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空間羣的选择定則*

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提　　要

本文在 J. L. Birman 方法的基础上，对布里渊区內跃迁和散射的选择定則，作了进一步的理論分析，在满足准动量守恒条件的情况下，提出了空間羣簡約系数的比較簡单的計算方法。并用这个方法計算了六角密积結构及纤維鋅矿結构的空間羣簡約系数，从而决定了这两个結构的布里渊区內跃迁和散射的选择定則。

一、引　　言

在固体中，特别是在半导体中的許多跃迁和散射过程，涉及电子和声子、电子和光子，以及电子同时和声子及光子的相互作用；例如在重要半导体鍺、硅及其他某些半导体中的光跃迁，就包括了沒有声子参与的直接光跃迁，和有声子参加的間接光跃迁[1]；通过和声子的相互作用，也可以引起載流子在能谷之間的散射[2]。此外，对于半导体中的激子能級及激子光譜，也有相当多的研究。由于半导体中的能态属于空間羣的不可約表示，因此利用羣論的方法，可以根据对称性，討論上述跃迁与散射的选择定則。

R. J. Elliott 和 R. Loudon[3] 首先利用空間羣性质，討論了半导体鍺、硅中載流子在能带极值之間的光跃迁和散射，以及激子的对称性。随后 M. Lax 和 J. J. Hopfield[4] 直接利用波矢羣的品格，避免构成新的公共羣品格表，討論了同一問題。最近 J. L. Birman[5] 在更加普遍的基础上，重新考虑了空間羣的选择定則，并将所发展的方法，应用于固体中其他問題，例如晶格振动，組态不稳定等。

本文在 J. L. Birman 工作的基础上，作了进一步的理論分析，提出了一个比較簡单的計算方法，并用这个方法計算了六角密积結构及纤維鋅矿結构的空間羣簡約系数。下面首先对計算方法作了簡单介紹，并列出六角密积結构及纤維鋅矿結构的空間羣簡約系数。用这个方法也可以得出金刚石及閃鋅矿結构的空間羣簡約系数，但因 J. L. Birman 已将全部結果列出，本文将不重述。

二、方 法 簡 介

为便于討論起見，先列出本文所用符号：

G　　空間羣，羣阶为 $g = h\alpha$；

T　　平移羣，羣阶为 α；

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G/T　空間羣的商羣，羣阶为 h；

$G^{\mathbf{k}_j}$　波矢羣，其波矢为 $\mathbf{k}_j$；

$T^{\mathbf{k}_j}$　波矢羣 $G^{\mathbf{k}_j}$ 的核；

$K_j^{(m)}(\phi\,|\,\boldsymbol{\tau}+\mathbf{R}_L)$　空間羣对称操作 $(\phi\,|\,\boldsymbol{\tau}+\mathbf{R}_L)$ 在商羣 $G^{\mathbf{k}_j}/T^{\mathbf{k}_j}$ 的第 m 个不可約表示中的品格，其中 ϕ 为轉动，$\boldsymbol{\tau}$ 和 $\mathbf{R}_L$ 为平移；

${}^*K_j=\{K_j, K_{j_2}, \cdots, K_{j_s}\}$　波矢 $\mathbf{K}_j$ 的星，具有 s 个不等价波矢；

${}^*K_j^{(m)}(\phi|\boldsymbol{\tau}+\mathbf{R}_L)$　空間羣对称操作 $(\phi|\boldsymbol{\tau}+\mathbf{R}_L)$ 在空間羣第 m 个不可約表示中的品格；

$\mathscr{K}_j$　矩陣羣 ${}^*K_j^{(m)}$ 的核；

${}^*K_j^{(m)}/\mathscr{K}_j$　矩陣羣 ${}^*K_j^{(m)}$ 的商羣；

$\mathscr{R}$　簡約羣，是三个商羣中羣阶最大的一个；

$(K_jK_{j'}|K_{j''})$　波矢星 ${}^*K_j$ 与 ${}^*K_{j'}$ 的直接乘积的簡約系数；

$(K_j^{(m)}K_{j'}^{(m')}\,|\,K_{j''}^{(m'')})$　两个空間羣不可約表示 ${}^*K_j^{(m)}$ 与 ${}^*K_{j'}^{(m')}$ 的直接乘积的簡約系数。

J. L. Birman 为了便于計算空間羣的簡約系数，把三个矩陣羣 ${}^*K_j^{(m)}$，${}^*K_{j'}^{(m')}$，${}^*K_{j''}^{(m'')}$ 及其核 $\mathscr{K}_j$，$\mathscr{K}_{j'}$，$\mathscr{K}_{j''}$ 組成商羣 ${}^*K_j^{(m)}/\mathscr{K}_j$，${}^*K_{j'}^{(m')}/\mathscr{K}_{j'}$，${}^*K_{j''}^{(m'')}/\mathscr{K}_{j''}$，羣阶各为 n_jh，$n_{j'}h$，$n_{j''}h$，如果 $n_{j''}>n_{j'}$ 或 n_j，則可扩展前两个商羣而得到三个同阶的矩陣羣 ${}^*K_j^{(m)}/\mathscr{K}_{j''}$，${}^*K_{j'}^{(m')}/\mathscr{K}_{j''}$，${}^*K_{j''}^{(m'')}/\mathscr{K}_{j''}$. 如矩陣羣的 $n_{j''}h$ 元素組成簡約羣 $\mathscr{R}$，且 ${}^*K_j^{(m)}(\mathscr{R})$，${}^*K_{j'}^{(m')}(\mathscr{R})$，${}^*K_{j''}^{(m'')}(\mathscr{R})$ 表示 $\mathscr{R}$ 在相应的空間羣不可約表示中的品格，則空間羣的簡約系数由下式所决定：

$$(K_j^{(m)}K_{j'}^{(m')}|K_{j''}^{(m'')})=\frac{1}{n_{j''}h}\sum_R {}^*K_j^{(m)}(R)\;{}^*K_{j'}^{(m')}(R)\;{}^*K_{j''}^{(m'')}(R)^*. \tag{1}$$

如果电子的初态属于不可約表示 ${}^*K_j^{(m)}$，末态属于不可約表示 ${}^*K_{j'}^{(m')}$，而且光子或声子等的微扰哈密頓属于不可約表示 ${}^*K_{j''}^{(m'')}$，則簡約系数不为零时，跃迁过程是允許的。

在利用 (1) 式計算簡約系数时，可以簡化. 因为如元素 $(\alpha_n|\mathbf{a}_n)$ 在商羣 G/T 中，則由附录 I[6,7]，可以把 (1) 式写成

$$\begin{aligned}(K_j^{(m)}K_{j'}^{(m')}|K_{j''}^{(m'')})&=\frac{1}{n_{j''}h}\sum_R {}^*K_j^{(m)}(R){}^*K_{j'}^{(m')}(R){}^*K_{j''}^{(m'')}(R)^*=\\&=\frac{1}{n_{j''}h}\sum_n\sum_l\Big\{\sum_{\mathbf{k}_j,\nu}[T_{\mathbf{k}_j}^{(m)}(\alpha_n|\mathbf{a}_n)]_{\nu\nu}\,e^{i\mathbf{k}_j\cdot\mathbf{t}_l}\sum_{\mathbf{k}_{j'},\mu}[T_{\mathbf{k}_{j'}}^{(m')}(\alpha_n|\mathbf{a}_n)]_{\mu\mu}\cdot\\&\quad\cdot e^{i\mathbf{k}_{j'}\cdot\mathbf{t}_l}\sum_{\mathbf{k}_{j''},\eta}[T_{\mathbf{k}_{j''}}^{(m'')}(\alpha_n|\mathbf{a}_n)]_{\eta\eta}^*\,e^{-i\mathbf{k}_{j''}\cdot\mathbf{t}_l}\Big\},\end{aligned} \tag{2}$$

其中 $\mathbf{t}_l$ 由

$$T=\sum_{l=1}^{n_{j''}}(\varepsilon|\mathbf{t}_l)K_{j''} \tag{3}$$

来决定. (2)式可写成

$$\begin{aligned}(K_j^{(m)}K_{j'}^{(m')}|K_{j''}^{(m'')})&=\frac{1}{n_{j''}h}\sum_n\sum_l\sum_{\mathbf{k}_j\mathbf{k}_{j'}\mathbf{k}_{j''}}\sum_{\nu,\mu,\eta}\{T_{\mathbf{k}_j}^{(m)}(\alpha_n|\mathbf{a}_n)\}_{\nu\nu}\{T_{\mathbf{k}_{j'}}^{(m')}(\alpha_n|\mathbf{a}_n)\}_{\mu\mu}\times\\&\quad\times\{T_{\mathbf{k}_{j''}}^{(m'')}(\alpha_n|\mathbf{a}_n)\}_{\eta\eta}^*\,e^{i(\mathbf{k}_j+\mathbf{k}_{j'}-\mathbf{k}_{j''})\cdot\mathbf{t}_l}.\end{aligned} \tag{4}$$

波矢羣 $G^{\mathbf{k}_j}$, $G^{\mathbf{k}_{j'}}$, $G^{\mathbf{k}_{j''}}$ 所共有元素組成公共羣 $G^{\mathbf{k}_j\mathbf{k}_{j'}\mathbf{k}_{j''}}$. 令在 $G^{\mathbf{k}_j\mathbf{k}_{j'}\mathbf{k}_{j''}}$ 中的 $(\alpha_n|\mathbf{a}_n)$ 为 $(\alpha_\lambda|\mathbf{a}_\lambda)$, 显然只有 $(\alpha_\lambda|\mathbf{a}_\lambda)$ 对于(4)式中的$(\mathbf{k}_j, \mathbf{k}_{j'}, \mathbf{k}_{j''})$項有貢献, 对 $G^{\mathbf{k}_j\mathbf{k}_{j'}\mathbf{k}_{j''}}$ 进行陪集分解,則

$$G = \sum_{\theta} (\alpha_\theta|\mathbf{a}_\theta)\, G^{\mathbf{k}_j\mathbf{k}_{j'}\mathbf{k}_{j''}} \qquad \left(\theta = 1\cdots\frac{h}{h_\lambda}\right), \tag{5}$$

其中 h_λ 是波矢羣 $G^{\mathbf{k}_j\mathbf{k}_{j'}\mathbf{k}_{j''}}/T$ 的阶. 如果把 $(\mathbf{k}_j, \mathbf{k}_{j'}, \mathbf{k}_{j''})$ 看成为一个波矢,則

$$\alpha_\theta(\mathbf{k}_j, \mathbf{k}_{j'}, \mathbf{k}_{j''}) \qquad \left(\theta = 1\cdots\frac{h}{h_\lambda}\right), \tag{6}$$

組成波矢 $(\mathbf{k}_j, \mathbf{k}_{j'}, \mathbf{k}_{j''})$ 的星 $^*(\mathbf{k}_j, \mathbf{k}_{j'}, \mathbf{k}_{j''})$, 而且 $(\alpha_\theta|\mathbf{a}_\theta)(\alpha_\lambda|\mathbf{a}_\lambda)(\alpha_\theta|\mathbf{a}_\theta)^{-1}$ 是公共羣 $G^{\alpha_\theta(\mathbf{k}_j,\mathbf{k}_{j'},\mathbf{k}_{j''})}$ 的元素, 且 $G^{\alpha_\theta(\mathbf{k}_j,\mathbf{k}_{j'},\mathbf{k}_{j''})}\left(\theta = 1\cdots\frac{h}{h_\lambda}\right)$ 是同构共軛子羣. 所以在(4)式中对 n 及 $(\mathbf{k}_j, \mathbf{k}_{j'}, \mathbf{k}_{j''})$ 的求和,可以用对 θ 及 λ 的求和来代替,(4)式写成

$$\begin{aligned}
(K_j^{(m)}K_{j'}^{(m')}|K_{j''}^{(m'')}) &= \left(\frac{1}{n_{j''}h}\right)\sum_{l}\sum_{\theta}\sum_{\lambda}\sum_{\nu,\mu,\eta}\{T^{(m)}_{\alpha_\theta\mathbf{k}_j}[(\alpha_\theta|a_\theta)(\alpha_\lambda|a_\lambda)(\alpha_\theta|a_\theta)^{-1}]\}_{\nu\nu}\times\\
&\times\{T^{(m')}_{\alpha_\theta\mathbf{k}_{j'}}[(\alpha_\theta|a_\theta)(\alpha_\lambda|a_\lambda)(\alpha_\theta|a_\theta)^{-1}]\}_{\mu\mu}\{T^{(m'')}_{\alpha_\theta\mathbf{k}_{j''}}[(\alpha_\theta|a_\theta)(\alpha_\lambda|a_\lambda)(\alpha_\theta|a_\theta)^{-1}]\}^*_{\eta\eta}\times\\
&\times e^{i\alpha_\theta(\mathbf{k}_j+\mathbf{k}_{j'}-\mathbf{k}_{j''})\cdot\mathbf{t}_l} =\\
&= \left(\frac{1}{n_{j''}h}\right)\sum_{\lambda}\sum_{\nu,\mu,\eta}\{T^{(m)}_{\mathbf{k}_j}(\alpha_\lambda|a_\lambda)\}_{\nu\nu}\{T^{(m')}_{\mathbf{k}_{j'}}(\alpha_\lambda|a_\lambda)\}_{\mu\mu}\{T^{(m'')}_{\mathbf{k}_{j''}}(\alpha_\lambda|a_\lambda)\}^*_{\eta\eta}\times\\
&\times\sum_{l,\theta}e^{i\alpha_\theta(\mathbf{k}_j+\mathbf{k}_{j'}-\mathbf{k}_{j''})\cdot\mathbf{t}_l},
\end{aligned}\tag{7}$$

由于准动量守恆,所以

$$\sum_{l,\theta} e^{i\alpha_\theta(\mathbf{k}_j+\mathbf{k}_{j'}-\mathbf{k}_{j''})\cdot\mathbf{t}_l} = n_{j''}\frac{h}{h_\lambda}. \tag{8}$$

由此得到

$$(K_j^{(m)}K_{j'}^{(m')}|K_{j''}^{(m'')}) = \frac{1}{h_\lambda}\sum_{\lambda}\sum_{\nu,\mu,\eta}\{T^{(m)}_{\mathbf{k}_j}(\alpha_\lambda|\mathbf{a}_\lambda)\}_{\nu\nu}\{T^{(m')}_{\mathbf{k}_{j'}}(\alpha_\lambda|\mathbf{a}_\lambda)\}_{\mu\mu}\{T^{(m'')}_{\mathbf{k}_{j''}}(\alpha_\lambda|\mathbf{a}_\lambda)\}^*_{\eta\eta}, \tag{9}$$

其中

$\mathbf{k}_j + \mathbf{k}_{j'} - \mathbf{k}_{j''} = 0$, 或 $\mathbf{K}_n$, $\mathbf{K}_n$ 是倒格矢.

