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DATA ANALYSIS OF CRYSTAL STRUCTURES OF POLYMORPHIC FORMS USING MATLAB PROGRAMMING

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Abstract:

Polymorphic form-I and form-II of (E) – 4 - bromo – 2 - [(Phenylimino)methyl] phenol [4B2PMP], commonly known as N-salicylidene, have been identified. Form-I and form-II, respectively synthesized at the temperature of 283 K and 333 K. In both forms, the molecules show some geometrical structure in different temperatures. In this paper, we employed MATLAB programming to visualize the formation of these molecules' structures and validated our findings via data analysis, hypothesis testing using MATLAB programming.

Keywords: Polymorphic, Testing of Hypothesis, Large Sample Test, MATLAB programming.

1. Introduction

Two or more crystal forms with similar element groupings or conformations in the crystal lattice are referred to as solid material polymorphism. The physicochemical properties of the medicine and, consequently, its therapeutic effects are significantly influenced by the physical structures of the constituents in the crystal lattice. Polymorphs are formed in the crystal by slight variations in the unit-cell parameter values. A single crystal of 4-bromo-2-[(phenylimino)methyl] phenol [9] was reported as an "orange-red" crystal produced at ambient temperature. An analysis has been carried out on two polymorphs (E)− 4-Bromo-2-[(phe nylimino) methyl] phenol (4B2PMP). Polymorphic Patterns of the 4B2PMP compound crystals were observed to have different colours at different temperatures. Therefore, one of the primary variables influencing crystal nucleation is temperature [10]. Variations in crystallization temperature between the two forms affect the packing arrangements of the molecular crystal structure. The related research was completed by Krishnapriya. B, Ida Malarselvi. R and et.al. [7] in 2023. The principal objective of this research is to evaluate the results on these forms by analysing the data of crystal polymorphs which may provide an improved structure. The structure of the crystals of polymorphic forms I and II are plotted by using MATLAB Programming [1 & 3] and the data set is analysed by hypothesis test [13] in MATLAB programming [5 & 6]. While performing the computation, we utilizing the peak point value which is obtained from the MATLAB plot.

This paper is organized as follows: Section 2 gives some preliminaries related to our research work. Our generated MATLAB Programming with plot organized in section 3. In section 4, Available numerical data are analysed by testing of hypothesis, also MATLAB programming for the hypothesis test is given. Finally, section 5, derives some conclusion. At last, some references provided in section 6.

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2. Preliminaries: [4]

In this section, we provide some preliminaries which are related to Testing of hypothesis.

2.1 Large Sample Test

When n is larger than 30 (n ≥30), it is referred to as a large sample. The sampling distribution is normal for large samples, as indicated by the Z test. Large sample theory is the study of the sampling distribution of statistics for a large sample.

2.2 Sample Mean

A measure of central tendency is the sample mean. To calculate the arithmetic average, random data or samples from the population are used. The evaluation method is involves dividing the total number of variables by the sum of all sample variables.

The following formula is used to compute sample mean:

$$\bar{x} = \frac{\sum a}{n}$$

Where “a is all sample values” and “n is the sample size”.

2.3 Population Mean

The average calculated from the entire group, distribution, or population is known as the population mean. It is calculated by dividing the total number of variables in the population by the sum of all the variables in the population.

Population Mean is denoted by

$$\mu = \frac{\sum p}{N}$$

Where “p is all the population values” and “N is the population size”.

3. MATLAB programming:

We generate a MATLAB program for available data, to visualize the crystal formation in different temperatures. Output plot graph given in figure 3.1.

```
clear all;
clc;
num1 = xlsread('crystal data1.xlsx','Sheet1','A2:A313');
num2 = xlsread('crystal data1.xlsx','Sheet1','B2:B313');
num3 = xlsread('crystal data1.xlsx','Sheet2','A2:A317');
num4 = xlsread('crystal data1.xlsx','Sheet2','B2:B317');
num5 = xlsread('crystal data1.xlsx','Sheet3','A2:A309');
```

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```
num6 = xlsread('crystal data1.xlsx','Sheet3','B2:B309');
num7 = xlsread('crystal data1.xlsx','Sheet4','A2:A313');
num8 = xlsread('crystal data1.xlsx','Sheet4','B2:B313');

subplot(2,2,1), plot(num1,num2,'g');
legend('5BSA 10','Location','best');
xlabel('Temperature','FontSize',12);
ylabel('Dsc','FontSize',12);
title('Polymorphic Form I Cooling graph','FontSize',12);
[peakVal1, idx1] = min(num2); % Find the peak for the first graph
peakTemp1 = num1(idx1);
hold on;
plot(peakTemp1, peakVal1, 'ro'); % Mark the peak point
text(peakTemp1, peakVal1, sprintf('(%0.2f, %0.2f)', peakTemp1, peakVal1), 'VerticalAlignment',
'bottom', 'HorizontalAlignment', 'right');

