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QUY T C L C L A CHO PH IR

$$[\mu_x]_{v',v''} = \int \psi_{v'}^*(Q_a) \mu_x \psi_{v''}(Q_a) dQ_a$$

$$[\mu_y]_{v',v''} = \int \psi_{v'}^*(Q_a) \mu_y \psi_{v''}(Q_a) dQ_a$$

$$[\mu_z]_{v',v''} = \int \psi_{v'}^*(Q_a) \mu_z \psi_{v''}(Q_a) dQ_a$$

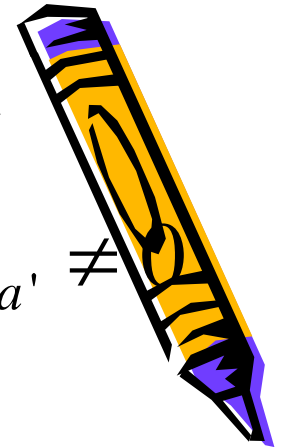
$$\mu_x = (\mu_x)_0 + \left(\frac{\delta \mu_x}{\delta Q_a} \right) Q_a + \dots$$

$$[\mu_x]_{v',v''} = (\mu_x)_0 \int \psi_{v'}^*(Q_a) \psi_{v''}(Q_a) dQ_a$$

$$+ \left(\frac{\delta \mu_x}{\delta Q_a} \right) \int \psi_{v'}^*(Q_a) Q_a \psi_{v''}(Q_a) dQ_a + \dots$$



QUY T C L C L A CHO PH IR



$$\left(\frac{\delta \mu_x}{\delta Q_a} \right) \neq 0 \quad \forall \quad \int \psi_{v'}^*(Q_a) Q_a \psi_{v''}(Q_a) dQ_a \neq 0$$

à

$$\left(\frac{\delta \mu_x}{\delta Q_a} \right) \int \psi_{v'}^*(Q_a) Q_a \psi_{v''}(Q_a) dQ_a \approx e \int \psi_{v'}^*(Q_a) Q_a \psi_{v''}(Q_a) dQ_a$$

$$v = 0, \psi_0 = \left(\frac{\alpha}{\pi} \right)^{1/4} e^{-\alpha Q_a^2 / 2}$$

$$v = 1, \psi_1 = \left(\frac{\alpha}{\pi} \right)^{1/4} 2^{1/2} Q_a e^{-\alpha Q_a^2 / 2}$$



$$\int f_A f_B f_C d\tau$$



QUY T C L C L A CHO PH RAHAN

$$[\alpha_{xx}]_{v',v''} = \int \psi_{v'}^*(Q_a) \alpha_{xx} \psi_{v''}(Q_a) dQ_a$$

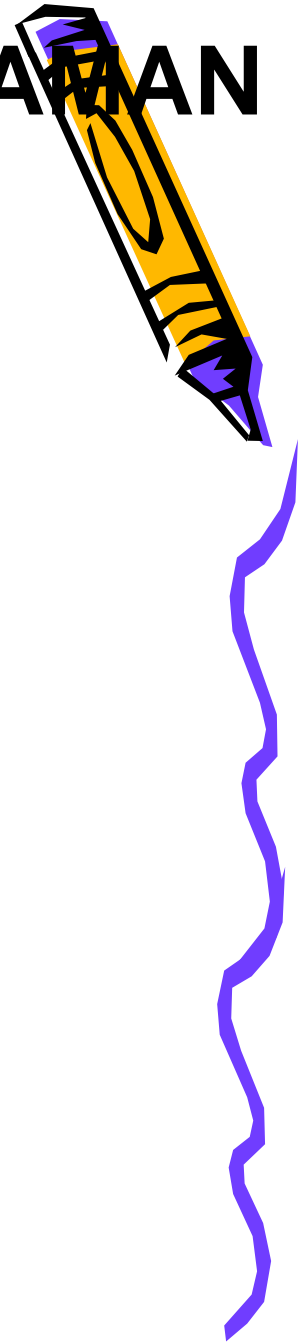
$$[\alpha_{xy}]_{v',v''} = \int \psi_{v'}^*(Q_a) \alpha_{xy} \psi_{v''}(Q_a) dQ_a$$

$$[\alpha_{xz}]_{v',v''} = \int \psi_{v'}^*(Q_a) \alpha_{xz} \psi_{v''}(Q_a) dQ_a$$

$$[\alpha_{yy}]_{v',v''} = \int \psi_{v'}^*(Q_a) \alpha_{yy} \psi_{v''}(Q_a) dQ_a$$

$$[\alpha_{yz}]_{v',v''} = \int \psi_{v'}^*(Q_a) \alpha_{yz} \psi_{v''}(Q_a) dQ_a$$

$$[\alpha_{zz}]_{v',v''} = \int \psi_{v'}^*(Q_a) \alpha_{zz} \psi_{v''}(Q_a) dQ_a$$



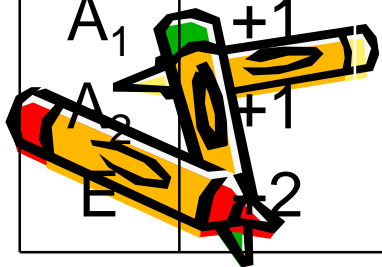
Ví dụ: phân tích NH_3 của nhóm điểm C_{3v}



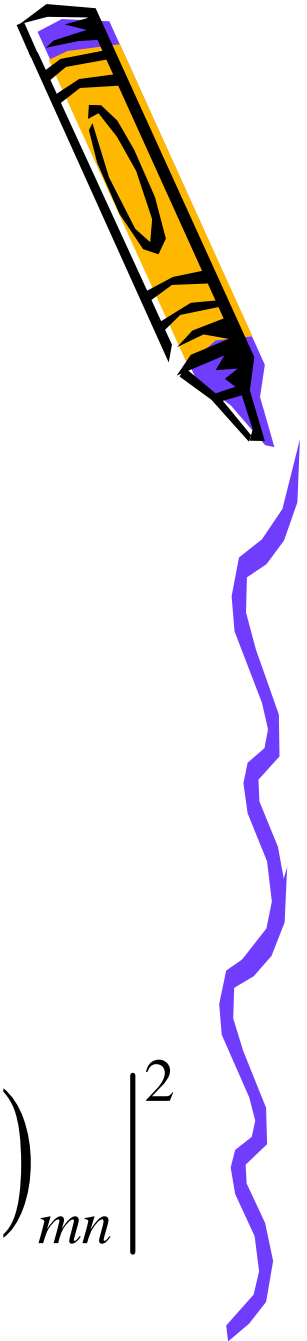
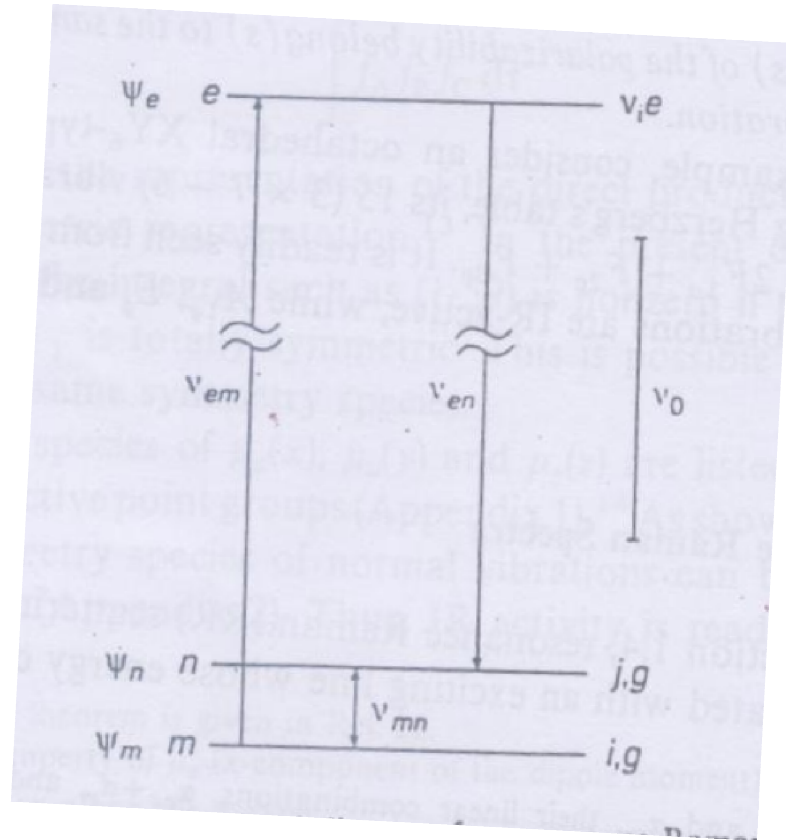
Dùng công thức Herzberg (phần 1 c 2) cho nhóm C_{3v} với $m=0, m_v=1, m_0=1$

