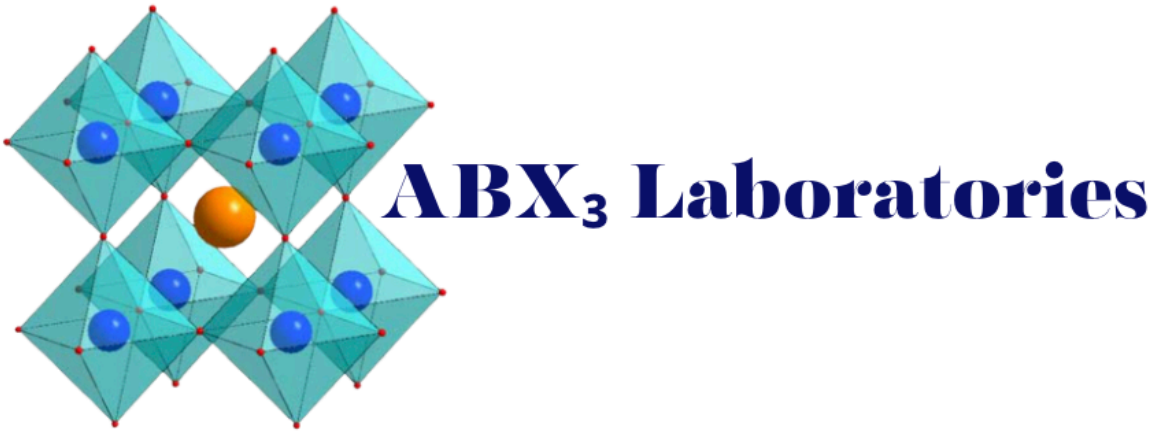
Machine Learning Molecular Structure Predictor



Overview

This project explores different machine learning algorithms to predict the lowest distortion in perovskite structures, which is a critical aspect in ceramic science, materials physics, and solid-state inorganic chemistry. Researchers have identified a total of 73 elements in the A and B cation sites of ABO3 structures, leading to numerous oxides of the perovskite type.

The objective is to develop models capable of accurately classifying perovskite structures based on features such as electronegativity, ionic radius, valence, and bond lengths of A-O and B-O pairs, thereby aiding in the prediction and optimization of material properties. Model performance is assessed using the Accuracy Score metric.

Business Problem

Here we will take a look at the [Kaggle Crystal Structure Dataset] (https://www.kaggle.com/datasets/meetnagadia/crystal-structure-dataset/data (https://www.kaggle.com/datasets/meetnagadia/crystal-structure-dataset/data)). Each record represents a different Perovskite structures based on their characteristics. The data consists of 4,165 ABO3 perovskite-type oxides. Each observation is described by 13 feature columns and 1 class column which identifies it to be either a cubic, tetragonal, orthorhombic, and rhombohedral structure.

A Research Laboratory has asked for an analysis of a dataset to help understand the relationships between various physical and chemical properties of perovskite materials and their crystal structure types.

This project will determine:

1. If there are any discernable patterns or correlations among the different variables and perovskite structure types?
2. How well features like the Glodschmidt tolerance factor, the electronegativity, and octahedral factor contribute to the predictive accuracy of the classification model?
3. Are there any limitations or challenges in interpreting the model's predictions based on the selected features?

Data Understanding

The data consists of 4,165 ABO3 perovskite-type oxides. Each observation is described by 13 feature columns and 1 class column which identifies it to be either a cubic, tetragonal, orthorhombic, and rhombohedral structure.(2)

Missing Values: In the case of data quality, missing or inconsistent data were handled on a case by case basis. Some considerations made were the relative importance of the variable in the analysis, how much data was needed, and finally, the possibility of filling data with a central measure of tendency and the statistical implications.

Data Preparation (EDA)

In [1]:

```
# Import the necessary packages

#Third Party Packages
import pandas as pd
import plotly.express as px
import seaborn as sns
import matplotlib.pyplot as plt
from sklearn.tree import DecisionTreeClassifier
from sklearn.model_selection import *
from sklearn.metrics import *
from sklearn.model_selection import GridSearchCV
from sklearn.metrics import confusion_matrix
from sklearn.metrics import accuracy_score
from sklearn.metrics import roc_curve, roc_auc_score
import numpy as np
from sklearn.ensemble import RandomForestClassifier
import time
from sklearn.svm import SVC
from sklearn.model_selection import cross_val_score
from sklearn.metrics import classification_report
from sklearn.inspection import permutation_importance
from sklearn.metrics import ConfusionMatrixDisplay

```

In [2]:

```
# Create DataFrame
prv_train = pd.read_csv("Data/Perovskite_train.csv")

# Display
print("Total number of results:", len(prv_train))
display(prv_train.head()) # Using display instead of print leads to a neater output

```

```
Total number of results: 4165
```

	v(A)	v(B)	r(AXII) (Å)	r(AVI) (Å)	r(BVI) (Å)	EN(A)	EN(B)	l(A-O)(Å)	l(B-O)(Å)	ΔENR	tG	τ	μ	Lowest distortion
0	0	0	0.52	0.52	0.93	2.18	2.54	2.214685	2.313698	-1.728214	0.582680	0.000000	0.664286	cubic
1	0	0	1.03	0.86	0.60	1.27	1.90	2.500930	0.000000	-1.768643	0.859135	0.000000	0.428571	cubic
2	2	4	0.92	0.67	0.53	1.83	1.88	2.290644	1.930311	-1.468464	0.849994	4.936558	0.378571	cubic
3	1	5	1.64	1.38	0.62	0.82	2.36	3.025719	1.745600	-1.974429	1.064161	3.977376	0.442857	orthorhombic
4	0	0	0.57	0.57	0.71	2.20	1.30	2.300109	2.027412	-1.622357	0.660190	0.000000	0.507143	cubic

In [3]:

```
# Rename columns in prv_train DataFrame
#(pep8 standard, a line of code should not exceed 79 characters
#so each renaming is it's own line)
prv_train = prv_train.rename(columns={'v(A)': 'vA'})
prv_train = prv_train.rename(columns={'v(B)': 'vB'})
prv_train = prv_train.rename(columns={'r(AXII)(Å)': 'r_A12'})
prv_train = prv_train.rename(columns={'r(AVI)(Å)': 'r_A6'})
prv_train = prv_train.rename(columns={'r(BVI)(Å)': 'r_B6'})
prv_train = prv_train.rename(columns={'EN(A)': 'EN_A'})
prv_train = prv_train.rename(columns={'EN(B)': 'EN_B'})
prv_train = prv_train.rename(columns={'l(A-O)(Å)': 'bond_len_AO'})
prv_train = prv_train.rename(columns={'l(B-O)(Å)': 'bond_len_BO'})
prv_train = prv_train.rename(columns={'ΔENR': 'ENR_diff'})
prv_train = prv_train.rename(columns={'τ': 'tau'})
prv_train = prv_train.rename(columns={'μ': 'mu'})
prv_train = prv_train.rename(columns={'Lowest distortion': 'lowest_distortion'})

```

In [4]:
```
# Get summary
display(prv_train.info())
```

```
 #   Column             Non-Null Count  Dtype
---  ------             --------------  -----
 0   vA                 4165 non-null   int64
 1   vB                 4165 non-null   int64
 2   r_A12              4165 non-null   float64
 3   r_A6               4165 non-null   float64
 4   r_B6               4165 non-null   float64
 5   EN_A               4165 non-null   float64
 6   EN_B               4165 non-null   float64
 7   bond_len_A0        4165 non-null   float64
 8   bond_len_B0        4165 non-null   float64
 9   ENR_diff           4165 non-null   float64
 10  tG                 4165 non-null   float64
 11  tau                4165 non-null   float64
 12  mu                 4165 non-null   float64
 13  lowest_distortion  4165 non-null   object
dtypes: float64(11), int64(2), object(1)
memory usage: 455.7+ KB
```

None

List of Feature (or attributes, either work) Descriptions

- `vA` : Valence of A
- `vB` : Valence of B
- `r_A6` : ionic radius of A cation (A6)
- `r_A12` : ionic radius of A cation (a second one, A12)
- `r_B6` : ionic radius of B cation
- `EN_A` : Average electronegativity value of A cation
- `EN_B` : Average electronegativity value of B cation
- `bond_len_A0` : Bond length of A-O pair
- `bond_len_B0` : Bond length of B-O pair
- `ENR_diff` : Electronegativity difference with radius
- `tG` : Goldschmidt tolerance factor
- `tau` : New tolerance factor
- `mu` : Octahedral factor

This is a multiclass, imbalanced dataset. The cubic structure is far more common than any other dataset.

$$\tau = \frac{r_A + r_B}{\sqrt{2}(r_O) + l_{B-O} - l_{A-O}}$$

- r_A is the ionic radius of the A-site cation.
- r_B is the ionic radius of the B-site cation.
- r_O is the radius of the oxygen ion.
- l_{A-O} is the bond length of the A-O pair.
- l_{B-O} is the bond length of the B-O pair.

Mathematically, the Goldschmidt tolerance factor (tG) is given by:

$$t_G = \frac{r_A + r_B}{2(r_O)}$$

- (r_A) is the ionic radius of the A-site cation.
- (r_B) is the ionic radius of the B-site cation.
- (r_O) is the radius of the oxygen ion.

Side quest (because it is interesting). The above formulas give context, which is extra data that many times won't be available.

Taking a closer look at the variables:

The only empirical data from the crystal structures here are `bond lengths` and `bond angles`.

Some may consider `valence electron` counts, but locking the atoms into formal charges when such things are assigned by convention might disrupt the algorithms (or not, charges probably aren't far off given it's oxygen).

`Ionic radii` are also, to some degree, just average values without someone/something to determine where those radii actually extend to across different combinations.

`Electronegativity` could be treated as an empirical parameter provided the different ways of obtaining those numbers don't produce significantly different results (collection methods were not provided) - in which case there would be a nice electronegativity/ionic radius predictor from enough data.

`tG`, `tau`, and `mu` are all things that should be able to be predicted from the structural parameters. It is suspected that `tG` and `tau` should be something that would fall out of a large dataset analysis easily.

In [5]:
```
# Select columns with data type 'object'
string_col = prv_train.select_dtypes(include="object").columns

# Convert selected columns to the 'string' data type
prv_train[string_col] = prv_train[string_col].astype("string")

```

In [6]:
```
# Get summary
display(prv_train.info())
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 4165 entries, 0 to 4164
Data columns (total 14 columns):
 #   Column             Non-Null Count  Dtype
---  ------             --------------  -----
 0   vA                 4165 non-null   int64
 1   vB                 4165 non-null   int64
 2   r_A12              4165 non-null   float64
 3   r_A6               4165 non-null   float64
 4   r_B6               4165 non-null   float64
 5   EN_A               4165 non-null   float64
 6   EN_B               4165 non-null   float64
 7   bond_len_AO        4165 non-null   float64
 8   bond_len_BO        4165 non-null   float64
 9   ENR_diff           4165 non-null   float64
 10  tG                 4165 non-null   float64
 11  tau                4165 non-null   float64
 12  mu                 4165 non-null   float64
 13  lowest_distortion  4165 non-null   string
dtypes: float64(11), int64(2), string(1)
memory usage: 455.7 KB

None
```

The object data has been converted to string.

It appears there are two measurements for the radius of the A cation, labeled as "r(AXII)(Å)" and "r(AVI)(Å)". This duplication could be due to different conventions or sources of data.

In short, there are two columns due to atomic arrangements; factors such as the types of ions present, their sizes, and their positions within the crystal lattice can influence the overall size of the perovskite structure. These variations in atomic arrangements and compositions can lead to different radii for perovskite structures.

Unfortunately, no atomic data is provided.

In [7]:
```
# Create a copy of the DataFrame to avoid altering the original
prv_train_num = prv_train.copy()

# Select columns with data type 'string'
string_col=prv_train_num.select_dtypes("string").columns.to_list()
```

In [8]:
```
# Extract column names of prv_train_num DataFrame and store them in num_col
num_col = prv_train_num.columns.to_list()


# Remove the column "Lowest distortion" from num_col
num_col.remove("lowest_distortion")
print(num_col)

```

```
['vA', 'vB', 'r_A12', 'r_A6', 'r_B6', 'EN_A', 'EN_B', 'bond_len_AO', 'bond_len_BO', 'ENR_diff',
'tG', 'tau', 'mu']
```

For this project, it doesn't really remove anything, but if there were hundreds of columns then the strings would get in the way of the data describe and so generally they would be removed this way before describing the data.

This line generates a summary statistics table for the DataFrame prv_train_num. The `.describe()` method calculates summary statistics for numerical columns by default. The `.T` at the end is a transpose operation, which swaps the rows and columns of the summary statistics table. This operation is performed to make the table more readable, with variables as rows and summary statistics as columns. This is often done to have a better visual representation of the data, especially when there are many columns, as is the case with this data set.

In [9]:
```
prv_train_num.describe().T
```

Out[9]:

	count	mean	std	min	25%	50%	75%	max
vA	4165.0	0.882353	1.672111	-1.000000	-1.000000	0.000000	2.000000	5.000000
vB	4165.0	1.385114	2.161707	-1.000000	-1.000000	0.000000	3.000000	5.000000
r_A12	4165.0	1.005570	0.336940	0.270000	0.730000	0.980000	1.240000	1.880000
r_A6	4165.0	0.841789	0.240549	0.270000	0.670000	0.860000	0.960000	1.670000
r_B6	4165.0	0.801999	0.234891	0.270000	0.630000	0.760000	0.940000	1.670000
EN_A	4165.0	1.547309	0.447277	0.790000	1.200000	1.500000	1.910000	2.540000
EN_B	4165.0	1.599059	0.442961	0.790000	1.220000	1.600000	1.960000	2.540000
bond_len_AO	4165.0	2.323011	0.635699	0.000000	2.294004	2.422517	2.582926	3.300176
bond_len_BO	4165.0	2.017219	0.555599	0.000000	1.956808	2.075849	2.284156	3.009747
ENR_diff	4165.0	-2.186093	0.636470	-5.411536	-2.570036	-2.084214	-1.734643	-0.601714
tG	4165.0	0.781040	0.135816	0.384648	0.680809	0.776944	0.873123	1.321062
tau	4165.0	1.332182	20.804362	-480.827696	0.000000	0.000000	3.892903	305.871348
mu	4165.0	0.572857	0.167778	0.192857	0.450000	0.542857	0.671429	1.192857

Looking at Tau, the zeros could be a problem. The max value is also 305 (which may likely be an outlier) with a listed mean of 1.3. Further investigation around this is needed. This column may need to be dropped.

EN(A) and EN(B) have the same values indicating that they are distributed the same.

Some of the bond lengths are displaying zero and will need to be investigated further (domain knowledge says that this is impossible).

If the valence(A) and (B) are both zero, in this dataset, it implies that both cations (A and B) are essentially neutral, meaning they have no charge. This scenario is highly unlikely and not physically meaningful in the context of perovskite compounds because A and B cations typically have non-zero valence states to contribute to the overall charge balance of the compound.

Therefore, in this dataset, the occurrence of both A and B having zero valence is likely an artifact or error rather than a meaningful data point. It's important to review the data and ensure its integrity, an occurrence like this may indicate issues with data collection

In [10]:
```
# Count the number of zeros in each column of the training dataset
zero_counts = prv_train.apply(lambda col: (col == 0).sum())
print("Count of zeros in each column:")
print(zero_counts)
```

```
Count of zeros in each column:
vA                    859
vB                    859
r_A12                   0
r_A6                    0
r_B6                    0
EN_A                    0
EN_B                    0
bond_len_AO           254
bond_len_BO           243
ENR_diff                0
tG                      0
tau                  2177
mu                      0
lowest_distortion       0
dtype: int64
```

The `tau` column, representing the New tolerance factor, is essential because:

Structural Stability Assessment: The New tolerance factor `tau` provides insight into the structural stability of perovskite compounds. It considers the ionic radii of the A and B cations and the oxygen ion as well as the bond lengths between these ions. By incorporating bond lengths, `tau` offers a comprehensive assessment of the compound's structural stability compared to the traditional Goldschmidt tolerance factor `t_G` .

So it would be worth our time to investigate the effectiveness of the model both with and without Tau.

In [11]:
```
# Create a copy of the DataFrame to avoid altering the original
prv_train_tau = prv_train.copy()

# Drop rows with zero values
prv_train_tau = prv_train_tau[prv_train_tau['tau'] != 0]

# Display
print("Total number of results:", len(prv_train_tau))
display(prv_train_tau.head())
```

```
Total number of results: 1988
```

	vA	vB	r_A12	r_A6	r_B6	EN_A	EN_B	bond_len_AO	bond_len_BO	ENR_diff	tG	tau	mu	lowest_distortion
2	2	4	0.92	0.67	0.53	1.83	1.88	2.290644	1.930311	-1.468464	0.849994	4.936558	0.378571	cubic
3	1	5	1.64	1.38	0.62	0.82	2.36	3.025719	1.745600	-1.974429	1.064161	3.977376	0.442857	orthorhombic
6	1	5	0.92	0.80	0.62	1.78	2.36	2.392362	1.745600	-1.484143	0.812123	5.017992	0.442857	cubic
10	3	3	1.36	1.03	0.90	1.10	1.23	2.689119	2.258656	-2.931286	0.848528	3.536265	0.642857	orthorhombic
11	2	4	1.19	0.99	0.61	1.22	1.54	2.550861	1.927849	-2.040571	0.911148	4.133678	0.435714	orthorhombic

In [12]:

```
# Count the number of zeros in each column of the training dataset with tolerance factor (tau)
zero_counts = prv_train_tau.apply(lambda col: (col == 0).sum())
print("Count of zeros in each column:")
print(zero_counts)
```

```
Count of zeros in each column:
vA                  0
vB                  0
r_A12               0
r_A6                0
r_B6                0
EN_A                0
EN_B                0
bond_len_AO         0
bond_len_BO         0
ENR_diff            0
tG                  0
tau                 0
mu                  0
lowest_distortion   0
dtype: int64
```

In [13]:

```
# Create a copy of the DataFrame to avoid altering the original
prv_train_no_tau = prv_train.copy()

# Drop tau column
prv_train_no_tau.drop(['tau'], axis=1, inplace=True)

# Display
print("Total number of results:", len(prv_train_no_tau))
display(prv_train_no_tau.head())
```

```
Total number of results: 4165
```

	vA	vB	r_A12	r_A6	r_B6	EN_A	EN_B	bond_len_AO	bond_len_BO	ENR_diff	tG	mu	lowest_distortion
0	0	0	0.52	0.52	0.93	2.18	2.54	2.214685	2.313698	-1.728214	0.582680	0.664286	cubic
1	0	0	1.03	0.86	0.60	1.27	1.90	2.500930	0.000000	-1.768643	0.859135	0.428571	cubic
2	2	4	0.92	0.67	0.53	1.83	1.88	2.290644	1.930311	-1.468464	0.849994	0.378571	cubic
3	1	5	1.64	1.38	0.62	0.82	2.36	3.025719	1.745600	-1.974429	1.064161	0.442857	orthorhombic
4	0	0	0.57	0.57	0.71	2.20	1.30	2.300109	2.027412	-1.622357	0.660190	0.507143	cubic

In [14]:
```
# Count the number of zeros in each column of the training dataset without tolerance factor (ta
zero_counts = prv_train_no_tau.apply(lambda col: (col == 0).sum())

# Print a message indicating the count of zeros in each column.
print("Count of zeros in each column:")

# Print the variable zero_counts, which contains the count of zeros in each column
# of the DataFrame prv_train_no_tau.
print(zero_counts)


```

```
Count of zeros in each column:
vA                   859
vB                   859
r_A12                  0
r_A6                   0
r_B6                   0
EN_A                   0
EN_B                   0
bond_len_AO          254
bond_len_BO          243
ENR_diff               0
tG                     0
mu                     0
lowest_distortion      0
dtype: int64
```

For consideration: Should these zero values be left to skew the data to be incorrect or should they be dropped?

vA and vB are crucial factors so zero values for those features would really not give any meaningful results. The dataset could be split here but then there would be multiple analyses on various datasets and not evaluations of various machine learning models. So these values will be dropped to limit the number of datasets and maximize the number of machine learning models.

