[——]

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($d_{h^*k^*l^*}$) ($\underline{a}$ $\underline{b}$ $\underline{c}$) (*h*k*l**)

$\frac{\underline{a}}{h^*}\times\frac{\underline{b}}{k^*}\bullet\frac{\underline{c}}{l^*}=|\underline{s}|d_{h^*k^*l^*}$ $d_{h^*k^*l^*}$ $d_{h^*k^*l^*}$ (

) $d_{h^*k^*l^*}$

($d_{h^*k^*l^*}$) $-d_{h^*k^*l^*}$

(a b c α β γ) ($h^*k^*l^*$)

$d_{h^*k^*l^*}$

( ) C_i 6 a b c α β γ $d_{h^*k^*l^*}$

(1) [1]

$$d_{h^*k^*l^*}=V/[h^{*2}b^2c^2\sin^2\alpha+k^{*2}a^2c^2\sin^2\beta+l^{*2}a^2b^2\sin^2\gamma$$
$$+2h^*k^*abc^2(\cos\alpha\cos\beta-\cos\gamma)$$
$$+2k^*l^*a^2bc(\cos\beta\cos\gamma-\cos\alpha)$$
$$+2h^*l^*ab^2c(\cos\alpha\cos\gamma-\cos\beta)]^{1/2}\cdots\cdots(1)$$

(1) $V=abc(1-\cos^2\alpha-\cos^2\beta-\cos^2\gamma+2\cos\alpha\cos\beta\cos\gamma)^{1/2}$

( ) D_{6h} 2 a c $a=b\neq c$ $\alpha=\beta=90^o$ $\gamma=$ 120^o (1) $d_{h^*k^*l^*}$

$$d_{h^*k^*l^*}=aac(1-\cos^2 90^o-\cos^2 90^o-\cos^2 120^o+2\cos90^o\cos90^o\cos120^o)^{1/2}$$
$$/[h^{*2}a^2c^2\sin^2 90^o+k^{*2}a^2c^2\sin^2 90^o+l^{*2}a^2a^2\sin^2 120^o$$
$$+2h^*k^*aac^2(\cos90^o\cos90^o-\cos120^o)$$
$$+2k^*l^*a^2ac(\cos90^o\cos120^o-\cos90^o)$$
$$+2h^*l^*aa^2c(\cos90^o\cos120^o-\cos90^o)]^{1/2}$$
$$=a/[\frac{4}{3}(h^{*2}+h^*k^*+k^{*2})+\frac{l^{*2}}{(c/a)^2}]^{1/2}\cdots\cdots(2)$$

(1) $d_{h^*k^*l^*}$

1 $\frac{\underline{a}}{h^*} \times \frac{\underline{b}}{k^*} \bullet \frac{\underline{c}}{l^*} = |\underline{s}| d_{h^*k^*l^*}$