Nhóm điểm	Tổng số nguyên tử	Đị xứng	S dao động
C_{3v}	$6m+3m_v+m_0$	A_1 A_2 E	$3m+2m_v+m_0-1=2$ $3m+m_v-1=0$ $6m+3m_v+m_0-2=0$
Bảng đặc trưng (phần 1 c 1)			

C_{3v}	E	$2C_3(z)$	$3\sigma_v$	Hoạt động IR	Hoạt động Raman
A_1	+1	+1	+1	T_z	$xx + yy, zz$
A_2	+1	+1	-1	R_z	
E	-2	-1	0	$(T_x, T_y), (R_x, R_y)$	$(xx - yy, xy), (yz, xz)$



PH RAMAN C NG H NG



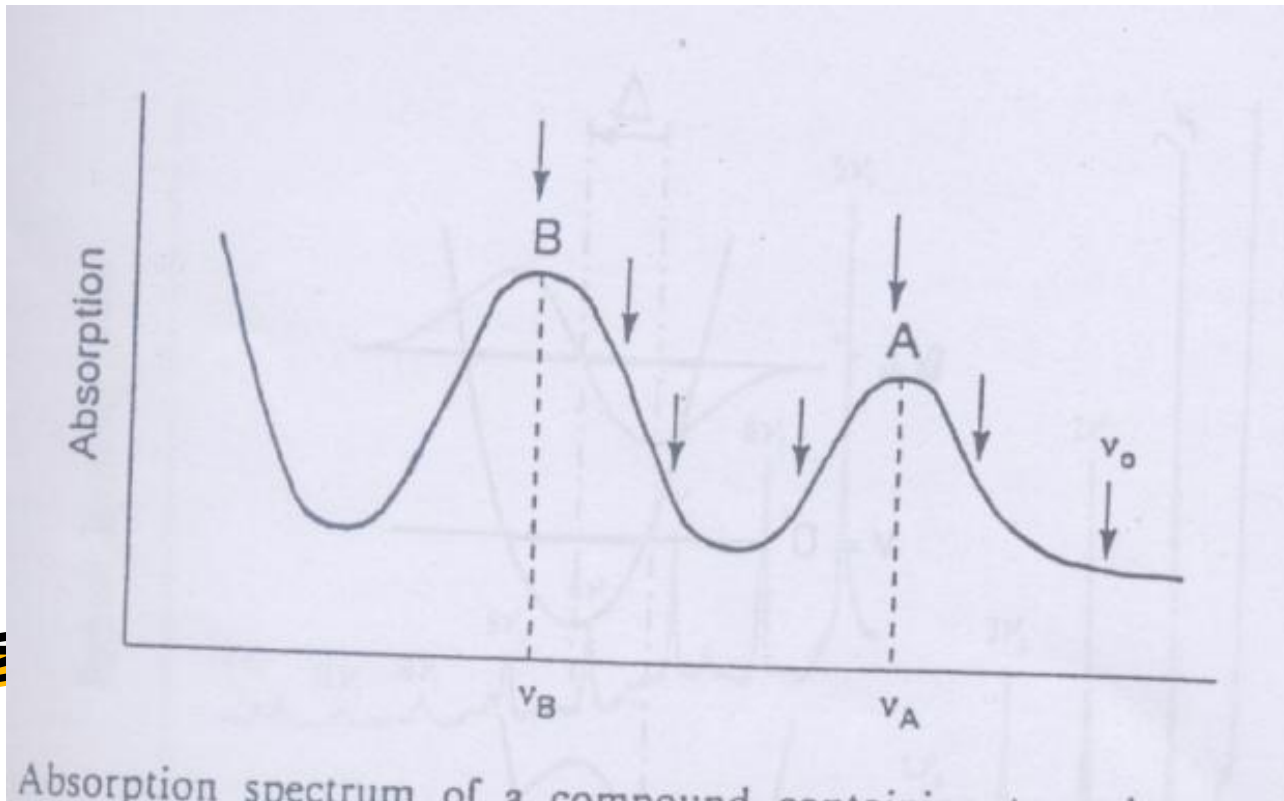
$$I = h \nu_0 I_0 (\nu_0 - \nu_{mn})^4 \sum_{p\sigma} \left| \left(\alpha_{p\sigma} \right)_{mn} \right|^2$$



PH RAMAN C NG H NG

$$(\alpha_{p\sigma})_{mn} = \frac{1}{h} \sum_e \left(\frac{M_{me} M_{en}}{\nu_{em} - \nu_0 + i\Gamma_e} + \frac{M_{me} M_{en}}{\nu_{en} + \nu_0 + i\Gamma_e} \right)$$

$$M_{me} = \int \Psi_m^* \mu_\sigma \Psi_e d\tau$$

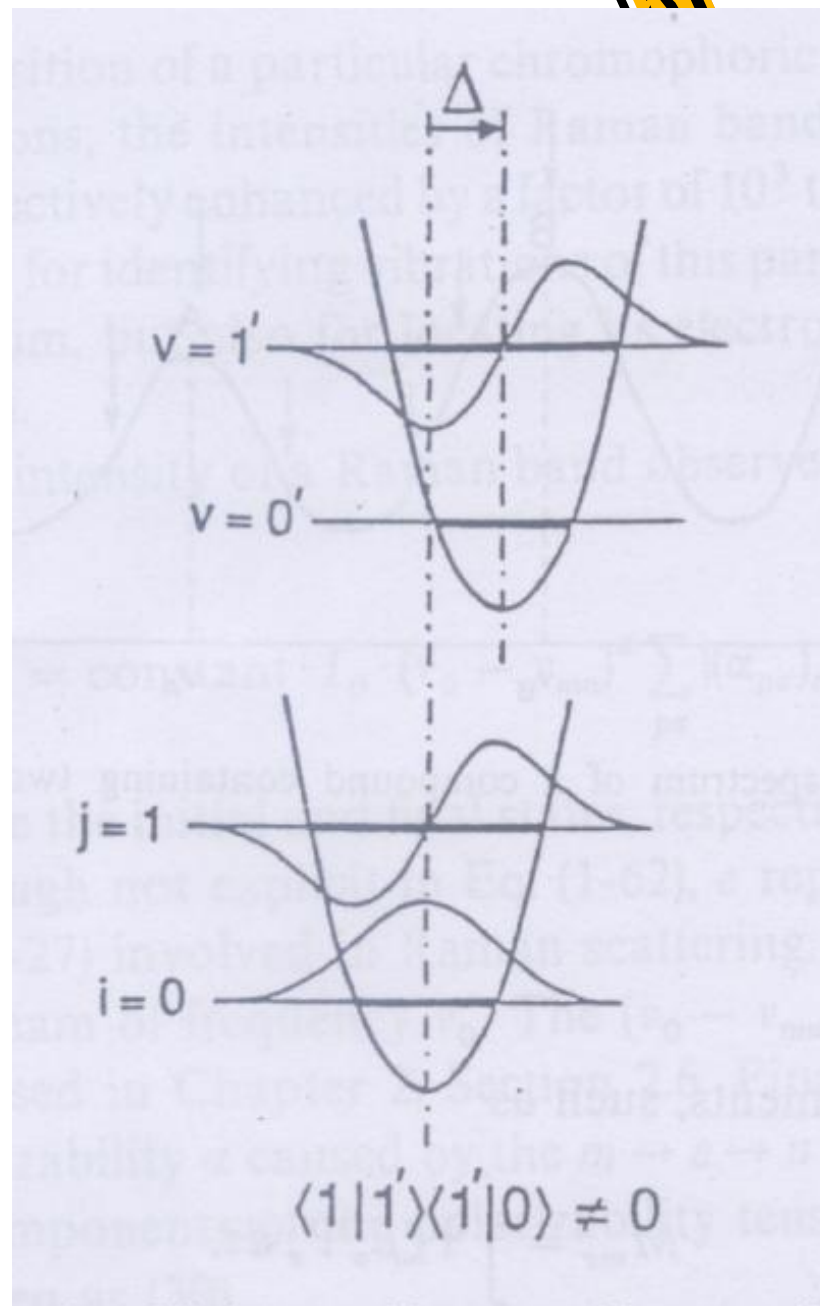
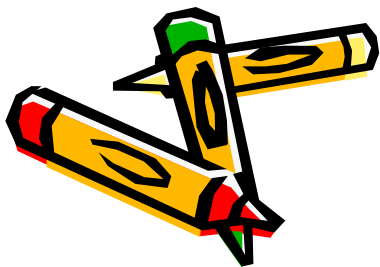