Every time there's a column or row with bad data there's an opportunity to drop that data. In this case, the zero count was so low, it was worth dropping the errors.

In [15]:
```
# Drop rows with zero values
prv_train_no_tau = prv_train_no_tau[prv_train_no_tau['vA'] != 0]

# Display
print("Total number of results:", len(prv_train_no_tau))
display(prv_train_no_tau.head())
```

```
Total number of results: 3306
```

	vA	vB	r_A12	r_A6	r_B6	EN_A	EN_B	bond_len_AO	bond_len_BO	ENR_diff	tG	mu	lowest_distortion
2	2	4	0.92	0.67	0.53	1.83	1.88	2.290644	1.930311	-1.468464	0.849994	0.378571	cubic
3	1	5	1.64	1.38	0.62	0.82	2.36	3.025719	1.745600	-1.974429	1.064161	0.442857	orthorhombic
6	1	5	0.92	0.80	0.62	1.78	2.36	2.392362	1.745600	-1.484143	0.812123	0.442857	cubic
10	3	3	1.36	1.03	0.90	1.10	1.23	2.689119	2.258656	-2.931286	0.848528	0.642857	orthorhombic
11	2	4	1.19	0.99	0.61	1.22	1.54	2.550861	1.927849	-2.040571	0.911148	0.435714	orthorhombic

In [16]:
```
# Count the number of zeros in each column of the training dataset without tolerance factor (ta
zero_counts = prv_train_no_tau.apply(lambda col: (col == 0).sum())
print("Count of zeros in each column:")
print(zero_counts)
```

```
Count of zeros in each column:
vA                  0
vB                  0
r_A12               0
r_A6                0
r_B6                0
EN_A                0
EN_B                0
bond_len_AO         0
bond_len_BO         0
ENR_diff            0
tG                  0
mu                  0
lowest_distortion   0
dtype: int64
```

Where vA was zero, it appears that vB and also bond_len_AO and bond_len_BO are all also zero. So only the zeros from vA needed to be dropped.

In [17]:
```
# Accessing -1 values
prv_train_no_tau.loc[prv_train_no_tau['vA'] == -1]

```

Out[17]:

	vA	vB	r_A12	r_A6	r_B6	EN_A	EN_B	bond_len_AO	bond_len_BO	ENR_diff	tG	mu	lowest_distortion
20	-1	-1	1.24	0.96	0.99	1.17	1.22	2.611965	2.255581	-3.002036	0.781072	0.707143	cubic
21	-1	-1	1.70	1.20	0.80	1.62	1.78	2.531967	2.147681	-2.510714	0.996378	0.571429	orthorhombic
23	-1	-1	0.27	0.27	0.27	2.04	2.04	1.891523	1.624662	-0.601714	0.707107	0.192857	cubic
24	-1	-1	0.63	0.63	0.90	2.20	2.02	2.311295	2.215655	-1.823786	0.624099	0.642857	cubic
30	-1	-1	0.90	0.63	1.52	1.88	0.82	2.233563	2.825997	-3.556429	0.556968	1.085714	rhombohedral
...	...	...	...	...	...	...	...	...	...	...	...	...	...
4137	-1	-1	0.68	0.68	0.90	2.05	2.02	2.361079	2.215655	-1.897357	0.639470	0.642857	cubic
4142	-1	-1	0.45	0.45	1.11	1.57	2.00	2.178342	2.323655	-2.336464	0.521174	0.792857	cubic
4143	-1	-1	0.87	0.75	0.62	1.36	1.55	2.417029	2.169994	-1.809536	0.794620	0.442857	cubic
4146	-1	-1	1.03	0.86	0.77	1.27	2.10	2.500930	2.115492	-2.035679	0.791829	0.550000	cubic
4148	-1	-1	0.54	0.54	0.94	1.61	1.30	2.186789	2.246056	-2.181929	0.586234	0.671429	cubic

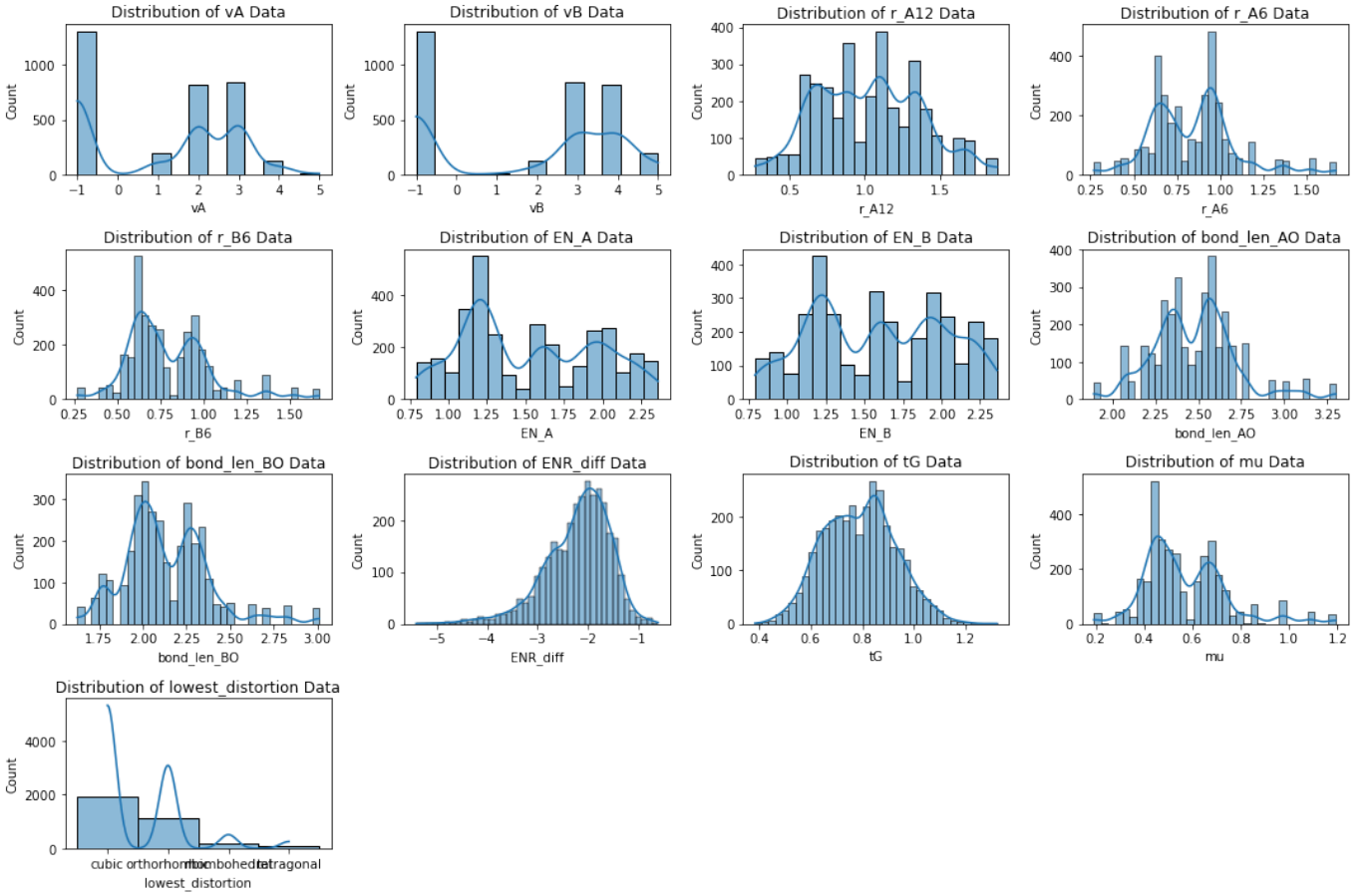
1299 rows × 13 columns

This might be two data sets combined. All perovskites contain two positively charged ions (A and B). Positively charged ions are called cations and are bonded to negatively charged atoms. A negative value for a valence electron count would indicate an overall negative charge. Since the compound will have a balance of charges, this value may indicate some inconsistency.

Data set 1: has valence electrons reported for each entry and a tau calculation. Data set 2: doesn't contain valence electrons or a calculated tau value.

In [18]:

```
# Set up the figure size for the plot
plt.figure(figsize=(15,10))

# Iterate over each column in the dataframe
for i, col in enumerate(prv_train_no_tau.columns, 1):
    # Create subplots in a 4x4 grid
    plt.subplot(4, 4, i)

    # Set title for each subplot indicating the distribution of data for the corresponding colu
    plt.title(f"Distribution of {col} Data")

    # Plot the histogram with kernel density estimation using seaborn's histplot function
    sns.histplot(prv_train_no_tau[col], kde=True)

    # Adjust subplot layout
    plt.tight_layout()

    # Ensure the plot is shown
    plt.plot()

```



The valence electrons should add up to 6. A '-1' value seems to be used as a placeholder. Drop all rows with a -1 value.

In [19]:
```
# Drop rows with -1 values
prv_train_no_tau = prv_train_no_tau[prv_train_no_tau['vA'] != -1]

# Display
print("Total number of results:", len(prv_train_no_tau))
display(prv_train_no_tau.head())
```

```
Total number of results: 2007
```

	vA	vB	r_A12	r_A6	r_B6	EN_A	EN_B	bond_len_AO	bond_len_BO	ENR_diff	tG	mu	lowest_distortion
2	2	4	0.92	0.67	0.53	1.83	1.88	2.290644	1.930311	-1.468464	0.849994	0.378571	cubic
3	1	5	1.64	1.38	0.62	0.82	2.36	3.025719	1.745600	-1.974429	1.064161	0.442857	orthorhombic
6	1	5	0.92	0.80	0.62	1.78	2.36	2.392362	1.745600	-1.484143	0.812123	0.442857	cubic
10	3	3	1.36	1.03	0.90	1.10	1.23	2.689119	2.258656	-2.931286	0.848528	0.642857	orthorhombic
11	2	4	1.19	0.99	0.61	1.22	1.54	2.550861	1.927849	-2.040571	0.911148	0.435714	orthorhombic

Next, let's take a look at maximizing the number of data points. What would the data set look like if the valence electron columns and the tau column were dropped? Would there be any zeros left in the data set?

In [20]:
```
# Create a copy of the DataFrame to avoid altering the original
prv_train_no_tau_no_v = prv_train.copy()

# Drop tau column
prv_train_no_tau_no_v.drop(['tau', 'vA', 'vB'], axis=1, inplace=True)

# Display
print("Total number of results:", len(prv_train_no_tau_no_v))
display(prv_train_no_tau_no_v.head())
```

```
Total number of results: 4165
```

	r_A12	r_A6	r_B6	EN_A	EN_B	bond_len_AO	bond_len_BO	ENR_diff	tG	mu	lowest_distortion
0	0.52	0.52	0.93	2.18	2.54	2.214685	2.313698	-1.728214	0.582680	0.664286	cubic
1	1.03	0.86	0.60	1.27	1.90	2.500930	0.000000	-1.768643	0.859135	0.428571	cubic
2	0.92	0.67	0.53	1.83	1.88	2.290644	1.930311	-1.468464	0.849994	0.378571	cubic
3	1.64	1.38	0.62	0.82	2.36	3.025719	1.745600	-1.974429	1.064161	0.442857	orthorhombic
4	0.57	0.57	0.71	2.20	1.30	2.300109	2.027412	-1.622357	0.660190	0.507143	cubic

In [21]:
```
# Count the number of zeros in each column of the training dataset without tolerance factor (ta
zero_counts = prv_train_no_tau_no_v.apply(lambda col: (col == 0).sum())
print("Count of zeros in each column:")
print(zero_counts)
```

```
Count of zeros in each column:
r_A12                0
r_A6                 0
r_B6                 0
EN_A                 0
EN_B                 0
bond_len_AO        254
bond_len_BO        243
ENR_diff             0
tG                   0
mu                   0
lowest_distortion    0
dtype: int64
```

Domain knowledge says that bond lengths cannot be zero so these values must be dropped. Also note that the bond length counts are different and may not occur in the same rows. The number of zero values is low so it is acceptable to drop these values.

In [22]:
```
# Drop rows with 0 values
prv_train_no_tau_no_v = prv_train_no_tau_no_v[prv_train_no_tau_no_v['bond_len_AO'] > 0]
prv_train_no_tau_no_v = prv_train_no_tau_no_v[prv_train_no_tau_no_v['bond_len_BO'] > 0]

# Display
print("Total number of results:", len(prv_train_no_tau_no_v))
display(prv_train_no_tau_no_v.head())

```

```
Total number of results: 3682
```

	r_A12	r_A6	r_B6	EN_A	EN_B	bond_len_AO	bond_len_BO	ENR_diff	tG	mu	lowest_distortion
0	0.52	0.52	0.93	2.18	2.54	2.214685	2.313698	-1.728214	0.582680	0.664286	cubic
2	0.92	0.67	0.53	1.83	1.88	2.290644	1.930311	-1.468464	0.849994	0.378571	cubic
3	1.64	1.38	0.62	0.82	2.36	3.025719	1.745600	-1.974429	1.064161	0.442857	orthorhombic
4	0.57	0.57	0.71	2.20	1.30	2.300109	2.027412	-1.622357	0.660190	0.507143	cubic
6	0.92	0.80	0.62	1.78	2.36	2.392362	1.745600	-1.484143	0.812123	0.442857	cubic

In [23]:
```
# Count the number of zeros in each column of the training dataset without tolerance factor (ta
zero_counts = prv_train_no_tau_no_v.apply(lambda col: (col == 0).sum())
print("Count of zeros in each column:")
print(zero_counts)
```

```
Count of zeros in each column:
r_A12                0
r_A6                 0
r_B6                 0
EN_A                 0
EN_B                 0
bond_len_AO          0
bond_len_BO          0
ENR_diff             0
tG                   0
mu                   0
lowest_distortion    0
dtype: int64
```

Choosing a final data set to train

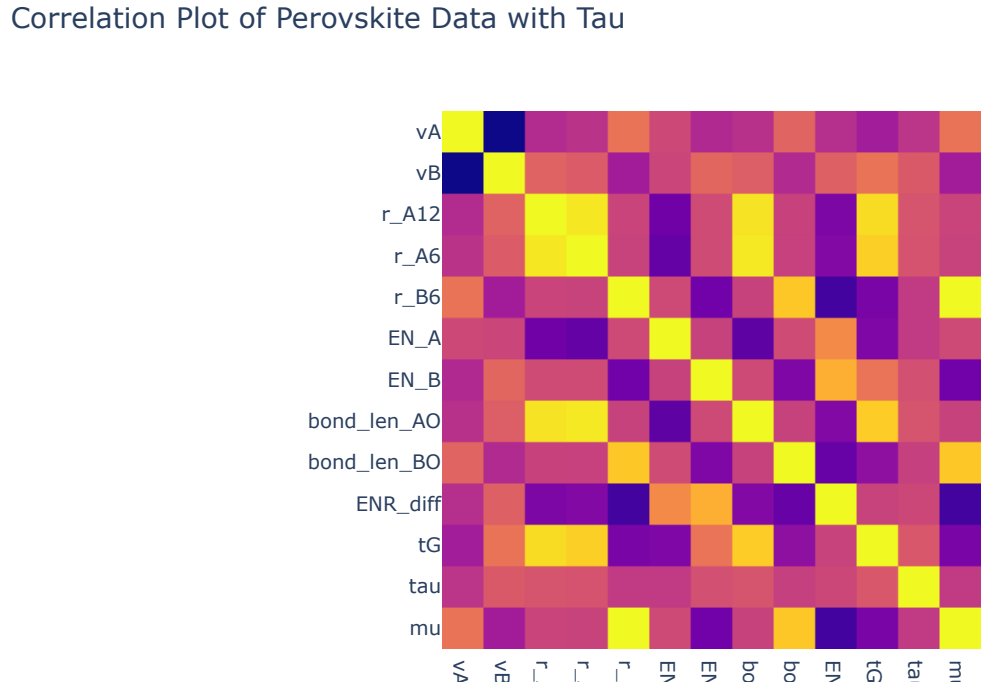
Comparing the perovskite data with tau and without tau.

