In [1]:

```
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
```

In [99]:

```
df = pd.read_csv('assignment3.txt')
```

In [ ]:

```

```

In [100]:

```
df.head()
```

Out[100]:

	Elements	Atomic Number	Electronegativity	Atomic Radius	Thermal Conductivity	Density	Crystal System
0	H	1	2.20	0.25	0.1805	0.09	HEX
1	He	2	0.00	1.20	0.1513	0.18	HCP
2	Li	3	0.98	1.45	85.0000	530.00	BCC
3	Be	4	1.57	1.05	190.0000	1850.00	HCP
4	B	5	2.04	0.85	27.0000	2340.00	RHO

In [21]:

```
df.dropna(subset=['Crystal System'],inplace=True)
```

In [31]:

```
df.isnull().value_counts()
```

Out[31]:

```
Elements  Atomic Number  Electronegativity  Atomic Radius  Thermal Conductivity  Density
Crystal System
False     False          False              False          False                 False
False              95
dtype: int64
```

Plot electronegativity, raddi, thermal conductivity and density values on the Y-axis vs. elements on the X-axis. You can make a separate plot for each of these features.

In [59]:

```
fig1 =px.line(df,x='Elements',y='Electronegativity',title='elements vs Electronegativity'
)
fig1.update_layout(paper_bgcolor='LightSteelBlue',plot_bgcolor='white')
```

In [ ]:

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```

In [26]:

```
import plotly.express as px
```

In [38]:

```
fig2 =px.line(df,x='Elements',y='Atomic Radius',title='elements vs Atomic radius')
fig2.update_layout(paper_bgcolor='LightSteelBlue',plot_bgcolor='white')
```

In [ ]:

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In [60]:

```
# Plotting thermal conductivity v/s Elements
fig3 =px.line(df,x='Elements',y='Thermal Conductivity',title='elements vs Thermal conduct
ivity')
fig3.update_layout(paper_bgcolor='LightSteelBlue',plot_bgcolor='white')
```

In [ ]:

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```

In [61]:

```
# Plot of  Density v/s Elements
fig4 =px.line(df,x='Elements',y='Density',title='elements vs Density')
fig4.update_layout(paper_bgcolor='LightSteelBlue',plot_bgcolor='white')
```

In [ ]:

```
```

Arrange in increasing order, divide the span of the values of each of these into 10 equal size bins, count the number of elements in each bin and plot number of elements on the Y-axis vs. bins on the X-axis. If you know another method of making bar chart for number distribution, you can use that. Is there any similarity between distributions of two features?

In [ ]:

```
```

In [41]:

```
from sklearn.preprocessing import KBinsDiscretizer
from sklearn.compose import ColumnTransformer
```

In [78]:

```
#kbin_age = KBinsDiscretizer(n_bins=10,encode='ordinal',strategy='quantile')
#kbin_fare = KBinsDiscretizer(n_bins=10,encode='ordinal',strategy='quantile')
```

In [82]:

```
def bin_counts(data, col):                                  # FUNCTION TO Calculate the eleme
nts in bins and dividing the column into equal sized bins
    data = data.sort_values(by=[col])
    col_range = data[col].max() - data[col].min()
    bin_size = col_range/10
    bins = np.linspace(data[col].min(), data[col].max(), num=11, endpoint=True)
    binned_col = np.digitize(data[col], bins)
    counts = [0]*10
    for i in range(1, len(bins)):
        counts[i-1] = (binned_col == i).sum()
    return bins, counts
```

In [83]:

```
# pd.qcut(df['Electronegativity'],q=10)
```

In [ ]:

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In [ ]:

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In [84]:

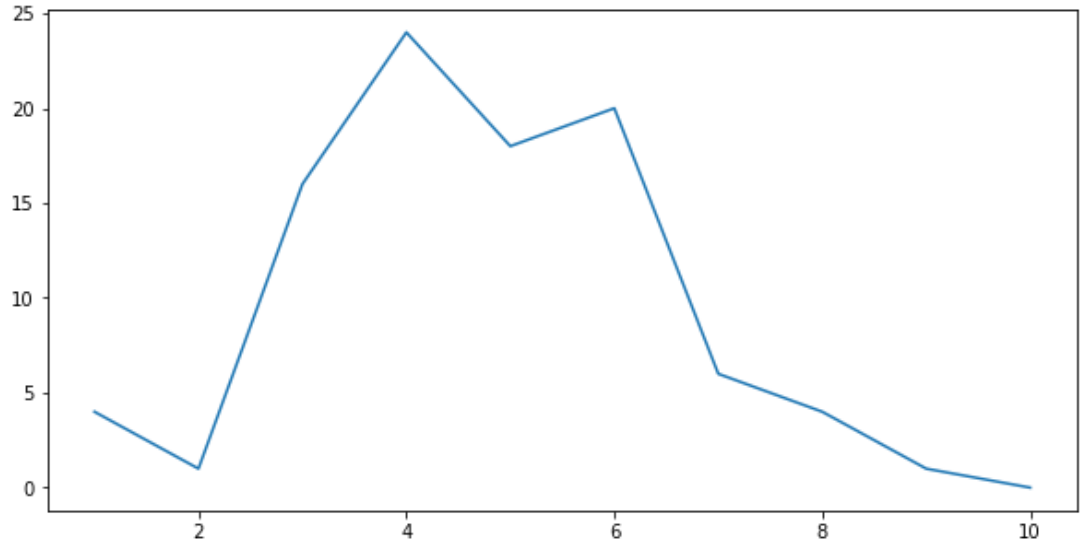
```
# Bins for electronegativity values
plt.figure(figsize=(10,5))
Electronegative_bins, Electronegative_counts = bin_counts(df, 'Electronegativity')
```

```
print(Electronegative_bins)
plt.plot(np.arange(1,11,1), Electronegative_counts)
```

```
[0.    0.398 0.796 1.194 1.592 1.99  2.388 2.786 3.184 3.582 3.98 ]
```

Out[84]:

```
[<matplotlib.lines.Line2D at 0x163f92f13d0>]
```



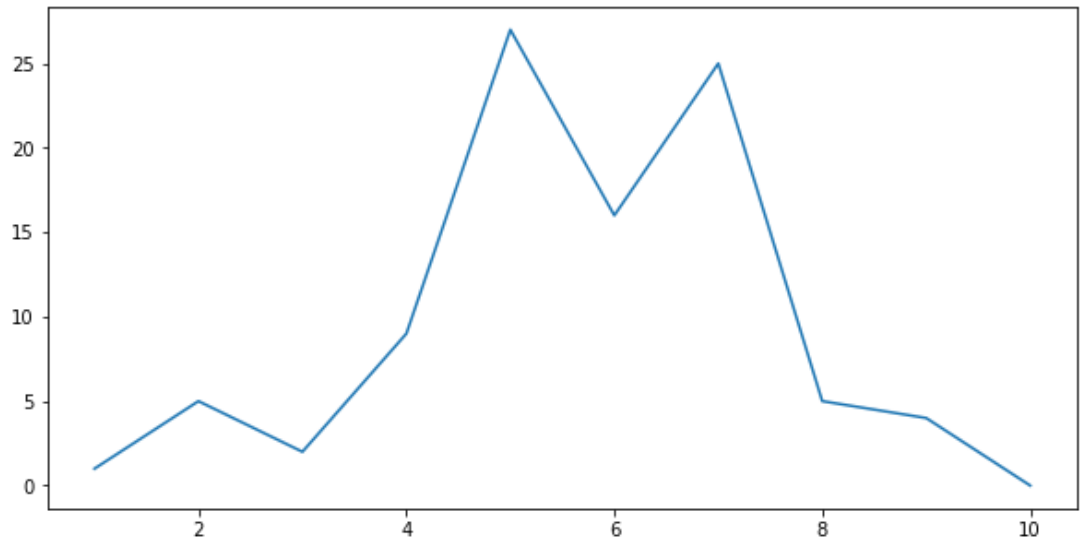
In [85]:

```
# Bins for Atomic Radii Values
plt.figure(figsize=(10,5))
ar_bins, ar_counts = bin_counts(df, 'Atomic Radius')
print(ar_bins)
plt.plot(np.arange(1,11,1), ar_counts)
```

```
[0.25  0.485 0.72  0.955 1.19  1.425 1.66  1.895 2.13  2.365 2.6  ]
```

