5. A rock specimen was analyzed for α-quartz. To correct for the unknown absorption of the specimen, an internal standard was used. The internal standard was chosen as KCl because of its excellent crystallinity, relatively simple diffraction pattern, and a strong reflection which is relatively close to the strong α-quartz reflection.

   Three samples were measured: pure KCl, pure quartz and a mixture of the rock specimen with KCl. The mixture was prepared by intimately mixing 200 mg of finely ground KCl with 1000 mg of the rock, also finely ground.

   The intensities of the 3.15 Å KCl reflection and the 3.34 Å quartz reflection were measured using CuKα radiation. The data are given below.

Phase	d (Å)	μ^{o}	Pure compound	Mixture
quartz	3.34	35.0	48360 cps	2648 cps
KCl	3.15	124.0	19072	6160

   For all intensities, the background was 240 cps. The dead time for the counting system was 1.0 μsec.

   The correction for the dead time, τ, makes use of the following equation:

$$\text{true counts/sec} = \frac{\text{observed counts/sec}}{1 - \tau \text{ observed counts/sec}}$$

   Calculate the concentration of quartz in the rock specimen.

   Note that:

$$\frac{I_\alpha}{I_\alpha^o} = \frac{\mu_\alpha^o}{\mu} X_\alpha$$

where:

I_α^o and I_α are the intensities for the pure compound and the mixture for phase α, respectively.

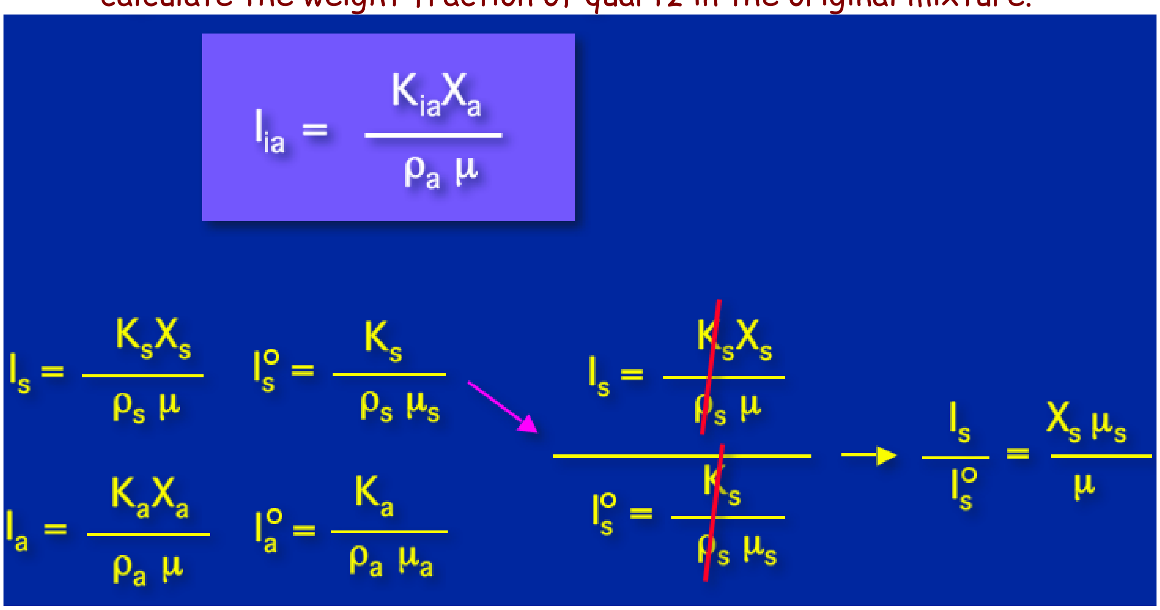
μ_α^o and μ are the mass attenuation coefficients for the pure compound and the mixture, respectively.

X_α is the weight fraction of phase α in the mixture.

An equation of this type can be written for both quartz and KCl. Combining these two equations to eliminate μ, the unknown mass attenuation coefficient for the mixture:

$$X_q = X_{KCl} \frac{I_{KCl}^o}{I_q^o} \frac{\mu_{KCl}^o}{\mu_q^o} \frac{I_q}{I_{KCl}}$$

First calculate the weight fraction X_q of quartz in the diluted specimen. Then, from the value of X_q and the dilution factor, calculate the weight fraction of quartz in the original mixture.



$$I_s = \frac{K_s X_s}{\rho_s \mu} \qquad I_s^o = \frac{K_s}{\rho_s \mu_s}$$

$$I_a = \frac{K_a X_a}{\rho_a \mu} \qquad I_a^o = \frac{K_a}{\rho_a \mu_a}$$

$$\frac{I_a = \dfrac{\cancel{K_a} X_a}{\cancel{\rho_a} \mu}}{I_a^o = \dfrac{\cancel{K_a}}{\cancel{\rho_a} \mu_a}} \rightarrow \frac{I_a}{I_a^o} = \frac{X_a \mu_a}{\mu}$$

$$\frac{\dfrac{I_s}{I_s^o} = \dfrac{X_s \mu_s}{\cancel{\mu}}}{\dfrac{I_a}{I_a^o} = \dfrac{X_a \mu_a}{\cancel{\mu}}} \rightarrow \frac{I_s \; I_a^o}{I_s^o \; I_a} = \frac{X_s \mu_s}{X_a \mu_a}$$

