
Crystallography

Bragg's Law

$$m \cdot \lambda = 2 \cdot d \cdot \sin(\theta)$$

$$k\alpha \lambda = 1.541874 \text{ \AA}$$

$$k\beta \lambda = 1.392250 \text{ \AA}$$

We can find d, d - spacing, by plugging in the observed peaks to θ .

Sample 4 from March 13, 2019

Measured on X' Pert Empréan

Rhodonite?

Here's the peak list, the underlined which I have manually taken out.

thetarhodonite1 (sample4-test) =

{20.8576,26.5242,26.6174,26.6814,36.5121,36.6108,38.3982,40.2851,44.6441,45.8763,45.9899,50.2079,50.331,54.8904,59.9781,60.1417,64.1266,64.307,65.0307,67.688,67.7750,67.898,67.967,68.3230,68.5224,75.8143,77.9293,79.9564,80.1681,81.4972,81.7570,83.8923}

thetarhodonite2 (sample4-test1)=

{20.8941,20.9501,26.6666,26.7386,36.4690,36.5483,38.4469,40.3007,42.4757,42.5929,44.6491,45.9710,50.1355,54.8927,55.0495,59.9773,60.1368,65.0635,67.7798,67.995,68.305,73.3738,78.2161,79.9069,80.152,83.9046,87.4697,87.769}

```
In[ ]:= m = 1;
```

```
lambda = 1.541874 * 10-10;
```

```
thetarhodonite = {20.8576, 26.5242, 26.6174, 26.6814, 36.5121, 36.6108, 44.6441, 45.8763, 45.9899, 50.2079, 50.331, 54.8904, 59.9781, 60.1417, 64.1266, 64.307, 65.0307, 67.688, 67.7750, 67.898, 67.967, 68.3230, 68.5224, 79.9564, 80.1681, 81.4972, 81.7570, 83.8923};
```

```
thetarhodonite2 = {20.8941, 20.9501, 26.6666, 26.7386, 36.4690, 36.5483, 38.4469, 40.3007, 42.4757, 42.5929, 44.6491, 45.9710, 50.1355, 54.8927, 55.0495, 59.9773, 60.1368, 65.0635, 67.7798, 67.995, 68.305, 73.3738, 78.2161, 79.9069, 80.152, 83.9046, 87.4697, 87.769};
```

For $k\alpha$ reference :

```
In[ ]:= d1rhodonite = m * 1.541874 / (2 * Sin[thetarhodonite * 0.5]);
```

```
d1rhodonite2 = m * 1.541874 / (2 * Sin[thetarhodonite2 * 0.5]);
```

```
In[ ]:= Dataset1 = Transpose[{Abs[d1rhodonite], thetarhodonite}];
```

```
Dataset2 = Transpose[{Abs[d1rhodonite2], thetarhodonite2}];
```

```
In[57]:= ListPlot[{Dataset1, Dataset2}, Background -> LightGray,  
  AxesStyle -> Black, ImageSize -> Large, PlotRange -> {{0, 40}, {0, 100}},  
  AxesLabel -> {HoldForm[d - spacing Angstrom], RowBoxes[RowBox[{"2", "\\theta"}]}},  
  PlotLabel -> HoldForm[Finding Periodicity in d - spacing], LabelStyle -> {GrayLevel[0]}]
```