PH RAMAN C NG H NG

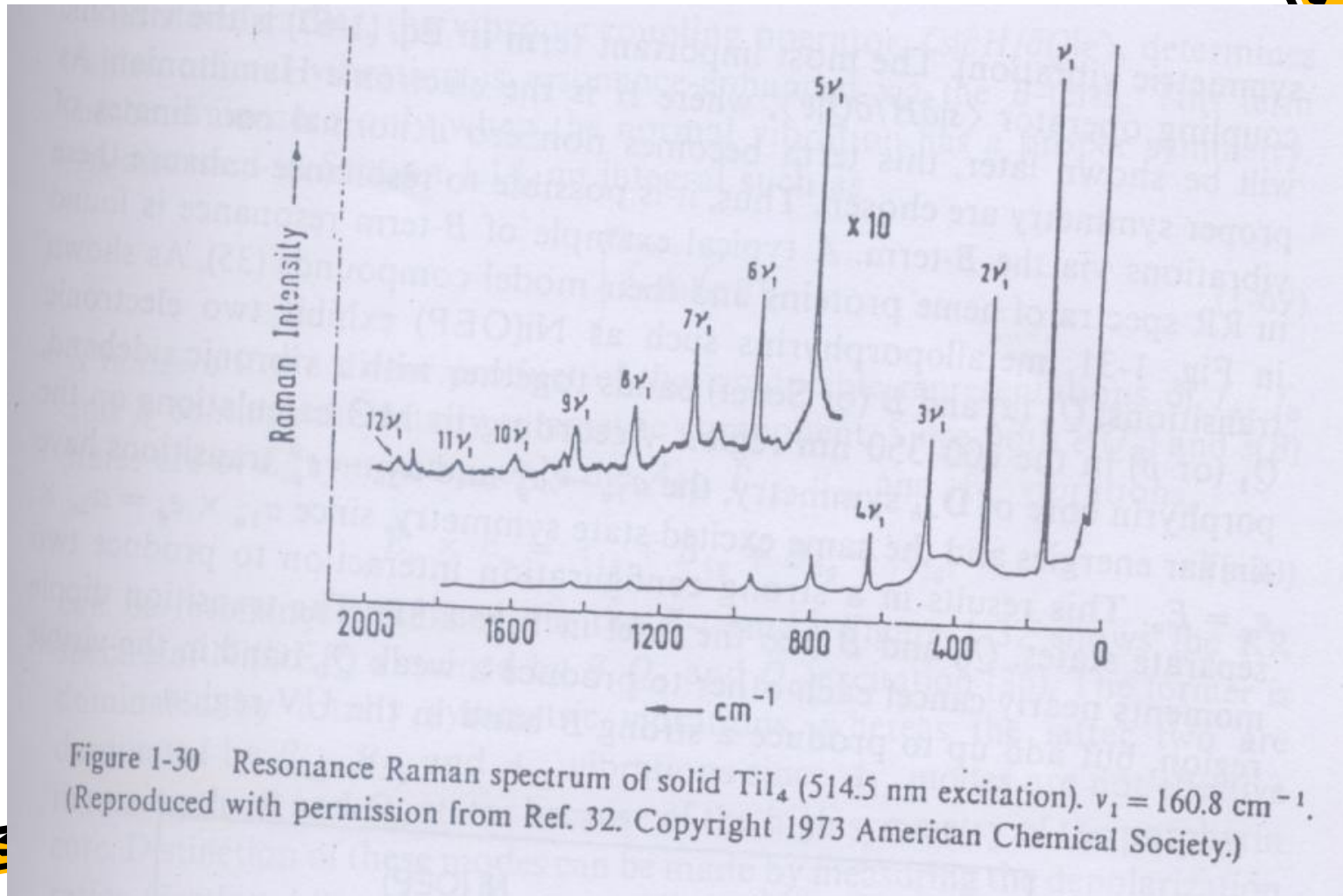
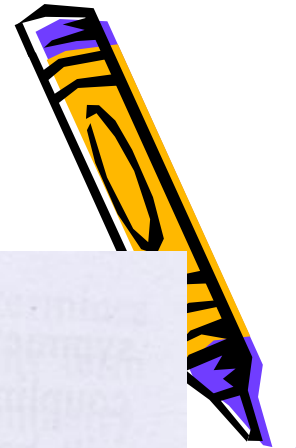


$$\left(\alpha_{p\sigma}\right)_{mn} \cong A + B$$

$$A \cong M_e^2 \frac{1}{h} \sum_{\nu} \frac{\langle j|\nu\rangle\langle\nu|i\rangle}{\nu_{\nu i} - \nu_0 + i\Gamma_e}$$



PH RAMAN C NG H NG



PH RAMAN C NG H NG

$$B \cong M_e M_e' \frac{1}{h} \sum_v \frac{\langle j|Q|v \rangle \langle v|i \rangle + \langle j|v \rangle \langle v|Q|i \rangle}{\nu_{vi} - \nu_0 + i\Gamma_v}$$

$$M_e' = \mu_s \langle s|\partial H / \partial Q|e \rangle / \langle \nu_s - \nu_e \rangle$$

