

Whisker Occurrence

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Student Researcher: Reid Haiger

Research Advisor: Dr. Rodekohr

Outline:

- Question
- Getting the data
- Cleaning the data
- Statistical Tests & Testing Hypotheses
- Visualizing Results
- Answer
- Acknowledgements

Question: Why do some elements whisker while others do not whisker?

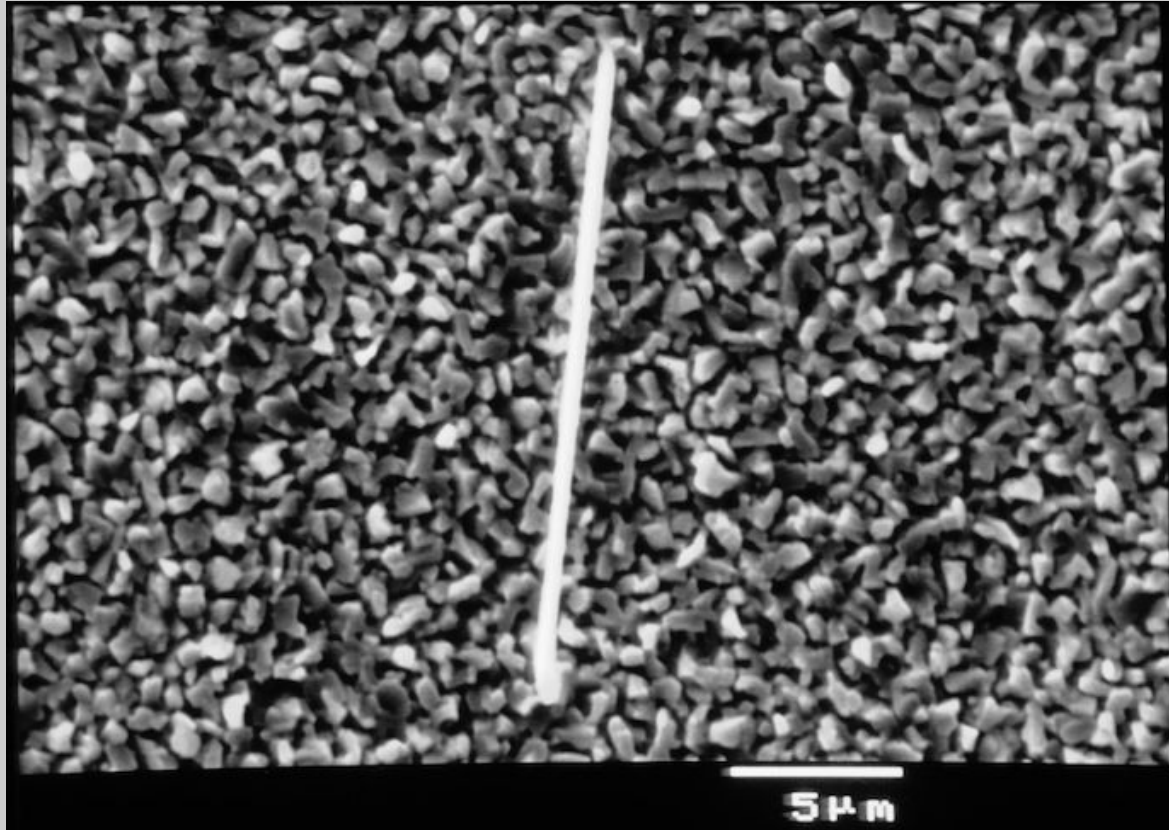


Photo Credit:
Dr. Rodekohr

- **Getting the data**

R Package “PeriodicTable”