Out[85]:

```
[<matplotlib.lines.Line2D at 0x163f9343310>]
```



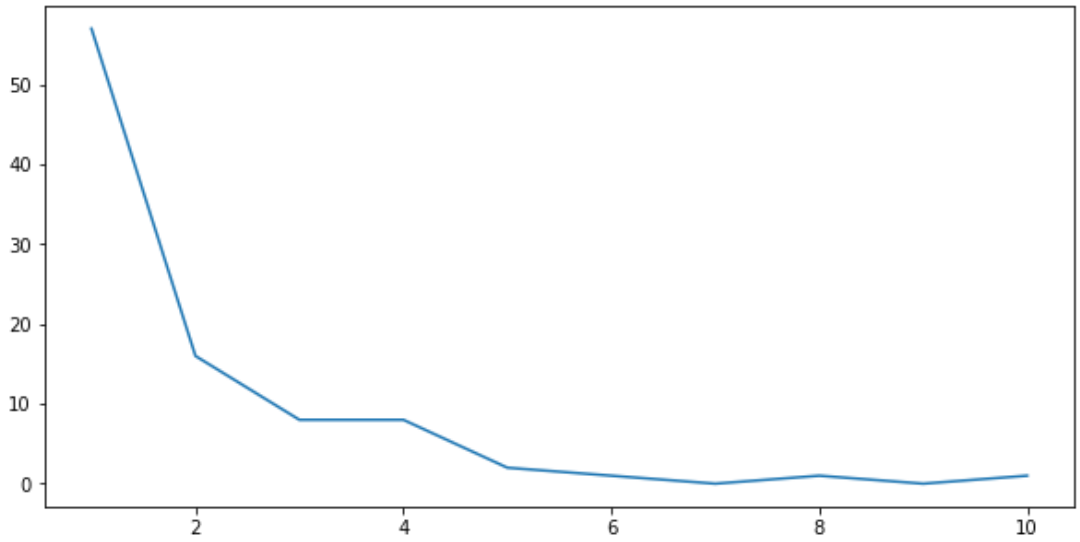
In [86]:

```
# Bins for Thermal Conductivity values
plt.figure(figsize=(10,5))
tc_bins, tc_counts = bin_counts(df, 'Thermal Conductivity')
print(tc_bins)
plt.plot(np.arange(1,11,1), tc_counts)
```

```
[3.61000000e-03 4.30032490e+01 8.60028880e+01 1.29002527e+02
 1.72002166e+02 2.15001805e+02 2.58001444e+02 3.01001083e+02
 3.44000722e+02 3.87000361e+02 4.30000000e+02]
```

Out[86]:

```
[<matplotlib.lines.Line2D at 0x163f9397580>]
```



In [ ]:

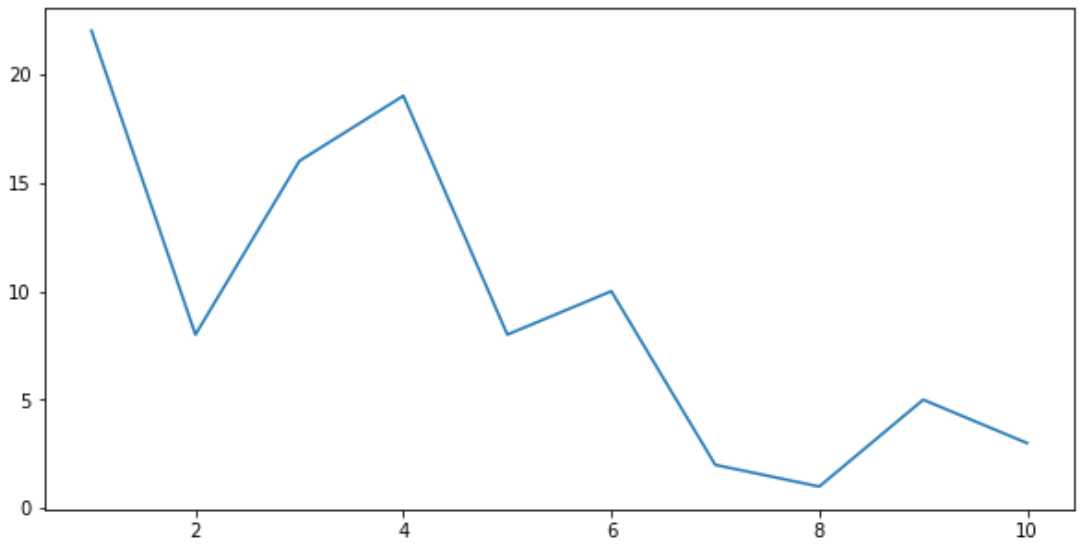
In [87]:

```
# Bins for density
plt.figure(figsize=(10,5))
tc_bins, tc_counts = bin_counts(df, 'Density')
print(tc_bins)
plt.plot(np.arange(1,11,1), tc_counts)
```

```
[9.0000000e-02 2.2600810e+03 4.5200720e+03 6.7800630e+03 9.0400540e+03
 1.1300045e+04 1.3560036e+04 1.5820027e+04 1.8080018e+04 2.0340009e+04
 2.2600000e+04]
```

Out[87]:

```
[<matplotlib.lines.Line2D at 0x163fa5311c0>]
```



There is similarity between Atomic radii and Electronegativity curves also the density and thermal conductivity In general, electronegativity tends to increase as atomic radius decreases. This is due to the fact that as the atomic radius decreases, the number of electrons in the outermost shell of the atom becomes more tightly bound to the nucleus. This results in a higher electron pull towards the nucleus and a corresponding increase in electronegativity. Here also the number of elements in each bins of electronegativty and atomic radii is kind of similar.

In [ ]:

In [ ]:

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In [89]:

```
data_crystal =  pd.DataFrame(df['Crystal System'].value_counts())
```

In [90]:

```
data_crystal
```

Out[90]:

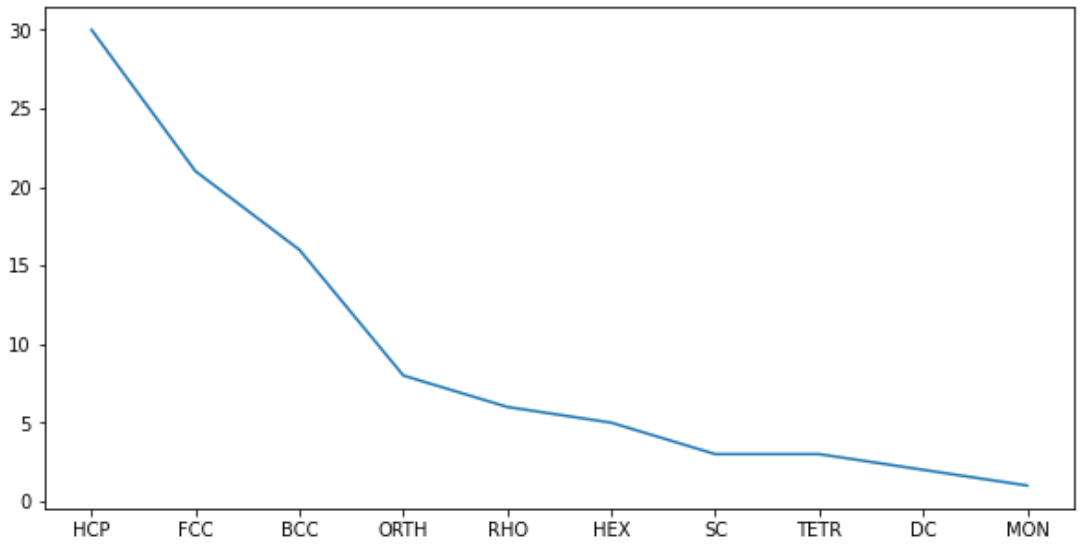
	Crystal System
HCP	30
FCC	21
BCC	16
ORTH	8
RHO	6
HEX	5
SC	3
TETR	3
DC	2
MON	1