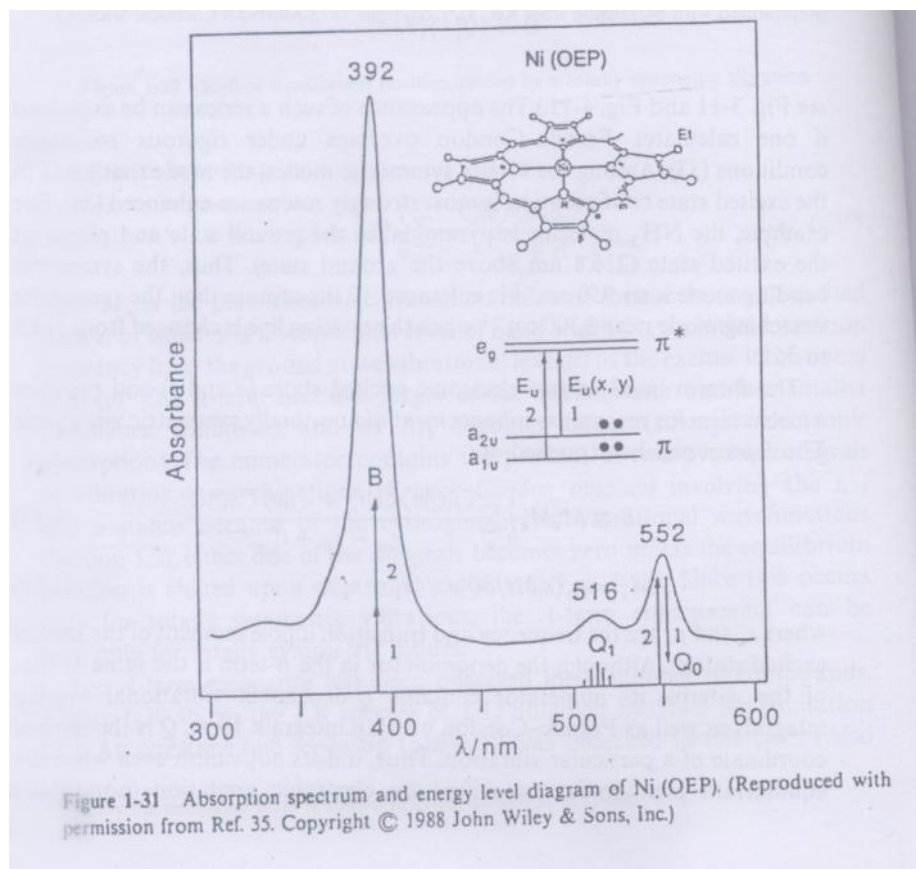
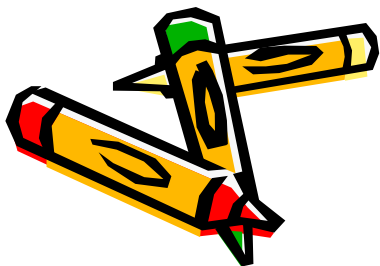
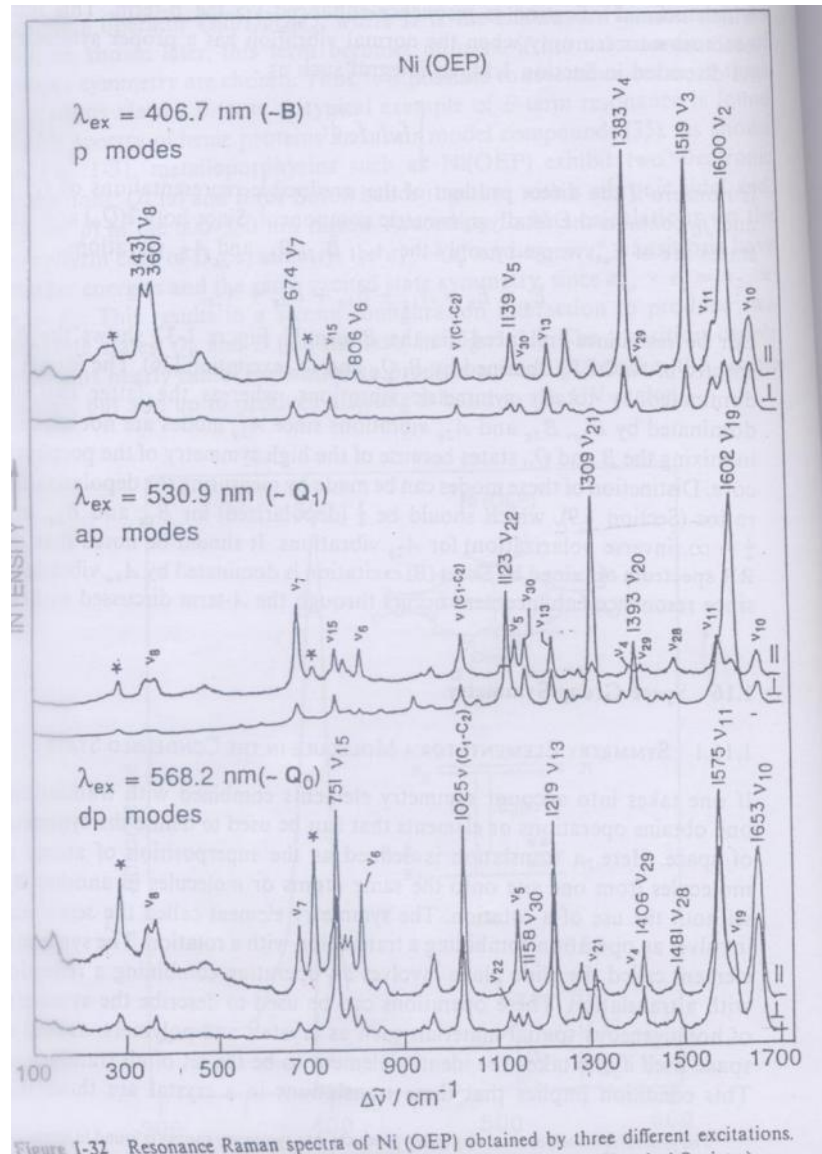
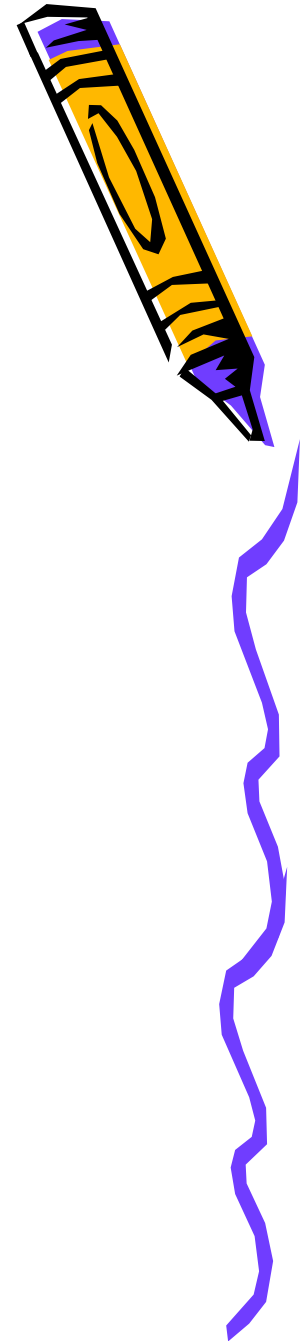


Figure 1-31 Absorption spectrum and energy level diagram of Ni(OEP). (Reproduced with permission from Ref. 35. Copyright © 1988 John Wiley & Sons, Inc.)