- Includes Chemical Properties of the Elements

● Cleaning the data

- create new dataframe by combining column named whisker with levels yes/no for whiskering ability (18 elements are known to whisker. There possibly could be more.)
- delete dummy row zero
- Remove higher number elements because of lots of missing data. (atomic numbers 85:117) !! We are analyzing hydrogen(A.N. 1) through polonium(A.N. 84)
- Remove columns with unnecessary or redundant variables: symbol, name, color, red, green, blue, discoverer, year, configuration, row, & col.
- Several numeric columns have just a couple missing values. So, fill empty values with mean value. Columns included: electronegativity, heat capacity, melting point, & ionic radii.
- change character variables to factor variables(type, phase, crystal, whisker)

● Statistical Tests & Testing Hypotheses

T-tests:

Atomic number v. whisker

Mass v. whisker

Covalent radii v. whisker

Van der Waals radii v. whisker

Ionic radii v. whisker

Electronegativity v. whisker

Ionization Potential v. whisker

Density v. whisker

Melting Point v. whisker

Boiling Point v. whisker

Chi-squared tests:

Period v. whisker

Group v. whisker

Type v. whisker

Phase v. whisker

Crystal v. whisker

Isotopes v. whisker

- Significant Results

```
> chisq.test(table.type)

      Pearson's Chi-squared test

data:  table.type
X-squared = 22.195, df = 8, p-value = 0.004567
```

Figure 11. χ^2 test on type v. whisker

- H_0 : The two variables are independent.
- H_1 : The two variables relate to each other.
- As $p\text{-value} = 0.004567 < 0.05$, we reject the null hypothesis

Therefore, the two variables relate to each other.

```
> chisq.test(table.crystal)

      Pearson's Chi-squared test

data:  table.crystal
X-squared = 14.145, df = 8, p-value = 0.07806
```

Figure 13. χ^2 test on crystal v. whisker

- H_0 : The two variables are independent.
- H_1 : The two variables relate to each other.
- As $p\text{-value} = 0.07806 > 0.05$, We do not reject the null hypothesis
- Therefore, the variables are independent

However, P-value is still less than .1, so it is still a interesting variable


```
> t.test(Eneg ~ whisker, data = newTable)

Welch Two Sample t-test

data:  Eneg by whisker
t = -1.9875, df = 58.998, p-value = 0.05151
alternative hypothesis: true difference in means is not equal to 0
95 percent confidence interval:
 -0.450446255  0.001519008
sample estimates:
mean in group no mean in group yes
      1.731647      1.956111
```

Figure 20. T-test Electronegativity v. whisker

- Is there a significant difference between the means of the numerical variable (Eneg) in two different categories of the categorical variable (whisker)?
- The p-value (0.05151) $>$ 0.05 means that the difference between the mean Eneg for “no” whisker and the mean Eneg for “yes” whisker is insignificant.