因此只要知道公共羣 $G^{\mathbf{k}_j\mathbf{k}_{j'}\mathbf{k}_{j''}}$ 的元素 $(\alpha_\lambda|\mathbf{a}_\lambda)$ 在有关的波矢羣中的品格, 便可求出空間羣的簡約系数,也就决定了选择定則.

以鍺导带能谷之間的散射, 說明利用(9)式計算空間羣的簡約系数 $(LL|X)$, 众所周知, 鍺的导带极値位于布里渊区的 L 对称点, 通过和声子相互作用, 由 $\frac{\pi}{a}(1, 1, 1)$ 能谷到 $\frac{\pi}{a}(-1, -1, 1)$ 能谷的散射,声子的波矢是 $\frac{2\pi}{a}(0, 0, 1)$. 如令 $L_{(1)} = \frac{\pi}{a}(1, 1, 1)$, $L_{(2)} = \frac{\pi}{a}(-1, -1, 1)$, $X_{(3)} = \frac{2\pi}{a}(0, 0, 1)$, 則这三个波矢羣的公共元素有 4 个, 即 $h_\lambda = 4$. 下表列出这些元素及相应的不可約表示的品格[1].

1) 在計算时应注意表 1 中共軛元素的品格并不相同. 例如操作$(\delta_{2\bar{x}y}|\tau_1)$在波矢羣 $L_{(2)}$ 的品格应为 $L_2(\delta_{2\bar{x}y}|\tau_1) = e^{i\mathbf{k}_{L_2}\cdot(\tau_1-\tau_4)}L_{(2)}(\delta_{2\bar{x}y}|\tau_4)$.

表 1 1)

$L_{(1)}$				$L_{(2)}$				$X_{(3)}$				
公共元素	L_1^+	L_2^+	L_3^+	公共元素	L_1^+	L_2^+	L_3^+	公共元素	X_1	X_2	X_3	X_4
$(\varepsilon\|0)$	1	1	2	$(\varepsilon\|0)$	1	1	2	$(\varepsilon\|0)$	2	2	2	2
$(\delta_{2\bar{x}y}\|\tau_1)$	1	-1	0	$(\delta_{2\bar{x}y}\|\tau_4)$	1	-1	0	$(\delta_{2\bar{x}y}\|\tau_1)$	0	0	-2	2
$(i\|\tau_1)$	±1	±1	±2	$(i\|\tau_4)$	±1	±1	±2	$(i\|\tau_1)$	0	0	0	0
$(\rho_{\bar{x}y}\|0)$	±1	∓1	0	$(\rho_{\bar{x}y}\|0)$	±1	∓1	0	$(\rho_{\bar{x}y}\|0)$	2	-2	0	0

利用(9)式及表 1 可以得到

$$(L_1^+L_1^+|X_1) = 1, \quad (L_1^+L_1^+|X_3) = 1,$$

即由 $\frac{\pi}{a}(1, 1, 1)$ 极值的 L_1^+ 对称能态到 $\frac{\pi}{a}(-1, -1, 1)$ 极值的 L_1^+ 对称能态之間的跃迁，是通过和具有对称性为 X_1 及 X_3 的声子的相互作用2)．其中 X_1 是 LA 及 LO，而 X_3 是 TA，X_4 是 TO．

三、六角密积結构空間羣 (D_{6h}^4) 簡約系数的計算3)

計算的步驟如下：

(i) 列出对称操作(表 2)及布里渊区內的对称点(軸)(表 3)．

(ii) 根据 J. L. Birman[5] 的方法計算波矢星的直接乘积簡約系数 (表 4)．

表 2　对称操作

基矢：

$$\mathbf{t}_1 = (0, 0, 1)\,c,\ \mathbf{t}_2 = (1, 0, 0)\,a,\ \mathbf{t}_3 = \left(-\frac{1}{2}, \frac{\sqrt{3}}{2}, 0\right)a,\ \mathbf{t}_4 = -(\mathbf{t}_2 + \mathbf{t}_3)$$

倒格子基矢：

$$\mathbf{b}_1 = (0, 0, 2\pi)\,\frac{1}{c},\ \mathbf{b}_2 = \left(2\pi, \frac{2\pi}{\sqrt{3}}, 0\right)\frac{1}{a},\ \mathbf{b}_3 = \left(0, \frac{4\pi}{\sqrt{3}}, 0\right)\frac{1}{a}$$

部分平移：

$$\boldsymbol{\tau}_2 = \left(0, -\frac{a}{\sqrt{3}}, \frac{c}{2}\right),\ \boldsymbol{\tau}_3 = \left(-\frac{a}{2}, \frac{a}{2\sqrt{3}}, \frac{c}{2}\right),\ \boldsymbol{\tau}_4 = \left(\frac{a}{2}, \frac{a}{2\sqrt{3}}, \frac{c}{2}\right)$$

对称操作	
$(\alpha\|0)$ 型	$(\alpha\|\tau)$ 型
ε：不变操作	i：反演
δ_3, δ_3^{-1}：繞 $\mathbf{t}_1$ 軸的三度轉动	δ_6, δ_6^{-1}：繞 $\mathbf{t}_1$ 軸的 6 度轉动
δ_{2i}''：$i = 2, 3, 4$，繞与 $\mathbf{t}_1$ 及 $\mathbf{t}_2, \mathbf{t}_3, \mathbf{t}_4$ 垂直的二度轉动	δ_{2i}'：$i = 2, 3, 4$，繞 $\mathbf{t}_2, \mathbf{t}_3, \mathbf{t}_4$ 的二度轉动
$\rho = i\delta_2$	δ_2：繞 $\mathbf{t}_1$ 軸的二度轉动
σ_3, σ_3^{-1}：$\sigma_3 = i\delta_6$	σ_6, σ_6^{-1}：$\sigma_6 = i\delta_3$
$\rho_i' = i\delta_{2i}'$　$i = 2, 3, 4$	$\rho_i'' = i\delta_{2i}''$　$i = 2, 3, 4$

1) 表 1 中金刚石結构对称操作同波矢羣品格表見文献[8]．

2) R. J. Elliott 及 R. Loudon[8] 得到的是 X_1 及 X_4 对称性的声子，M. Lax 已与 R. J. Elliott 討論了这个差异[4]．

3) 六角密积結构的波矢羣品格表見文献[8]．

(iii) 計算有关波矢羣的公共羣元素的品格，并根据 (9) 式計算簡約系数（表 5）．在表 5 中，Γ 与 M 是有奇表示和偶表示的，奇表示和偶表示的直接乘积得到奇表示，偶表示和偶表示得到偶表示等等，所以在表 5 中略去奇偶的标記．

下表列出六角密积結构及紆維鋅矿結构布里渊区內对称点坐标，不等价波矢星，只列出一个波矢，其他波矢由对称操作作用于这个波矢而得到．

表 3 六角密积及紆維鋅矿結构布里渊区內对称点坐标

对称点(軸)	坐 标	不等价波矢数[1]	对称点(軸)	坐 标	不等价波矢数
Γ	$(0, 0, 0)$	1	Σ	$\left(0, \frac{k}{\sqrt{3}a}, 0\right)2\pi$	6
A	$\left(0, 0, \frac{\pi}{c}\right)$	1	R	$\left(0, \frac{2k}{\sqrt{3}a}, \frac{1}{c}\right)\pi$	6
L	$\left(0, \frac{2\pi}{\sqrt{3}a}, \frac{\pi}{c}\right)$	3	S	$\left(\frac{2k}{a}, 0, \frac{1}{c}\right)\pi$	6
M	$\left(0, \frac{2\pi}{\sqrt{3}a}, 0\right)$	3	T	$\left(\frac{2k}{a}, 0, 0\right)\pi$	6
H	$\left(\frac{2}{3a}, \frac{2}{\sqrt{3}a}, \frac{1}{c}\right)\pi$	2	P	$\left(\frac{2\pi}{3a}, \frac{2\pi}{\sqrt{3}a}, \frac{k}{c}\right)$	4 (2)
K	$\left(\frac{2}{3a}, \frac{2}{\sqrt{3}a}, 0\right)\pi$	2	U	$\left(0, \frac{2\pi}{\sqrt{3}a}, \frac{k}{c}\right)$	6 (3)
Δ	$\left(0, 0, \frac{k}{c}\right)$	2 (1)			

表 4 六角密积結构波矢星的直接乘积簡約系数 $(K_jK_{j'}|K_{j''})$

$(\Gamma K_{j'}|K_{j'}) = 1$ 对于所有 $K_{j'}$

$(MM|\Gamma) = 3$

$(MM|M) = 2$

$(LL|\Gamma) = 3$

$(LL|M) = 2$

$(KK|\Gamma) = 2$

$(KK|K) = 1$

$(HH|\Gamma) = 2$

$(HH|K) = 1$

$(\Delta\Delta|\Gamma) = 2$

$(\Delta\Delta|\Delta') = 1 \quad \Delta_1' = \left(0, 0, \frac{2k}{c}\right)$

$(\Sigma\Sigma|\Gamma) = 6$

$(\Sigma\Sigma|T) = 2$

$(SS|T) = 2$

$(PP|P') = 1 \quad P_1' = \left(\frac{2\pi}{3a}, \frac{2\pi}{\sqrt{3}a}, \frac{2k}{c}\right)$

$(PP'|\Delta') = 2 \quad \Delta_1' = \left(0, 0, \frac{2k}{c}\right)$

$(PP|\Gamma) = 4$

$(PP|K) = 2$

$(UU|\Gamma) = 6$

$(UU|\Delta') = 3 \quad \Delta_1' = \left(0, 0, \frac{2k}{c}\right)$

$(UU|M) = 4$

$(UU|U') = 2 \quad U_1' = \left(0, \frac{2\pi}{\sqrt{3}a}, \frac{2k}{c}\right)$

$(\Delta M|U) = 1$

$(\Delta P|P') = 1 \quad P_1' = \left(\frac{2\pi}{3a}, \frac{2\pi}{\sqrt{3}a}, \frac{2k}{c}\right)$

$(\Delta P|K) = 2$

$(\Delta U|U') = 1 \quad U_1' = \left(0, \frac{2\pi}{\sqrt{3}a}, \frac{2k}{c}\right)$

$(\Delta U|M) = 2$

$(AM|L) = 1$

$(AK|H) = 1$

$(A\Sigma|R) = 1$

$(AT|S) = 1$

$(\Sigma\Sigma|\Sigma') = 1 \quad \Sigma_1' = \left(0, \frac{2k}{\sqrt{3}a}, 0\right)2\pi$

$(\Sigma\Sigma|\Sigma) = 2$

$(RR|\Gamma) = 6$

$(RR|T) = 2$

$(RR|\Sigma') = 1 \quad \Sigma_1' = \left(0, \frac{2k}{\sqrt{3}a}, 0\right)2\pi$

1) 括号內的数目系紆維鋅矿結构的不等价波矢数．

$(RR|\Sigma) = 2$

$(TT|\Gamma) = 6$

$(TT|\Sigma) = 2 \quad \Sigma_1 = \left(0,\ \frac{2\sqrt{3}\,k}{a},\ 0\right)\pi$

$(TT|T') = 1 \quad T_1' = \left(\frac{2k}{a},\ 0,\ 0\right)2\pi$

$(TT|T) = 2$

$(SS|\Gamma) = 6$

$(SS|\Sigma) = 2 \quad \Sigma_1 = \left(0,\ \frac{\sqrt{3}\,k}{a},\ 0\right)2\pi$

$(SS|T') = 1 \quad T_1' = \left(\frac{2k}{a},\ 0,\ 0\right)2\pi$

$(ML|L) = 2$

$(ML|A) = 3$

$(KH|H) = 1$

$(KH|A) = 2$

$(R\Sigma|A) = 6$

$(R\Sigma|S) = 2$

$(R\Sigma|R') = 1 \quad R_1' = \left(0,\ \frac{2k}{\sqrt{3}\,a},\ \frac{1}{2c}\right)2\pi$

$(R\Sigma|R) = 2$

$(ST|A) = 6$

$(ST|S') = 1 \quad S_1' = \left(\frac{4k}{a},\ 0,\ \frac{1}{c}\right)\pi$

$(ST|S) = 2$

$(ST|R) = 2$

$(AL|M) = 1$

$(AH|K) = 1$

$(AR|\Sigma) = 1$

$(AS|T) = 1$

$(AK|P) = 1$

表 5　六角密积結构空間羣簡約系数[1)]