$(h^*k^*l^*)$

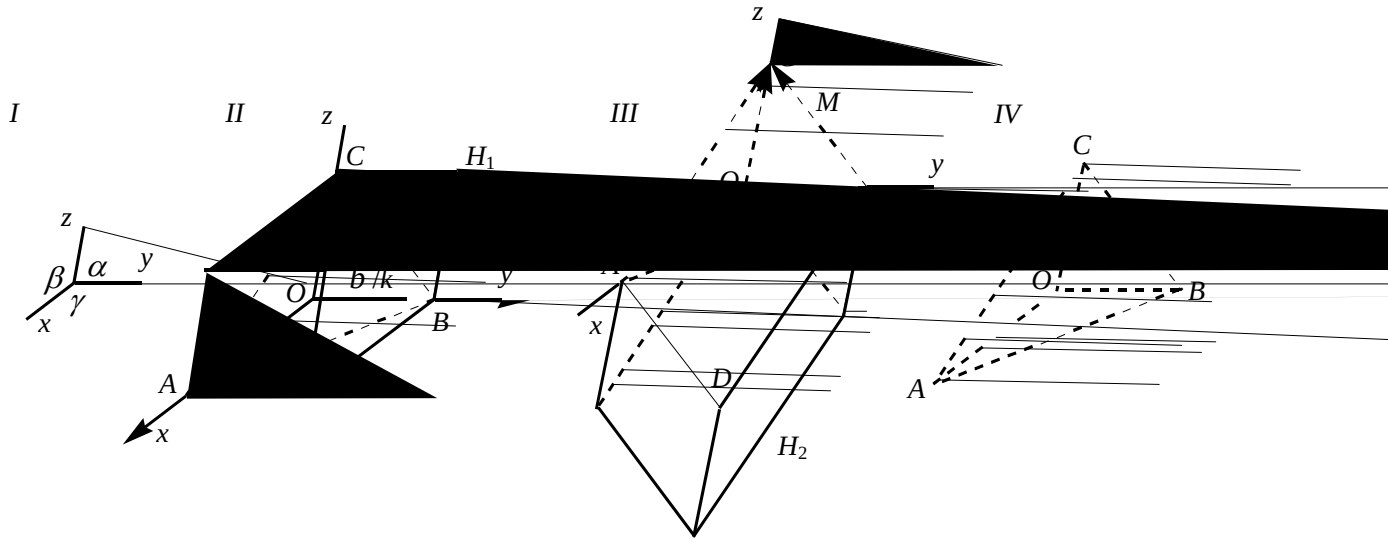
$$h^*x + k^*y + l^*z = N \cdots\cdots (3)$$

(3) $N = 0, \pm 1, \pm 2, \cdots\cdots$ $N = 1$ (3) $M\,(h^*x + k^*y + l^*z = 1)$

O M x y z $1/h^*$ $1/k^*$ $1/l^*$

$\underline{a}$ $\underline{b}$ $\underline{c}$ $\underline{a}/h^*$ $\underline{b}/k^*$ $\underline{c}/l^*$

1 ① $\underline{a}/h^*$ $\underline{b}/k^*$ $\underline{c}/l^*$ H_1 (1-*II*)



1 ***I*** $\boldsymbol{\alpha}$ $\boldsymbol{\beta}$ $\boldsymbol{\gamma}$ ***II*** $\underline{\boldsymbol{a}}/\boldsymbol{h}^*$ $\underline{\boldsymbol{b}}/\boldsymbol{k}^*$ $\underline{\boldsymbol{c}}/\boldsymbol{l}^*$ $\boldsymbol{H_1}$

II $\underline{\boldsymbol{AC}}$ $\underline{\boldsymbol{BC}}$ $\underline{\boldsymbol{OC}}$ $\boldsymbol{H_2}$ ***IV*** ***OABC***

H_1 V_1 $\underline{a}/h^*$ $\underline{b}/k^*$ $\underline{c}/l^*$

$$V_1 = \frac{\underline{a}}{h^*} \times \frac{\underline{b}}{k^*} \bullet \frac{\underline{c}}{l^*} \cdots\cdots (4)$$

② $\underline{AC}$ $(\underline{c}/l^* - \underline{a}/h^*)$ $\underline{BC}$ $(\underline{c}/l^* - \underline{b}/k^*)$ $\underline{OC}$ $(\underline{c}/l^*)$ H_2 (1-*III*)

H_2 V_2 $\underline{AC}$ $\underline{BC}$ $\underline{OC}$

$$\begin{aligned} V_2 &= \underline{AC} \times \underline{BC} \bullet \underline{OC} \\ &= (\frac{\underline{c}}{l^*} - \frac{\underline{a}}{h^*}) \times (\frac{\underline{c}}{l^*} - \frac{\underline{b}}{k^*}) \bullet \frac{\underline{c}}{l^*} \\ &= (\frac{\underline{a} \times \underline{b}}{h^*k^*} + \frac{\underline{b} \times \underline{c}}{k^*l^*} + \frac{\underline{c} \times \underline{a}}{l^*h^*}) \bullet \frac{\underline{c}}{l^*} \\ &= |\underline{s}| d_{h^*k^*l^*} \cdots\cdots (5) \end{aligned}$$