PH RAMAN C NG H NG



IX NG NHÓM KHÔNG GIAN

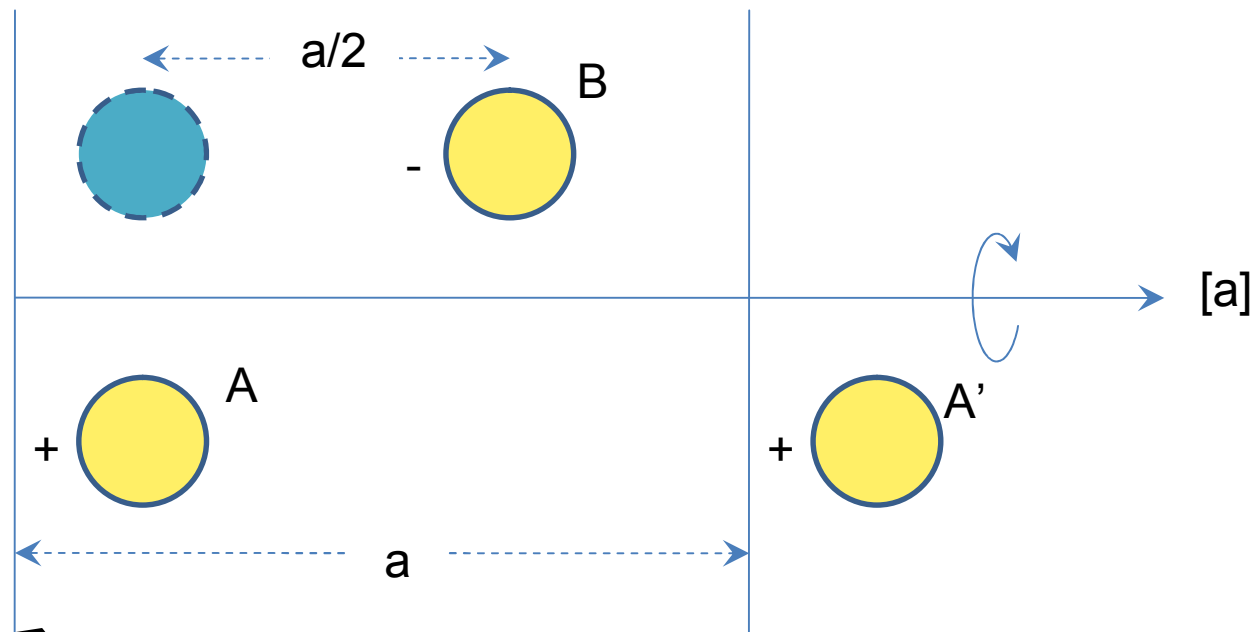


Y U T IX NG

Tr c x o n c (n_p)

$n = 2, 3, 4, 6$

$p = 1, 2, \dots, n-1$



Tr c x o n c b c 2

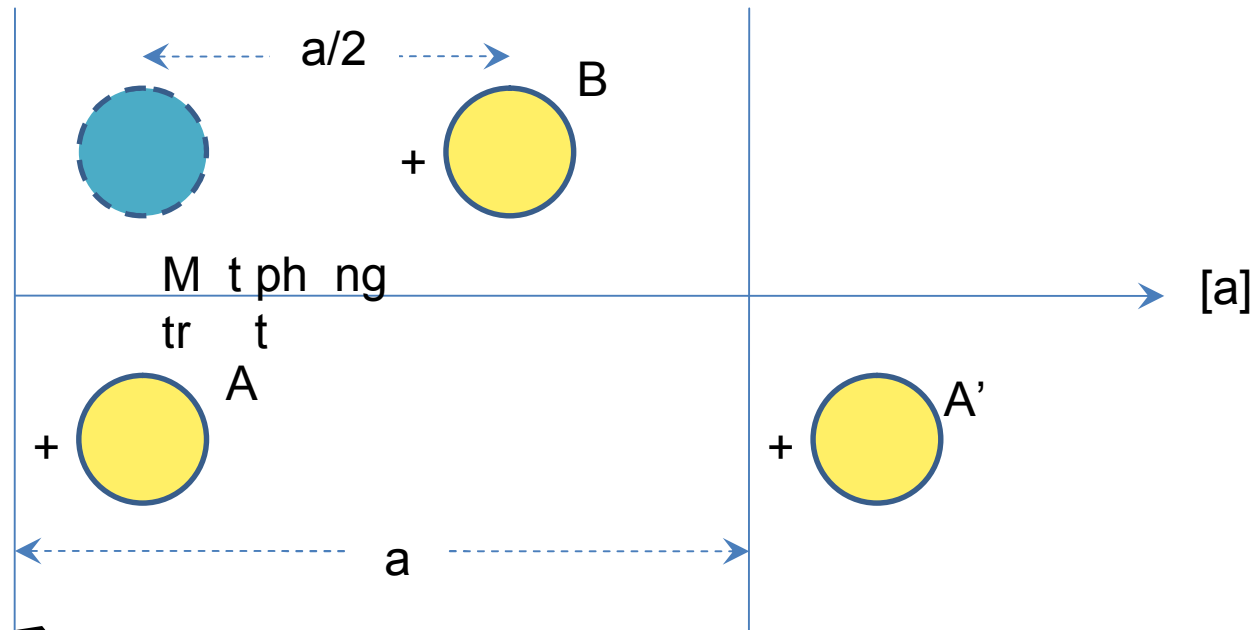


I X NG NHÓM KHÔNG GIAN

Y U T I X NG

Tr c x o n c (n_p)

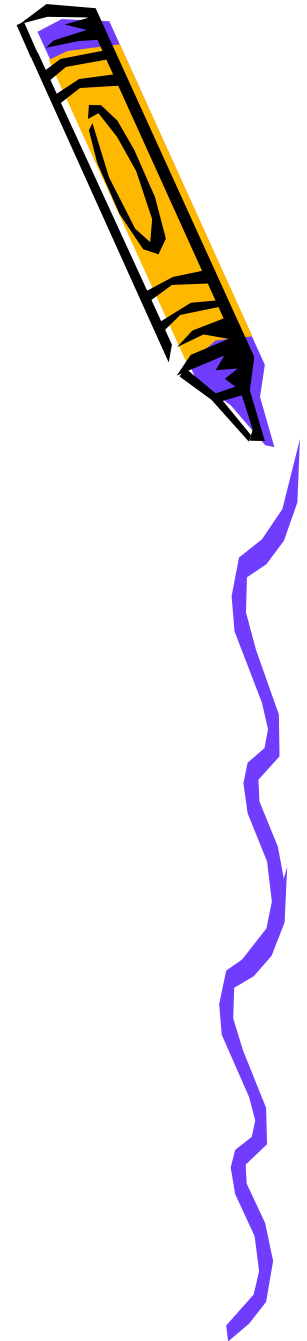
M t ph ng tr t



I X NG NHÓM KHÔNG GIAN

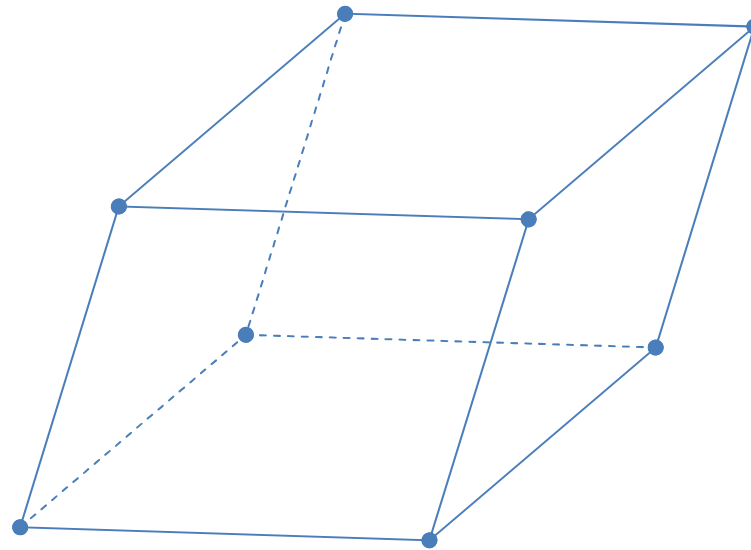
S phân b c a 230 nhóm không gian
vào 7 h th ng tinh th

H th ng tinh th	S nhóm không gian
Tam tà	2
n tà	13
Tr c thoi	59
Hình thoi	25
L c l ng	27
T giác	68
L p ph ng	36

