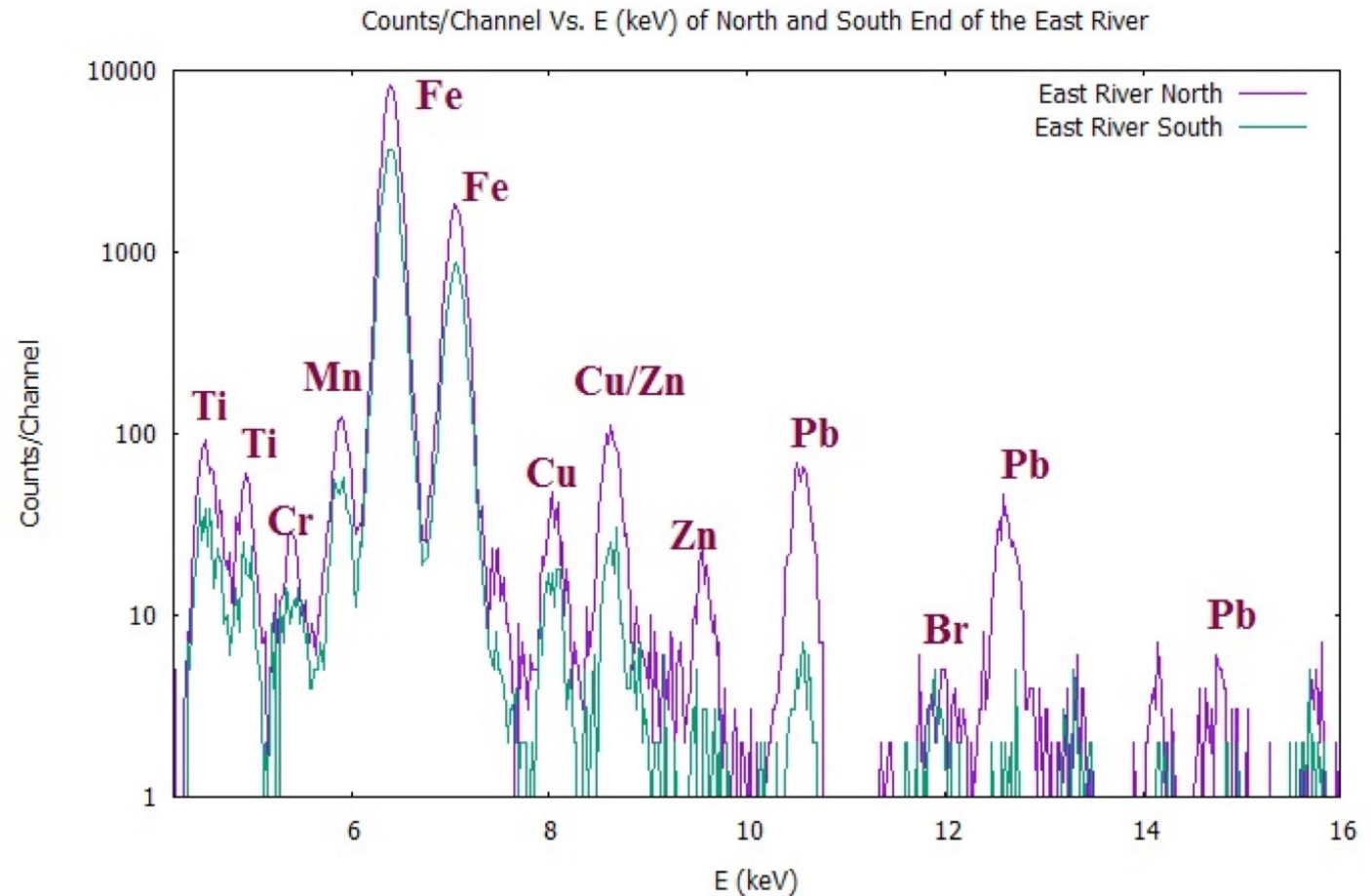
Characteristic X-Ray Energies (X-ray Energies in keV)

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.