$(\Gamma_1^+ K_j^{(m)}|K_j^{(m)}) = 1$

$(\Gamma_i\Gamma_i|\Gamma_1) = 1 \qquad i = 1, 2, 3, 4$

$(\Gamma_2\Gamma_3|\Gamma_4) = 1$

$(\Gamma_2\Gamma_4|\Gamma_3) = 1$

$(\Gamma_2\Gamma_5|\Gamma_5) = 1$

$(\Gamma_2\Gamma_6|\Gamma_6) = 1$

$(\Gamma_3\Gamma_4|\Gamma_2) = 1$

$(\Gamma_3\Gamma_5|\Gamma_6) = 1$

$(\Gamma_3\Gamma_6|\Gamma_5) = 1$

$(\Gamma_4\Gamma_5|\Gamma_6) = 1$

$(\Gamma_4\Gamma_6|\Gamma_5) = 1$

$(\Gamma_5\Gamma_5|\Gamma_1) = (\quad|\Gamma_2)$

$= (\quad|\Gamma_5)$

$= 1$

$(\Gamma_5\Gamma_6|\Gamma_3) = (\quad|\Gamma_4)$

$= (\quad|\Gamma_6)$

$= 1$

$(\Gamma_i\Gamma_i|\quad) = (\Gamma_1\Gamma_1|\quad) \qquad i = 1, 2, 3, 4$

$(\Gamma_1\Gamma_2|\quad) = (\Gamma_3\Gamma_4|\quad)$

$(\Gamma_1\Gamma_3|\quad) = (\Gamma_2\Gamma_4|\quad)$

$(\Gamma_1\Gamma_4|\quad) = (\Gamma_2\Gamma_3|\quad)$

$(\Gamma_1\Gamma_5|\quad) = (\Gamma_2\Gamma_5|\quad)$

$(\Gamma_1\Gamma_6|\quad) = (\Gamma_2\Gamma_6|\quad)$

$(\Gamma_3\Gamma_5|\quad) = (\Gamma_4\Gamma_5|\quad)$

$(\Gamma_5\Gamma_5|\quad) = (\Gamma_6\Gamma_6|\quad)$

$(A_1A_1|\Gamma_1^+) = (\quad|\Gamma_3^+)$

$= (\quad|\Gamma_2^-)$

$= (\quad|\Gamma_4^-)$

$= 1$

$(A_1A_2|\Gamma_1^-) = (\quad|\Gamma_2^+)$

$= (\quad|\Gamma_3^-)$

$= (\quad|\Gamma_4^+)$

$= 1$

$(A_1A_3|\Gamma_5^\pm) = (\quad|\Gamma_6^\pm)$

$= 1$

$(A_2A_2|\Gamma_1^+) = (\quad|\Gamma_2^-)$

$= (\quad|\Gamma_3^+)$

$= (\quad|\Gamma_4^-)$

$= 1$

$(A_2A_3|\Gamma_5^\pm) = (\quad|\Gamma_6^\pm)$

$= 1$

$(A_3A_3|\Gamma_1^\pm) = (\quad|\Gamma_2^\pm)$

$= (\quad|\Gamma_3^\pm)$

$= (\quad|\Gamma_4^\pm)$

$= (\quad|\Gamma_5^\pm)$

$= (\quad|\Gamma_6^\pm)$

$= 1$

$(A_1\Gamma_1^+|A_1) = (A_1\Gamma_3^+|\quad)$

$= (A_1\Gamma_2^-|\quad)$

$= (A_1\Gamma_4^-|\quad)$

$= 1$

$(A_1\Gamma_2^+|A_2) = (A_1\Gamma_4^+|\quad)$

$= (A_1\Gamma_1^-|\quad)$

$= (A_1\Gamma_3^-|\quad)$

$= 1$

$(A_1\Gamma_5^\pm|A_3) = (A_1\Gamma_6^\pm|\quad)$

$= 1$

$(A_2\Gamma_1^+|A_2) = (A_2\Gamma_3^+|\quad)$

$= (A_2\Gamma_2^-|\quad)$

1) 表中符号的含义与文献[5]相同.

$$= (A_2\Gamma_4^-|\quad)$$
$$= 1$$
$$(A_3\Gamma_1^\pm|A_3) = (A_3\Gamma_2^\pm|\quad)$$
$$= (A_3\Gamma_3^\pm|\quad)$$
$$= (A_3\Gamma_4^\pm|\quad)$$
$$= (A_3\Gamma_5^\pm|\quad)$$
$$= (A_3\Gamma_6^\pm|\quad)$$
$$= 1$$
$$(M_iM_i|\Gamma_1) = 1 \qquad i = 1, 2, 3, 4$$
$$(M_1M_2|\Gamma_4) = (\quad|\Gamma_6)$$
$$= 1$$
$$(M_1M_3|\Gamma_3) = (\quad|\Gamma_6)$$
$$= 1$$
$$(M_2M_3|\Gamma_2) = (\quad|\Gamma_5)$$
$$= 1$$
$$(M_1M_4|\Gamma_2) = (\quad|\Gamma_5)$$
$$= 1$$
$$(M_2M_4|\Gamma_3) = (\quad|\Gamma_6)$$
$$= 1$$
$$(M_3M_4|\Gamma_4) = (\quad|\Gamma_6)$$
$$= 1$$
$$(M_1M_2|\quad) = (M_3M_4|\quad)$$
$$(M_1M_3|\quad) = (M_2M_4|\quad)$$
$$(M_2M_3|\quad) = (M_1M_4|\quad)$$
$$(M_i\Gamma_1|M_i) = 1 \qquad i = 1, 2, 3, 4$$
$$(M_1\Gamma_4|M_2) = 1$$
$$(M_1\Gamma_6|M_2) = 1$$
$$(M_1\Gamma_3|M_3) = 1$$
$$(M_2\Gamma_2|M_3) = 1$$
$$(M_2\Gamma_5|M_3) = 1$$
$$(M_1\Gamma_2|M_4) = 1$$
$$(M_1\Gamma_5|M_4) = 1$$
$$(M_2\Gamma_3|M_4) = 1$$
$$(M_2\Gamma_6|M_4) = 1$$
$$(M_3\Gamma_4|M_4) = (M_3\Gamma_6|\quad)$$
$$= 1$$
$$(M_1\Gamma_6|M_3) = (M_2\Gamma_5|\quad)$$
$$= 1$$
$$(M_iM_i|M_1) = (\quad|M_4)$$
$$= 1 \qquad i = 1, 2, 3, 4$$
$$(M_1M_2|M_3) = (M_3M_4|\quad)$$
$$= (M_1M_3|\quad)$$
$$= (M_2M_4|\quad)$$
$$= 1$$
$$(M_1M_3|M_2) = (M_1M_2|\quad)$$
$$= (M_3M_4|\quad)$$
$$= (M_2M_4|\quad)$$
$$= 1$$
$$(M_1M_4|M_1) = (M_2M_3|\quad)$$
$$= 1$$
$$(M_1M_4|M_4) = (M_2M_3|\quad)$$
$$= 1$$
$$(L_iL_i|\Gamma_1^+) = (\quad|\Gamma_2^-)$$
$$= (\quad|\Gamma_3^+)$$
$$= (\quad|\Gamma_4^-)$$
$$= (\quad|\Gamma_5^\pm)$$
$$= (\quad|\Gamma_6^\pm)$$
$$= 1 \qquad i = 1, 2$$
$$(L_1L_2|\Gamma_1^-) = (\quad|\Gamma_2^+)$$
$$= (\quad|\Gamma_3^-)$$
$$= (\quad|\Gamma_4^+)$$
$$= (\quad|\Gamma_5^\pm)$$
$$= (\quad|\Gamma_6^\pm)$$
$$= 1$$
$$(L_i\Gamma_1^+|L_i) = (L_i\Gamma_2^-|\quad)$$
$$= (L_i\Gamma_3^+|\quad)$$
$$= (L_i\Gamma_4^-|\quad)$$
$$= (L_i\Gamma_5^\pm|\quad)$$
$$= (L_i\Gamma_6^\pm|\quad)$$
$$= 1 \qquad i = 1, 2$$
$$(L_1\Gamma_1^-|L_2) = (L_1\Gamma_2^+|\quad)$$
$$= (L_1\Gamma_3^-|\quad)$$
$$= (L_1\Gamma_4^+|\quad)$$
$$= (L_1\Gamma_5^\pm|\quad)$$
$$= (L_1\Gamma_6^\pm|\quad)$$
$$= 1$$
$$(L_iL_j|M_l^\pm) = 1 \qquad i, j = 1, 2; \qquad l = 1, 2, 3, 4$$
$$(K_iK_i|\Gamma_1^+) = (\quad|\Gamma_3^-)$$
$$= 1 \qquad i = 1, 2, 3, 4$$
$$(K_jK_j|\Gamma_1^+) = (\quad|\Gamma_2^+)$$
$$= (\quad|\Gamma_3^-)$$
$$= (\quad|\Gamma_4^-)$$
$$= (\quad|\Gamma_5^+)$$
$$= (\quad|\Gamma_6^-)$$
$$= 1 \qquad j = 5, 6$$
$$(K_1K_2|\Gamma_1^-) = (\quad|\Gamma_3^+)$$
$$= 1$$
$$(K_1K_3|\Gamma_2^+) = (\quad|\Gamma_4^-)$$
$$= 1$$
$$(K_1K_4|\Gamma_2^-) = (\quad|\Gamma_4^+)$$
$$= 1$$
$$(K_1K_5|\Gamma_5^+) = (\quad|\Gamma_6^-)$$
$$= 1$$
$$(K_1K_6|\Gamma_5^-) = (\quad|\Gamma_6^+)$$
$$= 1$$
$$(K_5K_6|\Gamma_1^-) = (\quad|\Gamma_2^-)$$
$$= (\quad|\Gamma_3^+)$$
$$= (\quad|\Gamma_4^+)$$
$$= 1$$
$$(K_2K_5|\Gamma_5^-) = (\quad|\Gamma_6^+)$$

$= 1$

$(K_2K_6|\Gamma_5^+) = (\quad |\Gamma_6^-)$

$= 1$

$(K_2K_3| \quad) = (K_1K_4| \quad)$

$(K_2K_4| \quad) = (K_1K_3| \quad)$

$(K_2K_5| \quad) = (K_4K_5| \quad)$

$(K_2K_6| \quad) = (K_4K_6| \quad)$

$(K_1K_5| \quad) = (K_3K_5| \quad)$

$(K_1K_6| \quad) = (K_3K_6| \quad)$

$(K_3K_4| \quad) = (K_1K_2| \quad)$

$(K_iK_i|K_1) = 1 \qquad i = 1, 2, 3, 4$

$(K_1K_4|K_4) = 1$

$(K_1K_6|K_6) = (K_2K_5| \quad)$

$= (K_3K_6| \quad)$

$= (K_4K_5| \quad)$

$= 1$

$(K_1K_5|K_5) = (K_2K_6| \quad)$

$= (K_3K_5| \quad)$

$= (K_4K_6| \quad)$

$= 1$

$(K_1K_3|K_3) = 1$

$(K_1K_2|K_2) = 1$

$(K_5K_5|K_1) = (\quad |K_3)$

$= (\quad |K_5)$

$= 1$

$(H_1H_2| \quad) = (H_1H_3| \quad)$

$(H_2H_2| \quad) = (H_3H_3| \quad)$

$(H_1H_1|\Gamma_1^\pm) = (\quad |\Gamma_2^\pm)$

$= (\quad |\Gamma_3^\pm)$

$= (\quad |\Gamma_4^\pm)$

$= 1$

$(H_2H_2|\Gamma_1^+) = (\quad |\Gamma_2^+)$

$= (\quad |\Gamma_3^-)$

$= (\quad |\Gamma_4^-)$

$= 1$

$(H_1H_2|\Gamma_5^\pm) = (\quad |\Gamma_6^\pm)$

$= 1$

$(H_2H_3|\Gamma_1^-) = (\quad |\Gamma_2^-)$

$= (\quad |\Gamma_3^+) = (\quad |\Gamma_4^+)$

$= 1$

$(H_1H_1|K_1) = (\quad |K_2)$

$= (\quad |K_3)$

$= (\quad |K_4)$

$= 1$

$(H_1H_2|K_5) = (\quad |K_6)$

$= 1$

$(H_2H_2|K_2) = (\quad |K_4)$

$= (\quad |K_5)$

$= 1$

$(H_2H_3|K_1) = (\quad |K_3)$

$= (\quad |K_6)$

$= 1$

$(\Delta_i\Delta_i| \quad) = (\Delta_1\Delta_1| \quad) \qquad i = 1, 2, 3, 4$

$(\Delta_5\Delta_5| \quad) = (\Delta_6\Delta_6| \quad)$

$(\Delta_1\Delta_2| \quad) = (\Delta_3\Delta_4| \quad)$

$(\Delta_1\Delta_3| \quad) = (\Delta_2\Delta_4| \quad)$

$(\Delta_1\Delta_4| \quad) = (\Delta_2\Delta_3| \quad)$

$(\Delta_1\Delta_5| \quad) = (\Delta_3\Delta_5| \quad)$

$(\Delta_1\Delta_6| \quad) = (\Delta_3\Delta_6| \quad)$

$(\Delta_2\Delta_5| \quad) = (\Delta_4\Delta_5| \quad)$

$(\Delta_2\Delta_6| \quad) = (\Delta_4\Delta_6| \quad)$

$(\Delta_1\Delta_2|\Gamma_3^+) = (\quad |\Gamma_4^-)$

$= 1$

$(\Delta_2\Delta_3|\Gamma_3^-) = (\quad |\Gamma_4^+)$

$= 1$

$(\Delta_1\Delta_3|\Gamma_1^-) = (\quad |\Gamma_2^+)$

$= 1$

$(\Delta_i\Delta_i|\Gamma_1^\pm) = (\quad |\Gamma_2^\pm) = (\quad |\Gamma_5^\pm) = 1$

