AAA

In[279]:=
```
ClearAll["Global`*"]
(*200*)
h = 2;
k = 0;
l = 0;
β = 90;
a = 7.784;
b = 8.201;
c = 10.380;
(*monoclinic*)
d = a b c / Sqrt[a^2 c^2 k^2 - 2 a b^2 c h l Cot[° β] Csc[° β] + b^2 c^2 h^2 Csc[° β]^2 + a^2 b^2 l^2 Csc[° β]^2];
(*---*)
λ = 1.541;
λ / (2 d);
θ = ArcSin[λ / (2 d)] * 180 / π;
2 θ;

Print["d(200)= ", d]
Print["2θ = ", 2 θ]
```

```
d(200)= 3.892
2θ = 22.8366
```

BBB

In[294]:=
```
ClearAll["Global`*"]
(*200*)
h = 2;
k = 0;
l = 0;
β = 90;
a = 7.784;
b = 8.201;
c = 10.380;
(*monoclinic*)
d = 1 / Sqrt[1/Sin[β Degree]^2 (h^2/a^2 + k^2*Sin[β Degree]^2/b^2 + l^2/c^2 - 2 h l Cos[β Degree]/(a c))];
λ = 1.541;
λ / (2 d);
θ = ArcSin[λ / (2 d)] * 180 / π;
2 θ;

Print["d(200)= ", d]
Print["2θ = ", 2 θ]
```

```
d(200)= 3.892
2θ = 22.8366
```

Storage

$$n\lambda = 2d\sin\theta$$

In[262]:=
```
ClearAll["Global`*"];
Solve[1/d^2 == 1/Sin[β Degree]^2 (h^2/a^2 + k^2 * Sin[β Degree]^2/b^2 + l^2/c^2 - 2 h l Cos[β Degree]/(a c)), d]
```

Out[263]=
$$\left\{\left\{d \to -\frac{a\,b\,c}{\sqrt{a^2\,c^2\,k^2 - 2\,a\,b^2\,c\,h\,l\,\text{Cot}[^\circ\beta]\,\text{Csc}[^\circ\beta] + b^2\,c^2\,h^2\,\text{Csc}[^\circ\beta]^2 + a^2\,b^2\,l^2\,\text{Csc}[^\circ\beta]^2}}\right\},\ \left\{d \to \frac{a\,b\,c}{\sqrt{a^2\,c^2\,k^2 - 2\,a\,b^2\,c\,h\,l\,\text{Cot}[^\circ\beta]\,\text{Csc}[^\circ\beta] + b^2\,c^2\,h^2\,\text{Csc}[^\circ\beta]^2 + a^2\,b^2\,l^2\,\text{Csc}[^\circ\beta]^2}}\right\}\right\}$$

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