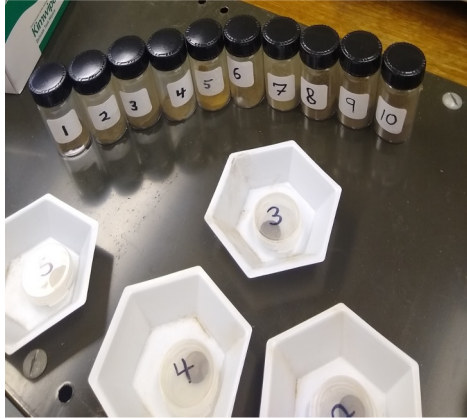
Source: <http://maps.google.com>

Environmental Pollution Along the East River in Queens, New York

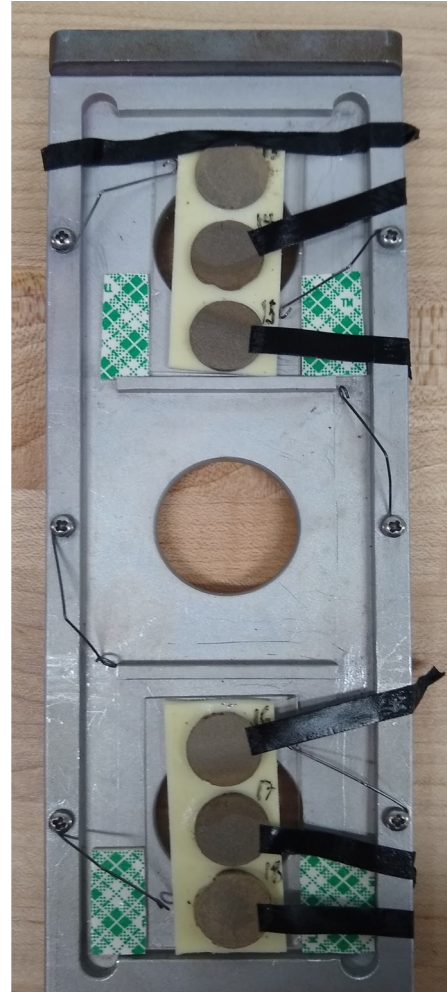


- Hell Gate Bridge is a 1000' railroad bridge built in 1916.
- Painted originally with Hell Gate Red, a lead-based paint.
- Sandblasted and repainted around 1990 with a non-lead-based paint.
- Is the bridge the source of the lead?

Environmental Pollution Along the East River in Queens, New York



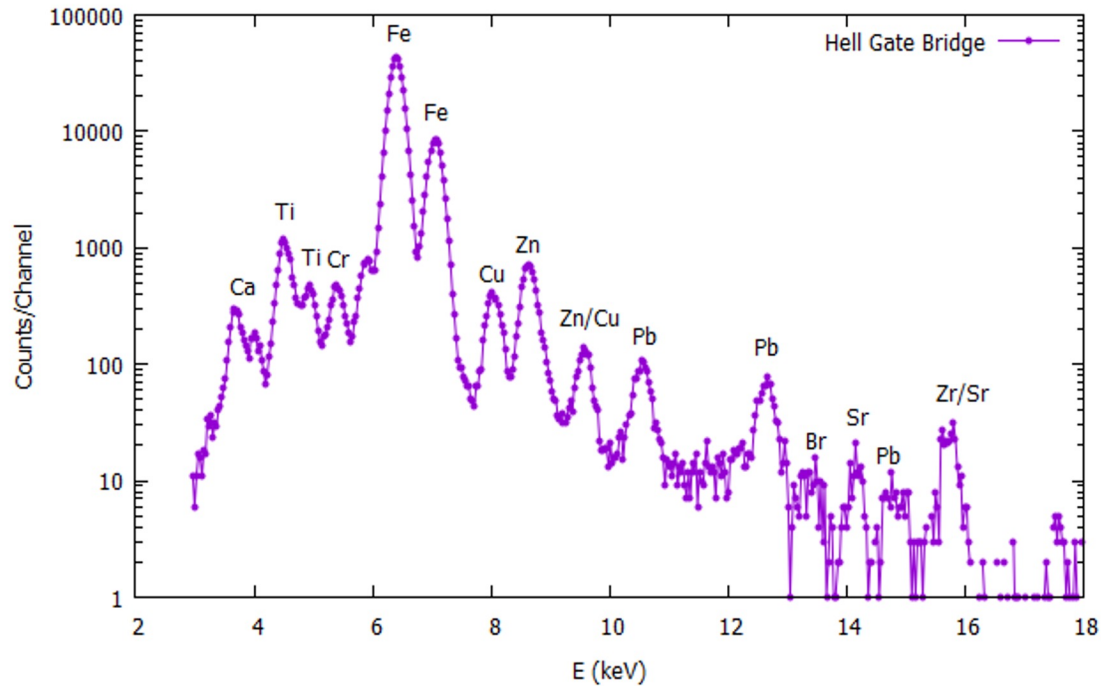
- We've taken 20 samples along the east river from Astoria to Gantry State park in 2018 – 2019.
- In the summer of 2019, we took 20 more samples surrounding the Hell Gate Bridge.
- Above are the soil samples from summer 2019 and on the right the soil pellets mounted on the target ladder.