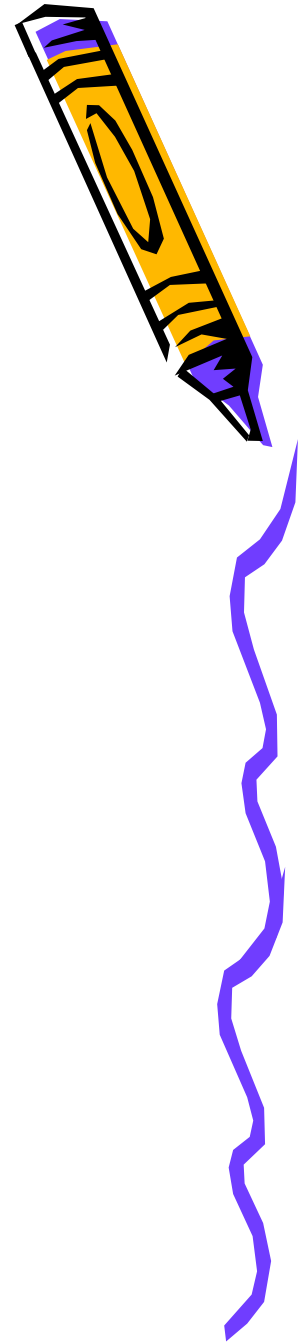
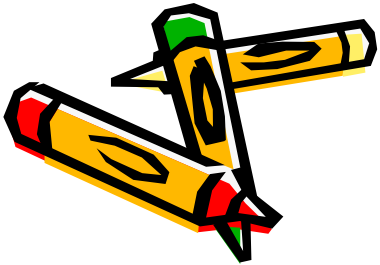


IX NHÓM KHÔNG GIAN

Các mạng Bravais

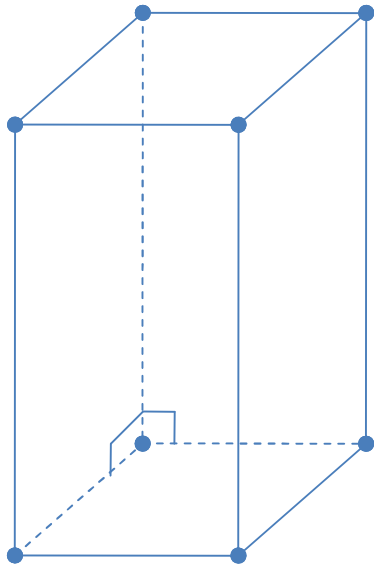


Triclinic – P
Tam tà - P

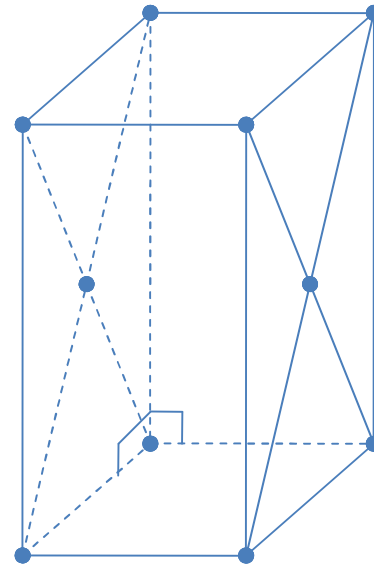


IX NHÓM KHÔNG GIAN

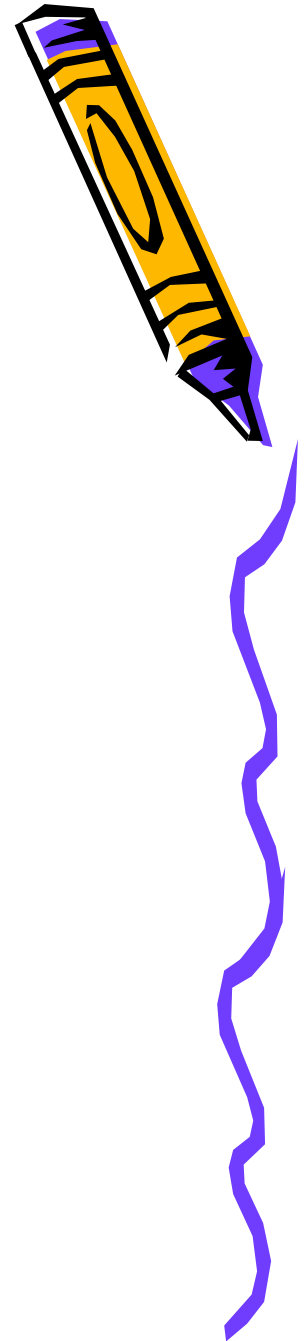
Các mạng Bravais



Monolonic – P
n tậ - P

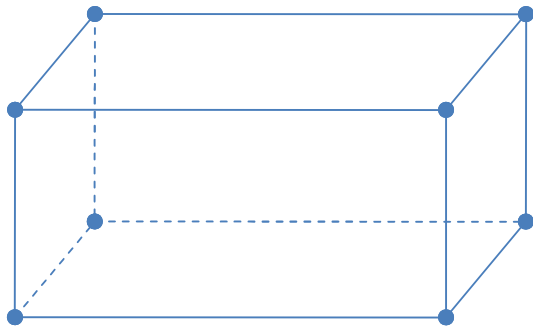


Monolonic – B
n tậ - B

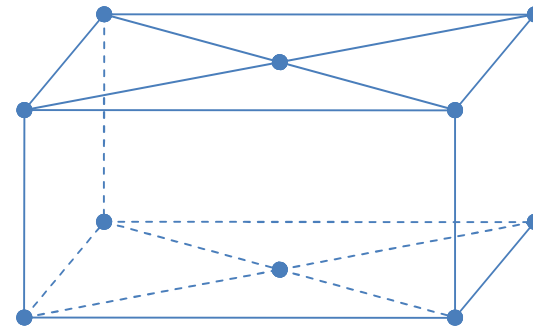


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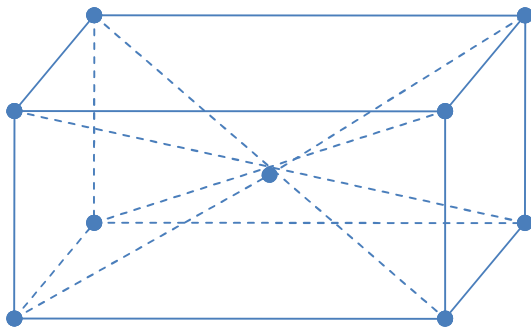
Các mạng Bravais



