

Bragg Diffraction Lab Report

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Abstract:

The phenomenon of bragg diffraction was explored in this lab report. The experiment was performed with an Li-Didactyl machine with two different mystery crystals. The estimated lattice constant value for Crystal 1 and crystal 2 was found to be $570 \pm 1.8 \text{ pm}$ and $403 \pm 1 \text{ pm}$. The true lattice constants were taken from OSF and then compared with the estimated values. NaCl crystals have a lattice constant of 564.02 pm while LiF crystals have a lattice constant of 402.7 pm. Modifying the theta arguments by $.15^\circ$ for crystal 1 resulted in a lattice constant value of $564.9 \pm .9 \text{ pm}$. Thus crystal 1 and crystal 2 were determined to be NaCl and LiF respectively.

Introduction:

It is first necessary to discuss the history of X-rays. An article by Iowa State Universities Center for Nondestructive evaluation showed that, in 1895, Wilhelm Conrad Roentgen was a university professor at Wurzburg university and was doing experiments with cathode ray tubes. He noticed that the tube produced a greenish glow when the air was evacuated from the tube and a large voltage was applied. He placed a piece of black material around the cathode tube and was astounded to find that the crystals a few feet away began to glow the same green color.

He posited that a new type of ray was being generated by the cathode tube. Further experiments uncovered that this new ray could pass through varied materials and cast shadows of these objects. This new ray could also pass-through human flesh which was of interest to the medical community. The ability for these rays to pass through matter allowed for new

discoveries in physics. Most importantly, the ability to investigate the internal structures of varied materials [1].

According to OpenStax University physics volume 3 chapter 4.6, In 1912, Max Von Laue convinced some colleagues of his to send X-Rays into a crystal structure. If a diffraction pattern could be acquired, that meant that X-Rays were waves. If they are waves, it is possible to extract wavelength properties. Thanks to this discovery, Max Von Laue won the Nobel Prize. This latest information was to be leveraged by the team of Sir William Lawrence Bragg and Sir William Henry Bragg to discover the science of X-Ray analysis which is conducted in a rudimentary form in this lab [2].

Theory:

If one were to zoom into a crystal, one would see ions spaced apart from each other an equal distance. This crystal acts as the diffraction grating one would see in a quintessential diffraction experiment. First, electrons are shot at a piece of molybdenum which generates X-ray emissions in response. These rays diffract off the atoms and constructively interfere with an integer multiple of the wavelength. The equation that represents this is shown below [2].

$$m * \lambda = 2 * d * \sin(\theta) \quad (1)$$

Where m is the diffraction order, λ is the wavelength, d is the and θ is the glancing angle. Figure 1 shows the physical scenario below.