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

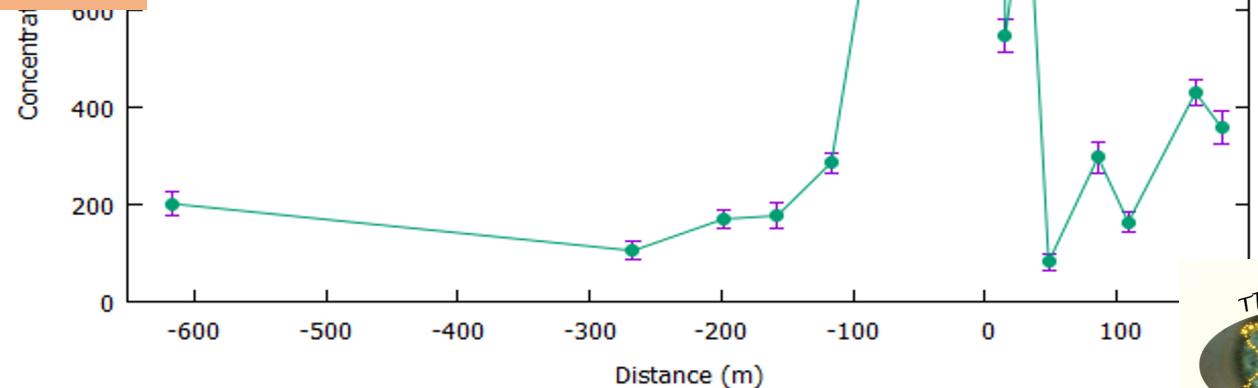


Environmental Pollution Along the East River in Queens, New York



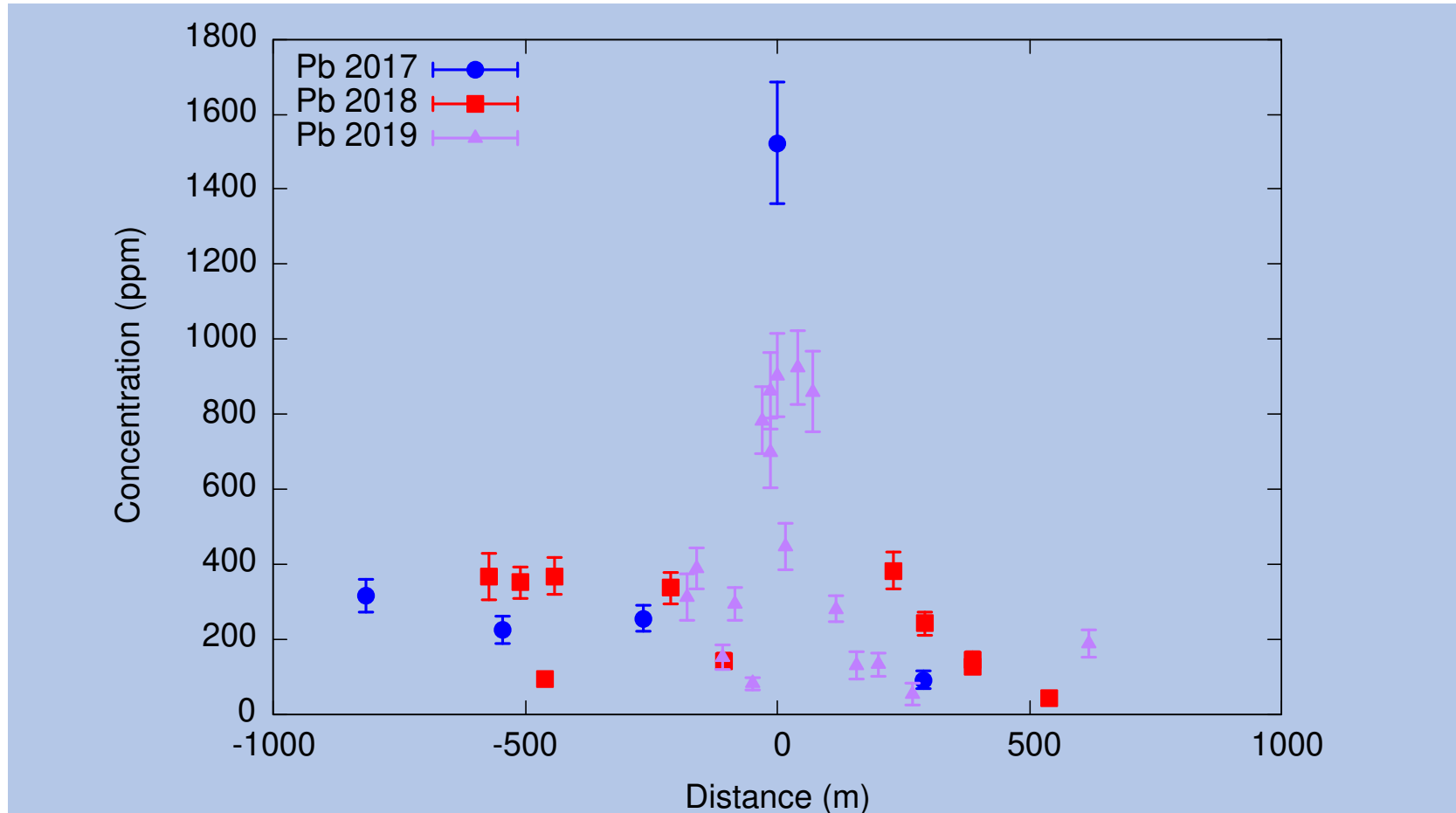
On the left, a typical PIXE spectrum for a soil sample taken near the Hell Gate Bridge, in Astoria, Queens, NY.

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?