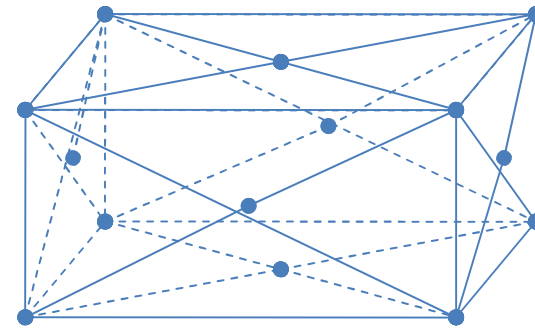
Orthorhombic – P
Tr c thoi - P



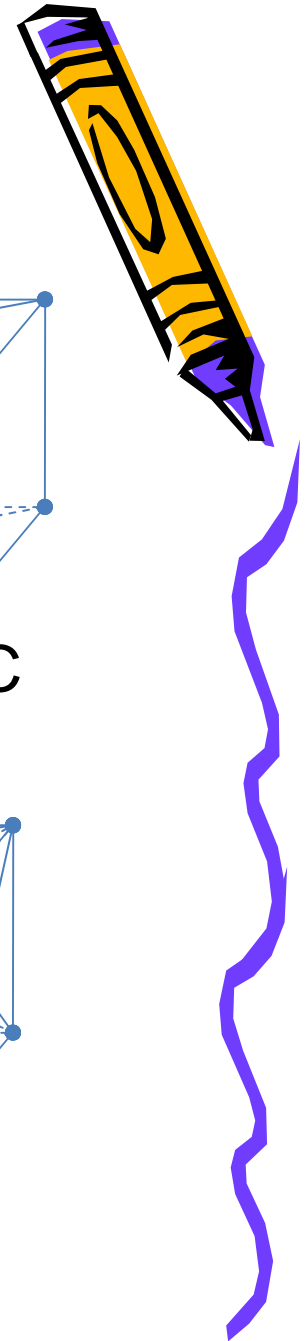
Orthorhombic – C
Tr c thoi - C



Orthorhombic – I
Tr c thoi - I

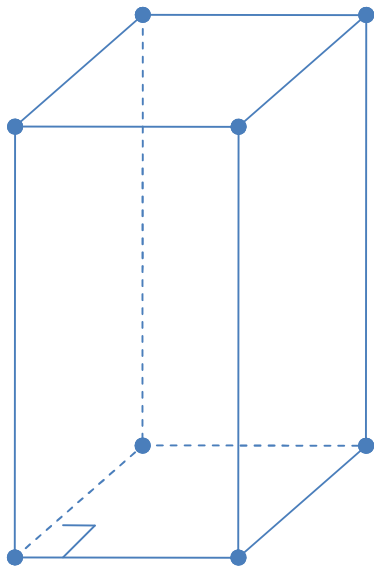


Orthorhombic – F
Tr c thoi - F

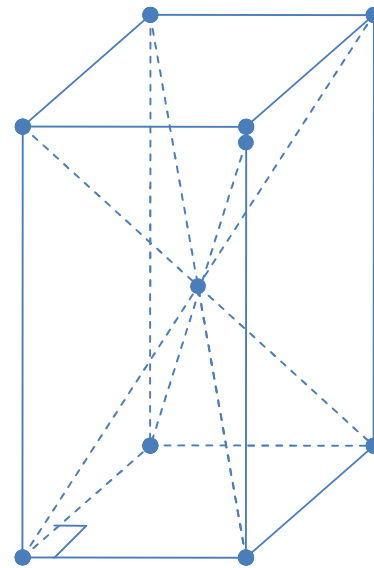


I X NG NHÓM KHÔNG GIAN

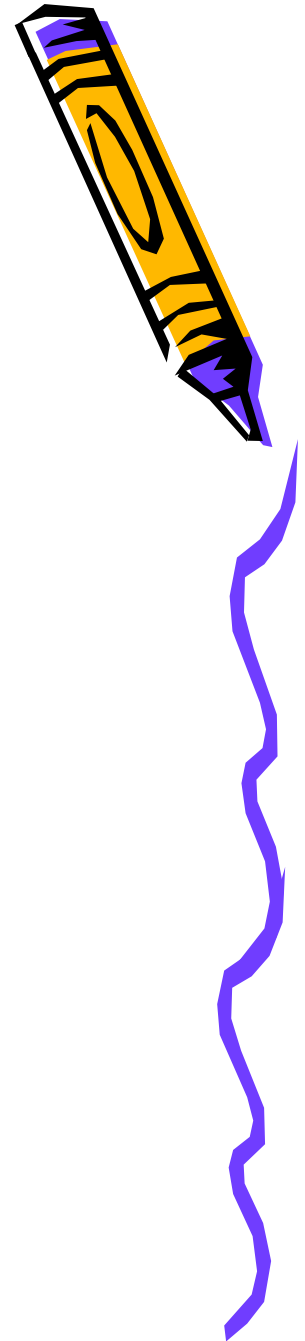
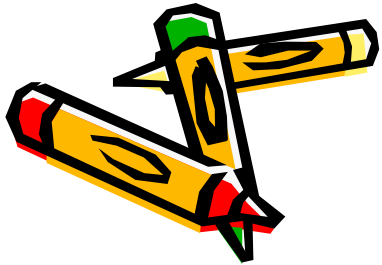
Các mạng Bravais