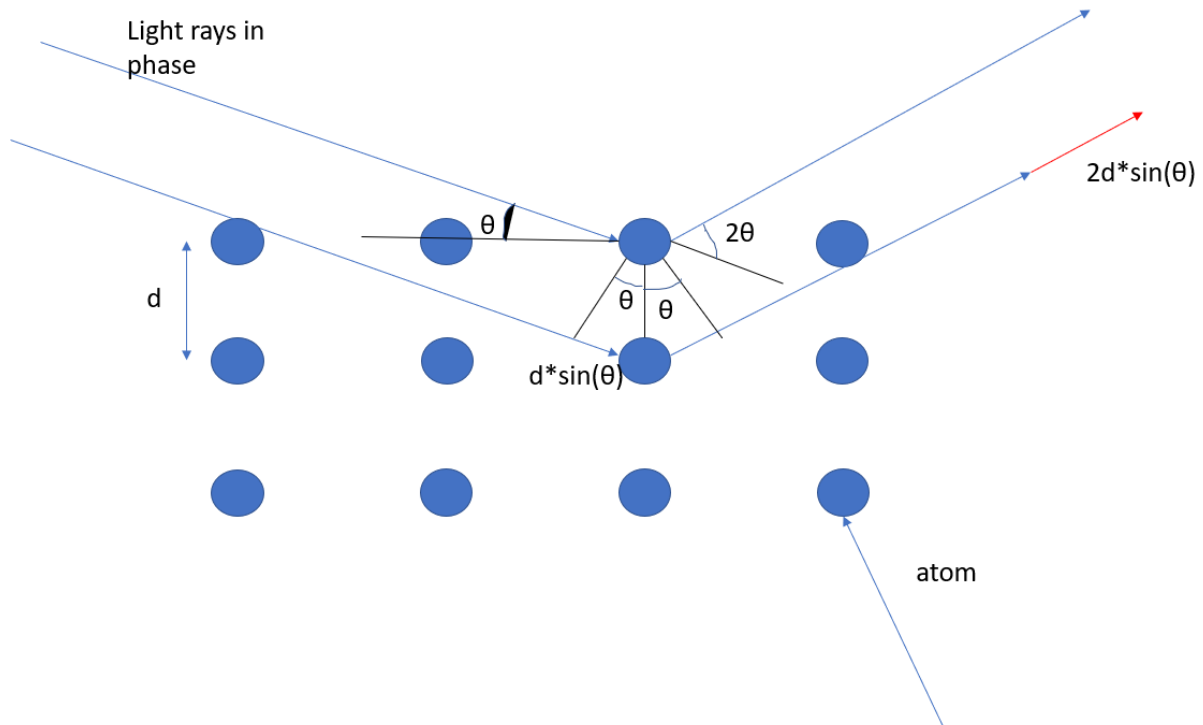


Figure 1: Model of light rays hitting crystal lattice.

This constructive interference of the line paths (i.e., the $2d \sin(\theta)$ term) at wavelengths yields valuable information about the crystals lattice structure. In this case the constructive interference happens when the line paths are integer multiples of the wavelengths.

An important quantity to look for is the lattice constant. This is denoted by the quantity a_0 . It is a measure of the distance between two of the same ions. This is related to the atomic spacing, d , by the relation shown in equation 2.

$$d = \frac{a_0}{2} \quad (2)$$

This transforms equation 1 into equation 3.

$$m\lambda = a_0 \sin(\theta) \quad (3)$$

Thus, it is possible to find the lattice constant of an unknown crystal by solving for a_0 and is shown in equation 4.

$$a_0 = \frac{m * \lambda}{\sin(\theta)} \quad (4)$$

The a_0 values will be compared with the true values to determine if the crystals are either NaCl or LiF.

The uncertainties for the emission lines were .005 pm for both emissions. The uncertainty for θ is shown in equation 5. Since its dependent on other variables by solving equation 1 for that variable the equation in 5 must be used and is taken from Taylor [3].

$$\theta_{unc} = \frac{df}{d\theta} * \theta = \cos(\theta) * a_0 * \theta \quad (5)$$

This was then used as an argument for arcsine for the uncertainty in the x variable for the ODR line of fit.

Setup/procedure:

The x-ray apparatus and two crystals were used to conduct the experiment. They are shown in figures 2, 3 and 4.