subplot(2,2,2), plot(num3,num4,'r');
legend('5BSA 60','Location','best');
xlabel('Temperature','FontSize',12);
ylabel('Dsc','FontSize',12);
title('Polymorphic Form II Cooling graph','FontSize',12);
[peakVal2, idx2] = min(num4); % Find the peak for the second graph
peakTemp2 = num3(idx2);
hold on;
plot(peakTemp2, peakVal2, 'ro');
text(peakTemp2, peakVal2, sprintf('(%0.2f, %0.2f)', peakTemp2, peakVal2), 'VerticalAlignment',
'bottom', 'HorizontalAlignment', 'right');

subplot(2,2,4), plot(num5,num6,'b');
legend('5BSA 10','Location','best');
xlabel('Temperature','FontSize',12);
ylabel('Dsc','FontSize',12);
title('Polymorphic Form I Heating graph','FontSize',12);
[peakVal3, idx3] = max(num6); % Find the peak for the third graph
```

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```
peakTemp3 = num5(idx3);
hold on;
plot(peakTemp3, peakVal3, 'ro');
text(peakTemp3, peakVal3, sprintf('(%0.2f, %0.2f)', peakTemp3, peakVal3), 'VerticalAlignment', 'bottom', 'HorizontalAlignment', 'right');

subplot(2,2,3), plot(num7,num8,'y');
legend('5BSA 60','Location','best');
xlabel('Temperature','FontSize',12);
ylabel('Dsc','FontSize',12);
title('Polymorphic Form II Heating graph','FontSize',12);
[peakVal4, idx4] = max(num8); % Find the peak for the fourth grap
peakTemp4 = num7(idx4);
hold on;
plot(peakTemp4, peakVal4, 'ro');
text(peakTemp4, peakVal4, sprintf('(%0.2f, %0.2f)', peakTemp4, peakVal4), 'VerticalAlignment', 'bottom', 'HorizontalAlignment', 'right');
```

3.1 Output Graphs:

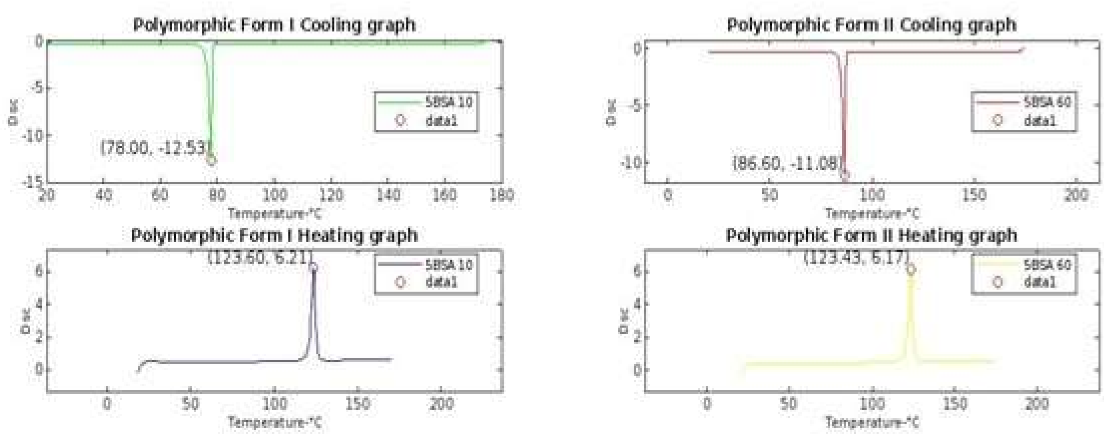

Figure 3.1

4. Numerical Example:

This section provides the numerical calculation for the available data, using MATLAB programming in Large Sample test.

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4.1 MATLAB Program for Testing of Hypothesis:

```
clear all;
clc;
sample_mean =  % Enter sample mean value
population_mean =  % Enter population mean value
standard_deviation =  % Enter standard deviation value
sample_size =  % Enter sample size value

z = (sample_mean - population_mean) / (standard_deviation / sqrt(sample_size));
alpha = 0.05; % significance level
critical_value = norminv(1 - alpha/2); % two-tailed test

if abs(z) > critical_value
   fprintf(' Reject H0 at %.2f%% level of significance.\n', alpha * 100);
   fprintf('\n Conclusion: There is a significant difference between the population mean and sample mean.\n');
else
   fprintf(' Accept H0 at %.2f%% level of significance.\n', alpha * 100);
   fprintf('\n Conclusion: mu = mu0. Therefore, the population mean value is equal to the crystallization point.\n');
end
```

4.1.1 Hypothesis Testing of Form I Cooling point

Given

Sample mean $(\bar{X}) = -0.4088$
Population mean $(\mu) = -0.3145$
Standard deviation $(s) = 0.8628$
Sample size $(n) = 311$

In this problem, the population parameter being tested is population mean. i.e., The peek point of crystal formation is – 0.3145. So our claim is $\mu = -0.3145$ and its complement is $\mu \neq -0.3145$.

Step I

$\boldsymbol{H_0}$: The population mean is $\mu = \mu_0$. i.e., $\mu = -0.3145$ (colling point of the crystal)

$\boldsymbol{H_1}$: $\mu \neq \mu_0$.

