Final Exam (AMIE352-00, Spring 2014)
June 16, 2014. 4:30 pm – 5:45 pm
Prof. Youngmin You

1. Answer following questions: (*6 points*)

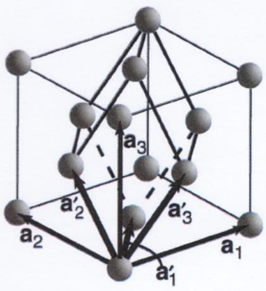
(1) Write the zone equation (Miller index (*hkl*)) for a [221] zone (*3 points*).

$2h + 2k + l = 0$

(2) Which of these planes belong to the [221] zone: $(1\bar{1}0), (\bar{1}13), (0\bar{1}2), (1\bar{3}2), (\bar{2}21), (\bar{1}\bar{1}4)$? (*3 points*)

$(1\bar{1}0)$, $\cancel{(\bar{1}\bar{1}2)}$, $(\bar{1}\bar{1}4)$
$(0\bar{1}2)$

2. Shown below is the face-centered cubic lattice (*cF*), wherein we can define a primitive rhombohedral (*R*) unit cell. Answer following questions: *(16 points)*.



(1) What is the transformation matrix for $cF \rightarrow R$? (*3 points*)

$$\alpha_{ij} = \frac{1}{2}\begin{pmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{pmatrix}$$

(2) What are the reciprocal basis vectors in *R*? (*3 points*)

Use this $\vec{a}_j'^{*} = \vec{a}_j^{*} \alpha_{ji}^{-1}$

$$= (\vec{a}_1^{*}\ \vec{a}_2^{*}\ \vec{a}_3^{*})\begin{pmatrix} 1 & -1 & 1 \\ 1 & 1 & -1 \\ -1 & 1 & 1 \end{pmatrix}$$

$\therefore \vec{a}_1'^{*} = \vec{a}_1^{*} + \vec{a}_2^{*} - \vec{a}_3^{*}$

$\vec{a}_2'^{*} = -\vec{a}_1^{*} + \vec{a}_2^{*} + \vec{a}_3^{*}$, $\vec{a}_3'^{*} = \vec{a}_1^{*} - \vec{a}_2^{*} + \vec{a}_3^{*}$

(3) What is the direct metric tensor in *R*? Use this for the direct metric tensor in *cF* (*4 points*):

$$\begin{pmatrix} a^2 & 0 & 0 \\ 0 & a^2 & 0 \\ 0 & 0 & a^2 \end{pmatrix} \Rightarrow g_{lk}$$

$$g_{ij}' = \alpha_{ik}\, g_{lk}\, \alpha_{jl}$$

$$= \frac{1}{2}\begin{pmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{pmatrix} \cdot \begin{pmatrix} a^2 & 0 & 0 \\ 0 & a^2 & 0 \\ 0 & 0 & a^2 \end{pmatrix} \frac{1}{2}\begin{pmatrix} 1 & 0 & 1 \\ 1 & 1 & 0 \\ 0 & 1 & 1 \end{pmatrix}$$

$$= \frac{a^2}{4}\begin{pmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{pmatrix}$$

(4) What is the translation vector of [001]c after the $cF \rightarrow R$ transformation? (*3 points*)

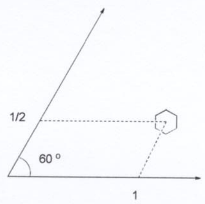
$$\vec{p_i}' = \vec{p_j}\,\alpha_{ij}^{-1}$$
$$= [001]\begin{pmatrix} 1 & -1 & 1 \\ 1 & 1 & -1 \\ -1 & 1 & 1 \end{pmatrix} = [-1\ 1\ 1]$$

(5) What is the Miller index of (110)c after the $cF \rightarrow R$ transformation? (*3 points*)

$$k_i'^{*} = \alpha_{ij}\,k_j^{*}$$
$$= \frac{1}{2}\begin{pmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{pmatrix}\begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 1/2 \\ 1/2 \end{pmatrix} \quad \therefore (211)$$

3. Calculate the W matrix for a $\pi/3$ rotation with respect to (1,1/2,0) point in the hexagonal reference frame shown below. You don't need to calculate the matrix multiplication to have a single matrix; leave the matrices in their multiplication form. (*7 points*)