In this section, it's really important to both consider removing columns or rows and how that impacts the integrity and completeness of the dataset. Specifically, we are considering different data set combinations that make use of different columns because that changes which rows are included in the dataset.

```
### 1. Correlation Plots
```

In [24]:

```
# Create a correlation plot of the training dataset with tolerance factor (tau)
px.imshow(prv_train_tau.corr(),title="Correlation Plot of Perovskite Data with Tau")
```



Some notes on the correlation matrix:

Strong Correlations:

Some variables exhibit strong correlations. For instance, there is a perfect negative correlation (-1) between vA and vB, indicating that they are inversely related. Similarly, r_A12 and r_A6, which likely represent different aspects of the same quantity, show a strong positive correlation (0.917346), suggesting they move in the same direction. Variables such as bond_len_AO and bond_len_BO also show strong positive correlations (0.923351), implying a strong relationship between the bond lengths of A-O and B-O pairs.

Moderate Correlations:

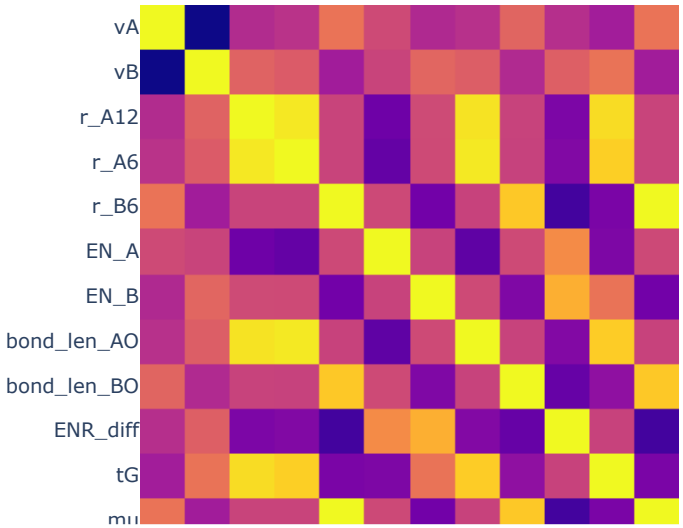
There are moderate correlations between certain variables, such as tG and bond_len_AO (0.785924) or tG and r_A12 (0.863578). These correlations suggest some degree of relationship between the variables but may not be as strong as the highly correlated ones.

Weak Correlations:

Some variables exhibit weak correlations or no significant correlation at all. For example, the correlation between EN_A and EN_B is relatively low (-0.034935), indicating a weak relationship between the electronegativities of A and B cations.

Correlation does not imply causation. While correlated variables may move together, it does not necessarily mean that changes in one variable cause changes in the other. Understanding the physical or chemical relationship between variables can provide insights into why certain correlations exist and their implications, such as in the case of the valence electrons.

In [25]:
```
# Create a correlation plot of the training dataset with tolerance factor (tau)
px.imshow(prv_train_no_tau.corr(),title="Correlation Plot of Perovskite Data without Tau")
```



In this correlation matrix, several noteworthy observations can be made:

Strong Positive Correlations:

Variables such as vA and vB (0.813366), r_A12 and r_A6 (0.935433), bond_len_AO and bond_len_BO (0.938676), and bond_len_BO and EN_diff (0.907513) exhibit strong positive correlations. These correlations suggest that changes in one variable tend to be associated with similar changes in the other variable. It is interesting that the EN_diff and the bond_len_BO are directly related while the EN_diff and the EN_A are inversely (see next statement).

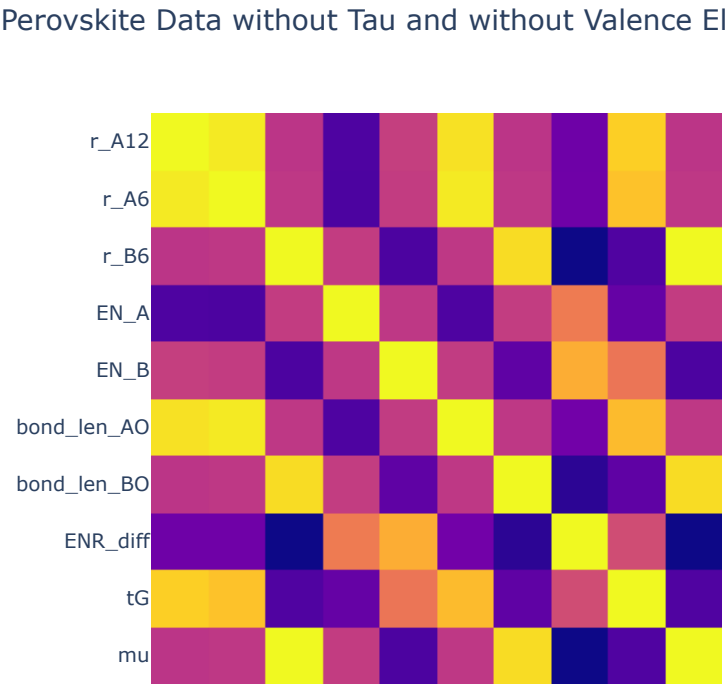
Strong Negative Correlations:

There are also strong negative correlations observed, such as between r_B6 and tG (-0.842273) or between EN_diff and EN_A (-0.842273). These negative correlations suggest an inverse relationship between the variables.

Moderate Correlations:

Moderate correlations are present between various pairs of variables, such as vA and tG (0.215130), vB and tG (0.342345), bond_len_AO and r_A12 (0.905104), or EN_B and EN_diff (0.674963). These moderate correlations indicate a discernible but not excessively strong relationship between the variables.

In [26]:
```
# Create a correlation plot of the training dataset without tolerance factor (tau) and valence
px.imshow(prv_train_no_tau_no_v.corr(),title="Correlation Plot of Perovskite Data without Tau a

```



Strong Positive Correlations:

Variables such as r_A12 and r_A6 (0.934533) exhibit a strong positive correlation. This suggests that changes in the radius at site A with a coordination number of 12 are strongly associated with similar changes in the radius at site A with a coordination number of 6, moving in the same direction. Another strong positive correlation is observed between bond_len_AO and bond_len_BO (0.894372), indicating that changes in the bond lengths between atoms A and oxygen are strongly associated with changes in the bond lengths between atoms B and oxygen, moving in the same direction.

Strong Negative Correlations:

A strong negative correlation is seen between r_B6 and tG (-0.584644). This suggests an inverse relationship, where increases in the radius at site B with a coordination number of 6 are associated with decreases in the value of parameter tG, and vice versa.

Moderate Correlations:

Moderate correlations are present between various pairs of variables, such as between r_A12 and EN_diff (-0.444288) or between EN_B and EN_diff (0.658368). These correlations indicate a discernible but not excessively strong relationship between the variables.

Summary of the three matrices:

Matrix 1 (with Tau):

This matrix includes all the variables along with the Tau variable. Strong positive correlations are observed between variables like vA and vB, bond_len_AO and r_A12, tG and r_A12, etc. Strong negative correlations are seen between EN_A and r_A12, EN_diff and r_B6, mu and r_B6, etc. The Tau variable shows moderate correlations with other variables. Overall, this matrix provides comprehensive information about the correlations, including Tau, with other variables.

Matrix 2 (without Tau):

Initially, Tau was excluded because of the large number of zeros in the data. This matrix is similar to Matrix 1 but excludes the Tau variable. The correlations remain quite similar to those in Matrix 1, except for the absence of correlations involving Tau. Strong positive and negative correlations between other variables remain intact. The removal of the Tau variable reduces the complexity of the matrix, making it easier to interpret if Tau is not a focus of the analysis.

Matrix 3 (without Tau and without Valence Electron Data):

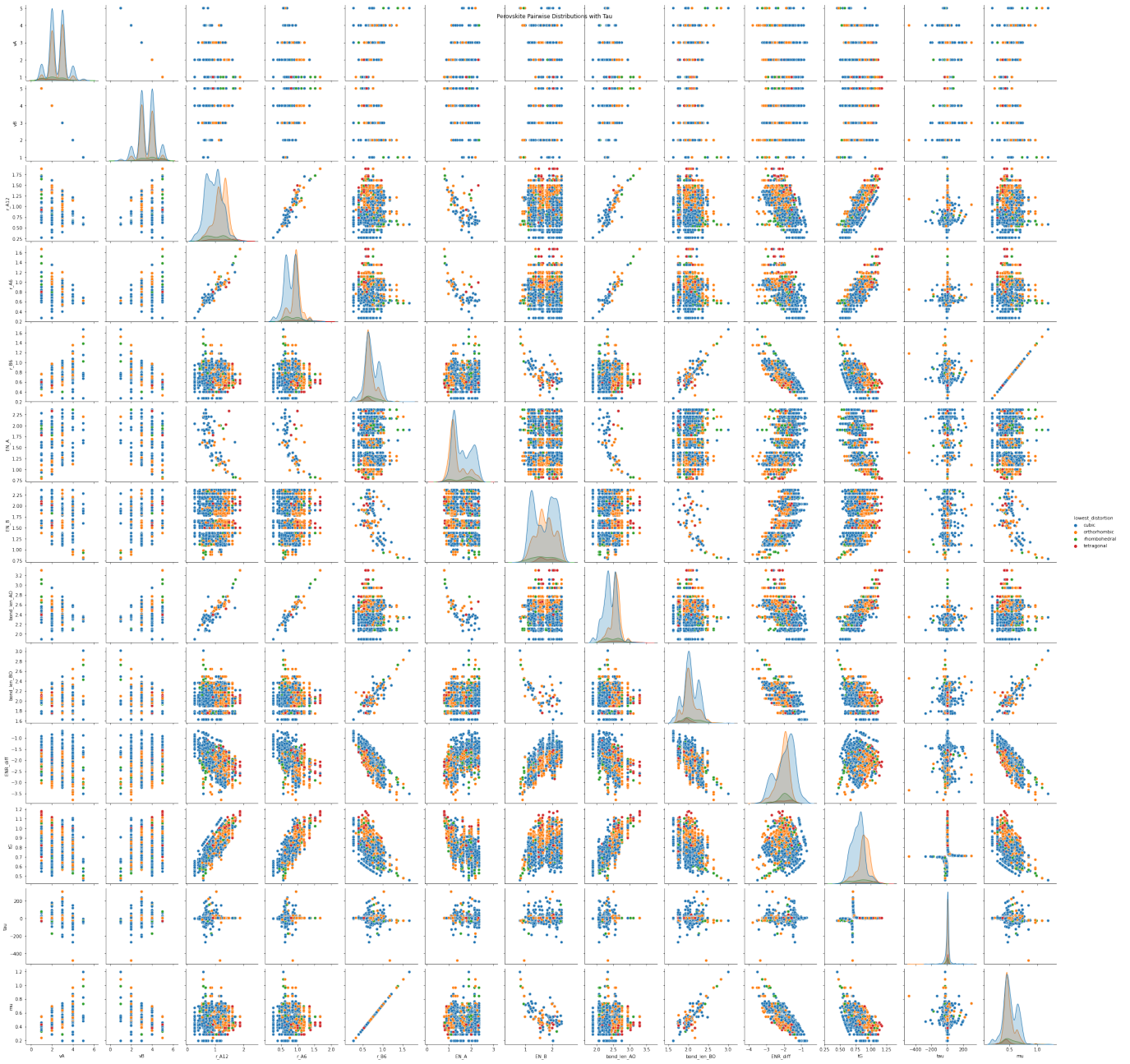
This matrix excludes both the Tau variable and the Valence Electron data in order to preserve more rows of data. The correlations presented here are limited to the remaining variables: r_A12, r_A6, r_B6, EN_A, EN_B, bond_len_AO, bond_len_BO, EN_diff, tG, and mu. Strong positive and negative correlations observed in the previous matrices persist in this matrix as well. This matrix provides a simplified view of the correlations among the selected variables, excluding additional information such as Tau and Valence Electron data.

Matrix 1 provides the most comprehensive view, Matrix 2 is useful when excluding Tau from consideration, and Matrix 3 offers a simplified view focusing only on the core variables.

Pair plots

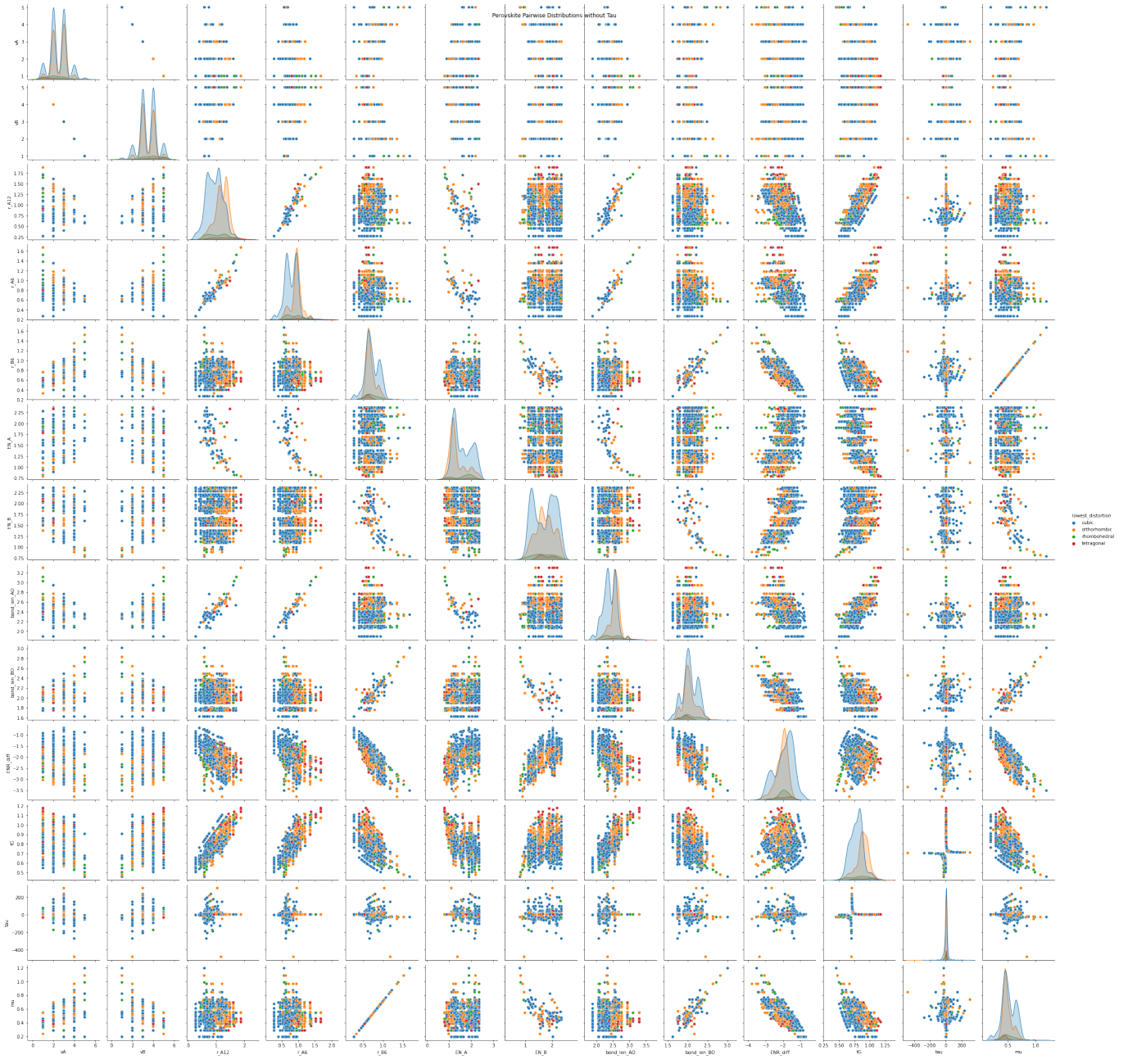
In [27]:

```
# Create a pairplot of the training dataset with tolerance factor (tau), distinguishing by lowe
pair_plot = sns.pairplot(prv_train_tau, hue="lowest_distortion")

# Set the title of the pairplot
pair_plot.fig.suptitle("Perovskite Pairwise Distributions with Tau")

# Save the pairplot as an image file
pair_plot.savefig("pairplot_perovskite_train_tau.jpg")

# Display the pairplot
plt.show()

```



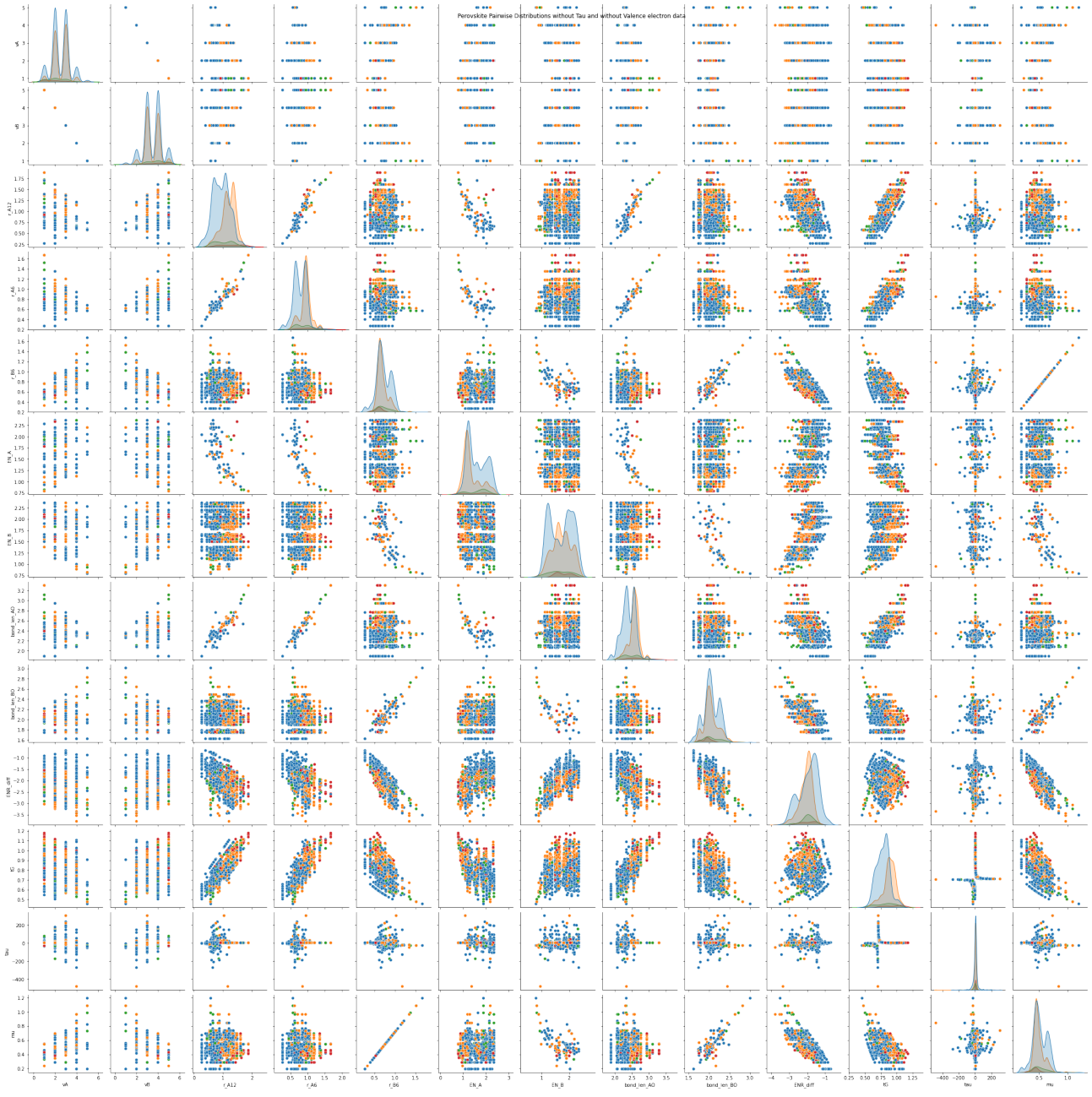
In [28]:

```
# Create a pair plot of the training dataset without tolerance factor (tau) with hue based on
pair_plot = sns.pairplot(prv_train_tau, hue="lowest_distortion")

# Set the title for the pair plot
pair_plot.fig.suptitle("Perovskite Pairwise Distributions without Tau")

# Save the pair plot as an image
pair_plot.savefig("pairplot_perovskite_train_without_tau.jpg")

# Display the pair plot
plt.show()