(5) $\underline{s}=\frac{\underline{a}\times\underline{b}}{h^*k^*}+\frac{\underline{b}\times\underline{c}}{k^*l^*}+\frac{\underline{c}\times\underline{a}}{l^*h^*}$ $|\underline{s}|$ *ACBD* $d_{h^*k^*l^*}$

③ H_1 H_2 *OABC* (1-*II*~*III*)

H_1 H_2 V_1 V_2 $V_1 = V_2$ (4) (5)

$$\frac{\underline{a}}{h^*}\times\frac{\underline{b}}{k^*}\bullet\frac{\underline{c}}{l^*}=|\underline{s}|d_{h^*k^*l^*}\cdots\cdots(6)$$

2 $d_{h^*k^*l^*}$

(6)

$$d^2_{h^*k^*l^*}=(\frac{\underline{a}}{h^*}\times\frac{\underline{b}}{k^*}\bullet\frac{\underline{c}}{l^*})^2/|\underline{s}|^2=(\frac{\underline{a}}{h^*}\times\frac{\underline{b}}{k^*}\bullet\frac{\underline{c}}{l^*})^2/\underline{s}\bullet\underline{s}\cdots\cdots(7)$$

(7) $d_{h^*k^*l^*}$ $(\frac{\underline{a}}{h^*}\times\frac{\underline{b}}{k^*}\bullet\frac{\underline{c}}{l^*})^2$ $\underline{s}\bullet\underline{s}$

$\underline{a}$ $\underline{b}$ $\underline{c}$ $\underline{d}$

$$(\underline{a}\times\underline{b}\bullet\underline{c})^2=\begin{vmatrix}\underline{a}\bullet\underline{a} & \underline{a}\bullet\underline{b} & \underline{a}\bullet\underline{c}\\ \underline{b}\bullet\underline{a} & \underline{b}\bullet\underline{b} & \underline{b}\bullet\underline{c}\\ c\bullet\underline{a} & \underline{c}\bullet\underline{b} & \underline{c}\bullet\underline{c}\end{vmatrix}\cdots\cdots(8)$$

$$(\underline{a}\times\underline{b})\bullet(\underline{c}\times\underline{d})=(\underline{a}\bullet\underline{c})(\underline{b}\bullet\underline{d})-(\underline{a}\bullet\underline{d})(\underline{b}\bullet\underline{c})\cdots\cdots(9)$$

1-*I*~*II* (8) (9) $(\frac{\underline{a}}{h^*}\times\frac{\underline{b}}{k^*}\bullet\frac{\underline{c}}{l^*})^2$ $\underline{s}\bullet\underline{s}$ $\underline{a}$ $\underline{b}$ $\underline{c}$

(7) $d_{h^*k^*l^*}$

$$\begin{aligned}(\frac{\underline{a}}{h^*}\times\frac{\underline{b}}{k^*}\bullet\frac{\underline{c}}{l^*})^2&=\frac{1}{(h^*k^*l^*)^2}(\underline{a}\times\underline{b}\bullet\underline{c})^2\\&=\frac{1}{(h^*k^*l^*)^2}V^2\\&=\frac{1}{(h^*k^*l^*)^2}\begin{vmatrix}\underline{a}\bullet\underline{a} & \underline{a}\bullet\underline{b} & \underline{a}\bullet\underline{c}\\ \underline{b}\bullet\underline{a} & \underline{b}\bullet\underline{b} & \underline{b}\bullet\underline{c}\\ c\bullet\underline{a} & \underline{c}\bullet\underline{b} & \underline{c}\bullet\underline{c}\end{vmatrix}\\&=\frac{1}{(h^*k^*l^*)^2}\{\underline{a}\bullet\underline{a}[(\underline{b}\bullet\underline{b})(\underline{c}\bullet\underline{c})-(\underline{c}\bullet\underline{b})(\underline{b}\bullet\underline{c})]\\&\quad-\underline{a}\bullet\underline{b}[(\underline{b}\bullet\underline{a})(\underline{c}\bullet\underline{c})-(c\bullet\underline{a})(\underline{b}\bullet\underline{c})]\\&\quad+\underline{a}\bullet\underline{c}[(\underline{b}\bullet\underline{a})(\underline{c}\bullet\underline{b})-(c\bullet\underline{a})(\underline{b}\bullet\underline{b})]\}\end{aligned}$$