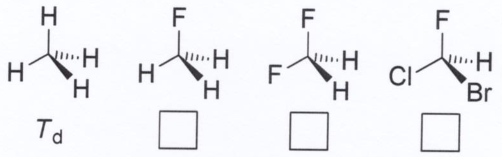
* Note that this is a hexagonal reference frame.



$$W = W_{translation}(origin \rightarrow (1, \tfrac{1}{2}, 0)) \cdot W_{\pi/3\ rotation} \cdot W_{translation}((1, \tfrac{1}{2}, 0) \rightarrow origin)$$

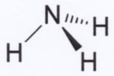
$$= \begin{bmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & \frac{1}{2} \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}\begin{bmatrix} 0 & -1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}\begin{bmatrix} 1 & 0 & 0 & -1 \\ 0 & 1 & 0 & -\frac{1}{2} \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

4. Substituted methanes can exist as four possible point groups. Identify their point groups (*one correct answer = 3 points, two = 6 points; three = 9 points*).



T_d C_{3v} C_{2v} C_1

5. Shown below it an ammonia molecule. Answer following questions: (*10 points*)



(1) List symmetry elements of ammonia (*2 points*)

one C_3 axis

three σ_v

(2) List symmetry operations of ammonia (*3 points*)

should be distinguishable ($\sigma_v, \sigma_v', \sigma_v''$)..

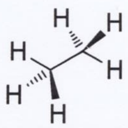
e, 3, 3^2, $\sigma_{v(1)}$, $\sigma_{v(2)}$, $\sigma_{v(3)}$

(C_3) (C_3^2)

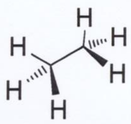
(3) What is the point group of ammonia? (*5 points*)

C_{3v}

6. Ethane (C_2H_6) can exist as two stable conformers, eclipsed and staggered forms. (*16 points*)



staggerd



eclipsed

(1) List (or indicate in the molecular structures) the symmetry elements of the staggered (*5 points*) and eclipsed (*5 points*) conformers.

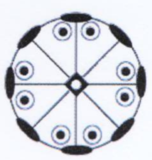
- staggered conformer: one C_3 axis, three C_2 axes, $3\sigma_d$, i, S_6
- elipsed conformer: one C_3 axis, three C_2 axes, σ_h, $3\sigma_d$

(2) Identify the point groups of both conformers (*3 point per each*)

- Staggered conformer : D_{3d}
- eclipsed conformer : D_{3h}

7. Shown below are stereographic projections of 3D crystallographic point groups. Determine their <u>Hermann–Mauguin and Schönflies notations</u> for each projection. (*5 points per each; no partial points*)

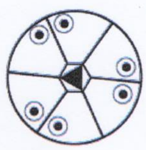
(1)



$4/mmm$ (H-M)

D_{4h} (S)

(2)



$\bar{6}m2$ (H-M)

D_{3h} (S)

(3)

$m\bar{3}$ (H-M)

T_h (S)

8. A 'polar point group' is a group in which there is at least one direction that has no symmetrically equivalent directions, and it happens only in non-centrosymmetric point groups with single rotation axes. (*10 points*)

(1) What are the highest-order point groups in the polar point groups? (*5 points*)

4mm (C_{4v}) and 6mm (C_{6v})

(2) List all of the polar points groups. (*5 points*)

4mm (C_{4v}), 6mm (C_{6v}), 6 (C_6), 4 (C_4), 3m (C_{3v}), 3 (C_3)
mm2 (C_{2v}), m (C_s), 2 (C_2), 1 (C_1)
} ten, total.

9. In our last class, we had an invited speaker who gave a talk about 'organic molecules for photodynamic therapy'. (*10 points*)

(1) What is photodynamic therapy? (*3 points*)

It is a non-invasive therapy using photosensitizers that produce toxic singlet oxygen ($^1O_2$) upon photoirradiation.

(2) Discuss about challenges that should be addressed for clinical applications of photodynamic therapy. (*7 points*)

- reduction in dark toxicity
- deep penetration of irradiation beam
- delivery of photosensitizers to concerous region
- efficient photosensitization of $^1O_2$
- & etc ...