```



In [29]:

```
# Create a pair plot of the training dataset without tolerance factor (tau) and without valence
pair_plot = sns.pairplot(prv_train_tau, hue="lowest_distortion")

# Set the title for the pair plot
pair_plot.fig.suptitle("Perovskite Pairwise Distributions without Tau and without Valence elect

# Save the pair plot as an image
pair_plot.savefig("pairplot_perovskite_train_without_tau_Ve.jpg")

# Display the pair plot
plt.show()

```



Summary

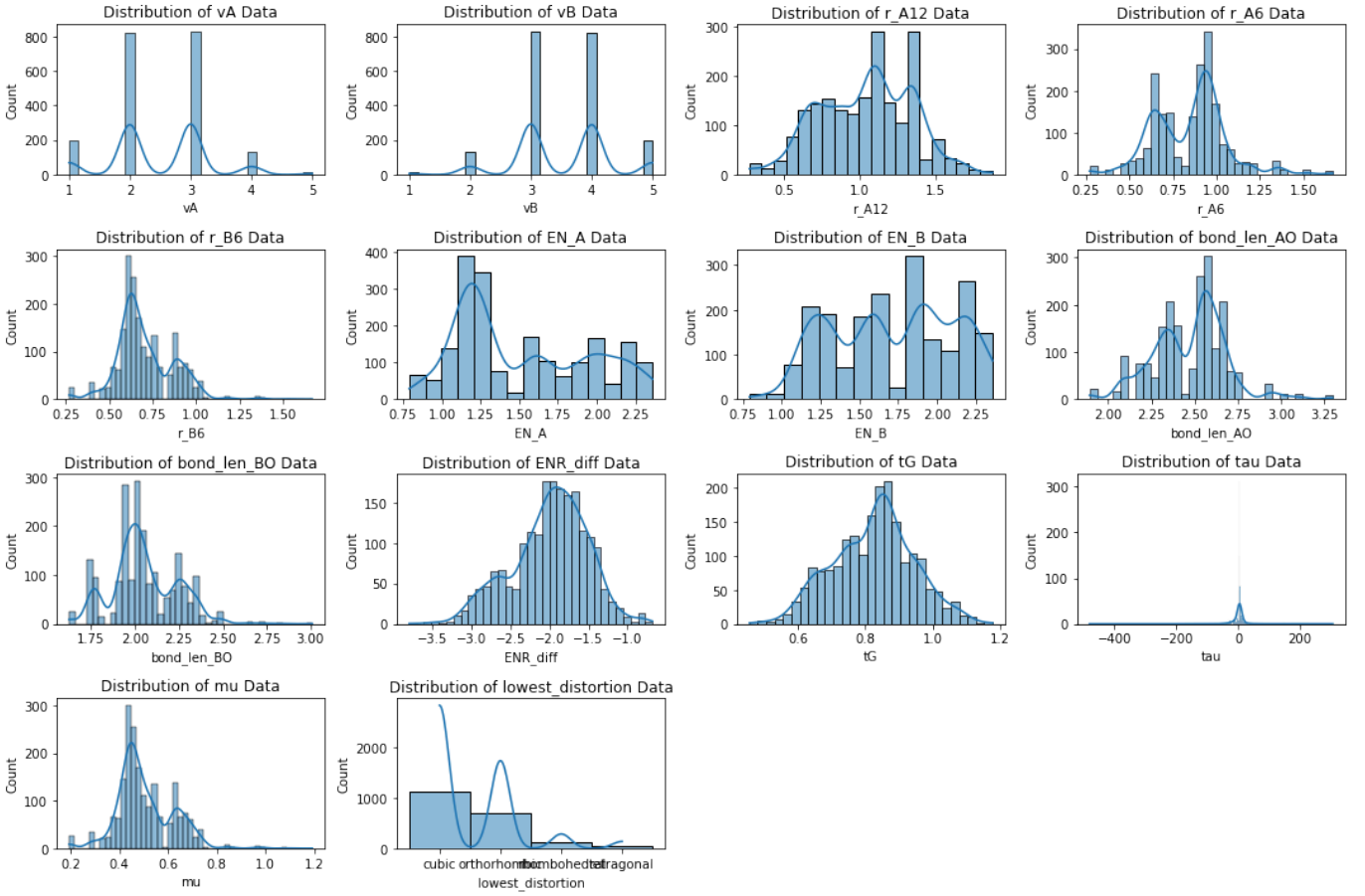
The pair plots are useful in quikly visualizing any data that may be problematic due to a directly linear relationship that would confuse the model. (multivariate)

It is a good practice to plot distribution graphs and look for skewness of features. Kernel density estimate (kde) is a useful tool for plotting the shape of a distribution. (univariate data view, zooming in).

No new or interesting correlations are noted from the pairplot distributions.

Histograms

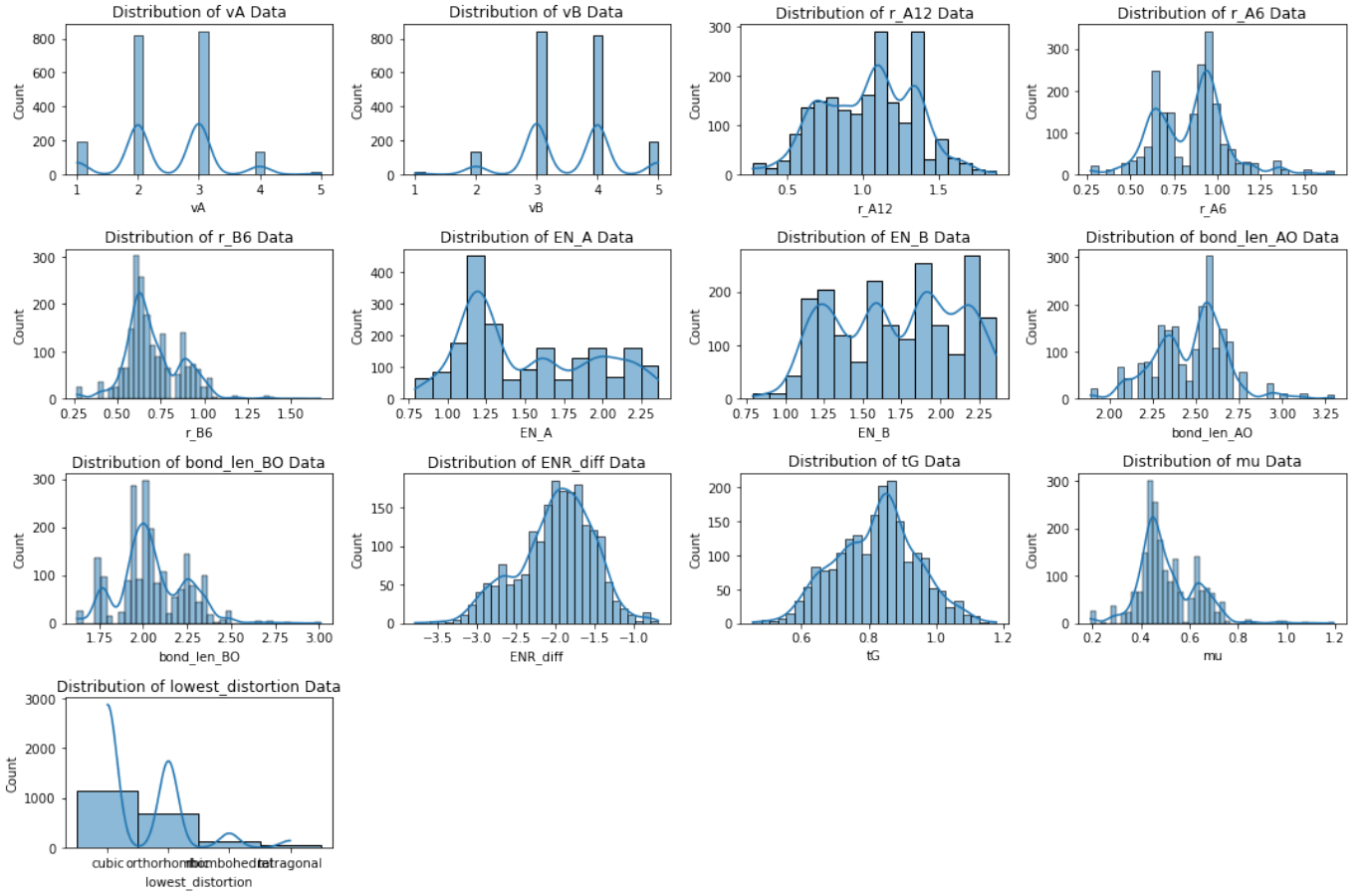
In [30]:
```
# Set up the figure size for the plot
plt.figure(figsize=(15,10))

# Iterate over each column in the dataframe
for i, col in enumerate(prv_train_tau.columns, 1):
    # Create subplots in a 4x4 grid
    plt.subplot(4, 4, i)

    # Set title for each subplot indicating the distribution of data for the corresponding colu
    plt.title(f"Distribution of {col} Data")

    # Plot the histogram with kernel density estimation using seaborn's histplot function
    sns.histplot(prv_train_tau[col], kde=True)

    # Adjust subplot layout
    plt.tight_layout()

    # Ensure the plot is shown
    plt.plot()

```



The valence electron data is showing a discrete pattern as expected and otherwise no notable outliers or abnormal distributions.

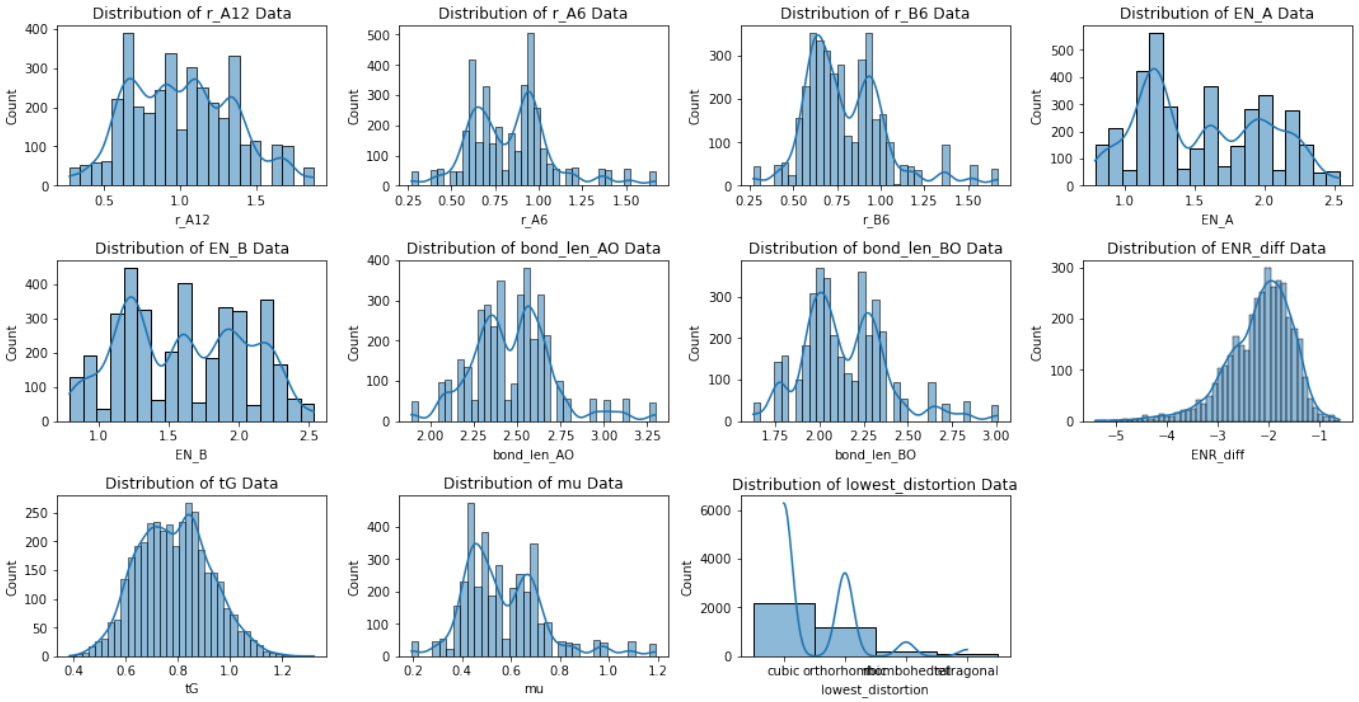
In [31]:

```
# Set up the figure size for the plot
plt.figure(figsize=(15,10))

# Iterate over each column in the dataframe
for i, col in enumerate(prv_train_no_tau.columns, 1):
    # Create subplots in a 4x4 grid
    plt.subplot(4, 4, i)

    # Set title for each subplot indicating the distribution of data for the corresponding colu
    plt.title(f"Distribution of {col} Data")

    # Plot the histogram with kernel density estimation using seaborn's histplot function
    sns.histplot(prv_train_no_tau[col], kde=True)

    # Adjust subplot layout
    plt.tight_layout()

    # Ensure the plot is shown
    plt.plot()

```



In [32]:

```
# Set up the figure size for the plot
plt.figure(figsize=(15,10))

# Iterate over each column in the dataframe
for i, col in enumerate(prv_train_no_tau_no_v.columns, 1):
    # Create subplots in a 4x4 grid
    plt.subplot(4, 4, i)

    # Set title for each subplot indicating the distribution of data for the corresponding colu
    plt.title(f"Distribution of {col} Data")

    # Plot the histogram with kernel density estimation using seaborn's histplot function
    sns.histplot(prv_train_no_tau_no_v[col], kde=True)

    # Adjust subplot layout
    plt.tight_layout()

    # Ensure the plot is shown
    plt.plot()
```



Summary

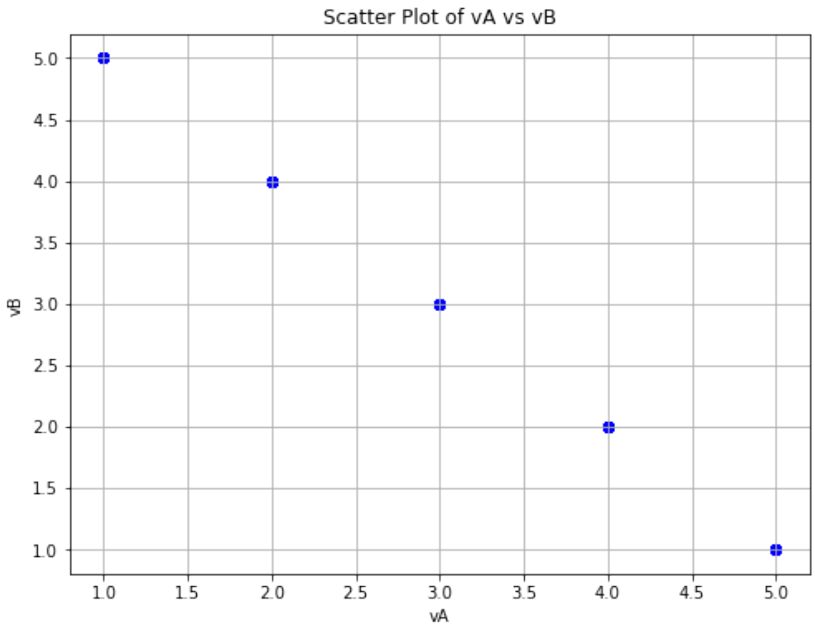
At this point, there doesn't seem to be a need to standardize or normalize the data.

Since the data already follows a Gaussian (normal) distribution, normalization might not provide significant benefits in terms of scaling the data to a fixed range. With this normally distributed data, standardization is a better choice, but doesn't seem necessary. Standardization could be beneficial for maintaining the integrity of the data's distribution while making it more compatible with algorithms that expect standardized inputs.