$i = 5, 6$

$(\Delta_i\Delta_i|\Gamma_1^+) = (\quad |\Gamma_2^-) = 1 \qquad i = 1, 2, 3, 4$

$(\Delta_3\Delta_4|\Gamma_3^+) = (\quad |\Gamma_4^-)$

$= 1$

$(\Delta_1\Delta_4|\Gamma_3^-) = (\quad |\Gamma_4^+)$

$= 1$

$(\Delta_2\Delta_4|\Gamma_1^-) = (\quad |\Gamma_2^+)$

$= 1$

$(\Delta_4\Delta_5|\Gamma_6^\pm) = 1$

$(\Delta_3\Delta_5|\Gamma_5^\pm) = 1$

$(\Delta_2\Delta_1|\Gamma_3^+) = (\quad |\Gamma_4^-)$

$= 1$

$(\Delta_5\Delta_6|\Gamma_3^\pm) = (\quad |\Gamma_4^\pm)$

$= 1$

$(\Delta_4\Delta_6|\Gamma_5^\pm) = (\Delta_3\Delta_5|\Gamma_5^\pm)$

$= 1$

$(\Delta_1\Gamma_3^+|\Delta_2) = (\Delta_1\Gamma_4^-| \quad)$

$= 1$

$(\Delta_2\Gamma_3^-|\Delta_3) = (\Delta_2\Gamma_4^+| \quad)$

$= 1$

$(\Delta_1\Gamma_1^-|\Delta_3) = (\Delta_1\Gamma_2^+| \quad)$

$= 1$

$(\Delta_3\Gamma_3^+|\Delta_4) = (\Delta_3\Gamma_4^-| \quad)$

$= 1$

$(\Delta_1\Gamma_3^-|\Delta_4) = (\Delta_1\Gamma_4^+| \quad)$

$= 1$

$(\Delta_2\Gamma_1^-|\Delta_4) = (\Delta_2\Gamma_2^+| \quad)$

$= 1$

$(\Delta_4\Gamma_6^\pm|\Delta_5) = 1$

$(\Delta_3\Gamma_5^\pm|\Delta_5) = 1$

$(\Delta_2\Gamma_3^+|\Delta_1) = (\Delta_2\Gamma_4^-| \quad)$

$$\begin{aligned}
&= 1 \\
(\triangle_5\Gamma_3^{\pm}|\triangle_6) &= (\triangle_5\Gamma_4^{\pm}|\quad) \\
&= 1 \\
(\triangle_4\Gamma_5^{\pm}|\triangle_6) &= (\triangle_3\Gamma_5^{\pm}|\triangle_5) \\
&= 1 \\
(\triangle_i\triangle_i|\triangle_1) &= 1 \\
&\quad i = 1, 2, 3, 4, 5, 6 \\
(\triangle_i\triangle_i|\triangle_3) &= (\triangle_i\triangle_i|\triangle_5) = 1, \qquad i = 5, 6 \\
(\triangle_1\triangle_2|\triangle_2) &= (\triangle_3\triangle_4|\quad) \\
&= 1 \\
(\triangle_1\triangle_3|\triangle_3) &= (\triangle_2\triangle_4|\quad) \\
&= 1 \\
(\triangle_1\triangle_4|\triangle_4) &= (\triangle_2\triangle_3|\quad) \\
&= 1 \\
(\triangle_1\triangle_5|\triangle_5) &= (\triangle_3\triangle_5|\quad) \\
&= 1 \\
(\triangle_1\triangle_6|\triangle_6) &= (\triangle_3\triangle_6|\quad) \\
&= 1 \\
(\triangle_2\triangle_5|\triangle_6) &= (\triangle_4\triangle_5|\quad) \\
&= 1 \\
(\triangle_2\triangle_6|\triangle_5) &= (\triangle_4\triangle_6|\quad) \\
&= 1 \\
(\Sigma_i\Sigma_i|\quad) &= (\Sigma_1\Sigma_1|\quad) \\
&\quad i = 1, 2, 3, 4 \\
(\Sigma_1\Sigma_2|\quad) &= (\Sigma_3\Sigma_4|\quad) \\
(\Sigma_1\Sigma_3|\quad) &= (\Sigma_2\Sigma_4|\quad) \\
(\Sigma_1\Sigma_4|\quad) &= (\Sigma_2\Sigma_3|\quad) \\
(\Sigma_i\Sigma_i|\Gamma_1^+) &= (\quad|\Gamma_4^-) \\
&= (\quad|\Gamma_5^+) \\
&= (\quad|\Gamma_6^-) \\
&= 1 \\
&\quad i = 1, 2, 3, 4 \\
(\Sigma_1\Sigma_2|\Gamma_1^-) &= (\quad|\Gamma_4^+) \\
&= (\quad|\Gamma_5^-) \\
&= (\quad|\Gamma_6^+) \\
&= 1 \\
(\Sigma_1\Sigma_3|\Gamma_2^-) &= (\quad|\Gamma_3^+) \\
&= (\quad|\Gamma_5^-) \\
&= (\quad|\Gamma_6^+) \\
&= 1 \\
(\Sigma_1\Sigma_4|\Gamma_2^+) &= (\quad|\Gamma_3^-) \\
&= 1 \\
(\Sigma_i\Sigma_i|\Sigma_1') &= 1^{1)} \\
&\quad i = 1, 2, 3, 4 \\
(\Sigma_1\Sigma_i|\Sigma_i') &= 1
\end{aligned}$$

$$\begin{aligned}
&\quad i = 1, 2, 3, 4 \\
(\Sigma_3\Sigma_4|\Sigma_2') &= 1 \\
(\Sigma_2\Sigma_4|\Sigma_3') &= 1 \\
(\Sigma_2\Sigma_3|\Sigma_4') &= 1 \\
(\Sigma_1\Sigma_2|\Sigma_2) &= (\Sigma_1\Sigma_3|\quad) \\
&= (\Sigma_2\Sigma_4|\quad) \\
&= (\Sigma_3\Sigma_4|\quad) \\
&= 1 \\
(\Sigma_1\Sigma_2|\Sigma_3) &= (\Sigma_1\Sigma_3|\quad) \\
&= (\Sigma_2\Sigma_4|\quad) \\
&= (\Sigma_3\Sigma_4|\quad) \\
&= 1 \\
(\Sigma_i\Sigma_i|\Sigma_1) &= (\quad|\Sigma_4) \\
&= 1 \\
&\quad i = 1, 2, 3, 4 \\
(\Sigma_2\Sigma_3|\Sigma_1) &= (\quad|\Sigma_4) \\
&= 1 \\
(\Sigma_1\Sigma_4|\Sigma_1) &= (\quad|\Sigma_4) \\
&= 1 \\
(\Sigma_i\Sigma_i|T_1) &= (\quad|T_4) \\
&= 1 \\
&\quad i = 1, 2, 3, 4 \\
(\Sigma_1\Sigma_2|T_2) &= (\Sigma_1\Sigma_3|\quad) \\
&= (\Sigma_2\Sigma_4|\quad) \\
&= (\Sigma_3\Sigma_4|\quad) \\
&= 1 \\
(\Sigma_1\Sigma_2|T_3) &= (\Sigma_1\Sigma_3|\quad) \\
&= (\Sigma_2\Sigma_4|\quad) \\
&= (\Sigma_3\Sigma_4|\quad) \\
&= 1 \\
(\Sigma_2\Sigma_3|T_1) &= (\Sigma_1\Sigma_4|\quad) \\
&= 1 \\
(\Sigma_2\Sigma_3|T_4) &= (\Sigma_1\Sigma_4|\quad) \\
&= 1 \\
(R_1R_2|\quad) &= (R_3R_4|\quad) \\
(R_1R_3|\quad) &= (R_2R_4|\quad) \\
(R_1R_4|\quad) &= (R_2R_3|\quad) \\
(R_iR_i|\quad) &= (R_1R_1|\quad) \\
&\quad i = 1, 2, 3, 4 \\
(R_iR_i|\Gamma_2^-) &= (\quad|\Gamma_3^+) \\
&= (\quad|\Gamma_5^-) \\
&= (\quad|\Gamma_6^+) \\
&= 1 \\
&\quad i = 1, 2, 3, 4 \\
(R_1R_2|\Gamma_2^+) &= (\quad|\Gamma_3^-)
\end{aligned}$$

---

1) Σ' 的波矢是 $4\pi\begin{pmatrix} 0 \\ \dfrac{k}{\sqrt{3}\,a} \\ 0 \end{pmatrix}$

$= (\quad | \Gamma_5^+)$
$= (\quad | \Gamma_6^-)$
$= 1$

$(R_1R_3 | \Gamma_1^+) = (\quad | \Gamma_4^-)$
$= (\quad | \Gamma_5^+)$
$= (\quad | \Gamma_6^-)$
$= 1$

$(R_1R_4 | \Gamma_1^-) = (\quad | \Gamma_4^+)$
$= (\quad | \Gamma_5^-)$
$= (\quad | \Gamma_6^+)$
$= 1$

$(R_iR_i | R_1) = 1 \qquad i = 1, 2, 3, 4$

$(R_1R_i | R_i) = 1 \qquad i = 1, 2, 3, 4$

$(R_3R_4 | R_2) = (R_1R_2 | \quad)$
$= 1$

$(R_2R_4 | R_3) = (R_1R_3 | \quad)$
$= 1$

$(R_2R_3 | R_4) = (R_1R_4 | \quad)$
$= 1$

$(R_iR_i | \Sigma_1) = (\quad | \Sigma_4)$
$= 1$
$i = 1, 2, 3, 4$

$(R_1R_2 | \Sigma_2) = (R_1R_3 | \quad)$
$= (R_2R_4 | \quad)$
$= (R_3R_4 | \quad)$
$= 1$

$(R_1R_2 | \Sigma_3) = (R_1R_3 | \quad)$
$= (R_2R_4 | \quad)$
$= (R_3R_4 | \quad)$
$= 1$

$(R_2R_3 | \Sigma_1) = (R_1R_4 | \quad)$
$= 1$

$(R_2R_3 | \Sigma_4) = (R_1R_4 | \quad)$
$= 1$

$(R_iR_i | T_2) = (\quad | T_3)$
$= 1$
$i = 1, 2, 3, 4$

$(R_1R_2 | T_1) = (R_1R_3 | \quad)$
$= (R_2R_4 | \quad)$
$= (R_3R_4 | \quad)$
$= 1$

$(R_1R_2 | T_4) = (R_1R_3 | \quad)$
$= (R_2R_4 | \quad)$
$= (R_3R_4 | \quad)$
$= 1$

$(R_2R_3 | T_2) = (R_1R_4 | \quad)$
$= 1$

$(R_2R_3 | T_3) = (R_1R_4 | \quad)$
$= 1$

$(T_1T_2 | \quad) = (T_3T_4 | \quad)$

$(T_1T_3 | \quad) = (T_2T_4 | \quad)$

$(T_1T_4 | \quad) = (T_2T_3 | \quad)$

$(T_iT_i | \quad) = (T_1T_1 | \quad)$
$i = 1, 2, 3, 4$

$(T_iT_i | \Gamma_1^+) = (\quad | \Gamma_3^-)$
$= (\quad | \Gamma_5^+)$
$= (\quad | \Gamma_6^-)$
$= 1$
$i = 1, 2, 3, 4$

$(T_1T_2 | \Gamma_1^-) = (\quad | \Gamma_3^+)$
$= (\quad | \Gamma_5^-)$
$= (\quad | \Gamma_6^+)$
$= 1$

$(T_1T_3 | \Gamma_2^-) = (\quad | \Gamma_4^+)$
$= (\quad | \Gamma_5^-)$
$= (\quad | \Gamma_6^+)$
$= 1$

$(T_1T_4 | \Gamma_2^+) = (\quad | \Gamma_4^-)$
$= (\quad | \Gamma_5^+)$
$= (\quad | \Gamma_6^-)$
$= 1$

$(T_iT_i | \Sigma_1) = (\quad | \Sigma_4)$
$= 1$
$i = 1, 2, 3, 4$

$(T_1T_2 | \Sigma_2) = (T_3T_4 | \quad)$
$= (T_1T_3 | \quad)$
$= (T_2T_4 | \quad)$
$= 1$

$(T_1T_2 | \Sigma_3) = (T_3T_4 | \quad)$
$= (T_1T_3 | \quad)$
$= (T_2T_4 | \quad)$
$= 1$

$(T_1T_4 | \Sigma_1) = (T_2T_3 | \quad)$
$= 1$

$(T_1T_4 | \Sigma_4) = (T_2T_3 | \quad)$
$= 1$

$(T_iT_i | T_1) = (\quad | T_4)$
$= 1$
$i = 1, 2, 3, 4$

$(T_1T_2 | T_2) = (T_3T_4 | \quad)$
$= (T_1T_3 | \quad)$
$= (T_2T_4 | \quad)$
$= 1$

$(T_1T_2 | T_3) = (T_3T_4 | \quad)$
$= (T_1T_3 | \quad)$
$= (T_2T_4 | \quad)$
$= 1$