In [92]:

```
plt.figure(figsize=(10,5))
plt.plot(data_crystal.index, data_crystal['Crystal System'])
```

Out[92]:

```
[<matplotlib.lines.Line2D at 0x163f91aeb20>]
```



In [ ]:

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In [ ]:

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Calculating the covariance

Calculating the covariance

Covariance can only be calculated for numerical variables, and the crystal system names are not numerical values. You cannot calculate covariance for categorical or nominal variables such as crystal system names.

To analyze the relationship between the crystal system and the count, you can use other methods such as contingency tables, chi-squared test, or a bar plot.

The p-value is the measure of the strength of the relationship between the two variables. If the p-value is less than a certain significance level (often 0.05), you can reject the null hypothesis and conclude that there is a relationship between the crystal system and the count.

In this case, the output of the code will give you the chi-squared statistic and the p-value, which you can use to determine whether there is a relationship between the crystal system and the count.

In [98]:

```
import pandas as pd
from scipy.stats import chi2_contingency

data = {'Crystal System': ['HCP', 'FCC', 'BCC', 'ORTH', 'RHO', 'HEX', 'SC', 'TETR', 'DC'
, 'MON'],
        'Count': [30, 21, 16, 8, 6, 5, 3, 3, 2, 1]}
df12 = pd.DataFrame(data)

table = pd.crosstab(index=df12["Crystal System"], columns="count", margins=True)

stat, p, dof, expected = chi2_contingency(table.iloc[:-1, :-1])

print("Chi-squared Statistic: ", stat)
print("p-value: ", p)
```

```
Chi-squared Statistic:  0.0
p-value:  1.0
```

A p-value of 1 means that there is no significant relationship between the crystal system and the count, and a chi-squared statistic of 0 means that the observed and expected counts are exactly the same.

This result indicates that the crystal system and the count are independent, meaning that the count of crystal systems does not depend on the type of crystal system. In other words, there is no relationship between the two variables.

This result is not surprising, given that the sample size is small and the data is not normally distributed. In general, with larger sample sizes and more representative data, you would expect to see more significant results from a chi-squared test.

In [ ]:

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In [ ]:

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In [102]:

```
def standardize(a):                     #a here is the input data
    mean = sum(a)/len(a)                #computing mean
    var = sum((a-mean)**2)/len(a)       #computing variance
    snd = (a-mean)/(var**0.5)           #compute zero mean for normalizating data
    return snd
```

In [105]:

```
Y =standardize(Electronegative_bins)
```

In [109]:

```
Y
```

Out[109]:

```
array([-1.58113883e+00, -1.26491106e+00, -9.48683298e-01, -6.32455532e-01,
       -3.16227766e-01,  1.76423792e-16,  3.16227766e-01,  6.32455532e-01,
        9.48683298e-01,  1.26491106e+00,  1.58113883e+00])
```

In [108]:

```
Electronegative_counts
```

Out[108]:

```
[4, 1, 16, 24, 18, 20, 6, 4, 1, 0]
```

In [110]:

```
def pca(X):
  # Add a functionality of adjusting X for zero mean for each column and normalize each c
olumn using variance.

  # Compute covariance matrix
    C = np.dot(X.T, X) / (11-1)
  # Eigen decomposition
    eigen_vals, eigen_vecs = np.linalg.eig(C)
  # Project X onto PC space
    X_pca = np.dot(X, eigen_vecs)
    return eigen_vecs,eigen_vals,X_pca
```

In [ ]:

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In [ ]:

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In [ ]:

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In [ ]:

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