Safety Check

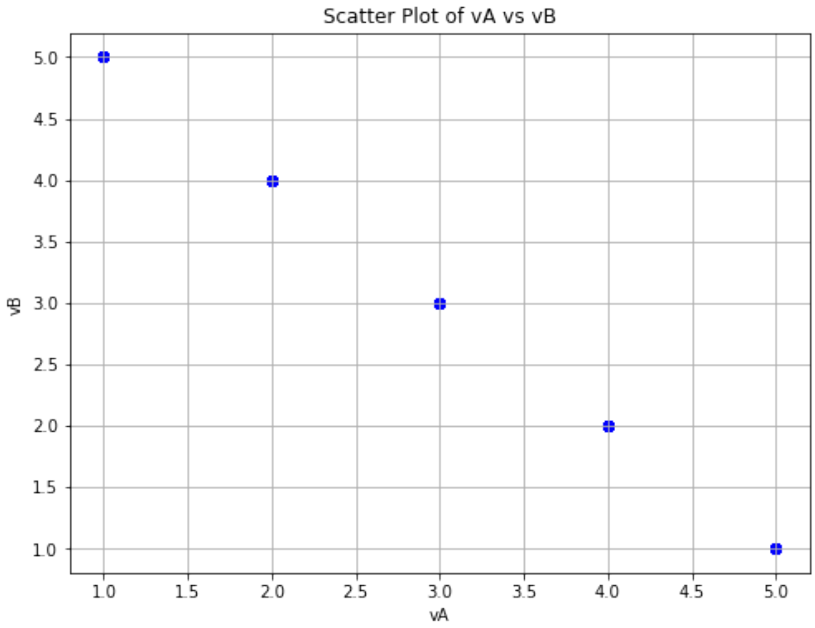
In [33]:

```
# Extracting the 'vA' and 'vB' columns from the training dataset
vA = prv_train_tau['vA']
vB = prv_train_tau['vB']

# Creating a scatter plot of 'vA' vs 'vB'
plt.figure(figsize=(8, 6))
plt.scatter(vA, vB, color='blue', alpha=0.5)

# Setting the labels for x and y axes
plt.xlabel('vA')
plt.ylabel('vB')

# Setting the title for the scatter plot
plt.title('Scatter Plot of vA vs vB')

# Displaying the grid
plt.grid(True)

# Showing the scatter plot
plt.show()

```



In [34]:

```
# Extracting the 'vA' and 'vB' columns from the training dataset without tolerance factor
vA = prv_train_no_tau['vA']
vB = prv_train_no_tau['vB']

# Creating a scatter plot of 'vA' vs 'vB'
plt.figure(figsize=(8, 6))
plt.scatter(vA, vB, color='blue', alpha=0.5)

# Setting the labels for x and y axes
plt.xlabel('vA')
plt.ylabel('vB')

# Setting the title for the scatter plot
plt.title('Scatter Plot of vA vs vB')

# Displaying the grid
plt.grid(True)

# Showing the scatter plot
plt.show()

```



These plots show the linear relationship between the valence electrons. This explicitly shows that vA and vB add up to the constant 6.

Final dataset choice:

It appears at this point that the dataset that is the most comprehensive would be best suited to answer our shareholders questions. The most comprehensive data set is the set that includes tau.

Perform a Train-Test Split

In [35]:
```
Extracting features (X_tau) and labels (y_tau) from the training dataset with tolerance factor
_tau = prv_train_tau.loc[:, 'vA':'mu']
_tau = prv_train_tau.loc[:, 'lowest_distortion']

Splitting the dataset into training and testing sets
X contains features and y contains labels/targets
X_train and y_train will contain the training data, while X_test and y_test will contain the testi
_train, X_test, y_train, y_test = train_test_split(X_tau, y_tau, test_size=0.2, random_state=42)

```

Here, test_size=0.2 specifies that 20% of the data will be held out for testing. The random_state is set for reproducibility, ensuring the same split is obtained each time the code is run.

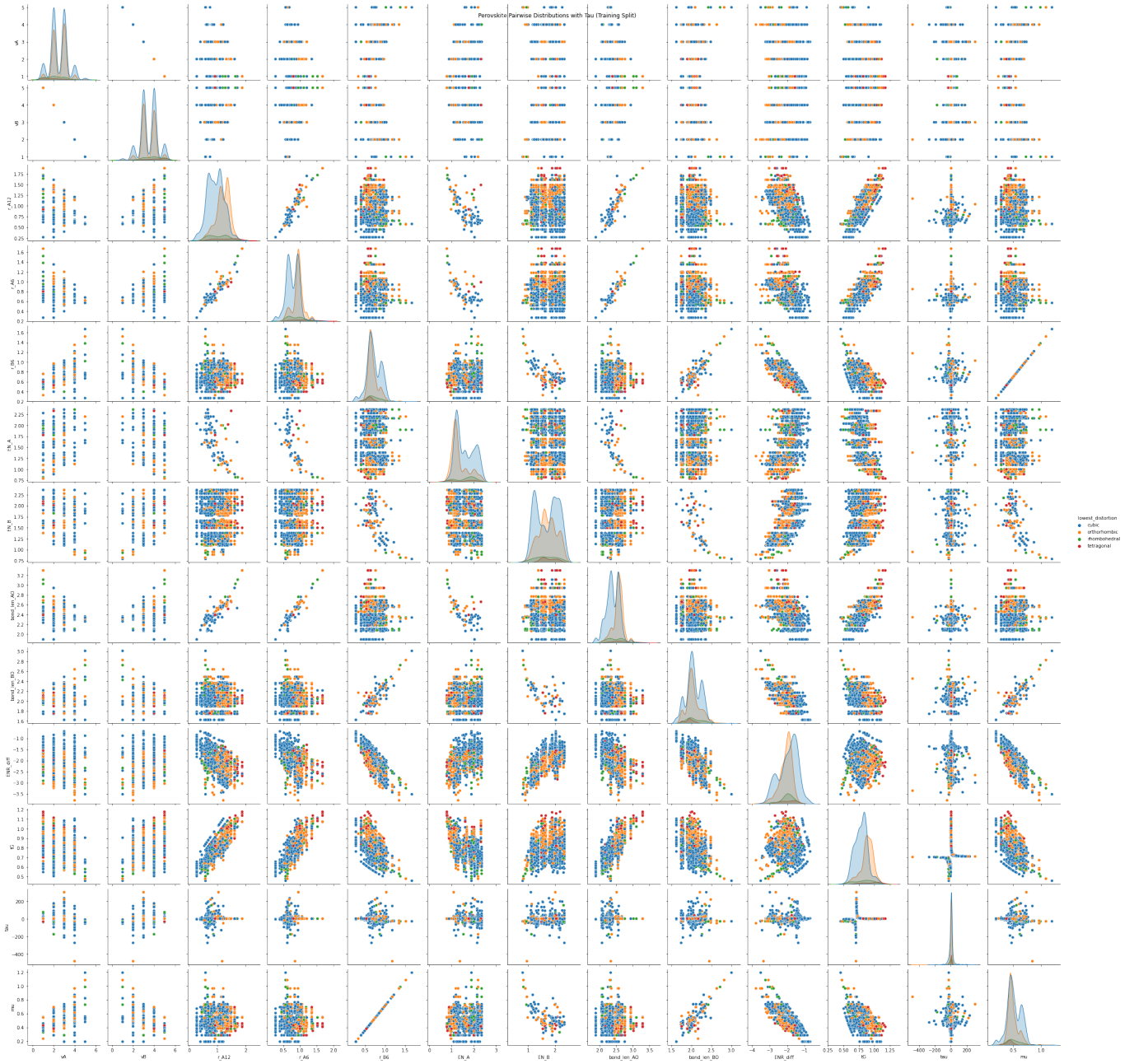
The test data must not be touched.

In [36]:
```
# Checking the lengths of the training and testing sets
len(X_train), len(X_test)
```

Out[36]: (1590, 398)

Verify that everything makes sense after the test-train split

In [37]:
```
#X_train and y_train are training feature and target variables

#Concatenate X_train and y_train along columns
train_data = pd.concat([X_train, y_train], axis=1)

#Creating a pair plot to visualize pairwise distributions of features in the training dataset with
pair_plot = sns.pairplot(prv_train_tau, hue="lowest_distortion")

#Adding a title to the pair plot
pair_plot.fig.suptitle("Perovskite Pairwise Distributions with Tau (Training Split)")

#Saving the pair plot as an image
pair_plot.savefig("pairplot_perovskite_tau_training_split.jpg")

#Displaying the pair plot
plt.show()
```



This is the primary indicator showing linear relationships that need to be monitored. Most linear relationships are not good for ML models because they often oversimplify the underlying patterns in the data and may not capture complex, non-linear relationships effectively (case by case basis, keep an eye on).

Asserting the dimensionality checks is not needed to verify in this case the size of the datasets (what they would asserted to be), because the lengths of the data confirmed that the test-train split did what it was told to do

Decision Tree Model with Stratified K-Fold Cross-Validation

A decision tree provides a good balance between interpretability, flexibility, and performance, making it a suitable choice for exploring the dataset and gaining insights before potentially exploring more complex models. (include stakeholders goals and how this model mighth meet it)

In [38]:

```
ists to store scores for each fold
es = []
= []

s = []

training
tratifiedKFold with 5 splits for cross-validation
dKFold(n_splits=5)

each fold
_, val_) in enumerate(kf.split(X=X_train, y=y_train)):

ata into training and validation sets for the current fold
old = X_train.iloc[trn_]
old = y_train.iloc[trn_]

Xtrain.iloc[val_]
ytrain.iloc[val_]

a Decision Tree classifier with specified hyperparameters
cisionTreeClassifier(criterion="entropy",max_depth = 10, random_state=42) #here is where we tune th

ecision Tree classifier on the training data for the current fold
Xtrain_Kfold, y_train_Kfold)

labels for the validation set
l = DTclf.predict(X_valid)

scores for the current fold
lassification_report(y_valid, y_pred_Kfold, output_dict=True)

recision, recall, F1-score, and accuracy scores to respective lists
scores.append(report['weighted avg']['precision'])
res.append(report['weighted avg']['recall'])
append(report['weighted avg']['f1-score'])
cores.append(report['accuracy'])
assification report for the current fold
e(f"Fold is: {fold}:")
sification_report(y_valid, y_pred_Kfold))

erage scores across all folds
=np.mean(precision_scores)
p.mean(recall_scores)
an(f1_scores)
np.mean(accuracy_scores)

evaluation metrics across all folds
e(f"Precision: {avg_precision}")
e(f"Recall: {avg_recall}")
e(f"F1-score: {avg_f1}")
e(f"Accuracy: {avg_accuracy}")
```

```
The fold is: 0:
              precision    recall  f1-score   support

       cubic       0.85      0.83      0.84       178
orthorhombic       0.69      0.77      0.72       113
rhombohedral       0.40      0.21      0.28        19
  tetragonal       0.33      0.38      0.35         8

    accuracy                           0.76       318
   macro avg       0.57      0.55      0.55       318
weighted avg       0.75      0.76      0.75       318

The fold is: 1:
              precision    recall  f1-score   support

       cubic       0.83      0.86      0.84       178
orthorhombic       0.76      0.71      0.73       112
rhombohedral       0.33      0.37      0.35        19
  tetragonal       0.38      0.33      0.35         9

    accuracy                           0.76       318
   macro avg       0.57      0.57      0.57       318
weighted avg       0.76      0.76      0.76       318

The fold is: 2:
              precision    recall  f1-score   support

       cubic       0.85      0.89      0.87       178
orthorhombic       0.75      0.79      0.77       112
rhombohedral       0.33      0.21      0.26        19
  tetragonal       1.00      0.44      0.62         9

    accuracy                           0.80       318
   macro avg       0.73      0.58      0.63       318
weighted avg       0.79      0.80      0.79       318

The fold is: 3:
              precision    recall  f1-score   support

       cubic       0.86      0.87      0.86       178
orthorhombic       0.72      0.75      0.74       112
rhombohedral       0.33      0.26      0.29        19
  tetragonal       0.38      0.33      0.35         9

    accuracy                           0.77       318
   macro avg       0.57      0.55      0.56       318
weighted avg       0.77      0.77      0.77       318

The fold is: 4:
              precision    recall  f1-score   support

       cubic       0.84      0.93      0.88       179
orthorhombic       0.83      0.71      0.77       112
rhombohedral       0.62      0.44      0.52        18
  tetragonal       0.20      0.22      0.21         9

    accuracy                           0.81       318
   macro avg       0.62      0.58      0.59       318
weighted avg       0.81      0.81      0.80       318

Average Precision: 0.7759573233355838
Average Recall: 0.779874213836478
Average F1-score: 0.7755647332614042
Average Accuracy: 0.779874213836478
```

In [39]:
```
print("Raw Counts")
print(prv_train_tau["lowest_distortion"].value_counts())
print()
print("Percentages")
print(prv_train_tau["lowest_distortion"].value_counts(normalize=True))
```

```
Raw Counts
cubic           1127
orthorhombic     692
rhombohedral     114
tetragonal        55
Name: lowest_distortion, dtype: Int64

Percentages
cubic           0.566901
orthorhombic    0.348089
rhombohedral    0.057344
tetragonal      0.027666
Name: lowest_distortion, dtype: float64
```

It is worth bringing up that the accuracy metric doesn't take into account an imbalanced dataset. If we had a model that always predicted a cubic crystal structure, the accuracy score would be only 56% (baseline, for uninformed decision, the worst it could be). (cell 39)

Using the Decision Tree Classifier (model), it is clear that the crystal structure accuracy score is performing better with the Stratified K Fold performace evaluation at 78%. (cell 38)

These are the example kfold scores (with default guess hyperparameterization) for each fold. At this point, the f1 score seems to be the most comprehensive. The closer the f1 score is to 1, the better the model will be at predicting the target. The closer to a score of 1 means that the model is doing well in both minimizing false positives and false negatives because both the precision and recall are high scores are well. The Decision Tree model was trained once for each of the 5 folds using a random seed of 42 so that the starting point for the randomness is chosen in a way that's consistent and predictable for the purposes of building this experiment.

Rhombohedral and tetragonal are training on little data so the scores are expected to be low compared to the cubic and orthorhombic which are training on a lot more data.

This presents a great opportunity to tune the hyperparameters and optimize the training before trying out different models.

Feature Engineering

In [40]:
```
# Create a copy of the test/train DataFrame to avoid altering the original
prv_train_tau_bin = prv_train_tau.copy()

# Calculate the absolute electronegativity difference between elements A and B
prv_train_tau_bin['abs_EN_diff']=abs(prv_train_tau_bin['EN_A'] - prv_train_tau_bin['EN_B'])

```

Does bond type influence the cyrstal structure shape?

The absolute value of the electronegativity difference between atoms A + B will be classified into different bond types from the describe method as shown here:

Electronegativity Difference	Bond Type Character	Label Number
0.0 - 0.4	Nonpolar Covalent	1
0.4 - 1.7	Polar Covalent	2
1.7 +	Ionic Bond	3

In [41]:
```
# Use the Pandas cut method to map the absolute value electronegativity between A+B into the ab

# Define cutoff for each bin
prv_train_tau_bin_edges = [0.0, 0.4, 1.7, 4]

# Name each bin
prv_train_tau_bin_names = [1, 2, 3]

# Make column for different ranges into which the values of the 'Electronegativty difference' c
prv_train_tau_bin['abs_EN_diff_bin'] = pd.cut(prv_train_tau_bin.abs_EN_diff, prv_train_tau_bin_

#Display df
print(len(prv_train_tau_bin))
display(prv_train_tau_bin.head())

```

1988

	vA	vB	r_A12	r_A6	r_B6	EN_A	EN_B	bond_len_AO	bond_len_BO	ENR_diff	tG	tau	mu	lowest_distortion
2	2	4	0.92	0.67	0.53	1.83	1.88	2.290644	1.930311	-1.468464	0.849994	4.936558	0.378571	cubic
3	1	5	1.64	1.38	0.62	0.82	2.36	3.025719	1.745600	-1.974429	1.064161	3.977376	0.442857	orthorhombic
6	1	5	0.92	0.80	0.62	1.78	2.36	2.392362	1.745600	-1.484143	0.812123	5.017992	0.442857	cubic
10	3	3	1.36	1.03	0.90	1.10	1.23	2.689119	2.258656	-2.931286	0.848528	3.536265	0.642857	orthorhombic
11	2	4	1.19	0.99	0.61	1.22	1.54	2.550861	1.927849	-2.040571	0.911148	4.133678	0.435714	orthorhombic

In [42]:
```
# Remove columns 'abs_EN_diff', 'EN_A', and 'EN_B' from the DataFrame to eliminate redundant o
prv_train_tau_bin.drop(columns=['abs_EN_diff', 'EN_A', 'EN_B'], inplace=True)

#reorder columns
new_order = ['vA', 'vB', 'r_A12', 'r_A6', 'r_B6', 'bond_len_AO', 'bond_len_BO', 'ENR_diff', 'tG

# Reorder the columns
prv_train_tau_bin = prv_train_tau_bin[new_order]

```

In [43]:
```
# Splitting the dataset into features (X_tau_bin) and target labels (y_tau_bin)
X_tau_bin = prv_train_tau_bin.loc[:, 'vA':'abs_EN_diff_bin']
y_tau_bin = prv_train_tau_bin.loc[:, 'lowest_distortion']

# Splitting the dataset into training and testing sets
# X_train_bin and y_train_bin will contain the training data, while X_test_bin and y_test_bin w
X_train_bin, X_test_bin, y_train_bin, y_test_bin = train_test_split(X_tau_bin, y_tau_bin, test_

```

In [44]:
```
# Print the lengths of training and testing data
len(X_train_bin), len(X_test_bin)
```

Out[44]: (1590, 398)