$(T_2T_3 | T_1) = (T_1T_4 | \quad)$
$= 1$

$(T_2T_3 | T_4) = (T_1T_4 | \quad)$

$= 1$

$(T_iT_i|T_1') = 1$[1]

$i = 1, 2, 3, 4$

$(T_1T_2|T_2') = 1$

$(T_2T_4|T_3') = 1$

$(T_2T_3|T_4') = 1$

$(T_3T_4|T_2') = 1$

$(T_1T_3|T_3') = 1$

$(T_1T_4|T_4') = 1$

$(S_1S_1|\Gamma_1^{\pm}) = (\quad|\Gamma_2^{\pm})$

$= (\quad|\Gamma_3^{\pm})$

$= (\quad|\Gamma_4^{\pm})$

$= 1$

$(S_1S_1|\Gamma_5^{\pm}) = (\quad|\Gamma_6^{\pm})$

$= 2$

$(S_1S_1|\Sigma_1) = (\quad|\Sigma_2)$

$= (\quad|\Sigma_3)$

$= (\quad|\Sigma_4)$

$= 2$

$(S_1S_1|T_1') = (\quad|T_2')$

$= (\quad|T_3')$

$= (\quad|T_4')$

$= 1$

$(S_1S_1|T_1) = (\quad|T_2)$

$= (\quad|T_3)$

$= (\quad|T_4)$

$= 2$

$(P_1P_1|\quad) = (P_2P_2|\quad)$

$(P_1P_3|\quad) = (P_2P_3|\quad)$

$(P_1P_1|\Gamma_1^{+}) = (\quad|\Gamma_2^{-})$

$= (\quad|\Gamma_3^{-})$

$= (\quad|\Gamma_4^{+})$

$= 1$

$(P_1P_2|\Gamma_1^{-}) = (\quad|\Gamma_2^{+})$

$= (\quad|\Gamma_3^{+})$

$= (\quad|\Gamma_4^{-})$

$= 1$

$(P_1P_3|\Gamma_5^{\pm}) = (\quad|\Gamma_6^{\pm})$

$= 1$

$(P_3P_3|\Gamma_1^{\pm}) = (\quad|\Gamma_2^{\pm})$

$= (\quad|\Gamma_3^{\pm})$

$= (\quad|\Gamma_4^{\pm})$

$= (\quad|\Gamma_5^{\pm})$

$= (\quad|\Gamma_6^{\pm})$

$= 1$

$(P_1P_1|P_1')$[2] $= (P_2P_2|\quad)$

$= 1$

$(P_1P_2|P_2') = 1$

$(P_2P_3|P_3') = (P_1P_3|\quad)$

$= 1$

$(P_3P_3|P_1') = (\quad|P_2')$

$= (\quad|P_3') = 1$

$(P_1P_1|K_1) = (P_2P_2|\quad)$

$= 1$

$(P_1P_1|K_4) = (\quad P_2P_2|\quad)$

$= 1$

$(P_1P_2|K_2) = (\quad|K_3)$

$= 1$

$(P_1P_3|K_5) = (\quad|K_6)$

$= 1$

$(P_2P_3|K_5) = (\quad|K_6)$

$= 1$

$(P_3P_3|K_i) = 1 \qquad i = 1, 2, 3, 4, 5, 6$

$(P_1P_1|\Delta_1')$[3] $= (P_2P_2|\quad)$

$= 1$

$(P_1P_1|\Delta_4') = (P_2P_2|\quad)$

$= 1$

$(P_1P_2|\Delta_2') = (\quad|\Delta_3')$

$= 1$

$(P_1P_3|\Delta_5') = (P_2P_3|\quad)$

$= 1$

$(P_1P_3|\Delta_6') = (P_2P_3|\quad)$

---

1) T' 的波矢是 $\frac{2\pi k}{a}\begin{pmatrix}2\\0\\0\end{pmatrix}$.

2) P' 的波矢是 $\begin{pmatrix}-\frac{2\pi}{3a}\\-\frac{2\pi}{\sqrt{3}\,a}\\\frac{2k}{c}\end{pmatrix}$.

3) $\Delta' = \begin{pmatrix}0\\0\\\frac{2k}{c}\end{pmatrix}$.

$$= 1$$
$$(P_3P_3|\Delta_1') = (\quad|\Delta_2')$$
$$= (\quad|\Delta_3')$$
$$= (\quad|\Delta_4')$$
$$= (\quad|\Delta_5') = (\quad|\Delta_6') = 1$$
$$(U_1U_2|\quad) = (U_3U_4|\quad)$$
$$(U_1U_3|\quad) = (U_2U_4|\quad)$$
$$(U_1U_4|\quad) = (U_2U_3|\quad)$$
$$(U_iU_i|\quad) = (U_1U_1|\quad)$$
$$i = 1, 2, 3, 4$$
$$(U_iU_i|\Gamma_1^+) = (\quad|\Gamma_2^-)$$
$$= (\quad|\Gamma_5^\pm)$$
$$= 1$$
$$i = 1, 2, 3, 4$$
$$(U_1U_2|\Gamma_3^+) = (\quad|\Gamma_4^-)$$
$$= (\quad|\Gamma_6^\pm)$$
$$= 1$$
$$(U_1U_3|\Gamma_3^-) = (\quad|\Gamma_6^\pm)$$
$$= (\quad|\Gamma_4^+)$$
$$= 1$$
$$(U_2U_3|\Gamma_1^-) = (\quad|\Gamma_2^+)$$
$$= (\quad|\Gamma_5^\pm)$$
$$= 1$$
$$(U_iU_i|U_1) = (\quad|U_4)$$
$$= 1$$
$$i = 1, 2, 3, 4$$
$$(U_1U_2|U_2) = (U_1U_3|\quad)$$
$$= (U_2U_4|\quad)$$
$$= (U_3U_4|\quad)$$
$$= 1$$
$$(U_1U_2|U_3) = (U_1U_3|\quad)$$
$$= (U_2U_4|\quad)$$
$$= (U_3U_4|\quad)$$
$$= 1$$
$$(U_1U_4|U_1) = (\quad|U_4)$$
$$= 1$$
$$(U_iU_i|M_1^\pm) = (\quad|M_4^\pm)$$
$$= 1$$
$$i = 1, 2, 3, 4$$
$$(U_1U_2|M_2^\pm) = (\quad|M_3^\pm)$$
$$= 1$$
$$(U_2U_3|M_1^\pm) = (\quad|M_4^\pm)$$
$$= 1$$
$$(U_1U_3|M_2^\pm) = (U_2U_4|\quad)$$
$$= (U_3U_4|\quad)$$
$$= 1$$
$$(U_1U_3|M_3^\pm) = (U_2U_4|\quad)$$
$$= (U_3U_4|\quad)$$
$$= 1$$
$$(U_1U_4|M_1^\pm) = (\quad|M_4^\pm)$$
$$= 1$$
$$(U_iU_i|\Delta_1) = (\quad|\Delta_5)$$
$$= 1$$
$$i = 1, 2, 3, 4$$
$$(U_1U_2|\Delta_2) = (\quad|\Delta_6)$$
$$= 1$$
$$(U_3U_4|\Delta_2) = (\quad|\Delta_6)$$
$$= 1$$
$$(U_1U_3|\Delta_4) = (\quad|\Delta_6)$$
$$= 1$$
$$(U_2U_4|\Delta_4) = (\quad|\Delta_6)$$
$$= 1$$
$$(U_1U_4|\Delta_3) = (\quad|\Delta_5)$$
$$= 1$$
$$(U_2U_3|\Delta_3) = (\quad|\Delta_5)$$
$$= 1$$

四、纖維鋅矿結构空間羣 (C_{6v}^4) 的簡約系数

計算步驟与前面相同．采用文献[9]所列的波矢羣品格表．

基矢，倒格子基矢，以及部分平移均和六角密积相同，見表 2．

布里渊区的对称点(軸)的坐标及不等价波矢数均見表 3．

表 6 轉动对称操作[1)]

$(\alpha\|0)$ 型	$(\alpha\|\tau)$ 型
ε：不变 δ_3, δ_3^{-1}：繞 $\mathbf{t}_1$ 軸的三度轉动 $\rho_i' = i\delta_{2i}'$ $i = 2, 3, 4$	δ_2：繞 $\mathbf{t}_1$ 軸二度轉动 δ_6, δ_6^{-1}：繞 $\mathbf{t}_1$ 軸 6 度轉动 $\rho_i'' = i\delta_{2i}''$ $i = 2, 3, 4$

1) 为与六角密积結构統一起見，操作符号引用六角密积結构的．

波矢星的直接乘积簡約系数 $(K_j K_{j'} | K_{j''})$ 大部分和六角密积結构相同，其和六角密积結构不同者，列于表 7．空間羣簡約系数列于表 8．

表 7 纤維鋅矿結构波矢星的直接乘积簡約系数 $(K_j K_{j'} | K_{j''})$

$(\Delta\Delta \| \Delta') = 1$	$(UU \| U') = 2$	$(\Delta K \| P) = 1$
$(PP \| P') = 1$	$(UU \| \Delta') = 3$	$(\Delta P \| P') = 1$
$(PP \| \Delta') = 2$	$(\Delta M \| U) = 1$	$(\Delta U \| U') = 1$

表 8 纤維鋅矿結构空間羣簡約系数 $(K_j^{(m)} K_{j'}^{(m')} | K_{j''}^{(m'')})$

$$
\begin{aligned}
&(\Gamma_1 k_j^{(m)} | k_j^{(m)}) = 1 \\
&(\Gamma_1\Gamma_2 | \quad) = (\Gamma_3\Gamma_4 | \quad) \\
&(\Gamma_1\Gamma_3 | \quad) = (\Gamma_2\Gamma_4 | \quad) \\
&(\Gamma_1\Gamma_4 | \quad) = (\Gamma_2\Gamma_3 | \quad) \\
&(\Gamma_1\Gamma_5 | \quad) = (\Gamma_2\Gamma_5 | \quad) \\
&(\Gamma_1\Gamma_6 | \quad) = (\Gamma_2\Gamma_6 | \quad) \\
&(\Gamma_3\Gamma_5 | \quad) = (\Gamma_4\Gamma_5 | \quad) \\
&(\Gamma_3\Gamma_6 | \quad) = (\Gamma_4\Gamma_6 | \quad) \\
&(\Gamma_i\Gamma_i | \quad) = (\Gamma_1\Gamma_1 | \quad) \\
&\qquad i = 1, 2, 3, 4 \\
&(\Gamma_5\Gamma_5 | \quad) = (\Gamma_6\Gamma_6 | \quad) \\
&(\Gamma_i\Gamma_i | \Gamma_1) = 1 \qquad i = 1, 2, 3, 4 \\
&(\Gamma_j\Gamma_j | \Gamma_1) = (\quad | \Gamma_2) = (\quad | \Gamma_5) \\
&\qquad = 1 \qquad j = 5, 6 \\
&(\Gamma_1\Gamma_2 | \Gamma_2) = 1 \\
&(\Gamma_2\Gamma_4 | \Gamma_3) = 1 \\
&(\Gamma_2\Gamma_5 | \Gamma_5) = 1 \\
&(\Gamma_2\Gamma_6 | \Gamma_6) = (\Gamma_4\Gamma_5 | \quad) \\
&\qquad = 1 \\
&(\Gamma_4\Gamma_6 | \Gamma_5) = (\Gamma_5\Gamma_5 | \quad) \\
&\qquad = (\Gamma_6\Gamma_6 | \quad) \\
&\qquad = 1 \\
&(\Gamma_5\Gamma_6 | \Gamma_3) = (\quad | \Gamma_4) \\
&\qquad = (\quad | \Gamma_6) \\
&\qquad = 1 \\
&(A_1A_2 | \quad) = (A_3A_4 | \quad) \\
&(A_1A_3 | \quad) = (A_2A_4 | \quad) \\
&(A_1A_4 | \quad) = (A_2A_3 | \quad) \\
&(A_1A_5 | \quad) = (A_2A_5 | \quad) \\
&(A_1A_6 | \quad) = (A_2A_6 | \quad) \\
&(A_3A_5 | \quad) = (A_4A_5 | \quad) \\
&(A_3A_6 | \quad) = (A_4A_6 | \quad) \\
&(A_iA_i | \quad) = (A_1A_1 | \quad) \\
&\qquad i = 1, 2, 3, 4 \\
&(A_5A_5 | \quad) = (A_6A_6 | \quad) \\
&(A_iA_i | \Gamma_3) = 1 \\
&\qquad i = 1, 2, 3, 4 \\
&(A_jA_j | \Gamma_3) = (\quad | \Gamma_4) \\
&\qquad = (\quad | \Gamma_6) \\
&\qquad = 1 \\
&\qquad j = 5, 6
\end{aligned}
$$

$$
\begin{aligned}
&(A_1A_2 | \Gamma_4) = 1 \\
&(A_1A_3 | \Gamma_1) = 1 \\
&(A_1A_4 | \Gamma_2) = 1 \\
&(A_1A_5 | \Gamma_6) = (A_3A_6 | \quad) \\
&\qquad = 1 \\
&(A_1A_6 | \Gamma_5) = (A_3A_5 | \quad) \\
&\qquad = 1 \\
&(A_5A_6 | \Gamma_1) = (\quad | \Gamma_2) = (\quad | \Gamma_5) \\
&\qquad = 1 \\
&(A_i\Gamma_1 | A_i) = 1 \\
&\qquad i = 1, 2, 3, 4 \\
&(A_5\Gamma_1 | A_5) = (A_5\Gamma_2 | A_5) \\
&\qquad = (A_6\Gamma_1 | A_6) \\
&\qquad = (A_6\Gamma_2 | A_6) \\
&\qquad = 1 \\
&(A_1\Gamma_2 | A_2) = 1 \\
&(A_1\Gamma_3 | A_3) = (A_2\Gamma_4 | \quad) \\
&\qquad = 1 \\
&(A_1\Gamma_4 | A_4) = (A_2\Gamma_3 | \quad) \\
&\qquad = 1 \\
&(A_1\Gamma_5 | A_5) = (A_2\Gamma_5 | \quad) \\
&\qquad = 1 \\
&(A_1\Gamma_6 | A_6) = (A_2\Gamma_6 | \quad) \\
&\qquad = 1 \\
&(A_3\Gamma_2 | A_4) = 1 \\
&(A_3\Gamma_6 | A_5) = (A_6\Gamma_4 | \quad) \\
&\qquad = 1 \\
&(A_3\Gamma_5 | A_6) = (A_5\Gamma_3 | \quad) \\
&\qquad = 1 \\
&(M_iM_i | \quad) = (M_1M_1 | \quad) \\
&\qquad i = 1, 2, 3, 4 \\
&(M_1M_2 | \quad) = (M_3M_4 | \quad) \\
&(M_1M_3 | \quad) = (M_2M_4 | \quad) \\
&(M_1M_4 | \quad) = (M_2M_3 | \quad) \\
&(M_iM_i | \Gamma_1) = (\quad | \Gamma_5) \\
&\qquad = 1 \\
&\qquad i = 1, 2, 3, 4 \\
&(M_1M_2 | \Gamma_4) = (\quad | \Gamma_6) \\
&\qquad = 1 \\
&(M_1M_3 | \Gamma_3) = (\quad | \Gamma_6) \\
&\qquad = 1
\end{aligned}
$$