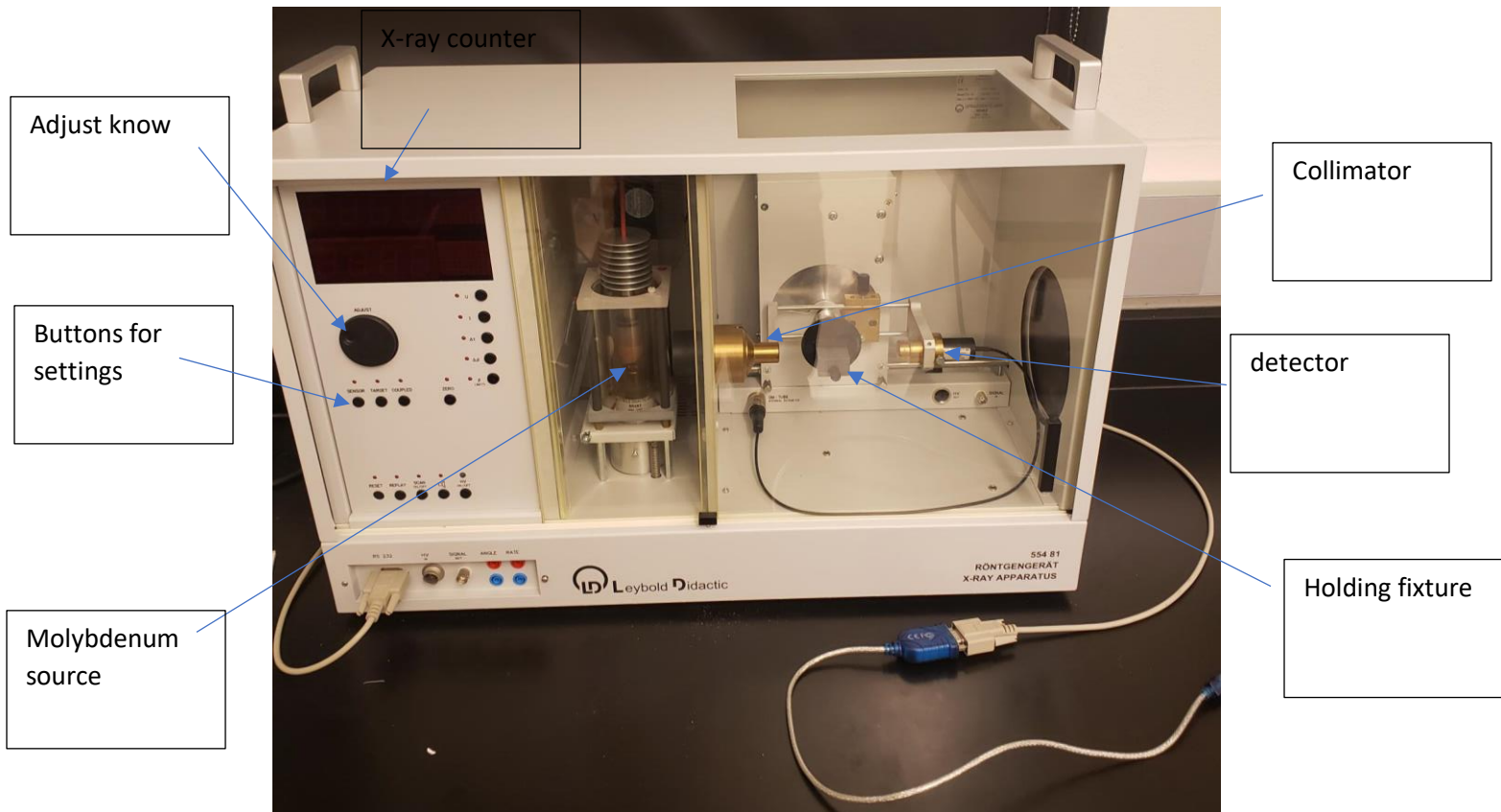


Figure 2: X-Ray Apparatus

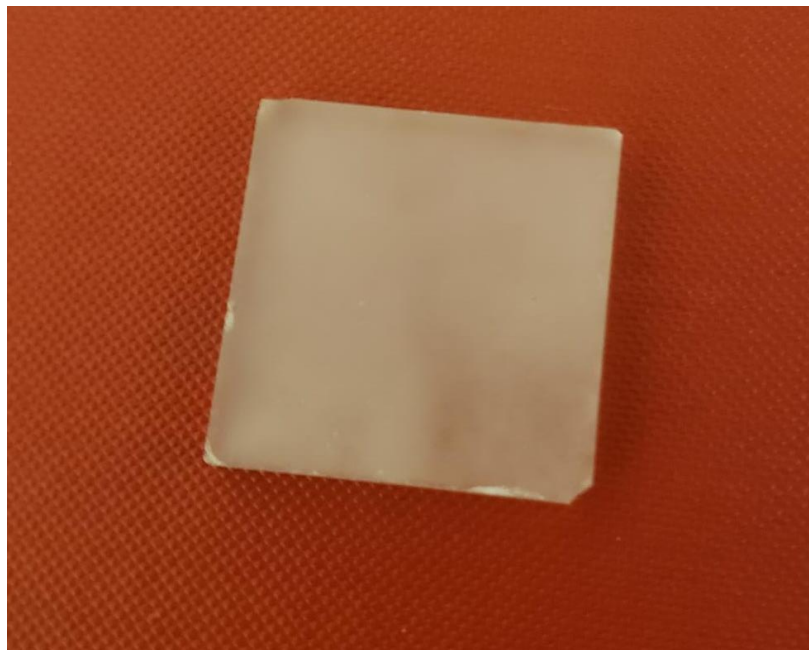


Figure 3: Crystal 1

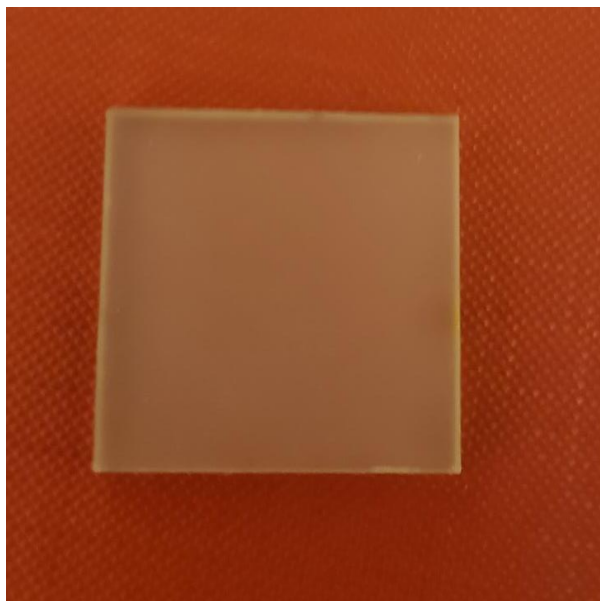


Figure 4: Crystal 2

First, the crystal was set into the holding fixture. The voltage and emission current were set to 35 kV and 1 mA. Using equation 1, the angles were calculated that would yield the $K\alpha$ and $K\beta$ lines. The target was set to this angle in coupled scanning mode with the adjust knob.

The “HV on/off” button was then pressed and then in sensor scanning mode, the angle of the detector was manually changed. There was an X-ray counter on the top of the machine that showed the number of X-rays per second. Once the maximum value was acquired, Target mode was initiated to determine the true maximum.

In coupled scanning mode, the target is moved back by the angle calculated previously. The position was then saved by setting the zero point by means of pressing TARGET, COUPLED and *B LIMITS* simultaneously. Then set the necessary parameters to conduct the scan to find the

different diffraction modes. B *LIMITS* was set according to the results acquired from equation 1 and is shown in table 1, Δt was set to 5 seconds and ΔB was set to .1 °.

The B limit parameters were found to be the following for both NaCl and LiF and are shown in table 1.

Mode	NaCl $\Delta\theta$ (°)	LiF $\Delta\theta$ (°)
1	6-8	8-12
2	11-15	17-21
3	18-23	27-33

Table 1: Calculated B Limits for NaCl and LiF crystals

Data:

The X-ray emission peaks are produced when energetic electrons hit a molybdenum target, these X-ray emissions can be used to determine a_0 and are listed below in table 2 [4].

Line	$\frac{\lambda}{pm}$
K_α	$71.08 \pm .005$
K_B	$63.09 \pm .005$

Table 2: X-ray emission peaks for molybdenum