Tetragonal – P
T giác - P

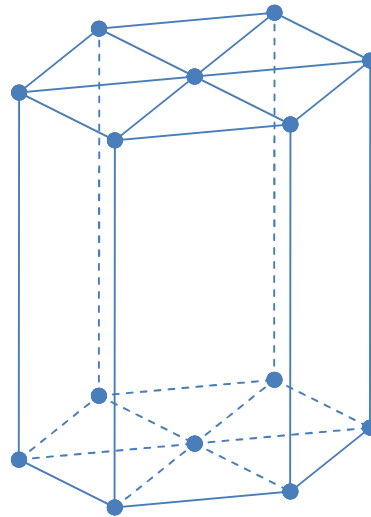


Tetragonal – I
T giác - I

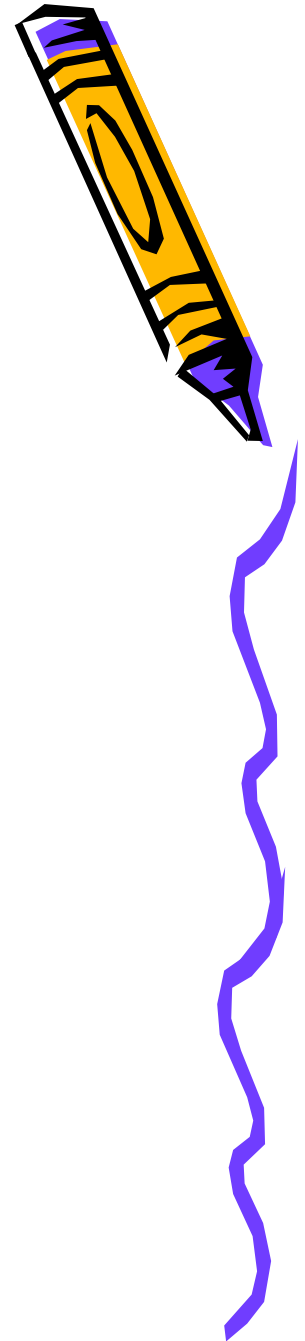


IX NHÓM KHÔNG GIAN

Các mạng Bravais

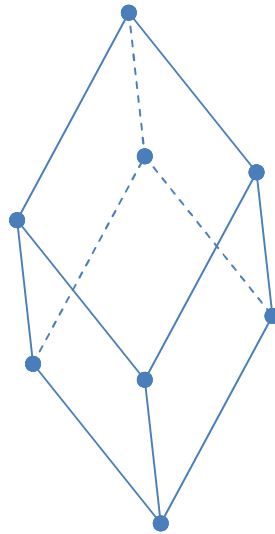


Hexagonal – P
L c l ng - P

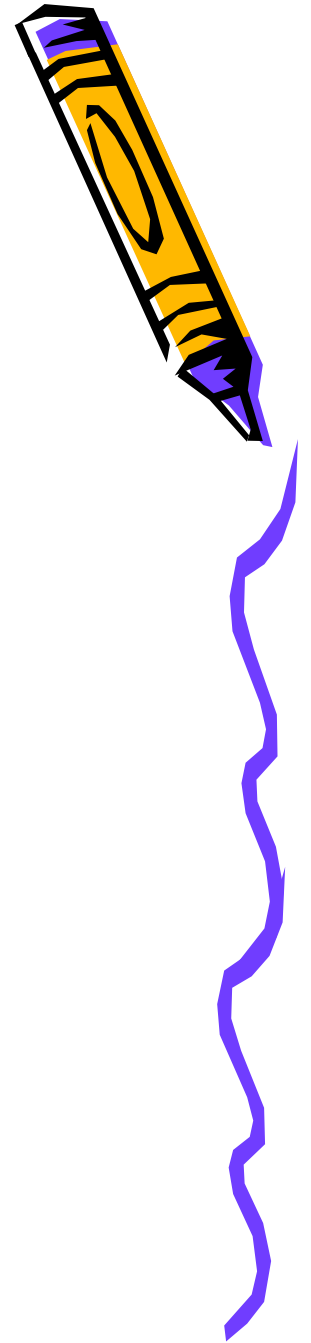


IX NHÓM KHÔNG GIAN

Các mạng Bravais

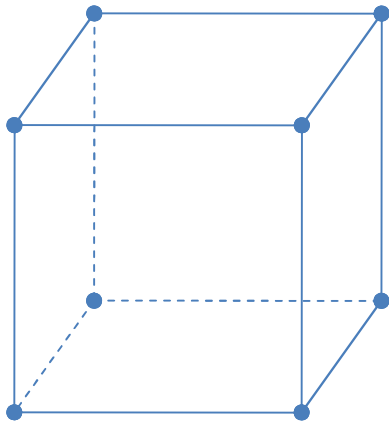


Trigonal – P
Hình thoi - P



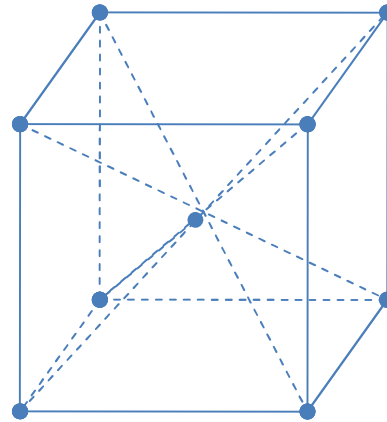
I X NG NHÓM KHÔNG GIAN

Các m ãng Bravais



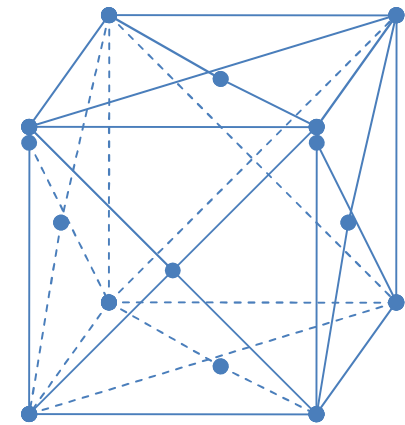
Cubic – P

L p ph ãng- P



Cubic – I

L p ph ãng- I

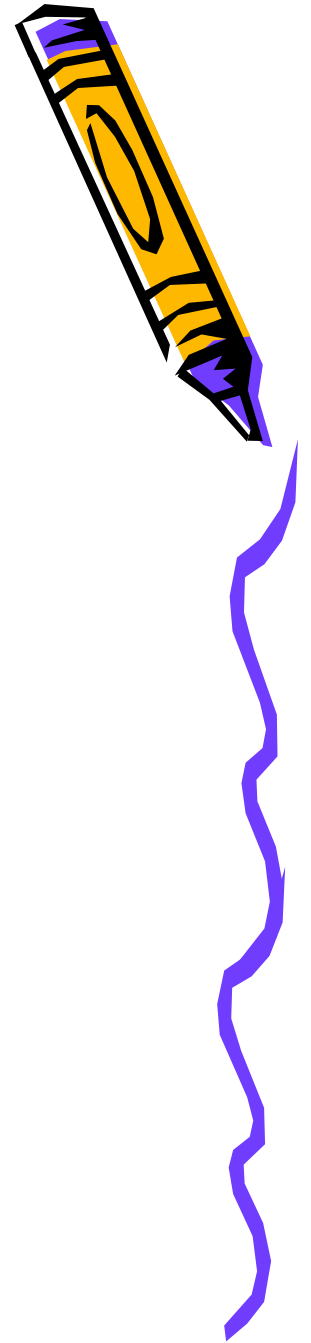


Cubic – F

L p ph ãng- F



I X NG NHÓM KHÔNG GIAN



Cách kí hi u nhóm không gian

P: m ng c b n

C: m ng nh tâm

F: m ng tâm m t

I: m ng tâm kh i

R: m ng hình thoi

Tr c quay c ký hi u n (b c c a tr c)

Tr c xo n c c ký hi u p/n

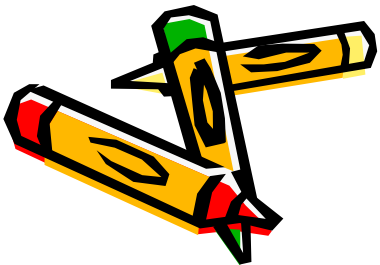
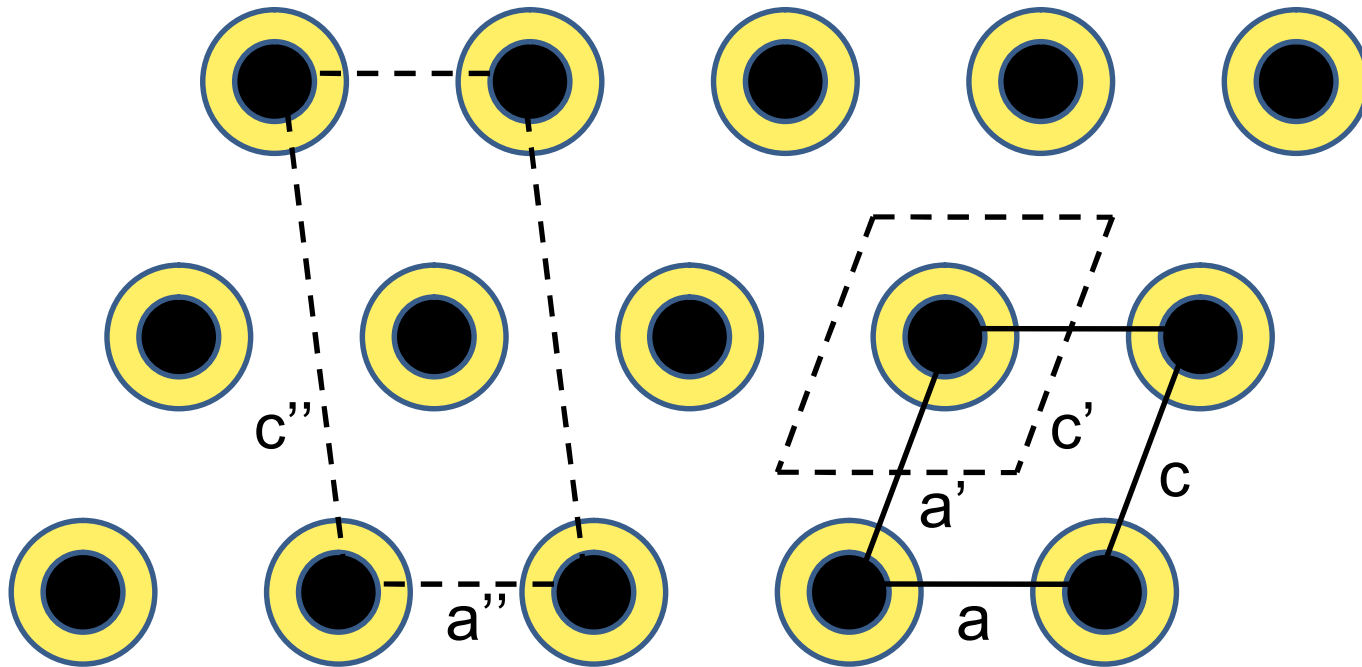
M t g ng c ký hi u m

M t ph ng tr t ký hi u a, b, c, n, d



I X NG NHÓM KHÔNG GIAN

Phân biệt các b n, không c b n, nh tâm



IX NG NHÓM KHÔNG GIAN



S n v l p l i trong m t ô

Lo i ô m ng	Ký hi u	S n v trong m t ô
C b n	P	1
Hình thoi	R	3 ho c 1
Tâm kh i	I	2
Tâm m t bên	A,B ho c C	2
Tâm m t	F	4

$Z' = s$ phân t trong ô c b n

$= (s$ phân t trong ô tinh th $) / (s$ n v l p l i trong ô)