$$(\frac{\underline{a}\times\underline{b}}{h^*k^*})\bullet(\frac{\underline{b}\times\underline{c}}{k^*l^*})=\frac{1}{h^*k^{*2}l^*}[(\underline{a}\times\underline{b})\bullet(\underline{b}\times\underline{c})]$$
$$=\frac{1}{h^*k^{*2}l^*}[(\underline{a}\bullet\underline{b})(\underline{b}\bullet\underline{c})-(\underline{a}\bullet\underline{c})(\underline{b}\bullet\underline{b})]$$
$$=\frac{ab^2c}{h^*k^{*2}l^*}(\cos\alpha\cos\gamma-\cos\beta)\cdots\cdots(15)$$

$$(\frac{\underline{b}\times\underline{c}}{k^*l^*})\bullet(\frac{\underline{c}\times\underline{a}}{l^*h^*})=\frac{1}{h^*k^*l^{*2}}(\underline{b}\times\underline{c})\bullet(\underline{c}\times\underline{a})$$
$$=\frac{1}{h^*k^*l^{*2}}[(\underline{b}\bullet\underline{c})(\underline{c}\bullet\underline{a})-(\underline{b}\bullet\underline{a})(\underline{c}\bullet\underline{c})]$$
$$=\frac{abc^2}{h^*k^*l^{*2}}(\cos\alpha\cos\beta-\cos\gamma)\cdots\cdots(16)$$

$$(\frac{\underline{c}\times\underline{a}}{l^*h^*})\bullet(\frac{\underline{a}\times\underline{b}}{h^*k^*})=\frac{1}{h^{*2}k^*l^*}(\underline{c}\times\underline{a})\bullet(\underline{a}\times\underline{b})$$
$$=\frac{1}{h^{*2}k^*l^*}[(\underline{c}\bullet\underline{a})(\underline{a}\bullet\underline{b})-(\underline{c}\bullet\underline{b})(\underline{a}\bullet\underline{a})]$$
$$=\frac{a^2bc}{h^{*2}k^*l^*}(\cos\beta\cos\gamma-\cos\alpha)\cdots\cdots(17)$$

(12) ~ (17) (11)

$$\underline{s}\bullet\underline{s}=\frac{b^2c^2}{(k^*l^*)^2}\sin^2\alpha+\frac{a^2c^2}{(h^*l^*)^2}\sin^2\beta+\frac{a^2b^2}{(h^*k^*)^2}\sin^2\gamma$$
$$+2\frac{ab^2c}{h^*k^{*2}l^*}(\cos\alpha\cos\gamma-\cos\beta)$$
$$+2\frac{abc^2}{h^*k^*l^{*2}}(\cos\alpha\cos\beta-\cos\gamma)$$
$$+2\frac{a^2bc}{h^{*2}k^*l^*}(\cos\beta\cos\gamma-\cos\alpha)\cdots\cdots(18)$$