$(M_1M_4|\Gamma_2) = (\quad\quad|\Gamma_5)$
$= 1$

$(M_iM_j|\quad\quad) = (M_jM_i|\quad\quad)$

$(M_i\Gamma_1|M_i) = (M_i\Gamma_5|M_i)$
$= 1$
$i = 1, 2, 3, 4$

$(M_1\Gamma_4|M_2) = (M_1\Gamma_6|M_2)$
$= 1$

$(M_1\Gamma_3|M_3) = (M_1\Gamma_6|M_3)$
$= 1$

$(M_1\Gamma_2|M_4) = (M_1\Gamma_5|M_4)$
$= 1$

$(M_iM_i|M_1) = (\quad\quad|M_4)$
$= 1$
$i = 1, 2, 3, 4$

$(M_1M_2|M_2) = (\quad\quad|M_3)$
$= 1$

$(M_1M_3|M_3) = (\quad\quad|M_2)$
$= 1$

$(M_1M_4|M_1) = (\quad\quad|M_4)$
$= 1$

$(M_3M_4|M_2) = (M_1M_3|\quad\quad)$
$= (M_2M_4|\quad\quad)$
$= 1$

$(M_3M_4|M_3) = (M_1M_3|\quad\quad)$
$= (M_2M_4|\quad\quad)$
$= 1$

$(M_2M_3|M_1) = (\quad\quad|M_4)$
$= 1$

$(L_iL_i|\quad\quad) = (L_1L_1|\quad\quad)$
$i = 1, 2, 3, 4$

$(L_1L_2|\quad\quad) = (L_3L_4|\quad\quad)$
$(L_1L_3|\quad\quad) = (L_2L_4|\quad\quad)$
$(L_1L_4|\quad\quad) = (L_2L_3|\quad\quad)$

$(L_iL_i|\Gamma_3) = (\quad\quad|\Gamma_6)$
$= 1 \qquad i = 1, 2, 3, 4$

$(L_1L_2|\Gamma_2) = (\quad\quad|\Gamma_5)$
$= 1$

$(L_1L_3|\Gamma_1) = (\quad\quad|\Gamma_5)$
$= 1$

$(L_1L_4|\Gamma_4) = (\quad\quad|\Gamma_6)$
$= 1$

$(L_i\Gamma_1|L_i) = (L_i\Gamma_5|L_i)$
$= 1$
$i = 1, 2, 3, 4$

$(L_1\Gamma_4|L_2) = (L_1\Gamma_6|L_2)$
$= 1$

$(L_1\Gamma_3|L_3) = (L_1\Gamma_6|L_3)$
$= 1$

$(L_1\Gamma_2|L_4) = (L_1\Gamma_5|L_4)$
$= 1$

$(L_2\Gamma_2|L_3) = (L_2\Gamma_5|L_3)$
$= 1$

$(L_2\Gamma_3|L_4) = (L_2\Gamma_6|L_4)$
$= (L_2\Gamma_6|\Gamma_1)$
$= 1$

$(L_iL_i|M_2) = (\quad\quad|M_3)$
$= 1$
$i = 1, 2, 3, 4$

$(L_1L_2|M_1) = (L_3L_4|\quad\quad)$
$= (L_1L_3|\quad\quad)$
$= (L_2L_4|\quad\quad)$
$= 1$

$(L_1L_2|M_4) = (L_3L_4|\quad\quad)$
$= (L_1L_3|\quad\quad)$
$= (L_2L_4|\quad\quad)$
$= 1$

$(L_2L_3|M_2) = (\quad\quad|M_3)$
$= 1$

$(L_1L_4|M_2) = (\quad\quad|M_3)$
$= 1$

$(K_1K_1|\quad\quad) = (K_2K_2|\quad\quad)$
$(K_1K_3|\quad\quad) = (K_2K_3|\quad\quad)$
$(K_iK_j|\quad\quad) = (K_jK_i|\quad\quad)$

$(K_iK_i|\Gamma_1) = (\quad\quad|\Gamma_4)$
$= 1 \qquad i = 1, 2$

$(K_3K_3|\Gamma_1) = (\quad\quad|\Gamma_2)$
$= (\quad\quad|\Gamma_3)$
$= (\quad\quad|\Gamma_4) = (\quad\quad|\Gamma_5) = (\quad\quad|\Gamma_6)$
$= 1$

$(K_1K_2|\Gamma_2) = (\quad\quad|\Gamma_3)$
$= 1$

$(K_1K_3|\Gamma_5) = (\quad\quad|\Gamma_6)$
$= 1$

$(K_2K_3|\Gamma_5) = (\quad\quad|\Gamma_6)$
$= 1$

$(K_i\Gamma_1|K_i) = (K_i\Gamma_4|K_i)$
$= 1$
$i = 1, 2$

$(K_3\Gamma_1|K_3) = (K_3\Gamma_2|\quad\quad)$
$= (K_3\Gamma_3|\quad\quad)$
$= (K_3\Gamma_4|\quad\quad) = (K_3\Gamma_5|\quad\quad)$
$= (K_3\Gamma_6|\quad\quad) = 1$

$(K_1\Gamma_2|K_2) = (K_1\Gamma_3|\quad\quad)$
$= 1$

$(K_1\Gamma_5|K_3) = (K_1\Gamma_6|\quad\quad)$
$= 1$

$$(K_2\Gamma_5|K_3)=(K_2\Gamma_6|\quad)$$
$$=1$$
$$(K_1K_1|K_1)=(K_2K_2|K_1)$$
$$=1$$
$$(K_1K_2|K_2)=1$$
$$(K_3K_3|K_1)=(\quad|K_2)=(\quad|K_3)$$
$$=1$$
$$(K_2K_3|K_3)=(K_1K_3|\quad)$$
$$=1$$

$$(H_1H_1|\quad)=(H_2H_2|\quad)$$
$$(H_1H_3|\quad)=(H_2H_3|\quad)$$
$$(H_iH_j|\quad)=(H_jH_i|\quad)$$
$$(H_iH_i|\Gamma_2)=(\quad|\Gamma_3)$$
$$=1\qquad i=1,2$$
$$(H_1H_2|\Gamma_1)=(\quad|\Gamma_4)$$
$$=1$$
$$(H_1H_3|\Gamma_5)=(\quad|\Gamma_6)$$
$$=1$$
$$(H_3H_3|\Gamma_1)=(\quad|\Gamma_2)$$
$$=(\quad|\Gamma_3)$$
$$=(\quad|\Gamma_4)$$
$$=1$$
$$(H_3H_3|\Gamma_5)=(\quad|\Gamma_6)$$
$$=1$$
$$(H_1\Gamma_2|H_2)=(H_1\Gamma_3|\quad)$$
$$=1$$
$$(H_1\Gamma_5|H_3)=(H_1\Gamma_6|\quad)$$
$$=1$$

$$(H_3\Gamma_1|H_3)=(H_3\Gamma_2|\quad)$$
$$=(H_3\Gamma_3|\quad)$$
$$=(H_3\Gamma_4|\quad)$$
$$=(H_3\Gamma_5|\quad)$$
$$=(H_3\Gamma_6|\quad)$$
$$=1$$

$$(H_2\Gamma_2|H_1)=(H_2\Gamma_3|\quad)$$
$$=1$$
$$(H_3\Gamma_5|H_1)=(H_3\Gamma_6|\quad)$$
$$=1$$

$$(H_3\Gamma_5|H_2)=(H_3\Gamma_6|H_2)=1$$
$$(H_iH_i|K_2)=1\qquad i=1,2$$
$$(H_3H_3|K_1)=(\quad|K_2)=(\quad|K_3)$$
$$=1$$
$$(H_1H_2|K_1)=1$$
$$(H_2H_3|K_3)=(H_1H_3|\quad)$$
$$=1$$

$$(\Delta_i\Delta_i|\quad)=(\Delta_1\Delta_1|\quad)$$
$$i=1,2,3,4$$
$$(\Delta_5\Delta_5|\quad)=(\Delta_6\Delta_6|\quad)$$
$$(\Delta_1\Delta_2|\quad)=(\Delta_3\Delta_4|\quad)$$
$$(\Delta_1\Delta_3|\quad)=(\Delta_2\Delta_4|\quad)$$
$$(\Delta_1\Delta_4|\quad)=(\Delta_2\Delta_3|\quad)$$
$$(\Delta_1\Delta_5|\quad)=(\Delta_2\Delta_5|\quad)$$
$$(\Delta_1\Delta_6|\quad)=(\Delta_2\Delta_6|\quad)$$
$$(\Delta_3\Delta_5|\quad)=(\Delta_4\Delta_5|\quad)$$
$$(\Delta_3\Delta_6|\quad)=(\Delta_4\Delta_6|\quad)$$
$$(\Delta_i\Delta_i|\Delta_1)=1\qquad i=1,2,3,4$$
$$(\Delta_5\Delta_6|\Delta_3)=(\quad|\Delta_4)=(\quad|\Delta_6)$$
$$=1$$

$$(\Delta_5\Delta_5|\Delta_1)=(\quad|\Delta_2)=(\quad|\Delta_5)$$
$$=1$$

$$(\Delta_1\Delta_2|\Delta_2)=1$$
$$(\Delta_2\Delta_4|\Delta_3)=1$$
$$(\Delta_2\Delta_3|\Delta_4)=1$$
$$(\Delta_1\Delta_5|\Delta_5)=1$$
$$(\Delta_1\Delta_6|\Delta_6)=(\Delta_3\Delta_5|\quad)$$
$$=1$$

$$(\Delta_4\Delta_6|\Delta_5)=1$$
$$(\Delta_i\Gamma_1|\Delta_i)=1\qquad i=1,2,3,4$$
$$(\Delta_j\Gamma_1|\Delta_j)=(\Delta_j\Gamma_2|\quad)$$
$$=1\qquad j=5,6$$

$$(\Delta_1\Gamma_2|\Delta_2)=1$$
$$(\Delta_1\Gamma_3|\Delta_3)=1$$
$$(\Delta_1\Gamma_4|\Delta_4)=1$$
$$(\Delta_1\Gamma_5|\Delta_5)=(\Delta_3\Gamma_6|\quad)$$
$$=1$$

$$(\Delta_1\Gamma_6|\Delta_6)=(\Delta_2\Gamma_6|\quad)$$
$$=1$$

$$(\Delta_3\Gamma_2|\Delta_4)=(\Delta_2\Gamma_3|\quad)$$
$$=1$$
$$(\Delta_2\Gamma_4|\Delta_3)=1$$
$$(\Delta_2\Gamma_5|\Delta_5)=(\Delta_4\Gamma_6|\quad)$$
$$=1$$

$$(\Sigma_1\Sigma_1|\quad)=(\Sigma_2\Sigma_2|\quad)$$
$$(\Sigma_1\Sigma_2|\quad)=(\Sigma_2\Sigma_1|\quad)$$
$$(\Sigma_i\Sigma_i|\Gamma_1)=(\quad|\Gamma_3)=(\quad|\Gamma_5)$$
$$=(\quad|\Gamma_6)=1\qquad i=1,2$$
$$(\Sigma_1\Sigma_2|\Gamma_2)=(\quad|\Gamma_4)=(\quad|\Gamma_5)$$
$$=(\quad|\Gamma_6)=1$$

$$(\Sigma_i\Gamma_1|\Sigma_i)=(\Sigma_i\Gamma_3|\quad)$$
$$=(\Sigma_i\Gamma_5|\quad)$$
$$=(\Sigma_i\Gamma_6|\quad)=1\qquad i=1,2$$

$$(\Sigma_1\Gamma_2|\Sigma_2)=(\Sigma_1\Gamma_4|\quad)=(\Sigma_1\Gamma_5|\quad)$$
$$=(\Sigma_1\Gamma_6|\quad)=1$$
$$(\Sigma_2\Gamma_3|\Sigma_1)=(\Sigma_2\Gamma_4|\quad)=(\Sigma_2\Gamma_5|\quad)$$
$$=(\Sigma_2\Gamma_6|\quad)=1$$