However, p-value is less than .1 so it is still an interesting variable

```
> t.test(density ~ whisker, data = newTable)

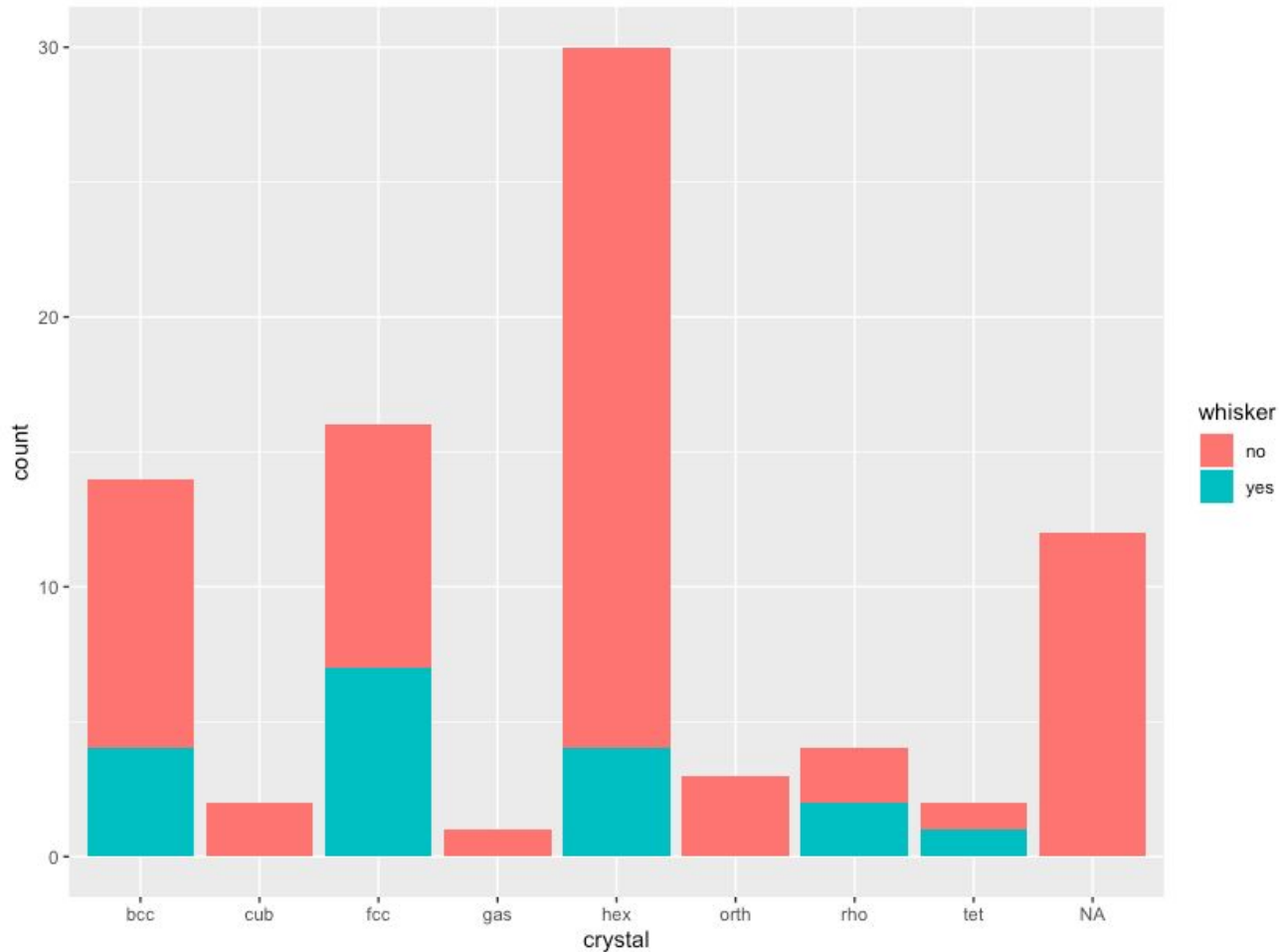
Welch Two Sample t-test

data: density by whisker
t = -3.2307, df = 26.096, p-value = 0.003329
alternative hypothesis: true difference in means is not equal to 0
95 percent confidence interval:
 -7.584211 -1.686677
sample estimates:
mean in group no mean in group yes
      5.943112      10.578556
```

Figure 22. T-test density v. whisker

- Is there a significant difference between the means of the numerical variable (density) in two different categories of the categorical variable (whisker)?
- The p-value ($0.003329 < 0.05$) means that the difference between the mean density for “no” whisker and the mean density for “yes” whisker is significant.

Count of Elements
by Crystalline Phases
and Whisker Ability



● Visualizing Results

Abbreviations:

Bcc = body centered
cubic

Cub = cubic

Fcc = face centered
cubic

Gas = gas

Orth = orthorhombic

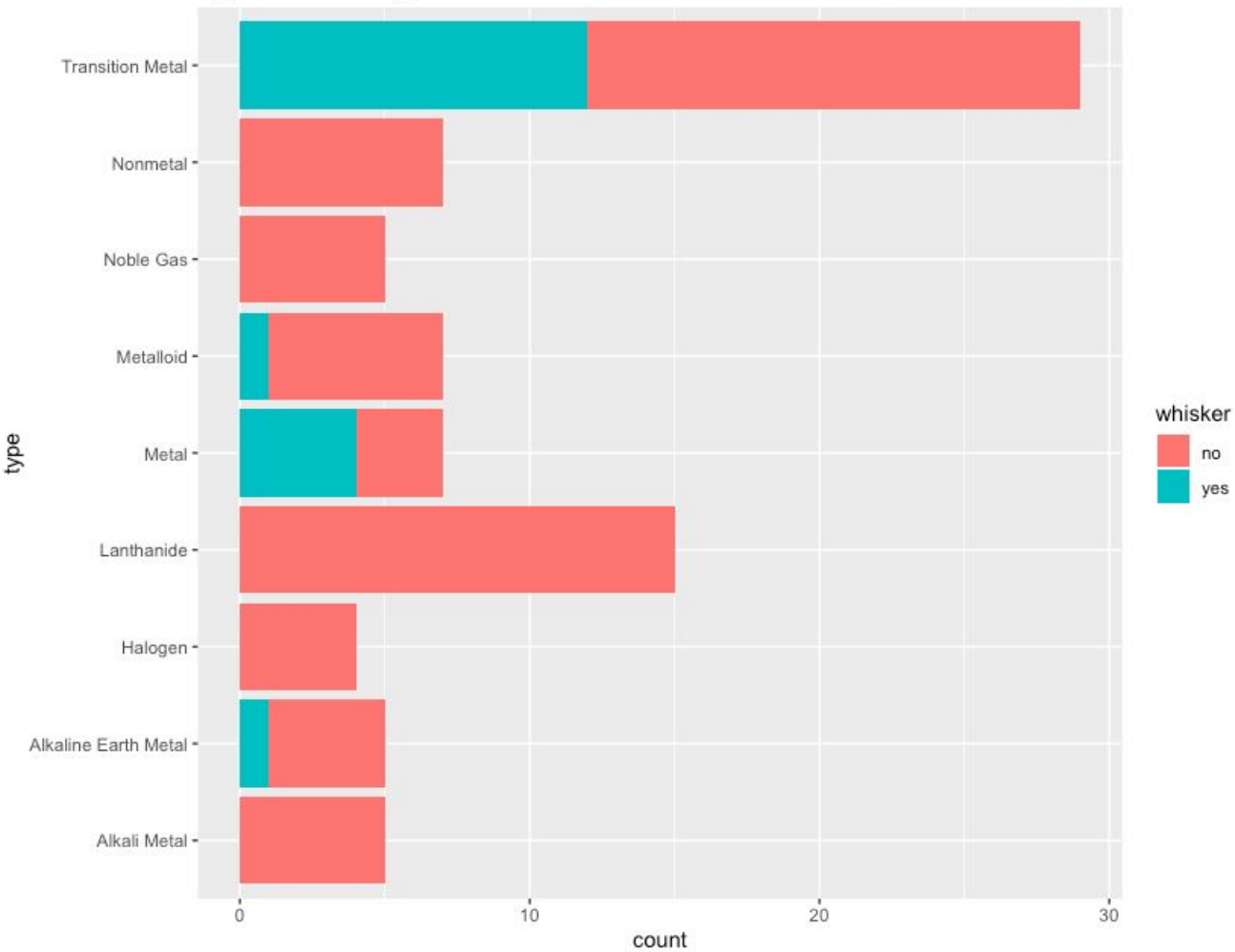
Rho = rhombohedral

