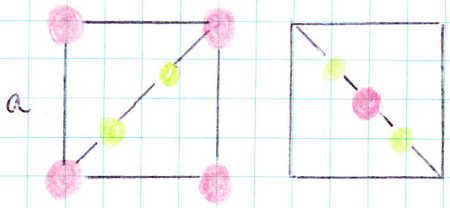
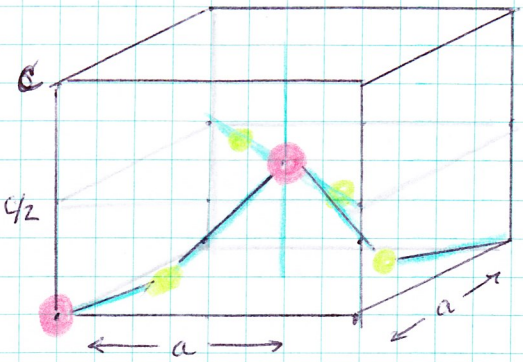
Calculate Peak Intensities of X-Ray Powder Diffraction: TiO_2 Rutile

$P4_2/mnm$ (#136) Rutile C4



Ae Bfd$_1$

Aen Bfd$_2$



$a = 4.5845\ \text{Å}$
$c = 2.9533\ \text{Å}$

$\lambda = 1.54056\ \text{Å}$

I	Z	Atom	fractional coord *	Form Factor
1	22	Ti	0, 0, 0	$18\sin\theta/\lambda$
2	8	O	+u, +u, 0	$10\sin\theta/\lambda$
3	8	O	-u, -u, 0	$10\sin\theta/\lambda$
~~4~~	~~8~~	~~O~~	~~2 2 2~~	~~$10\sin\theta/\lambda$~~
5	22	Ti	1/2, 1/2, 1/2	$18\sin\theta/\lambda$
6	8	O	1/2+u, 1/2-u, 1/2	$10\sin\theta/\lambda$
7	8	O	-1/2-u, -1/2+u, 1/2	$10\sin\theta/\lambda$
~~8~~	~~8~~	~~O~~	~~2 2 2~~	~~$10\sin\theta/\lambda$~~

Plane	Multiplicity	d	θ
(100)	4	4.5845Å	19.35°
(110)	4		
(101)	8		
(200)	4		
(111)	8		
(210)	8		

$\frac{1}{d^2} = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}$ $\quad \theta = \sin^{-1}\left(\frac{\lambda}{2d}\right)$

$\sin\theta/\lambda$

(100) 0.11

* Ma, App Surfaces Science 253, 2007

nmp =

if (n==m or n==0 or m==0) M=4

~~h k~~ h==k/h=0/k=0) M=4

~~if~~ if (h≠k/h>0/k>0) M=8

if (l≠0) M=2*m

Software & results attached...

what is charge?

Lambda=1.540560 Angstroms a=4.593600 c=2.958700 Angstroms u=0.300000

(h,k,l)	M	d(Ang)	T(Deg)	fTi	fO	nfTi	nfO	S(hkl)	LP(T)	Intensity
(1 0 0)	4	4.59360	19.31	1.96	1.09	0.00	-0.00	-0.00	8.53	0.0
(1 1 0)	4	3.24817	27.44	2.77	1.54	2.00	0.38	6.13	4.09	614.7
(1 0 1)	8	2.48740	36.08	3.62	2.01	2.00	-1.24	4.75	2.27	409.4
(2 0 1)	8	1.81429	50.25	4.96	2.76	0.00	0.00	0.00	1.08	0.0
(1 1 1)	8	2.18731	41.24	4.11	2.29	0.00	-3.62	-8.27	1.69	922.5
(2 1 0)	8	2.05432	44.04	4.38	2.43	0.00	2.24	5.44	1.45	344.7

Lambda=1.540560 Angstroms a=4.593600 c=2.958700 Angstroms u=0.333333

(h,k,l)	M	d(Ang)	T(Deg)	fTi	fO	nfTi	nfO	S(hkl)	LP(T)	Intensity
(1 0 0)	4	4.59360	19.31	1.96	1.09	0.00	-0.00	-0.00	8.53	0.0
(1 1 0)	4	3.24817	27.44	2.77	1.54	2.00	1.00	7.08	4.09	820.3
(1 0 1)	8	2.48740	36.08	3.62	2.01	2.00	-2.00	3.22	2.27	187.5
(2 0 1)	8	1.81429	50.25	4.96	2.76	0.00	0.00	0.00	1.08	0.0
(1 1 1)	8	2.18731	41.24	4.11	2.29	0.00	-3.00	-6.86	1.69	634.3
(2 1 0)	8	2.05432	44.04	4.38	2.43	0.00	3.00	7.30	1.45	620.4