$$(\Sigma_i\Sigma_i|\Sigma_1')^{1)} = 1 \qquad i = 1, 2$$

$$(\Sigma_1\Sigma_2|\Sigma_2') = (\Sigma_2\Sigma_1|\quad) = 1$$

$$\begin{aligned}(\Sigma_i\Sigma_i|\Sigma_1) &= (\quad|\Sigma_2)\\ &= 1 \qquad i = 1, 2\end{aligned}$$

$$\begin{aligned}(\Sigma_i\Sigma_i|T_1) &= (\quad|T_2)\\ &= 1 \qquad i = 1, 2\end{aligned}$$

$$\begin{aligned}(\Sigma_1\Sigma_2|\Sigma_1) &= (\quad|\Sigma_2)\\ &= 1\end{aligned}$$

$$\begin{aligned}(\Sigma_1\Sigma_2|T_1) &= (\quad|T_2)\\ &= 1\end{aligned}$$

$$\begin{aligned}(R_iR_i|\Gamma_1) &= (\quad|\Gamma_3) = (\quad|\Gamma_5)\\ &= (\quad|\Gamma_6) = 1 \qquad i = 1, 2\end{aligned}$$

$$\begin{aligned}(R_1R_2|\Gamma_2) &= (\quad|\Gamma_4) = (\quad|\Gamma_5)\\ &= (\quad|\Gamma_6) = 1\end{aligned}$$

$$(R_1R_1|\quad) = (R_2R_2|\quad)$$

$$(R_1R_2|\quad) = (R_2R_1|\quad)$$

$$\begin{aligned}(R_i\Gamma_1|R_i) &= (R_i\Gamma_3|\quad) = (R_i\Gamma_5|\quad)\\ &= (R_i\Gamma_6|\quad) = 1 \qquad i = 1, 2\end{aligned}$$

$$\begin{aligned}(R_1\Gamma_2|R_2) &= (R_1\Gamma_4|\quad) = (R_1\Gamma_5|\quad)\\ &= (R_1\Gamma_6|\quad) = 1\end{aligned}$$

$$\begin{aligned}(R_2\Gamma_2|R_1) &= (R_2\Gamma_4|\quad) = (R_2\Gamma_5|\quad)\\ &= (R_2\Gamma_6|\quad) = 1\end{aligned}$$

$$(R_iR_i|\Sigma_1')^{2)} = 1 \qquad i = 1, 2$$

$$\begin{aligned}(R_1R_2|\Sigma_2') &= (R_2R_1|\Sigma_2')\\ &= 1\end{aligned}$$

$$\begin{aligned}(R_iR_i|\Sigma_1) &= (\quad|\Sigma_2)\\ &= (\quad|T_1)\\ &= (\quad|T_2)\\ &= 1 \qquad i = 1, 2\end{aligned}$$

$$\begin{aligned}(R_1R_2|\Sigma_1) &= (\quad|\Sigma_2)\\ &= (\quad|T_1)\\ &= (\quad|T_2)\\ &= 1\end{aligned}$$

$$(T_1T_1|\quad) = (T_2T_2|\quad)$$

$$(T_1T_2|\quad) = (T_2T_1|\quad)$$

$$\begin{aligned}(T_iT_i|\Gamma_1) &= (\quad|\Gamma_4)\\ &= (\quad|\Gamma_5)\\ &= (\quad|\Gamma_6)\\ &= 1 \qquad i = 1, 2\end{aligned}$$

$$\begin{aligned}(T_1T_2|\Gamma_2) &= (\quad|\Gamma_3)\\ &= (\quad|\Gamma_5)\\ &= (\quad|\Gamma_6)\\ &= 1\end{aligned}$$

$$\begin{aligned}(T_i\Gamma_1|T_i) &= (T_i\Gamma_4|\quad)\\ &= (T_i\Gamma_5|\quad)\\ &= (T_i\Gamma_6|\quad)\\ &= 1 \qquad i = 1, 2\end{aligned}$$

$$\begin{aligned}(T_1\Gamma_2|T_2) &= (T_1\Gamma_3|\quad)\\ &= (T_1\Gamma_5|\quad)\\ &= (T_1\Gamma_6|\quad)\\ &= 1\end{aligned}$$

$$\begin{aligned}(T_2\Gamma_2|T_1) &= (T_2\Gamma_3|\quad)\\ &= (T_2\Gamma_5|\quad)\\ &= (T_2\Gamma_6|\quad)\\ &= 1\end{aligned}$$

$$(T_iT_i|T_1')^{3)} = 1 \qquad i = 1, 2$$

$$(T_1T_2|T_2') = (T_2T_1|\quad) = 1$$

$$\begin{aligned}(T_iT_i|\Sigma_1) &= (\quad|\Sigma_2)\\ &= (\quad|T_1)\\ &= (\quad|T_2)\\ &= 1 \qquad i = 1, 2\end{aligned}$$

$$\begin{aligned}(T_1T_2|\Sigma_1) &= (\quad|\Sigma_2)\\ &= (\quad|T_1)\\ &= (\quad|T_2)\\ &= 1\end{aligned}$$

$$(S_1S_1|\quad) = (S_2S_2|\quad)$$

$$(S_1S_2|\quad) = (S_2S_1|\quad)$$

$$\begin{aligned}(S_iS_i|\Gamma_2) &= (\quad|\Gamma_3) = (\quad|\Gamma_5)\\ &= (\quad|\Gamma_6)\\ &= 1 \qquad i = 1, 2\end{aligned}$$

$$\begin{aligned}(S_1S_2|\Gamma_1) &= (\quad|\Gamma_4) = (\quad|\Gamma_5)\\ &= (\quad|\Gamma_6) = 1\end{aligned}$$

$$\begin{aligned}(S_i\Gamma_1|S_i) &= (S_i\Gamma_4|\quad)\\ &= (S_i\Gamma_5|\quad)\\ &= (S_i\Gamma_6|\quad)\\ &= 1 \qquad i = 1, 2\end{aligned}$$

$$\begin{aligned}(S_1\Gamma_2|S_2) &= (S_1\Gamma_3|\quad)\\ &= (S_1\Gamma_5|\quad)\\ &= (S_1\Gamma_6|\quad) = 1\end{aligned}$$

$$\begin{aligned}(S_2\Gamma_2|S_1) &= (S_2\Gamma_3|\quad)\\ &= (S_2\Gamma_5|\quad)\end{aligned}$$

---

1) $\Sigma_1' = 2\pi\begin{pmatrix} 0 \\ \frac{2k}{\sqrt{3}\,a} \\ 0 \end{pmatrix}$.

2) 与 1) 相同.

3) $T_1' = \frac{\pi k}{a}\begin{pmatrix} 4 \\ 0 \\ 0 \end{pmatrix}$.

$$= (S_2\Gamma_6|\quad) = 1$$
$$(S_iS_i|T'_2) = 1 \qquad i = 1, 2$$
$$(S_1S_2|T'_1) = (S_2S_1|\quad)$$
$$= 1$$
$$(S_iS_i|\Sigma_1) = (\quad|\Sigma_2)$$
$$= (\quad|T_1)$$
$$= (\quad|T_2)$$
$$= 1 \qquad i = 1, 2$$
$$(S_1S_2|\Sigma_1) = (\quad|\Sigma_2) = (\quad|T_1)$$
$$= (\quad|T_2) = 1$$
$$(P_1P_1|\quad) = (P_2P_2|\quad)$$
$$(P_1P_3|\quad) = (P_3P_3|\quad)$$
$$(P_iP_i|P'_1)^{1)} = 1 \qquad i = 1, 2$$
$$(P_1P_2|P'_2) = 1$$
$$(P_2P_3|P'_3) = 1$$
$$(P_3P_3|P'_1) = (\quad|P'_2)$$
$$= (\quad|P'_3)$$
$$= 1$$
$$(P_iP_i|\Delta'_1)^{2)} = (\quad|\Delta'_4)$$
$$= 1 \qquad i = 1, 2$$
$$(P_1P_3|\Delta'_5) = (\quad|\Delta'_6)$$
$$= 1$$
$$(P_3P_3|\Delta'_1) = (\quad|\Delta'_2)$$
$$= (\quad|\Delta'_3)$$
$$= (\quad|\Delta'_4)$$
$$= (\quad|\Delta'_5)$$
$$= (\quad|\Delta'_6)$$
$$= 1$$
$$(P_1P_2|\Delta'_2) = (\quad|\Delta'_3)$$
$$= 1$$
$$(U_1U_2|\quad) = (U_3U_4|\quad)$$
$$(U_1U_3|\quad) = (U_2U_4|\quad)$$
$$(U_1U_4|\quad) = (U_2U_3|\quad)$$
$$(U_iU_i|\quad) = (U_1U_1|\quad)$$
$$i = 1, 2, 3, 4$$
$$(U_iU_i|U'_1)^{3)} = (\quad|U'_4)$$
$$= 1$$
$$i = 1, 2, 3, 4$$
$$(U_1U_2|U'_2) = (U_1U_3|\quad)$$
$$= (U_2U_4|\quad)$$
$$= (U_3U_4|\quad)$$
$$= 1$$
$$(U_1U_2|U'_3) = (U_1U_3|\quad) = (U_2U_4|\quad)$$
$$= (U_3U_4|\quad) = 1$$
$$(U_1U_4|U'_1) = (U_2U_3|U'_1)$$
$$= 1$$
$$(U_1U_4|U'_4) = (U_2U_3|\quad)$$
$$= 1$$
$$(U_iU_i|\Delta'_1)^{2)} = (|\Delta'_5)$$
$$= 1 \qquad i = 1, 2, 3, 4$$
$$(U_1U_2|\Delta'_4) = (\quad|\Delta'_6)$$
$$= 1$$
$$(U_1U_3|\Delta'_3) = (\quad|\Delta'_6)$$
$$= 1$$
$$(U_1U_4|\Delta'_2) = (\quad|\Delta'_5)$$
$$= 1$$
$$(U_3U_4|\Delta'_4) = (\quad|\Delta'_6)$$
$$= 1$$
$$(U_2U_4|\Delta'_3) = (\quad|\Delta'_6)$$
$$= 1$$
$$(U_2U_3|\Delta'_2) = (\quad|\Delta'_5)$$
$$= 1$$

五、討　　論

1）由結构的对称性来看，六角密积比纤維鋅矿多了反演心，和金刚石及閃鋅矿情況相似；这两个空間羣具有羣与子羣的关系，因此从对称性出发，可得到它們的波矢羣不可約表示之間有下列的对应关系.

---

1) $P'_1 = \begin{pmatrix} \frac{2\pi}{3a} \\ \frac{2\pi}{\sqrt{3}\,a} \\ \frac{2k}{c} \end{pmatrix}$.　　2) $\Delta'_1 = \begin{pmatrix} 0 \\ 0 \\ \frac{2k}{c} \end{pmatrix}$.

3) $U'_1 = \begin{pmatrix} 0 \\ \frac{2\pi}{\sqrt{3}\,a} \\ \frac{2k}{c} \end{pmatrix}$.

C_{6v}^4	D_{6h}^4	C_{6v}^4	D_{6h}^4	C_{6v}^4	D_{6h}^4	C_{6v}^4	D_{6h}^4
Γ_1	Γ_1^+, Γ_2^-	H_1	H_1	L_1	L_1	Σ_1	Σ_1
Γ_2	Γ_2^+, Γ_1^-	H_2		L_3		Σ_2	Σ_2
Γ_3	Γ_3^+, Γ_4^-	H_3	H_2	L_2	L_2	Σ_1	Σ_3
Γ_4	Γ_4^+, Γ_3^-			L_4		Σ_2	Σ_4
Γ_5	Γ_5^+, Γ_5^-	H_3	H_3	R_1	R_1	P_1	P_1
Γ_6	Γ_6^+, Γ_6^-	K_1	K_1	R_2	R_2	P_2	P_2
M_1	M_1^+, M_4^-	K_2	K_2	R_1	R_3	P_3	P_3
		K_2	K_3	R_2	R_4	U_1	U_1
M_2	M_2^+, M_3^-	K_1	K_4	S_1	S_1	U_3	U_2
M_3	M_3^+, M_2^-	K_3	K_5	S_2		U_2	U_3
M_4	M_4^+, M_1^-	K_3	K_6	T_1	T_1	U_4	U_4
A_1	A_1	Δ_1	Δ_1	T_2	T_2		
A_3		Δ_3	Δ_2	T_1	T_3		
A_2	A_2	Δ_2	Δ_3	T_2	T_4		
A_4		Δ_4	Δ_4				
A_5	A_3	Δ_5	Δ_5				
A_6		Δ_6	Δ_6				

利用这些不可約表示之間的对应关系，可以由六角密积結构的空間羣簡約系数直接得到纤維鋅矿結构的空間羣簡約系数，这对于$\Gamma, K, M, \Delta, \Sigma, R, T, P, U$等对称点(軸)是非常明显的；但是对于$A, L, H, S$則不是簡单的一一对应关系，例如由六角密积的

$$(A_1A_1|\Gamma_1^+) = (\qquad|\Gamma_2^-) = (\qquad|\Gamma_3^+) = (\qquad|\Gamma_4^-) = 1$$

可以得到纤維鋅矿的

$$(A_1A_1|\Gamma_3) = (A_3A_3|\Gamma_3) = 1,$$
$$(A_1A_3|\Gamma_1) = 1$$

等等.