(10) (18) (7)

$$d^2_{h^*k^*l^*}=(\frac{\underline{a}}{h^*}\times\frac{\underline{b}}{k^*}\bullet\frac{\underline{c}}{l^*})^2/\underline{s}\bullet\underline{s}=\frac{1}{(h^*k^*l^*)^2}V^2/|\underline{s}|^2$$
$$=V^2/[h^{*2}b^2c^2\sin^2\alpha+k^{*2}a^2c^2\sin^2\beta+l^{*2}a^2b^2\sin^2\gamma$$
$$+2h^*l^*ab^2c(\cos\alpha\cos\gamma-\cos\beta)$$
$$+2h^*k^*abc^2(\cos\alpha\cos\beta-\cos\gamma)$$
$$+2k^*l^*a^2bc(\cos\beta\cos\gamma-\cos\alpha)]\cdots\cdots(19)$$

$$V^2=(abc)^2(1-\cos^2\alpha-\cos^2\beta-\cos^2\gamma+2\cos\alpha\cos\beta\cos\gamma)\cdots\cdots(20)$$

(19) (20) $d_{h^*k^*l^*}$ V

$$d_{h^*k^*l^*} = V/[h^{*2}b^2c^2\sin^2\alpha + k^{*2}a^2c^2\sin^2\beta + l^{*2}a^2b^2\sin^2\gamma + 2h^*l^*ab^2c(\cos\alpha\cos\gamma - \cos\beta) + 2h^*k^*abc^2(\cos\alpha\cos\beta - \cos\gamma) + 2k^*l^*a^2bc(\cos\beta\cos\gamma - \cos\alpha)]^{1/2} \cdots\cdots(1)$$

$$V = abc(1 - \cos^2\alpha - \cos^2\beta - \cos^2\gamma + 2\cos\alpha\cos\beta\cos\gamma)^{1/2}$$

$2d_{hkl}\sin\theta_{hkl} = \lambda$ (*Bragg*) $d_{hkl} = \dfrac{d_{h^*k^*l^*}}{n}$ $h = nh^*$ $k = nk^*$ $l = nl^* \cdots\cdots(21)$

(21) θ_{hkl} *Bragg* λ *X-* *n* (*hkl*) *Laue*

$$d_{hkl} = \frac{d_{h^*k^*l^*}}{n} = V/n[h^{*2}b^2c^2\sin^2\alpha + k^{*2}a^2c^2\sin^2\beta + l^{*2}a^2b^2\sin^2\gamma + 2h^*l^*ab^2c(\cos\alpha\cos\gamma - \cos\beta) + 2h^*k^*abc^2(\cos\alpha\cos\beta - \cos\gamma) + 2k^*l^*a^2bc(\cos\beta\cos\gamma - \cos\alpha)]^{1/2} = V/[h^2b^2c^2\sin^2\alpha + k^2a^2c^2\sin^2\beta + l^2a^2b^2\sin^2\gamma + 2hlab^2c(\cos\alpha\cos\gamma - \cos\beta) + 2hkabc^2(\cos\alpha\cos\beta - \cos\gamma) + 2kla^2bc(\cos\beta\cos\gamma - \cos\alpha)]^{1/2} \cdots\cdots(22)$$

(1) (22) ($h^*k^*l^*$) (hkl) $d_{h^*k^*l^*}$ d_{hkl}

3 $d_{h^*k^*l^*}$

( ) C_{2h} 4 a b c β $a \neq b \neq c$ $\beta > 90^o$ $\alpha = \gamma = 90^o$ (1) $d_{h^*k^*l^*}$

$$d_{h^*k^*l^*} = abc(1 - \cos^2 90^o - \cos^2\beta - \cos^2 90^o + 2\cos 90^o\cos\beta\cos 90^o)^{1/2} /[h^{*2}b^2c^2\sin^2 90^o + k^{*2}a^2c^2\sin^2\beta + l^{*2}a^2b^2\sin^2 90^o + 2h^*l^*ab^2c(\cos 90^o\cos 90^o - \cos\beta) + 2h^*k^*abc^2(\cos 90^o\cos\beta - \cos 90^o) + 2k^*l^*a^2bc(\cos\beta\cos 90^o - \cos 90^o)]^{1/2} = \sin\beta/[(\frac{h^*}{a})^2 + (\frac{k^*}{b})^2\sin^2\beta + (\frac{l^*}{c})^2 - 2\frac{h^*l^*}{ac}\cos\beta]^{1/2} \cdots\cdots(23)$$