In [45]:

```python
from sklearn.metrics import classification_report

# Initialize lists to store scores for each fold
precision_scores_bin = []
recall_scores_bin = []
f1_scores_bin = []
accuracy_scores_bin = []

#Step 1, start training
# Initialize StratifiedKFold with 5 splits for cross-validation
kf = StratifiedKFold(n_splits=5)

# Iterate over each fold
for fold, (trn_, val_) in enumerate(kf.split(X=X_train_bin, y=y_train_bin)):

    # Split the data into training and validation sets for the current fold
    X_train_Kfold_bin = X_train_bin.iloc[trn_]
    y_train_Kfold_bin = y_train_bin.iloc[trn_]

    X_valid_bin = X_train_bin.iloc[val_]
    y_valid_bin = y_train_bin.iloc[val_]

    # Initialize a Decision Tree classifier with specified hyperparameters
    DTclf_bin = DecisionTreeClassifier(criterion="entropy",max_depth=10, random_state=42)#here

    # Train the Decision Tree classifier on the training data for the current fold
    DTclf_bin.fit(X_train_Kfold_bin, y_train_Kfold_bin)

    # Predict labels for the validation set
    y_pred_Kfold_bin = DTclf_bin.predict(X_valid_bin)

    # Calculate scores for the current fold
    report_bin = classification_report(y_valid_bin, y_pred_Kfold_bin, output_dict=True)

    # Append precision, recall, F1-score, and accuracy scores to respective lists
    precision_scores_bin.append(report_bin['weighted avg']['precision'])
    recall_scores_bin.append(report_bin['weighted avg']['recall'])
    f1_scores_bin.append(report_bin['weighted avg']['f1-score'])
    accuracy_scores_bin.append(report_bin['accuracy'])

    # Print classification report for the current fold
    print(f"The fold is: {fold}:")
    print(classification_report(y_valid_bin, y_pred_Kfold_bin))

# Calculate average scores across all folds
avg_precision_bin = np.mean(precision_scores_bin)
avg_recall_bin = np.mean(recall_scores_bin)
avg_f1_bin = np.mean(f1_scores_bin)
avg_accuracy_bin = np.mean(accuracy_scores_bin)

# Print average evaluation metrics across all folds
print(f"Average Precision Bin: {avg_precision_bin}")
print(f"Average Recall Bin: {avg_recall_bin}")
print(f"Average F1-score Bin: {avg_f1_bin}")
print(f"Average Accuracy Bin: {avg_accuracy_bin}")


```

```
The fold is: 0:
              precision    recall  f1-score   support

       cubic       0.84      0.81      0.83       178
orthorhombic       0.70      0.71      0.70       113
rhombohedral       0.23      0.26      0.24        19
  tetragonal       0.25      0.25      0.25         8

    accuracy                           0.73       318
   macro avg       0.50      0.51      0.51       318
weighted avg       0.74      0.73      0.73       318

The fold is: 1:
              precision    recall  f1-score   support

       cubic       0.79      0.84      0.81       178
orthorhombic       0.75      0.66      0.70       112
rhombohedral       0.29      0.32      0.30        19
  tetragonal       0.33      0.33      0.33         9

    accuracy                           0.73       318
   macro avg       0.54      0.54      0.54       318
weighted avg       0.73      0.73      0.73       318

The fold is: 2:
              precision    recall  f1-score   support

       cubic       0.82      0.84      0.83       178
orthorhombic       0.70      0.71      0.71       112
rhombohedral       0.56      0.47      0.51        19
  tetragonal       0.67      0.44      0.53         9

    accuracy                           0.76       318
   macro avg       0.69      0.62      0.65       318
weighted avg       0.76      0.76      0.76       318

The fold is: 3:
              precision    recall  f1-score   support

       cubic       0.86      0.83      0.84       178
orthorhombic       0.72      0.79      0.75       112
rhombohedral       0.35      0.32      0.33        19
  tetragonal       0.57      0.44      0.50         9

    accuracy                           0.77       318
   macro avg       0.62      0.59      0.61       318
weighted avg       0.77      0.77      0.77       318

The fold is: 4:
              precision    recall  f1-score   support

       cubic       0.82      0.89      0.86       179
orthorhombic       0.77      0.70      0.73       112
rhombohedral       0.43      0.33      0.38        18
  tetragonal       0.25      0.22      0.24         9

    accuracy                           0.77       318
   macro avg       0.57      0.54      0.55       318
weighted avg       0.77      0.77      0.77       318

Average Precision Bin: 0.7521560849621787
Average Recall Bin: 0.7528301886792453
Average F1-score Bin: 0.7513915936097715
Average Accuracy Bin: 0.7528301886792453
```

This is a transformation and evaluation of whether or not the bins helped or not. The addition of the electronegativity difference column is feature engineering with the data.

The bins do not seem to improve the cross validation scores so we will move forward with the chosen dataset and not the binned dataset. Because most of the data is continuous and numeric (some of which derived) then it isn't expected that any other binning would have much of an impact.

Hyperparameter Tuning

In [46]:

```
# Start measuring the time taken for grid search
start_time = time.time()

# Set the random seed
N_SEED = 42

# Define the cross-validation strategy
cv = StratifiedKFold(n_splits=5, shuffle=True, random_state=N_SEED)

# Define the Decision Tree classifier
DTclf = DecisionTreeClassifier(random_state=N_SEED)

# Define the hyperparameters grid
param_grid = {
    'criterion': ['gini', 'entropy'],
    'max_depth': [None, 5, 10, 15],
    'min_samples_split': [2, 5, 10],
    'min_samples_leaf': [1, 2, 4]
}

# Perform grid search
grid_search_cv = GridSearchCV(
    estimator=DTclf,
    param_grid=param_grid,
    scoring='accuracy',
    n_jobs=-1,
    cv=cv)

grid_search_cv.fit(X_train, y_train)

# Measure the time taken for grid search
end_time = time.time()
elapsed_time = end_time - start_time
print("Grid search completed in {:.2f} seconds".format(elapsed_time))

# Print the best hyperparameters found
print(grid_search_cv.best_params_)


```

```
Grid search completed in 1.62 seconds
{'criterion': 'entropy', 'max_depth': 15, 'min_samples_leaf': 1, 'min_samples_split': 2}
```

This hyperparameter tuning is interesting. It could be assumed that unlimited depth (layers/decisions on each branch of the tree) in a tree would be best at producing the highest accuracy, but in this case the hypertuning suggests that only 15 tree layers are needed to optimize the model. This might be because the data set is so small, so it seems like tuning hyperparameters may not make a huge difference.

Train the Decision Tree Model

The next step will be to train all of the training data not just a piece (split).

In [47]:
```
# Define the Decision Tree classifier with tuned hyperparameters
all_DTclf = DecisionTreeClassifier(criterion="entropy", max_depth=15, random_state=42, min_samp

# Train the classifier on the entire training set
all_DTclf.fit(X_train, y_train)  # Final step of training

```

Out[47]:
```
DecisionTreeClassifier(criterion='entropy', max_depth=15, random_state=42)
```

Performace Evaluation

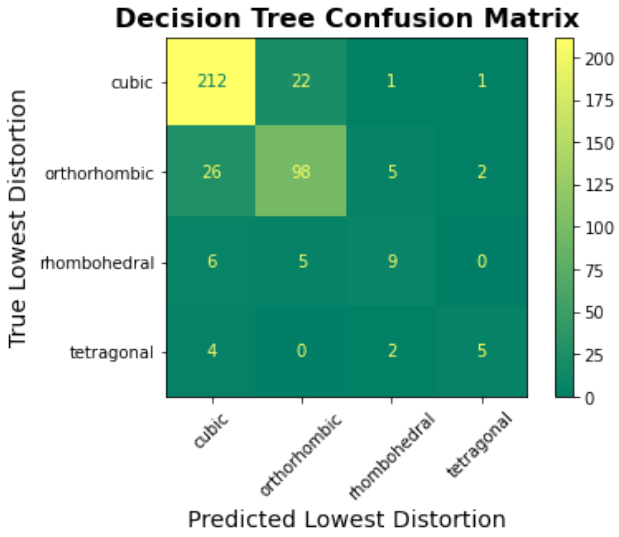
Does the prediction x data match real-life y?

In [48]:
```
# Step 1: Apply the trained model to the holdout data to make predictions
y_pred_final_DT = all_DTclf.predict(X_test)

# Step 2: Assess the performance of the classifier

# Compute the confusion matrix to evaluate the classification performance
DTconf_matrix = confusion_matrix(y_test, y_pred_final_DT)
print("Confusion Matrix:\n", DTconf_matrix)

```

```
Confusion Matrix:
 [[212  22   1   1]
 [ 26  98   5   2]
 [  6   5   9   0]
 [  4   0   2   5]]
```

In [49]:
```
# Create a ConfusionMatrixDisplay object with the confusion matrix and display labels
disp = ConfusionMatrixDisplay(confusion_matrix=DTconf_matrix, display_labels=all_DTclf.classes_

# Set the size of the plot
plt.figure(figsize=(40, 35))

# Plot the confusion matrix
disp.plot(cmap='summer')

# Rotate x-axis labels
plt.xticks(rotation=45)

# Set the title of the plot
plt.title("Decision Tree Confusion Matrix", fontsize=16, fontweight='bold')

# Set the axis labels
plt.xlabel("Predicted Lowest Distortion", fontsize=14)
plt.ylabel("True Lowest Distortion", fontsize=14)

# Visualize confusion matrix
plt.show()
```

```
<Figure size 2880x2520 with 0 Axes>
```




```
It would appear that the classifier is only able to classify cubic shape with the most
accuracy - it's optimized for this shape. This makes sense because the majority of the data
points relate to the cubic shape.
```

In [50]:
```
# Calculate the accuracy of the classifier
DTaccuracy = accuracy_score(y_test, y_pred_final_DT)

# Print the accuracy score
print("Accuracy:", DTaccuracy)


```

```
Accuracy: 0.8140703517587939
```

This is great! Tuning the hyperpapameters to maximize the accuracy increased the accuracy from 78% to 81%.

In [51]:

```
#Generate and print the classification report
DTreport = classification_report(y_test, y_pred_final_DT)
print("Classification Report:\n", DTreport)

```

```
Classification Report:
               precision    recall  f1-score   support

       cubic       0.85      0.90      0.88       236
orthorhombic       0.78      0.75      0.77       131
rhombohedral       0.53      0.45      0.49        20
  tetragonal       0.62      0.45      0.53        11

    accuracy                           0.81       398
   macro avg       0.70      0.64      0.66       398
weighted avg       0.81      0.81      0.81       398
```

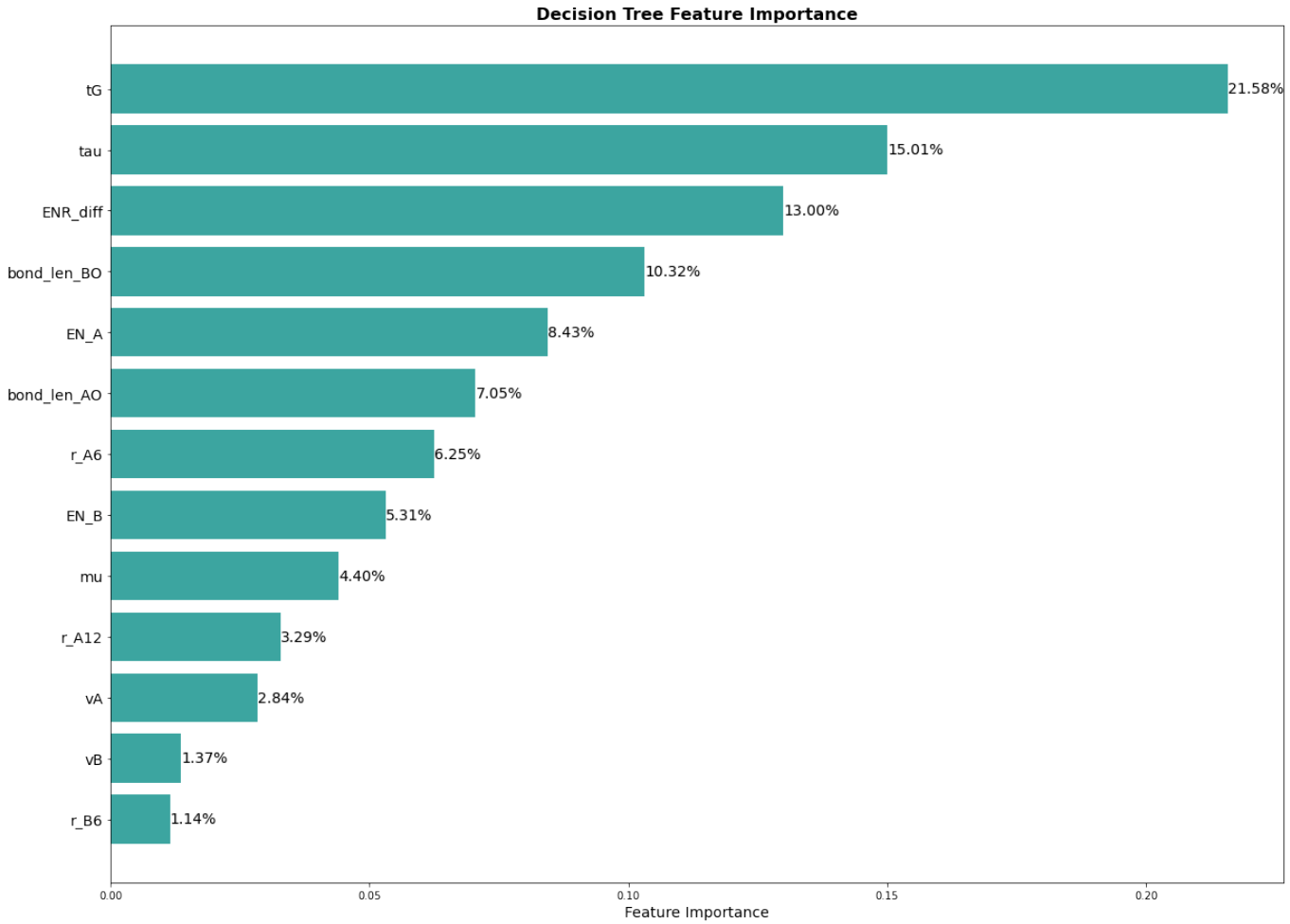
```
This supports the conclusion above with the confusion matrix. This is reasonable given the
size of the data set and the simplicity of the decision tree model.

Potentially, a feature could be dropped and this may improve the accuracy of the model.

```

Feature Importance

In [53]:

```
#Step 3, feature importance and printing a visualization

## Checking Feature importance

# Create a figure with a specific size for the plot
plt.figure(figsize=(20, 15))

# Obtain feature importance from the trained decision tree classifier
DTimportance = all_DTclf.feature_importances_

# Sort the indices of features based on their importance
idxs = np.argsort(DTimportance)

# Set the title of the plot
plt.title("Decision Tree Feature Importance", fontsize=16, fontweight='bold')

# Create horizontal bar plot for feature importance
bars = plt.barh(range(len(idxs)), DTimportance[idxs], align="center", color='#40A6A3')

# Set y-axis labels to feature names based on their importance order
plt.yticks(range(len(idxs)), [X_train.columns[i] for i in idxs], fontsize=14)

# Set x-axis label
plt.xlabel("Feature Importance", fontsize=14)

# Add percentage labels to the bars
for i, bar in zip(idxs, bars):
    yval = DTimportance[i]
    plt.text(yval, bar.get_y() + bar.get_height()/2, "{:.2%}".format(yval), va='center', fonts

# Print feature importance list
print("Feature Importance List:")
for i, feature_name in enumerate(X_train.columns[idxs]):
    yval = DTimportance[idxs[i]]
    print(f"{i + 1}. {feature_name}: {yval}")

#Display the plot
plt.show()
```

```
Feature Importance List:
1. r_B6: 0.0114442161757059
2. vB: 0.013655687954807967
3. vA: 0.028397715225330956
4. r_A12: 0.03292281355697572
5. mu: 0.0440063280003429
6. EN_B: 0.05309493888597719
7. r_A6: 0.06250300628790516
8. bond_len_AO: 0.07051139761566444
9. EN_A: 0.08434850271968457
10. bond_len_BO: 0.10320230050295497
11. ENR_diff: 0.13001005750909686
12. tau: 0.1500696911609554
13. tG: 0.21583334440459806
```



Decision Tree Model Summary

This feature importance output shows gaps in the percentages for the top features. This may be highlighting some linear relationships and should be investigated in a future analysis.

Although tau doesn't show separation in the pairwise plot, it does seem to be a significant feature. Since tau is determined by factors of radii and bond lengths of A and B, the importance may also change and be dependent on the size of atom A or B.

The top 5 feature importance really highlights the relationship between the ENR_diff and its relationship to EN_A and bond_len_BO. The electronegativity radius difference most certainly is strongly related to the electronegativity of atom A because the stronger A is the shorter the bond length to A and the longer the bond length is to B.

Random Forest Model with Stratified K-Fold Cross-Validation

The random forest machine learning model is a similar algorithm however it's ensemble classifier which should provide an improvement from the decision tree classifier.

In [54]:

```python
#start over! #Step 1, start training a different type of algorithm
# Define cross-validation strategy
kf = StratifiedKFold(n_splits=5)

# Iterate over each fold
for fold, (trn_, val_) in enumerate(kf.split(X=X_train, y=y_train)):

    # Split data into training and validation sets
    X_train_Kfold = X_train.iloc[trn_]
    y_train_Kfold = y_train.iloc[trn_]

    X_valid = X_train.iloc[val_]
    y_valid = y_train.iloc[val_]

    # Define Random Forest classifier
    RFclf = RandomForestClassifier(n_estimators=200, criterion="entropy")  # Tuning hyperparame
    RFclf.fit(X_train_Kfold, y_train_Kfold)  # Train the model
    y_pred_Kfold = RFclf.predict(X_valid)  # Make predictions

    # Print classification report for the current fold
    print(f"The fold is: {fold}:")
    print(classification_report(y_valid, y_pred_Kfold))

```

The fold is: 0:

	precision	recall	f1-score	support
cubic	0.86	0.94	0.90	178
orthorhombic	0.79	0.80	0.79	113
rhombohedral	0.60	0.16	0.25	19
tetragonal	0.75	0.38	0.50	8
accuracy			0.83	318
macro avg	0.75	0.57	0.61	318
weighted avg	0.81	0.83	0.81	318

The fold is: 1:

	precision	recall	f1-score	support
cubic	0.86	0.90	0.88	178
orthorhombic	0.79	0.82	0.81	112
rhombohedral	0.80	0.42	0.55	19
tetragonal	0.75	0.33	0.46	9
accuracy			0.83	318
macro avg	0.80	0.62	0.68	318
weighted avg	0.83	0.83	0.82	318

The fold is: 2:

	precision	recall	f1-score	support
cubic	0.88	0.94	0.91	178
orthorhombic	0.82	0.80	0.81	112
rhombohedral	0.53	0.42	0.47	19
tetragonal	1.00	0.33	0.50	9
accuracy			0.84	318
macro avg	0.81	0.62	0.67	318
weighted avg	0.84	0.84	0.84	318

The fold is: 3:

	precision	recall	f1-score	support
cubic	0.84	0.96	0.89	178
orthorhombic	0.84	0.76	0.80	112
rhombohedral	0.73	0.42	0.53	19
tetragonal	1.00	0.33	0.50	9
accuracy			0.84	318
macro avg	0.85	0.62	0.68	318
weighted avg	0.84	0.84	0.83	318

The fold is: 4:

	precision	recall	f1-score	support
cubic	0.84	0.96	0.90	179
orthorhombic	0.87	0.79	0.83	112
rhombohedral	0.80	0.44	0.57	18
tetragonal	0.75	0.33	0.46	9
accuracy			0.85	318
macro avg	0.82	0.63	0.69	318
weighted avg	0.85	0.85	0.84	318

Hyperparameter Tuning

In [55]:
```
#next step, hyperparameter tuning
start_time = time.time()

# Define random seed and cross-validation strategy
N_SEED = 42
cv = StratifiedKFold(n_splits=5, shuffle=True, random_state=N_SEED)

# Define Random Forest Classifier
RFclf = RandomForestClassifier(random_state=N_SEED)

# Define the hyperparameters grid
param_grid = {
    'criterion': ['gini', 'entropy'],
    'max_depth': [None, 5, 10, 15],
    'min_samples_split': [2, 5, 10],
    'min_samples_leaf': [1, 2, 4],
    'n_estimators': [50, 150, 200, 500]
}

#Perform grid search
grid_search_cv = GridSearchCV(
    estimator=RFclf,
    param_grid=param_grid,
    scoring='accuracy',
    n_jobs=-1,
    cv=cv)

grid_search_cv.fit(X_train, y_train)

# Calculate and print elapsed time for grid search
end_time = time.time()
elapsed_time = end_time - start_time
print("Grid search completed in {:.2f} seconds".format(elapsed_time))

# Print best hyperparameters found
print(grid_search_cv.best_params_)


```

```
Grid search completed in 71.81 seconds
{'criterion': 'entropy', 'max_depth': None, 'min_samples_leaf': 1, 'min_samples_split': 5, 'n_est
imators': 500}
```

The impact of hyperparameter tuning might be less pronounced here compared to larger datasets. However, it's still valuable to perform hyperparameter tuning.