Tet = tetragonal

NA = not applicable

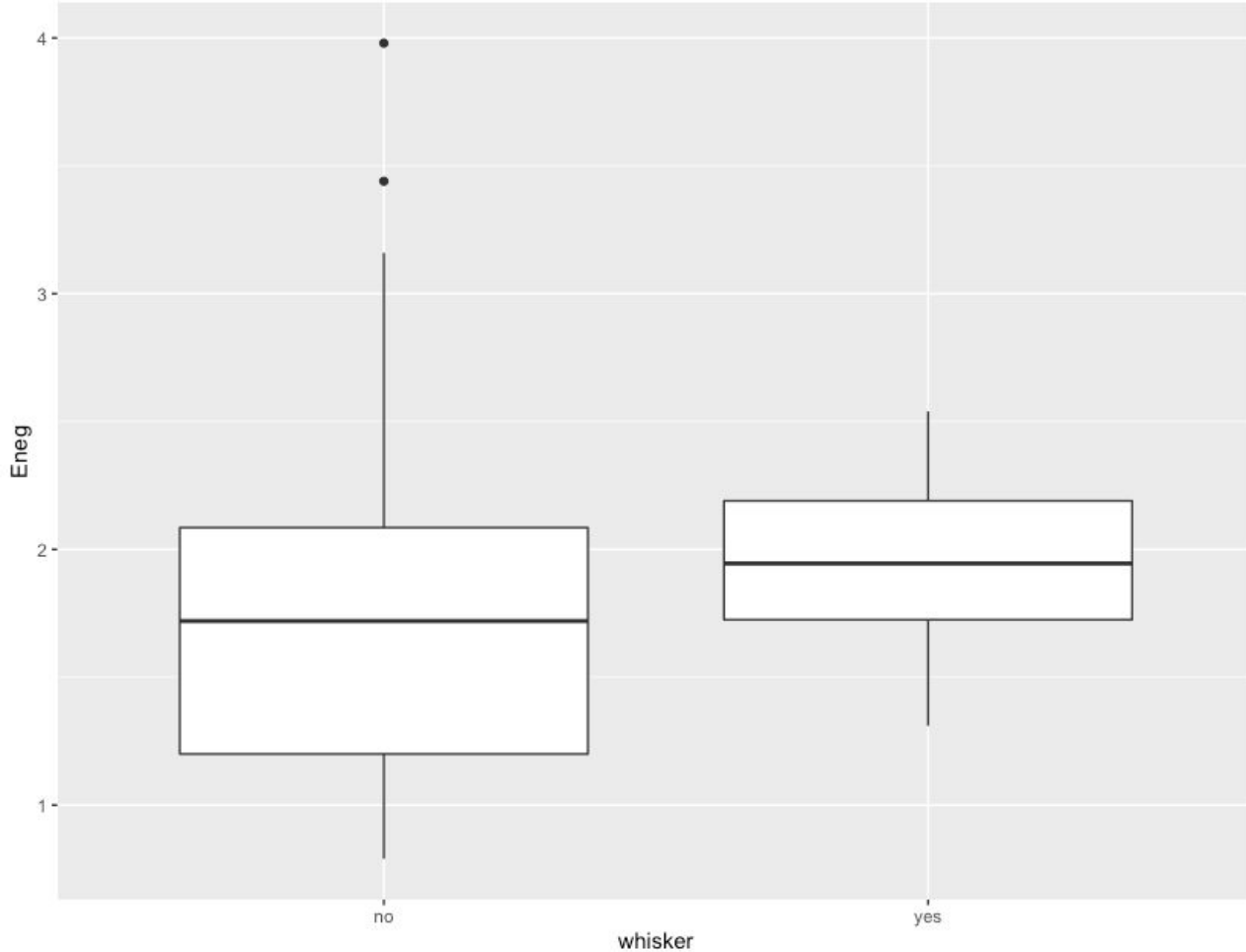
Graph 1. Count of Elements by
Crystalline Phases and Whisker
Ability