Crystal 1 had the following data showing the $\sin(\theta)$ and λ for both emission peaks from the molybdenum that were organized from smallest to largest and is shown in table 3.

Mode	$\sin(\theta) \pm \sigma_{\sin(\theta)}$	$m * \lambda \pm \sigma_\lambda$ (pm)
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1	$.1080 \pm .0009$	$63.09 \pm .005$
1	$.1219 \pm .0009$	$71.08 \pm .005$
2	$.2215 \pm .0009$	$126.18 \pm .005$
2	$.2489 \pm .0009$	$142.60 \pm .005$
3	$.3338 \pm .0009$	$189.27 \pm .005$
3	$.3746 \pm .0009$	$213.24 \pm .005$

Table 3: sorted values for crystal 1

Crystal 2 had the following data showing the $\sin(\theta)$ and λ for both emission peaks from the molybdenum that were organized from smallest to largest and is shown in table 4.

Mode	$\sin(\theta) \pm \sigma_{\sin(\theta)}$	$m * \lambda \pm \sigma_{\lambda}$ (pm)
1	$.1547 \pm .0009$	$63.090 \pm .005$
1	$.1771 \pm .0009$	$71.080 \pm .005$
2	$.3140 \pm .0009$	$126.180 \pm .005$
2	$.3518 \pm .0009$	$142.600 \pm .005$
3	$.4710 \pm .0009$	$189.270 \pm .005$
3	$.5270 \pm .0009$	$213.240 \pm .005$

Table 4: sorted values for crystal 2

Analysis:

ODR was applied to the data which allows for a line of best fit that accounts not only for uncertainties in the x-data but in the y-data as well. $\sin(\theta)$ was used for the X values. The $m *$

λ values for both emission lines were used for the Y values. Of course, the appropriate uncertainties were used with each of these values.

This was then followed by analyzing how many standard deviations the true value of the lattice constant was from the calculated value using the formula shown in equation 6.

$$Z = \frac{x - \mu}{\sigma} \quad (6)$$

The Z-scores would be able to determine whether a value had a high propensity of being found.

These values were found in a z-score table to determine their probability.

The graph for crystal 1 is shown below with associated error bars in figure 5.