( ) D_{2h} 3 a b c $a \neq b \neq c$ $\alpha = \beta = \gamma = 90^{o}$

(1) (23) $d_{h^*k^*l^*}$ (23)

$$d_{h^*k^*l^*} = \sin 90^{o} / [(\frac{h^*}{a})^2 + (\frac{k^*}{b})^2 \sin^2 90^{o} + (\frac{l^*}{c})^2 - 2\frac{h^*l^*}{ac}\cos 90^{o}]^{1/2}$$
$$= 1/[(\frac{h^*}{a})^2 + (\frac{k^*}{b})^2 + (\frac{l^*}{c})^2]^{1/2} \cdots\cdots (24)$$

( ) D_{4h} 2 a c ($a = b \neq c$) ( )

O_h 1 a ($a = b = c$) 3 90^{o}

$\alpha = \beta = \gamma = 90^{o}$ (24) $d_{h^*k^*l^*}$

$$d_{h^*k^*l^*} = 1/[(\frac{h^*}{a})^2 + (\frac{k^*}{a})^2 + (\frac{l^*}{c})^2]^{1/2}$$
$$= 1/(\frac{h^{*2} + k^{*2}}{a^2} + \frac{l^{*2}}{c^2})^{1/2} \cdots\cdots (25)$$

$$d_{h^*k^*l^*} = 1/[(\frac{h^*}{a})^2 + (\frac{k^*}{a})^2 + (\frac{l^*}{a})^2]^{1/2}$$
$$= a/(h^{*2} + k^{*2} + l^{*2})^{1/2} \cdots\cdots (26)$$

$d_{h^*k^*l^*}$ d_{hkl} $d_{h^*k^*l^*}$

d_{hkl} (hP D_{6h}) 3

—R (hR D_{3d}) $d_{h^*k^*l^*}$ $d_{h^*k^*l^*}$

1 (D_{3d}) a α $a = b = c$ $\alpha = \beta$ $= \gamma \neq 90^{o}$ $d_{h^*k^*l^*}$ (1)

$$d_{h^*k^*l^*} = aaa(1 - \cos^2\alpha - \cos^2\alpha - \cos^2\alpha + 2\cos\alpha\cos\alpha\cos\alpha)^{1/2}$$
$$/[h^{*2}a^2a^2\sin^2\alpha + k^{*2}a^2a^2\sin^2\alpha + l^{*2}a^2a^2\sin^2\alpha$$
$$+ 2h^*l^*aa^2a(\cos\alpha\cos\alpha - \cos\alpha)$$
$$+ 2h^*k^*aaa^2(\cos\alpha\cos\alpha - \cos\alpha)$$
$$+ 2k^*l^*a^2aa(\cos\alpha\cos\alpha - \cos\alpha)]^{1/2}$$
$$= a(1 - 3\cos^2\alpha + 2\cos^3\alpha)^{1/2}$$
$$/[(h^{*2} + k^{*2} + l^{*2})\sin^2\alpha + 2(h^*l^* + h^*k^* + k^*l^*)(\cos\alpha - 1)\cos\alpha]^{1/2} \cdots\cdots (27)$$

4

$d_{h^*k^*l^*}$ $d_{h^*k^*l^*}$

7 $d_{h^*k^*l^*}$ $d_{h^*k^*l^*}$ X-

$d_{h^*k^*l^*}$

$d_{h^*k^*l^*}$ $d_{h^*k^*l^*}$

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