Type of Element
by Whisker Ability



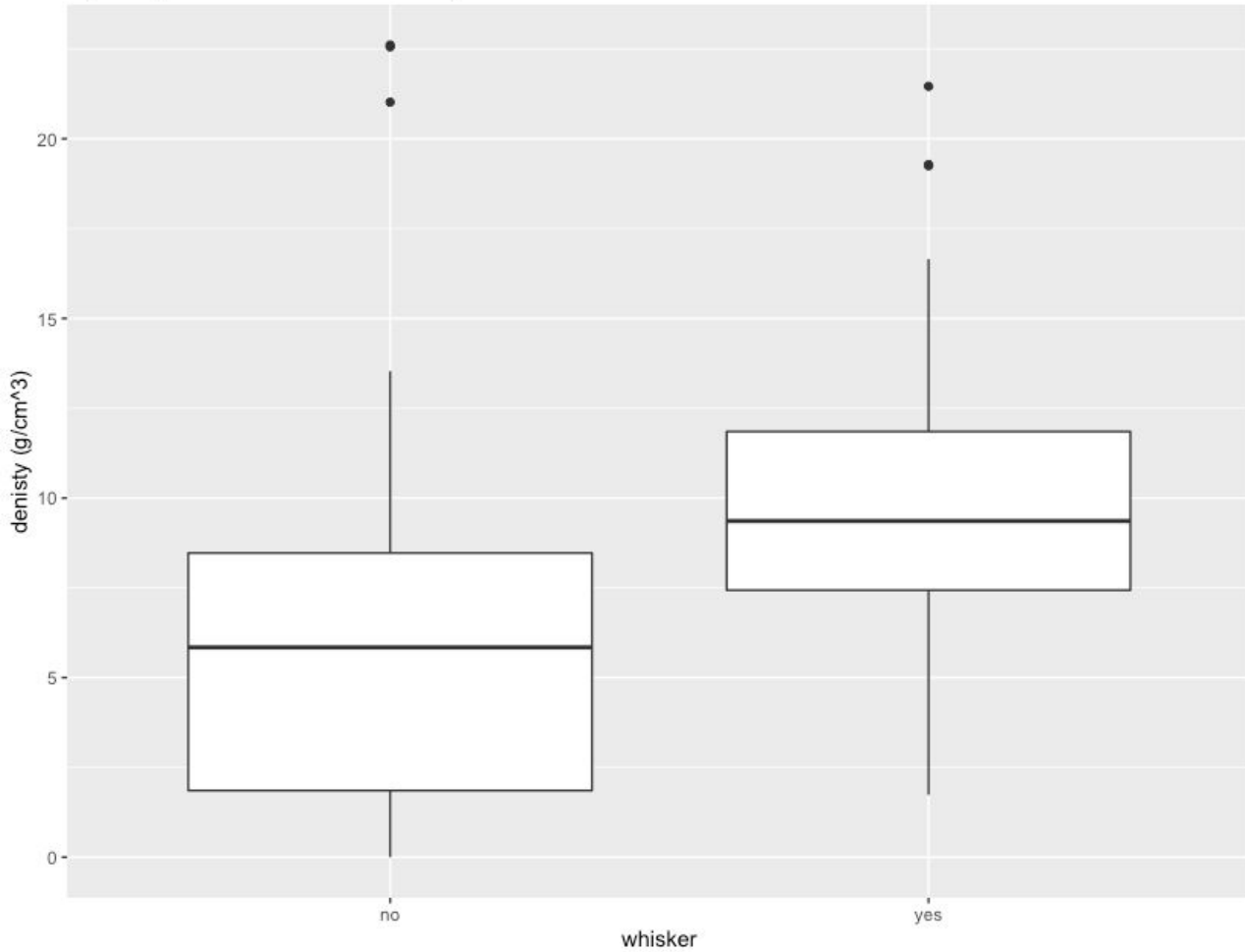
Graph 2. Type of
Element by Whisker
Ability

Whisker Ability
by Electronegativity Boxplot Distribution



Graph 3. Whisker
Ability by
Electronegativity
Boxplot Distribution

Whisker Ability
by Boxplot Distribution of Density



Graph 4. Whisker
Ability by Density

- Answer

Remember The Question: Why do some elements whisker while others do not whisker?

Answer: We do not know for certain. We do know that elements that whisker are denser and more electronegative than elements that don't whisker. We also know that whiskering is only seen in transition metals, metals, metalloids, and alkaline earth metals. Also, whiskering only seen in crystalline phases bcc, fcc, hex, rho, and tet.

- Acknowledgements

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