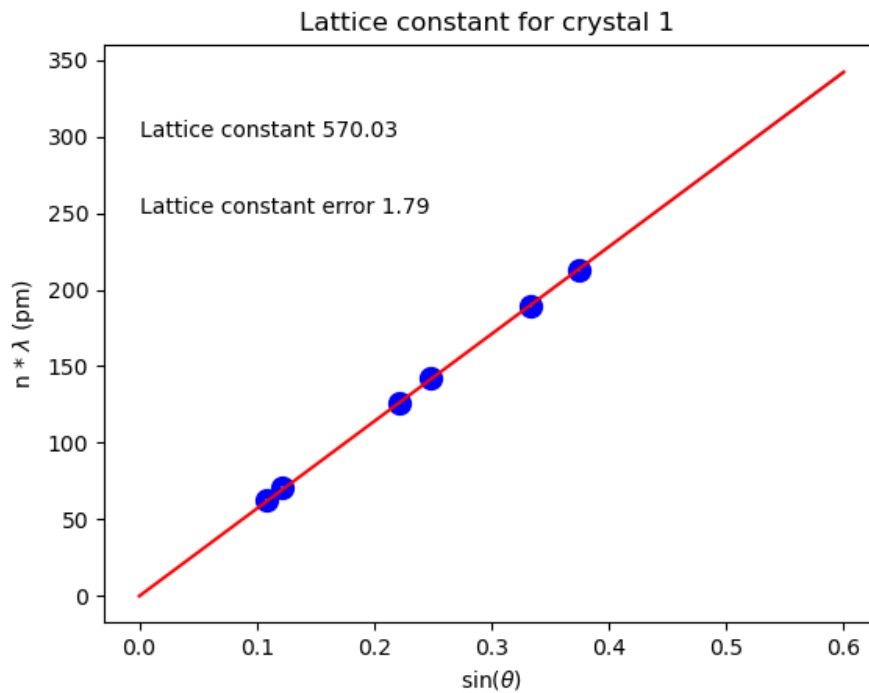


Figure 5: Lattice constant for crystal 1

The lattice constant for this crystal 1 was found to be $570.0 \pm 1.8 \text{ pm}$.

When calculating the Z-score for the true value of the lattice constant and odd result surfaced. The true value was 3.35 standard deviations away from the mean. This value would be very unlikely to occur. The probability of getting a value larger than that is

$$P(x > 3.33) = .000434 \rightarrow .0434 \%$$

Thus the true value would be extremely rare. This leads to the belief that systematic error is present.

The theta values were tweaked so that they were increased by .15 degrees each. The new graph is shown below in figure 6 that used the modified theta values.

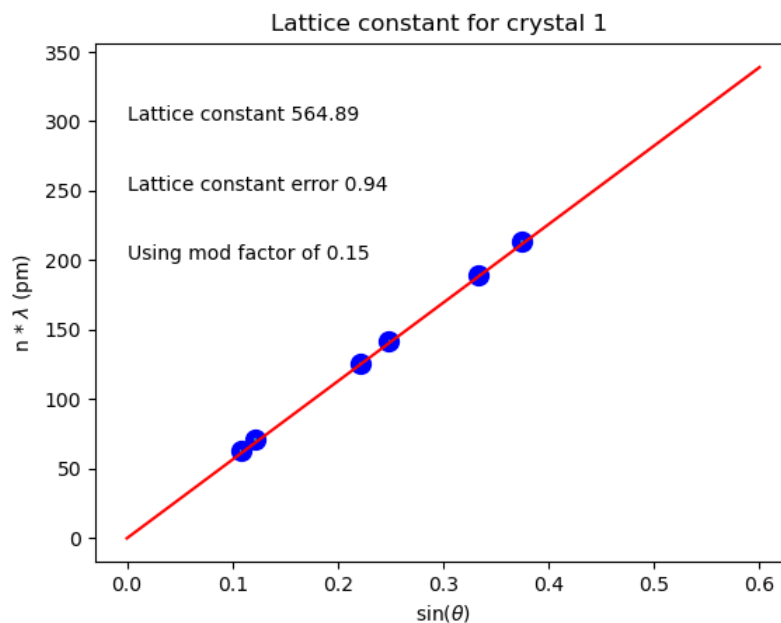


Figure 6: New lattice constant for Crystal 1 with modified theta

The lattice crystal constant for this scenario was found to be $564.9 \pm .9 \text{ pm}$.