2）本方法的优点是：从基本原理出发，得到空間羣的直接乘积簡約系数，因而决定了布里渊区内的跃迁选择定則；与 R. J. Elliott 和 R. Loudon 相比，可以不必計算 $G^{\mathbf{k}}/T^{\mathbf{k}}$ 品格表，与 Birman 相比，可以不必計算空間羣的品格，而只須計算同构共軛波矢羣的品格.

3）在附录中，除給出空間羣品格的計算方法外，并以M点的空間羣表示为例，通过品格的計算，說明用直接观察法也可以比較容易地得到簡約系数.

附　录　I

設 ${}^{(m)}e_\nu^{(1)}$ $(\nu = 1, \cdots, \nu)$ 是波矢羣 $G^{\mathbf{k}_{i1}}$ 的第m个不可約表示的基矢，如K表波矢羣 $G^{\mathbf{k}_{i1}}$，則

$$G = \sum_r (\alpha_r|\mathbf{a}_r)K$$

于是

$$(\alpha_r|\mathbf{a}_r)^{(m)}e_\nu^{(1)} = {}^{(m)}e_\nu^{(r)} \quad \begin{array}{l} \nu = 1, \cdots, \nu \\ r = 1, \cdots, r \end{array} \tag{1}$$

組成空間羣 G 的不可約表示的基矢[6]. 如果 $(\alpha|\mathbf{a})$ 是空間羣 G 的某任一元素,且

$$(\alpha|\mathbf{a})^{(m)}e_{\nu'}^{(p)} = \sum_{\mu=1}^{\nu} C_{\mu\nu'}{}^{(m)}e_\mu^{(q)},$$

式中 $C_{\mu\nu'}$ 是系数,則 $(\alpha_0|\mathbf{a}_0) = (\alpha_q|\mathbf{a}_q)^{-1}(\alpha|\mathbf{a})(\alpha_p|\mathbf{a}_p)$ 是波矢羣 $G^{\mathbf{k}j_1}$ 的元素,因为

$$(\alpha_q|\mathbf{a}_q)^{-1}(\alpha|\mathbf{a})(\alpha_p|\mathbf{a}_p)^{(m)}e_{\nu'}^{(1)} = (\alpha_q|\mathbf{a}_q)^{-1}(\alpha|\mathbf{a})^{(m)}e_{\nu}^{(p)} =$$
$$= (\alpha_q|\mathbf{a}_q)^{-1}\sum_{\mu=1}^{\nu} C_{\mu\nu'}{}^{(m)}e_\mu^{(q)} = \sum_{\mu=1}^{\nu} C_{\mu\nu'}{}^{(m)}e_\mu^{(1)}.$$

所以 $(\alpha|\mathbf{a})$ 可写成[7]

$$(\alpha|\mathbf{a}) = (\alpha_q|\mathbf{a}_q)(\alpha_0|\mathbf{a}_0)(\alpha_p|\mathbf{a}_p)^{-1} = (\alpha_q|\mathbf{a}_q)(\alpha_0|\mathbf{a}_0)(\alpha_q|\mathbf{a}_q)^{-1}(\alpha_q|\mathbf{a}_q)(\alpha_p|\mathbf{a}_p)^{-1}. \tag{3}$$

由于 $G^{\mathbf{k}jr}$ $(r = 1, \cdots, r)$ 是同构共軛子羣,如 $(\alpha_0|\mathbf{a}_0)$ 是 $G^{\mathbf{k}j_1}$ 的元素,則 $(\alpha_q|\mathbf{a}_q)(\alpha_0|\mathbf{a}_0)(\alpha_q|\mathbf{a}_q)^{-1}$ 是波矢羣 $G^{\mathbf{k}jq}$ 的元素,所以

$$\begin{aligned}(\alpha|\mathbf{a})^{(m)}e_\nu^{(p)} &= (\alpha_q|\mathbf{a}_q)(\alpha_0|\mathbf{a}_0)(\alpha_q|\mathbf{a}_q)^{-1}(\alpha_q|\mathbf{a}_q)(\alpha_p|\mathbf{a}_p)^{-1\,(m)}e_\nu^{(p)} \\ &= (\alpha_q|\mathbf{a}_q)(\alpha_0|\mathbf{a}_0)(\alpha_q|\mathbf{a}_q)^{-1}(\alpha_q|\mathbf{a}_q)^{(m)}e_\nu^{(1)} = \\ &= (\alpha_q|\mathbf{a}_q)(\alpha_0|\mathbf{a}_0)(\alpha_q|\mathbf{a}_q)^{-1\,(m)}e_\nu^{(q)} = \\ &= \sum_\mu \{T_{\mathbf{k}jq}^{(m)}(\alpha_q|\mathbf{a}_q)(\alpha_0|\mathbf{a}_0)(\alpha_q|\mathbf{a}_q)^{-1}\}_{\mu\nu}{}^{(m)}e_\mu^{(q)},\end{aligned} \tag{4}$$

其中 $T_{\mathbf{k}jq}^{(m)}$ 是波矢羣 $G^{\mathbf{k}jq}$ 的第 m 个不可約表示. 因此以(1)式作为基矢,空間羣任一元素 $(\alpha|\mathbf{a})$ 的不可約表示的品格可写成

$$\begin{aligned}K_j^m(\alpha|\mathbf{a}) &= \sum_{p=1}^{r}\sum_{\nu=1}^{\nu}\int {}^{(m)}e_\nu^{(p)*}(\alpha|\mathbf{a})^{(m)}e_\nu^{(p)}\,d\tau = \\ &= \sum_{p=1}^{r}\sum_{\nu=1}^{\nu}\sum_\mu \{T_{\mathbf{k}jq}^{(m)}(\alpha_q|\mathbf{a}_q)(\alpha_0|\mathbf{a}_0)(\alpha_q|\mathbf{a}_q)^{-1}\}_{\mu\nu}\int {}^{(m)}e_\nu^{(p)*(m)}e_\mu^{(q)}\,d\tau = \\ &= \sum_{p\,\nu\,\mu}\{T_{\mathbf{k}jq}^{(m)}(\alpha_q|\mathbf{a}_q)(\alpha_0|\mathbf{a}_0)(\alpha_q|\mathbf{a}_q)^{-1}\}_{\mu\nu}\delta_{\mu\nu}\delta_{pq} = \\ &= \begin{cases}\sum_\mu \{T_{\mathbf{k}jq}^{(m)}(\alpha|\mathbf{a})\}_{\mu\mu} & \{\alpha|\mathbf{a}\}\ \text{是波矢羣}\ G^{\mathbf{k}jq}\ \text{的元素}, \\ 0 & \text{其他情況}.\end{cases}\end{aligned} \tag{5}$$

附 录 II

这里列出利用附录 I 所計算得的空間羣不可約表示 $^*K_M^{(m)}$ 的品格1). $^*K_M$ 的矢量如下:

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1) 所列出的不是空間羣的全部元素.

$$M_1=\begin{pmatrix}0\\ \dfrac{2\pi}{\sqrt{3}\,a}\\ 0\end{pmatrix},\quad M_2=\begin{pmatrix}-\dfrac{\pi}{a}\\ -\dfrac{\pi}{\sqrt{3}\,a}\\ 0\end{pmatrix},\quad M_3=\begin{pmatrix}\dfrac{\pi}{a}\\ \dfrac{-\pi}{\sqrt{3}\,a}\\ 0\end{pmatrix}$$

	$M_1^\pm$	$M_2^\pm$	$M_3^\pm$	$M_4^\pm$
$(\varepsilon\|0,\mathbf{t}_1)$	3	3	3	3
$(\delta_2\|\boldsymbol{\tau}_2,\boldsymbol{\tau}_2+\mathbf{t}_1)$	-1	1	1	-1
$(\delta''_{22}\|0,\mathbf{t}_1)$	1	1	-1	-1
$(\delta'_{22}\|\boldsymbol{\tau}_2,\boldsymbol{\tau}_2+\mathbf{t}_1)$	1	-1	1	-1
$(i\|\boldsymbol{\tau}_2,\boldsymbol{\tau}_2+\mathbf{t}_1)$	∓ 1	∓ 1	∓ 1	∓ 1
$(\rho\|0,\mathbf{t}_1)$	± 3	∓ 3	∓ 3	± 3
$(\rho'_2\|0,\mathbf{t}_1)$	± 1	∓ 1	± 1	∓ 1
$(\rho''_2\|\boldsymbol{\tau}_2+\mathbf{t}_1)$	± 1	± 1	∓ 1	∓ 1
$(\delta_6,\delta_6^{-1}\|\boldsymbol{\tau},\boldsymbol{\tau}+\mathbf{t}_1)$	0	0	0	0
$(\delta_3,\delta_3^{-1}\|\sigma,\mathbf{t}_1)$	0	0	0	0
$(\sigma_6,\sigma_6^{-1}\|\boldsymbol{\tau},\boldsymbol{\tau}+\mathbf{t}_1)$	0	0	0	0
$(\sigma_3,\sigma_3^{-1}\|0,\mathbf{t}_1)$	0	0	0	0

用 $^*K_M^{(m)}$ 及 $^*K_\Gamma^{(m')}$ 的品格可以用直接观察法，即利用关系式

$$^*K_j^{(m)}(R)\,^*K_{j'}^{(m')}(R)=\sum_{j''}\sum_{m''}(K_j^{(m)}K_{j'}^{(m')}|K_{j''}^{(m'')})\,^*K_{j''}^{(m'')}(R)$$

可求出空間羣的簡約系数[1]，其中 R 是空間羣中任意元素.

元素 ＼ 直接乘积的品格	$M_1^+M_2^+$	$M_1^+M_3^+$	$M_1^+M_4^+$	$M_2^+M_3^+$	$M_2^+M_4^+$	$M_3^+M_4^+$
$(\varepsilon\|0,\mathbf{t}_1)$	9	9	9	9	9	9
$(\delta_2\|\boldsymbol{\tau}_2,\boldsymbol{\tau}_2+\mathbf{t}_1)$	-1	-1	1	1	-1	-1
$(\delta''_{22}\|0,\mathbf{t}_1)$	1	-1	-1	-1	-1	1
$(\delta''_{23}\|0,\mathbf{t}_1)$	1	-1	-1	-1	-1	1
$(\delta''_{24}\|0.\mathbf{t}_1)$	1	-1	-1	-1	-1	1
$(\delta'_{22}\|\boldsymbol{\tau}_2,\boldsymbol{\tau}_2+\mathbf{t}_1)$	-1	1	-1	-1	1	-1
$(\delta'_{23}\|\boldsymbol{\tau}_4,\boldsymbol{\tau}_4+\mathbf{t}_1)$	-1	1	-1	-1	1	-1
$(\delta'_{24}\|\boldsymbol{\tau}_3,\boldsymbol{\tau}_3+\mathbf{t}_1)$	-1	1	-1	-1	1	-1
$(i\|\boldsymbol{\tau}_2,\boldsymbol{\tau}_2+\mathbf{t}_1)$	1	1	1	1	1	1
$(\rho\|0,\mathbf{t}_1)$	-9	-9	9	9	-9	-9
$(\rho'_2\|0,\mathbf{t}_1)$	-1	1	-1	-1	1	-1
$(\rho'_3\|0,\mathbf{t}_1)$	-1	1	-1	-1	1	-1
$(\rho'_4\|0,\mathbf{t}_1)$	-1	1	-1	-1	1	-1
$(\rho''_2\|\boldsymbol{\tau}_2,\boldsymbol{\tau}_2+\mathbf{t}_1)$	1	-1	-1	-1	-1	1
$(\rho''_3\|\boldsymbol{\tau}_4,\boldsymbol{\tau}_4+\mathbf{t}_1)$	1	-1	-1	-1	-1	1
$(\rho''_4\|\boldsymbol{\tau}_3,\boldsymbol{\tau}_3+\mathbf{t}_1)$	1	-1	-1	-1	-1	1
$(\delta_6,\delta_6^{-1}\|\boldsymbol{\tau},\boldsymbol{\tau}+\mathbf{t}_1)$	0	0	0	0	0	0
$(\delta_3,\delta_3^{-1}\|0,\mathbf{t}_1)$	0	0	0	0	0	0
$(\sigma_6,\sigma_6^{-1}\|\boldsymbol{\tau},\boldsymbol{\tau}+\mathbf{t}_1)$	0	0	0	0	0	0
$(\sigma_3,\sigma_3^{-1}\|0,\mathbf{t}_1)$	0	0	0	0	0	0

1) 一般只利用 $^*K_j^{(m)}$, $^*K_{j'}^{(m')}$, $^*K_{j''}^{(m'')}$ 的共有元素就可得到所要求的簡約系数.

利用上面品格表及Γ的品格表,显然可得

$$M_1^+ \otimes M_2^+ = M_3^+ \otimes M_4^+ = \Gamma_4^+ \oplus \Gamma_6^+ \oplus M_2^+ \oplus M_3^+,$$
$$M_1^+ \otimes M_3^+ = M_2^+ \otimes M_4^+ = \Gamma_3^+ \oplus \Gamma_6^+ \oplus M_2^+ \oplus M_3^+,$$
$$M_1^+ \otimes M_4^+ = M_2^+ \otimes M_3^+ = \Gamma_2^+ \oplus \Gamma_5^+ \oplus M_1^+ \oplus M_4^+.$$

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SPACE GROUP SELECTION RULES

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Abstract

Based on the general methods for the reduction of direct products of space group irreducible representations developed by Birman, a simpler method of finding the wave vector selection rules is derived. The method is applied here to the hexagonal close-packed and the wurtzite space groups. The coupling coefficients for the reduction of the direct products of two space group irreducible representations are given explicitly.