

$$d = \frac{a b c}{\sqrt{a^2 c^2 k^2 - 2 a b^2 c h l \cot[\circ \beta] \csc[\circ \beta] + b^2 c^2 h^2 \csc[\circ \beta]^2 + a^2 b^2 l^2 \csc[\circ \beta]^2}}$$

In cellulose I β crystal, (b->c), (c->b), (k->l), (l->k), (β -> γ), (γ -> β)

Monoclinic

```
In[73]:= ClearAll["Global`*"]
λ = 1.5418; (*Kα1&Kα2*)
calc[h_, k_, l_, α_, β_, γ_, a_, b_, c_] := Module[{ },
    d = 
$$\frac{a b c}{\sqrt{a^2 b^2 l^2 - 2 a c^2 b h k \cot[\circ \gamma] \csc[\circ \gamma] + c^2 b^2 h^2 \csc[\circ \gamma]^2 + a^2 c^2 k^2 \csc[\circ \gamma]^2}}$$
;
    θ = ArcSin[λ / (2 d)] * 180 / π;
];

In[76]:= calc[1, 1, 0, 90, 90, 96.5, 7.784, 8.201, 10.380];
Print["2θ(110)= ", Round[2 θ, 0.1], ", d(110)= ", d]

calc[1, -1, 0, 90, 90, 96.5, 7.784, 8.201, 10.380];
Print["2θ(1-10)= ", Round[2 θ, 0.1], ", d(1-10)= ", d]

calc[2, 0, 0, 90, 90, 96.5, 7.784, 8.201, 10.380];
Print["2θ(200)= ", Round[2 θ, 0.1], ", d(200)= ", d]

calc[0, 0, 4, 90, 90, 96.5, 7.784, 8.201, 10.380];
Print["2θ(004)= ", Round[2 θ, 0.1], ", d(004)= ", d]

2θ(110)= 16.7, d(110)= 5.317
2θ(1-10)= 14.9, d(1-10)= 5.95626
2θ(200)= 23., d(200)= 3.86698
2θ(004)= 34.6, d(004)= 2.595
```

```

In[84]:= (*lattice 'a' dependence*)
temp = 7.784;
t110 = {}; (*110*)
t110b = {}; (*1-10*)
t200 = {}; (*200*)
n = Table[temp + i, {i, -1, 1, 0.1}];
For[j = 1, j ≤ Length[n], j++,
  {h, k, l} = {1, 1, 0};
  calc[h, k, l, 90, 90, 96.5, n[[j]], 8.201, 10.380];
  AppendTo[t110, 2 θ];
  {h, k, l} = {1, -1, 0};
  calc[h, k, l, 90, 90, 96.5, n[[j]], 8.201, 10.380];
  AppendTo[t110b, 2 θ];
  {h, k, l} = {2, 0, 0};
  calc[h, k, l, 90, 90, 96.5, n[[j]], 8.201, 10.380];
  AppendTo[t200, 2 θ];
]
tta2 = Table[{n[[j]], t110[[j]], t110b[[j]], t200[[j]]}, {j, 1, Length[n]}];

In[91]:= (*lattice 'b' dependence*)
temp = 8.201;
t110 = {}; (*110*)
t110b = {}; (*1-10*)
t200 = {}; (*200*)
n = Table[temp + i, {i, -1, 1, 0.1}];
For[j = 1, j ≤ Length[n], j++,
  {h, k, l} = {1, 1, 0};
  calc[h, k, l, 90, 90, 96.5, 7.784, n[[j]], 10.380];
  AppendTo[t110, 2 θ];
  {h, k, l} = {1, -1, 0};
  calc[h, k, l, 90, 90, 96.5, 7.784, n[[j]], 10.380];
  AppendTo[t110b, 2 θ];
  {h, k, l} = {2, 0, 0};
  calc[h, k, l, 90, 90, 96.5, 7.784, n[[j]], 10.380];
  AppendTo[t200, 2 θ];
]
ttb2 = Table[{n[[j]], t110[[j]], t110b[[j]], t200[[j]]}, {j, 1, Length[n]}];

```

```

In[98]:= (*lattice 'γ' dependence*)
temp = 96.5;
t110 = {}; (*110*)
t110b = {}; (*1-10*)
t200 = {}; (*200*)
n = Table[temp + i, {i, -10, 10, 1}];
For[j = 1, j ≤ Length[n], j++,
  {h, k, l} = {1, 1, 0};
  calc[h, k, l, 90, 90, n[[j]], 7.784, 8.201, 10.380];
  AppendTo[t110, 2 θ];
  {h, k, l} = {1, -1, 0};
  calc[h, k, l, 90, 90, n[[j]], 7.784, 8.201, 10.380];
  AppendTo[t110b, 2 θ];
  {h, k, l} = {2, 0, 0};
  calc[h, k, l, 90, 90, n[[j]], 7.784, 8.201, 10.380];
  AppendTo[t200, 2 θ];
]
ttg2 = Table[{n[[j]], t110[[j]], t110b[[j]], t200[[j]]}, {j, 1, Length[n]}];

```

plotting

plot

Storage