Train the Random Forest Model

In [56]:
```
# Initialize a Random Forest classifier with tuned hyperparameters
all_RFclf = RandomForestClassifier(criterion="entropy",max_depth = None, random_state=42, min_sam

# Fit the classifier to the training data
all_RFclf.fit(X_train, y_train) #last step of training

```

Out[56]:
```
RandomForestClassifier(criterion='entropy', min_samples_split=5,
                       n_estimators=500, random_state=42)
```

Performance Evaluation

Does the prediction x data match real-life y?

In [57]:
```
# Step 1: Apply the holdout data to the trained classifier
y_pred_final_RF = all_RFclf.predict(X_test)

#Step 2: assess the performance of the classifier

# Calculate the confusion matrix
RFconf_matrix = confusion_matrix(y_test, y_pred_final_RF)
print("Confusion Matrix:\n", RFconf_matrix)

```

```
Confusion Matrix:
 [[220  15   0   1]
 [ 21 108   1   1]
 [  7   4   9   0]
 [  4   0   3   4]]
```

This matrix is better. The error in row 2 decreased from about 1/3 to 1/5.

In [58]:
```
#still step 2, measures the proportion of correctly classified instances out of the total insta

# Calculate and print the accuracy score
RFaccuracy = accuracy_score(y_test, y_pred_final_RF)
print("Accuracy:", RFaccuracy)
```

```
Accuracy: 0.8567839195979899
```

In [59]:
```
step 2, These metrics provide insights into the classifier's performance, especially when dealing

late and print the classification report
rt = classification_report(y_test, y_pred_final_RF)
"Classification Report:\n", RFreport)

```

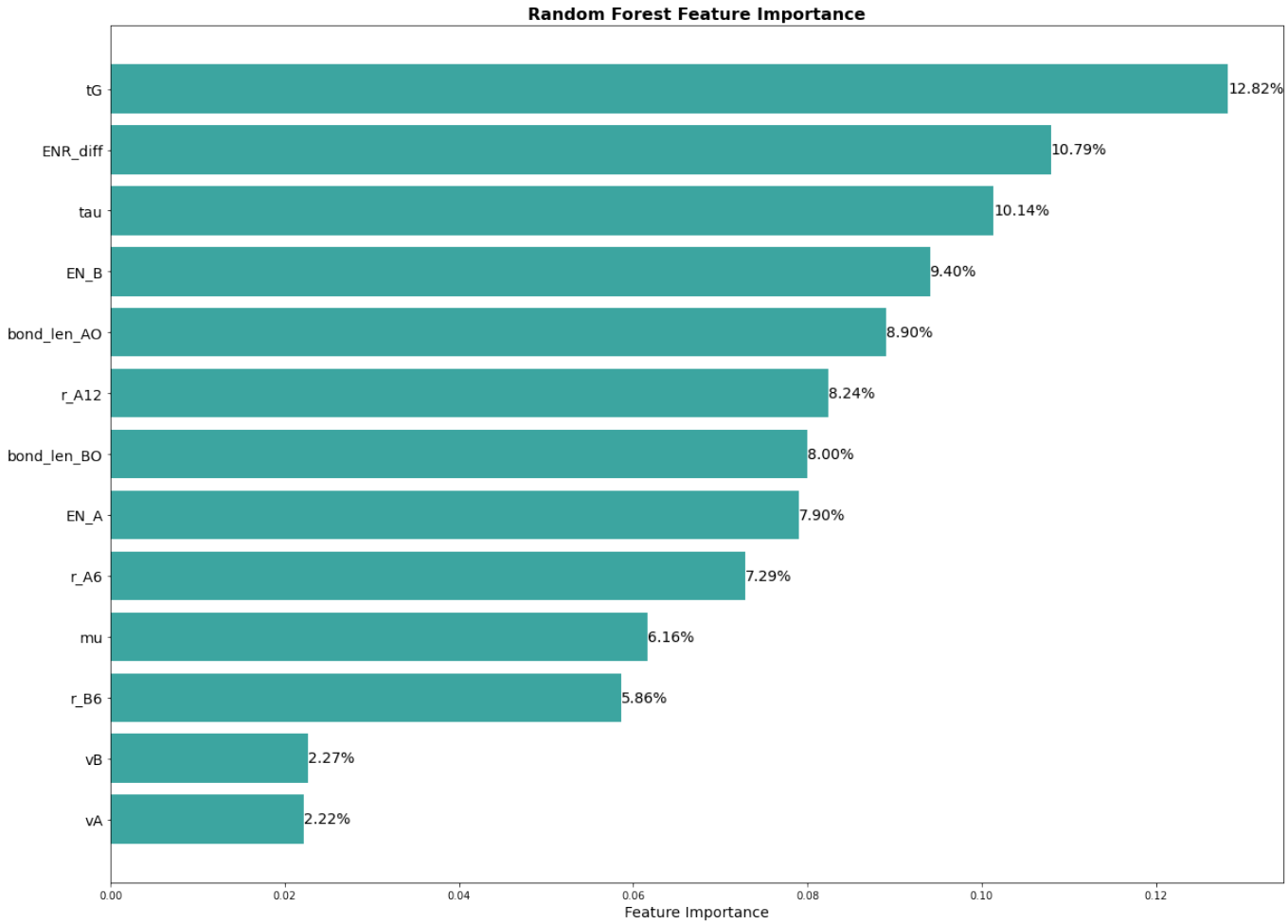
```
Classification Report:
               precision    recall  f1-score   support

       cubic       0.87      0.93      0.90       236
orthorhombic       0.85      0.82      0.84       131
rhombohedral       0.69      0.45      0.55        20
  tetragonal       0.67      0.36      0.47        11

    accuracy                           0.86       398
   macro avg       0.77      0.64      0.69       398
weighted avg       0.85      0.86      0.85       398
```

Feature Importance

In [60]:

```
#Step 3, feature importance and printing a visualization

## Checking Feature importance

# Set plot size
plt.figure(figsize=(20, 15))

# Get feature importance from the trained random forest classifier
RFimportance = all_RFclf.feature_importances_

# Sort indices based on feature importance
idxs = np.argsort(RFimportance)

# Set title
plt.title("Random Forest Feature Importance", fontsize=16, fontweight='bold')

# Create horizontal bar plot for feature importance
bars = plt.barh(range(len(idxs)), RFimportance[idxs], align="center", color='#40A6A3')

# Set y-ticks labels with feature names based on the sorted indices
plt.yticks(range(len(idxs)), [X_train.columns[i] for i in idxs], fontsize=14)  # Assuming X_tra

# Set label for x-axis
plt.xlabel("Feature Importance", fontsize=14)

# Add percentage labels to the bars
for i, bar in zip(idxs, bars):
    feature_name = X_train.columns[i]
    yval = RFimportance[i]
    plt.text(yval, bar.get_y() + bar.get_height()/2, "{:.2%}".format(yval), va='center', fonts

# Print feature importance list
print("Feature Importance List:")
for i, feature_name in enumerate(X_train.columns[idxs]):
    yval = RFimportance[idxs[i]]
    print(f"{i + 1}. {feature_name}: {yval}")

#Show plot
plt.show()

```

```
Feature Importance List:
1. vA: 0.022160397419173736
2. vB: 0.022682457628388688
3. r_B6: 0.05859750987072454
4. mu: 0.06159343483801437
5. r_A6: 0.07288902998776703
6. EN_A: 0.078963615009264
7. bond_len_BO: 0.08001388535701298
8. r_A12: 0.08244603789897259
9. bond_len_AO: 0.08904365790781456
10. EN_B: 0.09404402383463224
11. tau: 0.1013717550249592
12. ENR_diff: 0.10794889624140462
13. tG: 0.12824529898187145
```



Random Forest Model Summary

This feature importance output shows much closer percentages for the top features than the decision tree model. This may be highlighting some linear relationships and should be investigated in a future analysis.

Although tau doesn't show separation in the pairwise plot, it does seem to be a significant feature. Since tau is determined by factors of radii and bond lengths of A and B, the importance may also change and be dependent on the size of atom A or B.

The top 5 feature importance really highlights the relationship between the ENR_diff and its relationship to EN_B and bond_len_AO. The electronegativity radius difference most certainly is strongly related to the electronegativity of atom B because the stronger B is the shorter the bond length to B and the longer the bond length is to A.

Finally, it is interesting that the Decision tree model prioritized the ENR_diff, EN_A, and bond_len_BO while the random forest model prioritizes the oppsite.

Support Vector Machine Model with Cross-Validation Score Method

Support Vector Machines (SVM) is a non tree classifier. It was chosen to compare the results of tree and nontree based models.

Support Vector Machines (SVM) are an effective solution for capturing complex nonlinear relationships in data. Because SVMs have margin maximization objective and regularization parameters, they preform well in high-dimensional or noisy datasets.

SVMs offer the ability to handle non-linear data through kernel functions, making them a valuable choice after decision trees and random forests in multiclassification problems.

In [61]:

```python
#third model, Hyperparameter Tuning

# Define the list of kernels to try
kernels = ['linear', 'poly', 'rbf', 'sigmoid']

# Define hyperparameters grid for each kernel
param_grids = {
    'linear': {'C': [0.1, 1, 10, 100]},
    'poly': {'C': [1], 'degree': [3], 'gamma':['scale', 'auto']},
    'rbf': {'C': [0.1, 1, 10, 100], 'gamma': [0.01, 0.1, 1, 10, 'scale', 'auto']},
    'sigmoid': {'C': [0.1, 1, 10, 100], 'gamma': [0.01, 0.1, 1, 10, 'scale', 'auto']}
}

# Iterate over each kernel and perform hyperparameter tuning
for kernel in kernels:
    print(f"Tuning hyperparameters for SVM with {kernel} kernel")

    # Start time for performance measurement
    start_time = time.time()

    # Define SVM classifier
    SVMclf = SVC(kernel=kernel)

    # Define hyperparameters grid
    param_grid = param_grids[kernel]

    # Perform grid search
    grid_search_cv = GridSearchCV(
        estimator=SVMclf,
        param_grid=param_grid,
        scoring='accuracy',
        n_jobs=-1,
        cv=cv
    )

    grid_search_cv.fit(X_train, y_train)

    # End time and elapsed calculation for performance measurement
    end_time = time.time()
    elapsed_time = end_time - start_time

    #Print results
    print("Grid search for {} kernel completed in {:.2f} seconds".format(kernel, elapsed_time))
    print(f"Best parameters for {kernel} kernel: {grid_search_cv.best_params_}")

```

```
Tuning hyperparameters for SVM with linear kernel
Grid search for linear kernel completed in 798.62 seconds
Best parameters for linear kernel: {'C': 100}
Tuning hyperparameters for SVM with poly kernel
Grid search for poly kernel completed in 4544.59 seconds
Best parameters for poly kernel: {'C': 1, 'degree': 3, 'gamma': 'auto'}
Tuning hyperparameters for SVM with rbf kernel
Grid search for rbf kernel completed in 2.66 seconds
Best parameters for rbf kernel: {'C': 10, 'gamma': 10}
Tuning hyperparameters for SVM with sigmoid kernel
Grid search for sigmoid kernel completed in 0.78 seconds
Best parameters for sigmoid kernel: {'C': 10, 'gamma': 0.01}
```

Hyperparameter Tuning

In [62]:
```
#assess the performance of each SVM classifier with different kernels using cross-validation

# Start time for performance measurement
start_time = time.time()

# Define SVM classifiers with the best parameters for each kernel
svm_linear = SVC(kernel='linear', C=100)
svm_poly = SVC(kernel='poly', C=1, degree=3, gamma='auto')
svm_rbf = SVC(kernel='rbf', C=10, gamma=10)
svm_sigmoid = SVC(kernel='sigmoid', C=10, gamma=0.01)

# Perform cross-validation for each SVM classifier
svm_linear_scores = cross_val_score(svm_linear, X_train, y_train, cv=5)
svm_poly_scores = cross_val_score(svm_poly, X_train, y_train, cv=5)
svm_rbf_scores = cross_val_score(svm_rbf, X_train, y_train, cv=5)
svm_sigmoid_scores = cross_val_score(svm_sigmoid, X_train, y_train, cv=5)

# End time and elapsed calculation for performance measurement
end_time = time.time()
elapsed_time = end_time - start_time
print("Grid search for {} kernel completed in {:.2f} seconds".format(kernel, elapsed_time))

# Print average cross-validation scores
print("Average cross-validation scores:")
print(f"Linear SVM: {svm_linear_scores.mean()}")
print(f"Polynomial SVM: {svm_poly_scores.mean()}")
print(f"RBF SVM: {svm_rbf_scores.mean()}")
print(f"Sigmoid SVM: {svm_sigmoid_scores.mean()}")

```

```
Grid search for sigmoid kernel completed in 8987.58 seconds
Average cross-validation scores:
Linear SVM: 0.7132075471698112
Polynomial SVM: 0.7459119496855345
RBF SVM: 0.7874213836477988
Sigmoid SVM: 0.6553459119496855
```

These scores provide insights into how well each SVM classifier generalizes to unseen data. The grid search results were used to tune the hyperparameters that are hard coded here.

The best performing SVM classifer is RBF SVM. The reason for this could be that polynomials may not effectively describe all boundaries, whereas the RBF kernel, being more robust, can accommodate a wider range of boundary shapes and variations.

Ranking the SVM classifiers in order of performance from best to worst would be

RBF (Gaussian), Polynomial, Linear, Sigmoid

Train the SVM Model

In [63]:

```
#Model Training

# Start time for performance measurement
start_time = time.time()

# Train SVM classifiers with the best hyperparameters for each kernel
svm_linear_best = SVC(kernel='linear', C=100)
svm_rbf_best = SVC(kernel='rbf', C=10, gamma=10)
svm_sigmoid_best = SVC(kernel='sigmoid', C=10, gamma=0.01)
svm_poly_best = SVC(kernel='poly', C=100, degree=3)

svm_linear_best.fit(X_train, y_train)
svm_rbf_best.fit(X_train, y_train)
svm_sigmoid_best.fit(X_train, y_train)
svm_poly_best.fit(X_train, y_train)

# Model Evaluation

# Evaluate the trained SVM classifiers on the test set
svm_linear_accuracy = svm_linear_best.score(X_test, y_test)
svm_rbf_accuracy = svm_rbf_best.score(X_test, y_test)
svm_sigmoid_accuracy = svm_sigmoid_best.score(X_test, y_test)
svm_poly_accuracy = svm_poly_best.score(X_test, y_test)

print("Accuracy on the test set:")
print(f"Linear SVM: {svm_linear_accuracy}")
print(f"RBF SVM: {svm_rbf_accuracy}")
print(f"Sigmoid SVM: {svm_sigmoid_accuracy}")
print(f"Poly SVM: {svm_poly_accuracy}")

# End time and elapsed calculation for performance measurement
end_time = time.time()
elapsed_time = end_time - start_time

print("Grid search for {} kernel completed in {:.2f} seconds".format(kernel, elapsed_time))

```

```
Accuracy on the test set:
Linear SVM: 0.6984924623115578
RBF SVM: 0.8291457286432161
Sigmoid SVM: 0.6155778894472361
Poly SVM: 0.592964824120603
Grid search for sigmoid kernel completed in 348.22 seconds
```

In the future, instead of training all models individually, I may explore advanced ensemble methods that combine predictions from multiple models, in the next steps.

Ensemble methods include: bagging, boosting, and stacking

In retrospect, I should have chosen advanced ensemble methods like gradient boosting, XGBoost, and LightGBM where the algorithms are specifically designed to handle imbalanced datasets.