Sample dead time correction:

$$R_{true} = \frac{48360}{1 - 48360 \cdot 10^{-6}} = 50818$$

Phase	μ	I_{pure}	I_{pure}^{corr}	I_{mix}	I_{mix}^{corr}
Quartz	35.0	48360	50578	2648	2415
KCl	124.0	19072	19203	6160	5958

$$\frac{I_s \; I_a^{o}}{I_s^{o} \; I_a} = \frac{X_s \, \mu_s}{X_a \, \mu_a}$$

$$X_q = X_{KCl} \frac{I_{KCl}^{o}}{I_q^{o}} \frac{I_q}{I_{KCl}} \frac{\mu_{KCl}}{\mu_q}$$

$$X_{KCl} = \frac{200 \text{ mg}}{(200+1000) \text{ mg}} = 0.1667$$

$$X_q = 0.1667 \frac{19203}{50578} \frac{2415}{5958} \frac{124.0}{35.0}$$

$$X_q = 0.091$$

$X_q = 0.091$

This is wt. fraction quartz in KCl + rock mixture

Wt. fraction quartz in rock:

$$X_q^{rock} = 0.091 \frac{1200}{1000} = 0.109$$

6. MoB is $I4_1/amd$ with a = 3.110, c = 16.95 Å, and Mo and B atoms in 8e, z = 0.196 and 0.352, respectively.

Calculate F_{001} and F_{004}.

F_{001} = __0____I centered – (001) is extinct

$$F_{hkl} = \sum_{j=1}^{N} f_j \exp(2\pi i(hx_j + ky_j + lz_j)).$$

$$F_{004} = 2 \sum_{1}^{N/2} f_j \exp(2\pi i(4z_j))$$ since I centered

What must be calculated?

f_{Mo} and f_B

d_{004} = ____ c/4 = 16.95/4 = 4.2375 _____

$(\sin\theta)/\lambda$ = _____1/(2d) = 0.1180_____

	0.1	0.2
Mo	38.2	32.6
B	3.5	2.4

f_{Mo} = __37.2______

f_B = ____3.4_____

8e: $(00z)$ $(0,\frac{1}{2},\frac{1}{4}+z)$ $(\frac{1}{2},0,\frac{3}{4}-z)$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2}-z)$

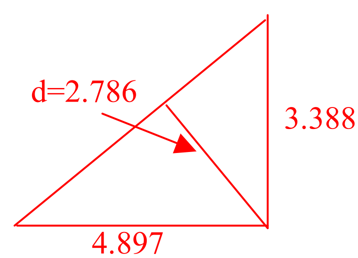
$$F_{004} = 2\,(37.2\,(\exp(2\pi i \times 4 \times 0.196) + \exp(2\pi i \times 4 \times 0.196) + \exp(-2\pi i \times 4 \times 0.196) + \exp(-2\pi i \times 4 \times 0.196)) + 3.4\,(\exp(2\pi i \times 4 \times 0.352) + \exp(2\pi i \times 4 \times 0.352) + \exp(-2\pi i \times 4 \times 0.352) + \exp(-2\pi i \times 4 \times 0.352)))$$

$$= 8\,(37.2 \cos(8\pi \times 0.196) + 3.4 \cos(8\pi \times 0.352))$$

$$= 8\,((37.2 \times 0.333) - (3.4 \times 0.598)) = 82.78$$

7. β-Np is $P42_12$ with a = 4.897, c = 3.388 Å, and Np in 2a ((000) and $(\frac{1}{2}\frac{1}{2}0)$) and 2c ($(0\frac{1}{2}z)$ and $(\frac{1}{2}0\bar{z})$), z = 0.375. Find I_{101} for CuKα radiation. Ignore scale factor, absorption and temperature factor.

f calculation:



$(\sin\theta)/\lambda = 1/(2 \times 2.786) = 0.1795$

$f = 87 - 9 \times 0.795 = 79.84$

$(\sin\theta)/\lambda$	0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.7
f	93	87	78	69	60	53	48	44

F calculation:

$F_{101} = 79.84\ (1 + e^{\pi i} + e^{0.75\pi i} + e^{\pi i\,(1 - 0.75)})$

$F_{101} = 79.84\ (e^{0.75\pi i} + e^{\pi i\,(0.25)})$

$F_{101} = 79.84\ (\cos 0.75\pi + i \sin 0.75\pi + \cos 0.25\pi + i \sin 0.25\pi)$

$F_{101} = 79.84 \times 1.414\ i = 112.89\ i$

What is p?

8

(101) (011) (-101) (10-1) (-10-1) (0-11) (01-1) (0-1-1)

LP calculation:

$\theta = 16.07°$

$LP = (1 + \cos^2 2\theta)/(\sin^2\theta \cos\theta) = 1.717/(0.0766 \times 0.961) = 23.32$

I calculation:

$I = 8 \times 23.32 \times 112.89^2 = 2.38 \times 10^6$