The Z – score for the true value using this new lattice constant was found to be .925. The probability of getting a z-score larger than .925 is

$$P(x > Z) = .1774$$

So this value is more likely to appear and thus could be considered as an actual value.

Systematic error would seem plausible because the improvement happened after modifying all the theta values by the same amount. The tuning procedure for the maximum amount of x-rays needed to be done more carefully. It seems that crystal 1 is NaCl.

The ion sizes in the NaCl crystal are 98 pm for Na^+ and 181 pm for Cl^- . This shows that 285.9 pm is comprised of empty space. Nearly half of the lattice constant is taken up by the ions.

Crystal 2 was then analyzed and the graph is shown below in figure 7.

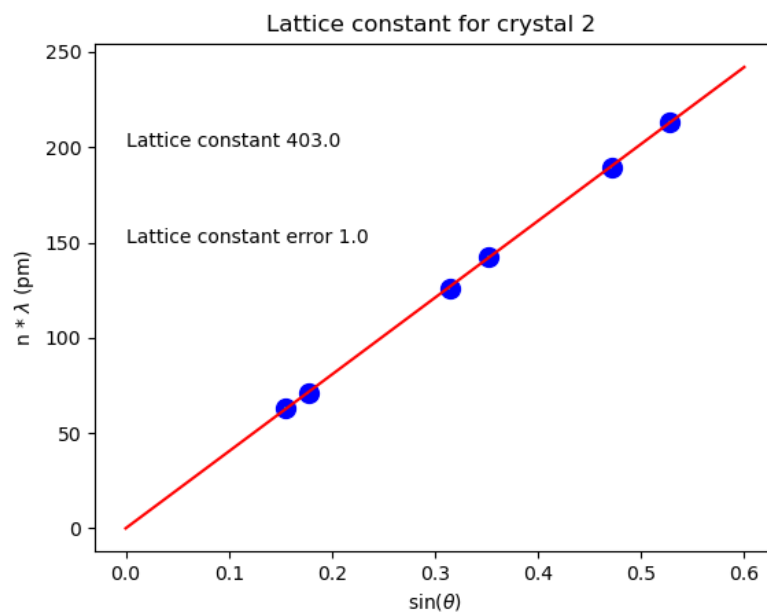


Figure 7: Lattice constant for crystal 2

The lattice constant for this crystal was found to be $403.0 \pm 1.0 \text{ pm}$. The lattice crystal constant for LiF is 402.6 pm. The true value is in the bounds of the estimated value.

The Z score was found to be .399. The probability of getting a value larger than .399 is

$$P(x > .399) = .344$$

This value would be very common in a gaussian distribution. Therefore, there is ample evidence to suggest that crystal 2 is LiF.

The ion sizes in the LiF crystal are 68 pm for Li^+ and 133 pm for F^- . The size of the ions takes up half of the space in the lattice constant and 202 pm is solely empty space.

Conclusion:

The estimated lattice constant for crystal 1 was found to be $570.0 \pm 1.8 \text{ pm}$. The lattice crystal constant for salt was found to be 564.02 pm [5]. The estimated value did not match up with this value. In fact, it was 3.33 standard deviations from the mean. The probability of getting a value larger than that was .0044 percent which means this was a fringe value.

The estimated lattice crystal constant for crystal 2 was found to be $403.0 \pm 1.0 \text{ pm}$. The lattice crystal constant for LiF was found to be 402.7 pm [5]. The true value was within the boundaries of the estimated value. The true value was .923 standard deviations from the mean. The probability of getting a value larger than that was 34.4%. The true value would be a common value that would be seen quite a bit.

Looking at the fact that the conclusions for crystal 1 were not as certain as crystal 2, led to the belief that there was systematic error present. If the theta arguments for the x values were

incremented by .15 degrees, a new lattice constant for crystal 1 was acquired. This value was $564 \pm .90 \text{ pm}$. The true lattice constant for salt was only .91 standard deviations away from the estimated value. So even a small deviation of .15 degrees gives a lattice constant that deviates by 4 pm. It was determined that crystal 1 was NaCl and crystal 2 was LiF. It was also interesting to see that the ions for both crystals take up half of the distance stated in the lattice constants and the other half was solely empty space.

Sources:

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2. Ling, S. J., Sanny, J., & Moebis, W. (2016, July 29). *4.6 X-Ray Diffraction - University Physics Volume 3 / OpenStax*. OpenStax. Retrieved April 11, 2022, from <https://openstax.org/books/university-physics-volume-3/pages/4-6-x-ray-diffraction>
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