Performance Evaluation

In [64]:

```
# More Model Evaluation

# Start time for performance measurement
start_time = time.time()

# Confusion matrix and classification report for each SVM classifier
svm_classifiers = {
    'Linear SVM': svm_linear_best,
    'Polynomial SVM': svm_poly_best,
    'RBF SVM': svm_rbf_best,
    'Sigmoid SVM': svm_sigmoid_best
}

for name, clf in svm_classifiers.items():
    print(f"\nEvaluation metrics for {name}:")
    y_pred = clf.predict(X_test)
    print("Confusion Matrix:")
    print(confusion_matrix(y_test, y_pred))
    print("\nClassification Report:")
    print(classification_report(y_test, y_pred, zero_division=0.0))

# End time for performance measurement
end_time = time.time()
elapsed_time = end_time - start_time

print("Grid search for {} kernel completed in {:.2f} seconds".format(kernel, elapsed_time))

```

```
Evaluation metrics for Linear SVM:
Confusion Matrix:
[[189  47   0   0]
 [ 42  89   0   0]
 [ 11   9   0   0]
 [  3   8   0   0]]

Classification Report:
              precision    recall  f1-score   support

       cubic       0.77      0.80      0.79       236
orthorhombic       0.58      0.68      0.63       131
rhombohedral       0.00      0.00      0.00        20
  tetragonal       0.00      0.00      0.00        11

    accuracy                           0.70       398
   macro avg       0.34      0.37      0.35       398
weighted avg       0.65      0.70      0.67       398


Evaluation metrics for Polynomial SVM:
Confusion Matrix:
[[236   0   0   0]
 [131   0   0   0]
 [ 19   1   0   0]
 [ 11   0   0   0]]

Classification Report:
              precision    recall  f1-score   support

       cubic       0.59      1.00      0.75       236
orthorhombic       0.00      0.00      0.00       131
rhombohedral       0.00      0.00      0.00        20
  tetragonal       0.00      0.00      0.00        11

    accuracy                           0.59       398
   macro avg       0.15      0.25      0.19       398
weighted avg       0.35      0.59      0.44       398


Evaluation metrics for RBF SVM:
Confusion Matrix:
[[221  11   1   3]
 [ 32  93   6   0]
 [  6   2  11   1]
 [  5   0   1   5]]

Classification Report:
              precision    recall  f1-score   support

       cubic       0.84      0.94      0.88       236
orthorhombic       0.88      0.71      0.78       131
rhombohedral       0.58      0.55      0.56        20
  tetragonal       0.56      0.45      0.50        11

    accuracy                           0.83       398
   macro avg       0.71      0.66      0.68       398
weighted avg       0.83      0.83      0.82       398


Evaluation metrics for Sigmoid SVM:
Confusion Matrix:
[[176  55   5   0]
 [ 40  69  22   0]
 [ 13   7   0   0]
 [  4   7   0   0]]

Classification Report:
              precision    recall  f1-score   support
```

```
       cubic       0.76      0.75      0.75       236
orthorhombic       0.50      0.53      0.51       131
rhombohedral       0.00      0.00      0.00        20
  tetragonal       0.00      0.00      0.00        11

    accuracy                           0.62       398
   macro avg       0.31      0.32      0.32       398
weighted avg       0.61      0.62      0.61       398

Grid search for sigmoid kernel completed in 0.09 seconds
```

Based on the evaluation metrics for different SVM kernels, the RBF SVM achieves the highest accuracy of 83%, indicating good performance in distinguishing between different crystal structures.

All SVM kernels seem to struggle with correctly classifying samples from the 'rhombohedral' and 'tetragonal' classes, as indicated by low precision and recall scores. This might happen because the characteristics of these classes might be very similar or subtly different but challenging to distinguish. Further investigation into improving classification for these classes is needed.

Feature Importance

For non-linear SVM models (e.g., polynomial, RBF, sigmoid), interpreting feature importance in terms of coefficients is not applicable because these models do not directly produce coefficients like linear SVMs.

Since the best kernel was RBF, permutation importance will be used.

Permutation importance is compatible with various models and is a technique that measures the increase in model error when a feature's values are randomly shuffled. By permuting feature values and observing the impact on model performance, the importance of each feature can be assessed. This technique is applicable to any machine learning model, including SVMs.

In [65]:
```
# Calculate permutation importance for the RBF SVM classifier
result = permutation_importance(svm_classifiers['RBF SVM'], X_test, y_test, n_repeats=10, rando
rbf_svm_importance = result.importances_mean

# Loop through each feature and its importance score, displaying them sequentially
for i, (feature, importance_score) in enumerate(zip(X_test.columns, rbf_svm_importance)):
    print(f"{i + 1}. {feature}: {importance_score}")

# Print feature importance for the RBF SVM classifier
print("\nPermutation Importance for RBF SVM:")


```

```
1. vA: 0.1520100502512563
2. vB: 0.1520100502512563
3. r_A12: 0.10427135678391966
4. r_A6: 0.052261306532663344
5. r_B6: 0.02412060301507544
6. EN_A: 0.11005025125628146
7. EN_B: 0.12085427135678395
8. bond_len_AO: 0.06281407035175884
9. bond_len_BO: 0.04170854271356787
10. ENR_diff: 0.12286432160804021
11. tG: 0.011055276381909585
12. tau: 0.19849246231155784
13. mu: 0.0037688442211055717

Permutation Importance for RBF SVM:
```

Support Vector Machine Model Summary

The most to least important permutation scores are:

1. tau: 0.19849246231155784

2. vA: 0.1520100502512563
3. vB: 0.1520100502512563
4. EN_B: 0.12085427135678395
5. ENR_diff: 0.12286432160804021
6. EN_A: 0.11005025125628146
7. r_A12: 0.10427135678391966
8. bond_len_AO: 0.06281407035175884
9. r_A6: 0.052261306532663344
10. bond_len_BO: 0.04170854271356787
11. r_B6: 0.02412060301507544
12. tG: 0.011055276381909585
13. mu: 0.0037688442211055717

Looking at the Permutation Importance scores, the larger the decrease in performance when a particular feature is shuffled, the more important that feature is considered to be. So in this case the RBF SVM is relying on tau, vA, vB, EN_B, and ENR_diff to make accurate predictions.

This has brough a new insight. When looking at the pairwise plot, the tau feature doesn't show any distinctive separation in the univariate plot, this agrees with the histogram data as well. However, looking at the tau/tG pairwise plot, there is a distinctive nonlinear separation (possibly a inverse relationship) which means that SVM brought an advantage over the decision tree and random forest when highlighting this relationship.

Simply looking at the pairwise univariate plot the top expected features would be: tG, ENR_diff, EN_B, r_A6 and r_A12. While the pairwise plot is useful, the machine learning models are required to fully construct an understadning of the data.

It is surprising to see three discrete values ranked in the top 5 most important features according to the RBF SVM and that r_A12 and tG ranked so low.

Discrete data is likely to be further from the boundary lines and so this result might suggest that RBF SVM handles the discrete values really well and is adept at capturing and utilizing the nonlinear relationships between these categorical features and the target variable. This capability allows the model to effectively discriminate between different 'lowest distortion' structures, leading to accurate predictions even in datasets with complex, nonlinear structures.

Compare at all 3 models

Below is a table that compares the accuracy, recall, and weighted avg f1-score of each model.

make a dataframe or matrix compare metrics of the different models.

Machine Learning Model Comparison

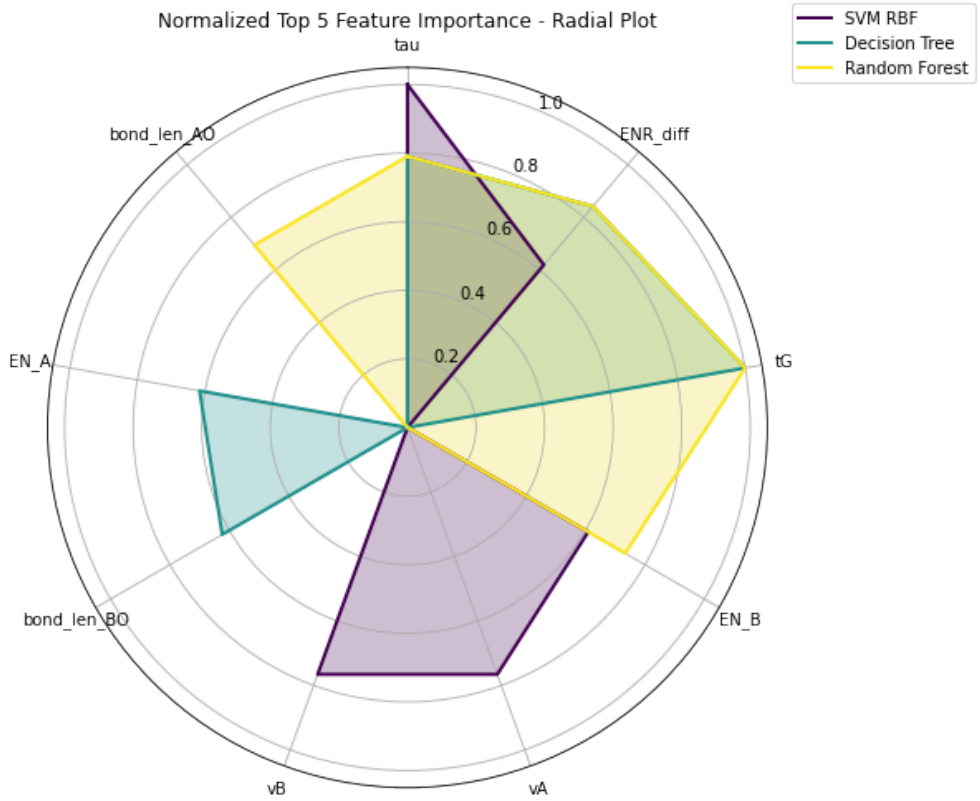
Model	Precision	Recall	Accuracy	F1-Score
Decision Tree	81%	81%	81%	81%
Random Forest	85%	86%	86%	85%
RBF Support Vector Machine	83%	83%	83%	82%

These percentages show the best possible 'lowest distortion' structural prediction performance from the featured data.

In [74]:

```
#Final visualization

# Define all features
all_features = ['tau', 'ENR_diff', 'tG', 'EN_B', 'vA', 'vB',  'bond_len_BO', 'EN_A', 'bond_len_

# Define the top 5 ranked features and their importance scores for SVM RBF
svm_rbf_features = ['tau', 'vA', 'vB', 'EN_B', 'ENR_diff']
svm_rbf_scores = [0.19849246231155784, 0.1520100502512563, 0.1520100502512563, 0.12085427135678

# Define the top 5 ranked features and their importance scores for Decision Tree
decision_tree_features = ['tG', 'tau', 'ENR_diff', 'bond_len_BO', 'EN_A']
decision_tree_scores = [0.12824529898187145, 0.1013717550249592, 0.10794889624140462, 0.080013

# Define the top 5 ranked features and their importance scores for Random Forest
random_forest_features = ['tG', 'ENR_diff', 'tau', 'EN_B', 'bond_len_AO']
random_forest_scores = [0.12824529898187145, 0.10794889624140462, 0.1013717550249592, 0.094044

# Normalize scores for each model
max_score_svm_rbf = max(svm_rbf_scores)
normalized_svm_rbf_scores = [score / max_score_svm_rbf for score in svm_rbf_scores]

max_score_decision_tree = max(decision_tree_scores)
normalized_decision_tree_scores = [score / max_score_decision_tree for score in decision_tree_s

max_score_random_forest = max(random_forest_scores)
normalized_random_forest_scores = [score / max_score_random_forest for score in random_forest_s

# Initialize lists to store adjusted scores for each model
adjusted_svm_rbf_scores = []
adjusted_decision_tree_scores = []
adjusted_random_forest_scores = []

# Iterate over all features
for feature in all_features:
    # Check if the feature is in the top 5 ranked features for SVM RBF
    if feature in svm_rbf_features:
        # If present, append its score
        adjusted_svm_rbf_scores.append(normalized_svm_rbf_scores[svm_rbf_features.index(feature
    else:
        # If not present, append zero
        adjusted_svm_rbf_scores.append(0)

    # Repeat the same process for Decision Tree and Random Forest
    if feature in decision_tree_features:
        adjusted_decision_tree_scores.append(normalized_decision_tree_scores[decision_tree_feat
    else:
        adjusted_decision_tree_scores.append(0)

    if feature in random_forest_features:
        adjusted_random_forest_scores.append(normalized_random_forest_scores[random_forest_feat
    else:
        adjusted_random_forest_scores.append(0)

# Convert to DataFrame
adjusted_df = pd.DataFrame({
    'SVM RBF': adjusted_svm_rbf_scores,
    'Decision Tree': adjusted_decision_tree_scores,
    'Random Forest': adjusted_random_forest_scores
}, index=all_features)

# Plotting Radial Chart
angles = np.linspace(0, 2 * np.pi, len(all_features), endpoint=False).tolist()
angles += angles[:1]  # Close the plot
fig, ax = plt.subplots(figsize=(8, 8), subplot_kw=dict(polar=True))
colors = plt.cm.viridis(np.linspace(0, 1, len(adjusted_df.columns)))

for i, (model, scores) in enumerate(adjusted_df.iteritems()):
    ax.plot(angles, scores.tolist() + scores[:1].tolist(), color=colors[i], label=model, linew
    ax.fill(angles, scores.tolist() + scores[:1].tolist(), color=colors[i], alpha=0.25)  # Fil
ax.set_theta_offset(np.pi / 2)
```

```
ax.set_theta_direction(-1)
plt.xticks(angles[:-1], all_features)
ax.legend(loc='upper right', bbox_to_anchor=(1.3, 1.1))
plt.title('Normalized Top 5 Feature Importance - Radial Plot')
plt.show()

```



Conclusion

This analysis reveals that the Random Forest model outperforms the other models tested, making it the best choice for predicting molecular structures from this analysis. Random Forest, an ensemble learning method, harnesses the power of multiple decision trees, combining their outputs to produce more accurate predictions. This ensemble approach is advantageous compared to standalone models, as it reduces the risk of overfitting and improves generalization by averaging the predictions of individual trees.

Tau's Importance, Simplicity, and Overfitting:

The consistent presence of 'tau' among the top 5 important features across different models highlights its significance in predicting the target variable. As a simple 1D descriptor, 'tau' offers efficiency and effectiveness in capturing patterns without introducing unnecessary complexity. Its simplicity makes it less prone to overfitting, contributing to model robustness and generalization.

Goldschmidt as a Descriptor:

Goldschmidt's tolerance factor involves multiple dimensions, making it more complex. This complexity could potentially impact its performance in predictive modeling compared to simpler descriptors like 'tau'. While Goldschmidt may provide comprehensive insights into molecular structures, its complexity may pose challenges in model interpretation and generalization.

Final thoughts:

Both Random Forest and RBF Support Vector Machine models offer unique features. Random Forest excels in handling complex datasets. For instance, in the dataset, with features such as bond lengths, bond angles, and electronegativity values, Random Forest effectively captures the complex relationships among these features to predict molecular properties.

RBF SVM demonstrates proficiency in capturing complex patterns within the data, including potential nonlinear relationships. While 'tau' and 'vA' are important features in the model, it's important to note that the relationship between these features and the target variable may exhibit complexity. For example, 'tau', despite being a one-dimensional descriptor, ranks highly in importance for RBF SVM, suggesting its relevance in capturing nuanced variations in molecular structures.

However, when considering predictive performance and generalization across diverse features like those present in molecular structures, Random Forest's ensemble approach may offer superior capabilities. This is evidenced by its ability to handle complex feature interactions and provide robust predictions across various structural parameters, ultimately enhancing the model's accuracy

Summary

The objective was to develop a predictive model for molecular structure determination, leveraging machine learning algorithms. The analysis involved three models: Decision Tree, Random Forest, and Support Vector Machine with Radial Basis Function (RBF) kernel.

Key Findings:
Feature Importance Analysis with Evaluation Scores:

1. Decision Tree Model: Top 5 feature importance 'tG', 'tau', 'ENR_diff', 'bond_len_BO', and 'EN_A'. Notably, 'ENR_diff' and 'EN_A' exhibited strong relationships with 'bond_len_BO'.
   Decision Tree: Precision: 81% Recall: 81% Accuracy: 81% F1-Score: 81%
2. Random Forest Model: Highlighted 'tG', 'ENR_diff', 'tau', 'EN_B', and 'bond_len_AO' as important predictors, suggesting correlations between 'ENR_diff' and 'EN_B' with 'bond_len_AO'.
   Random Forest: Precision: 85% Recall: 86% Accuracy: 86% F1-Score: 85%
3. RBF Support Vector Machine: Found 'tau', 'vA', 'vB', 'EN_B', and 'ENR_diff' as key features, indicating the model's capability to handle discrete values effectively.
   RBF Support Vector Machine: Precision: 83% Recall: 83% Accuracy: 83% F1-Score: 82%

Recommendations

- Utilize the Random Forest model.
- Enhance dataset with additional empirical data.
- Address missing values and discrepancies using insights from feature importance analysis to ensure data quality.
- Strategically target discrete values: Leverage RBF SVM's proficiency in capturing nonlinear relationships to target molecules with discrete values for improved predictive accuracy.

Next Steps

There are several directions that could be explored in the next phase of this project.

1. Gather Additional Empirical Data

- Focus on collecting empirical data, especially experimental data related to molecular structures. Bond lengths, bond angles, valences are critical empirical parameters.
- Consider expanding the dataset to include a wide range of molecular structures and variations to capture diverse structural characteristics.

2. Improve Electronegativity and Ionic Radius Estimates:

- Investigate methods to improve the accuracy of electronegativity and ionic radius estimates using data-driven approaches. Machine learning models can be trained to refine and optimize these parameters based on observed structural characteristics.
- Assess the impact of adjusted electronegativity and ionic radius values on predictive model performance and molecular structure determination.

3. Feature Segmentation

- Utilize unsupervised machine learning techniques like clustering to identify patterns and group similar molecular structures. This can help in segmenting the dataset into distinct clusters without relying on labeled data.
- Explore the use of clustering algorithms such as K-means or hierarchical clustering to identify structural similarities and differences.

4. Utilize Structural Parameters for Prediction:

- Leverage structural parameters such as tG, tau, and mu to predict molecular properties and behaviors. These parameters can serve as valuable predictors in machine learning models.

- Explore existing relationships between structural parameters and molecular properties, and consider incorporating them into the feature set for predictive modeling.

5. Deep Learning

- Investigate the application of deep learning models, such as neural networks, for molecular structure determination. Deep learning techniques can effectively capture complex relationships and patterns in the data.
- Explore the use of deep learning architectures like convolutional neural networks (CNNs) or recurrent neural networks (RNNs) for feature extraction and classification tasks.

5. Analyze Halides for Big Data Processing:

- Explore the inclusion of halides in the dataset for big data processing and analysis. Investigate how variations in halide compositions contribute to structural diversity and affect predictive model outcomes.
- Consider incorporating halide-specific features or parameters into the dataset to enhance the predictive capabilities of

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