Step II

Here Z-test of two-tailed test can be used to test the hypothesis.

Step III

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The test statistic is

$$Z = \frac{\bar{x} - \mu}{s/\sqrt{n}}$$

Where $\bar{x}$ – Sample mean, μ –Population mean, s – Standard deviation, n – Sample size
Using MATLAB Program for the calculation given in 4.1.

Step IV- Output:

sample_mean =
 -0.4088

population_mean =
 -0.3145

standard_deviation =
 0.8628

sample_size =
 311

Accept H0 at 5.00% level of significance.

Conclusion: mu = mu0. Therefore, the population mean value is equal to the crystallization point.

Step V

We conclude that, the population mean is – 0.3145. That is, the cooling point of the crystal is – 0.3145.

4.1.2 Hypothesis Testing of Form I Heating point:

Given

Sample mean $(\bar{X}) = 0.6399$
Population mean $(\mu) = 0.4951$
Standard deviation $(s) = 0.6256$
Sample size $(n) = 315$

In this problem, the population parameter being tested is population mean. i.e., The peek point of crystal formation is 0.4951. So our claim is $\mu = 0.4951$ and its complement is $\mu \neq 0.4951$.

Step I

$\boldsymbol{H_0}$: *There is a significant difference between the population mean and sample mean.*
$\boldsymbol{H_1}$: *There is no significant difference between the population mean and sample mean.*

Step II

Here Z-test of two-tailed test can be used to test the hypothesis.

Step III

The test statistic is

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$$Z = \frac{\bar{x} - \mu}{s/\sqrt{n}}$$

Where $\bar{x}$ – Sample mean, μ –Population mean, s – Standard deviation, n – Sample size
Using MATLAB Program for the calculation given in 4.1.

Step IV- Output:

sample_mean =
0.6399

population_mean =
0.4951

standard_deviation =
0.6256

sample_size =
315

Reject H0 at 5.00% level of significance.

Conclusion: There is a significant difference between the population mean and sample mean.

Step V

We conclude that, *there is no significant difference between the population mean and sample mean.*

4.1.3 Hypothesis Testing of Form II Cooling point:

Given

Sample mean $(\bar{X}) = -0.3884$
Population mean $(\mu) = -9.8849$
Standard deviation $(s) = 0.8171$
Sample size $(n) = 311$

In this problem, the population parameter being tested is population mean. i.e., The peek point of crystal formation is – 9.8849. So our claim is $\mu = -9.8849$ and its complement is $\mu \neq -9.8849$.

Step I

H_0 : *There is a significant difference between the population mean and sample mean*
H_1: *There is no significant difference between the population mean and sample mean*

Step II

Here Z-test of two-tailed test can be used to test the hypothesis.

Step III

The test statistic is

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$$Z = \frac{\bar{x} - \mu}{s/\sqrt{n}}$$

Where $\bar{x}$ – Sample mean, μ –Population mean, s – Standard deviation, n – Sample size
Using MATLAB Program for the calculation given in 4.1.

Step IV- Output:

sample_mean =
-0.3884

population_mean =
-9.8849

standard_deviation =
0.8171

sample_size =
311

Reject H0 at 5.00% level of significance.

Conclusion: There is a significant difference between the population mean and sample mean.

Step V

We conclude that, *There is no significant difference between the population mean and sample mean*.

4.1.4 Hypothesis Testing of Form II Heating point:

Given

Sample mean $(\bar{X}) = 0.5923$
Population mean $(\mu) = 6.16678$
Standard deviation $(s) = 0.6442$
Sample size $(n) = 308$

In this problem, the population parameter being tested is population mean. i.e., The peek point of crystal formation is 6.16678. So, our claim is $\mu = 6.16678$ and its complement is $\mu \neq 6.16678$.

Step I

$\boldsymbol{H_0}$: *There is a significant difference between the population mean and sample mean*
$\boldsymbol{H_1}$: *There is no significant difference between the population mean and sample mean*

Step II

Here Z-test of two-tailed test can be used to test the hypothesis.

Step III

The test statistic is

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$$Z = \frac{\bar{x} - \mu}{s/\sqrt{n}}$$

Where $\bar{x}$ – Sample mean, μ –Population mean, s – Standard deviation, n – Sample size.
Using MATLAB Program for the calculation given in 4.1.

Step IV - Output:

```
sample_mean =
   0.5923

population_mean =
   6.1668

standard_deviation =
   0.6442

sample_size =
  308

 Reject H0 at 5.00% level of significance.

 Conclusion: There is a significant difference between the population mean and sample mean.
```

Step V

We conclude that, *there is no significant difference between the population mean and sample mean.*

5. Conclusion:

A vital aspect in the formation of crystals is temperature. Therefore, the primary value of the crystal formation cooling and heating temperature points have been calculated and presented in this study. A MATLAB programming is generated to plot the available data and display the peak point of crystal formation as a function of temperature in order to perform further computations. The attained results are verified using Hypothesis testing with the peak point of the crystals. Also, a MATLAB programming for the large sample is developed which simplifies the computation part. Finally, with our calculations it is confirmed that the result got in this research work is accurate.

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