Lambda=1.540560 Angstroms a=4.584500 c=2.953300 Angstroms u=0.300000

(h,k,l)	M	d(Ang)	T(Deg)	fTi	fO	nfTi	nfO	S(hkl)	LP(T)	Intensity
(1 0 0)	4	4.58450	19.35	1.96	1.09	0.00	-0.00	-0.00	8.49	0.0
(1 1 0)	4	3.24173	27.49	2.78	1.54	2.00	0.38	6.14	4.07	614.5
(1 0 1)	8	2.48274	36.15	3.63	2.01	2.00	-1.24	4.76	2.26	409.2
(2 0 1)	8	1.81081	50.35	4.97	2.76	0.00	0.00	0.00	1.07	0.0
(1 1 1)	8	2.18316	41.32	4.12	2.29	0.00	-3.62	-8.29	1.68	921.9
(2 1 0)	8	2.05025	44.14	4.39	2.44	0.00	2.24	5.45	1.45	344.4

Lambda=1.540560 Angstroms a=4.584500 c=2.953300 Angstroms u=0.333333

(h,k,l)	M	d(Ang)	T(Deg)	fTi	fO	nfTi	nfO	S(hkl)	LP(T)	Intensity
(1 0 0)	4	4.58450	19.35	1.96	1.09	0.00	-0.00	-0.00	8.49	0.0
(1 1 0)	4	3.24173	27.49	2.78	1.54	2.00	1.00	7.09	4.07	820.1
(1 0 1)	8	2.48274	36.15	3.63	2.01	2.00	-2.00	3.22	2.26	187.4
(2 0 1)	8	1.81081	50.35	4.97	2.76	0.00	0.00	0.00	1.07	0.0
(1 1 1)	8	2.18316	41.32	4.12	2.29	0.00	-3.00	-6.87	1.68	633.9
(2 1 0)	8	2.05025	44.14	4.39	2.44	0.00	3.00	7.32	1.45	620.0

Should also do 200

```
function TiO2Rutile_PeakIntensity

Lambda = 1.54056;
u = [0.3; 1.0/3.0];
LC = [[4.5936,2.9587];[4.5845,2.9533]];

for i = 1:2
    for j = 1:2
        fprintf(1,'\n');
        fprintf(1,'Lambda=%f Angstroms a=%f c=%f Angstroms u=%f
\n',Lambda,LC(i,1),LC(i,2),u(j));
        fprintf(1,'(h,k,l) M d(Ang)  T(Deg)  fTi    fO  nfTi   nfO  S
(hkl) LP(T) Intensity\n');
        TiO2Rutile_PeakIntensity2(1,0,0,u(j),Lambda,LC(i,1),LC(i,2));
        TiO2Rutile_PeakIntensity2(1,1,0,u(j),Lambda,LC(i,1),LC(i,2));
        TiO2Rutile_PeakIntensity2(1,0,1,u(j),Lambda,LC(i,1),LC(i,2));
        TiO2Rutile_PeakIntensity2(2,0,1,u(j),Lambda,LC(i,1),LC(i,2));
        TiO2Rutile_PeakIntensity2(1,1,1,u(j),Lambda,LC(i,1),LC(i,2));
        TiO2Rutile_PeakIntensity2(2,1,0,u(j),Lambda,LC(i,1),LC(i,2));
    end
end

function TiO2Rutile_PeakIntensity2(h,k,l,u,Lambda,a,c)
if (h==k || h==0 | k==0)
    Multiplicity = 4;
else
    Multiplicity = 8;
end
if (l ~= 0)
    Multiplicity = Multiplicity*2;
end
d = 1.0/sqrt( (h^2)/(a^2) + (k^2)/(a^2) + (l^2)/(c^2) );
Theta = asin(Lambda/(2*d));
fTi = 18*sin(Theta)/Lambda;fO = 10*sin(Theta)/Lambda;
LP = (1.0  + (cos(2*Theta))^2)/(8*cos(Theta)*(sin(Theta))^2);
nfTi = 1 + real(exp(-i*pi*(h+k+l)));
nfO = 0;
nfO = nfO + real(exp(-i*2*pi*(  h*u + k*u )));
nfO = nfO + real(exp(-i*2*pi*( -h*u - k*u )));
nfO = nfO + real(exp(-i*2*pi*( h*(0.5+u) + k*(0.5-u) + l/2)));
nfO = nfO + real(exp(-i*2*pi*(-h*(0.5+u) - k*(0.5-u) - l/2)));
S = nfTi*fTi + nfO*fO;
fprintf(1,'(%d %d %d) %d %.5f', h, k, l, Multiplicity, d);
fprintf(1,' %5.2f', 360.0*Theta/pi);
fprintf(1,' %5.2f %5.2f %5.2f %5.2f',fTi,fO,nfTi,nfO);
fprintf(1,' %7.2f',S);
fprintf(1,' %5.2f',LP);
fprintf(1,' %9.1f\n',S*S*Multiplicity*LP);
```