

CHEM 373
Chemical Physics

Test: 19 August 2009

Time allowed: 50 minutes

Answer ALL questions

1. Provide group theoretical definitions for the following:

- (a) multiplication table
- (b) isomorphic groups
- (c) matrix representatives
- (d) class of symmetry operations
- (e) representation

2. A basis $\{\phi\}$ has the following representatives under symmetry operations A and B;

$$D_A(\phi) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \qquad D_B(\phi) = \begin{pmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

- (a) What is the dimensionality of the basis $\{\phi\}$?
 - (b) What are the characters, $\chi_A(\phi)$ and $\chi_B(\phi)$ for this basis under A and B?
 - (c) What are the representative and character for $\{\phi\}$ under the identity operation (E)?
 - (d) What are the representative and character for $\{\phi\}$ under the operation $C = AB$?
3. The following equation is of significant utility in chemical application of group theory. Define all of the parameters that appear in the equations and explain how the equation is used.

$$a_q = \frac{1}{h} \sum_R n_R \chi(R) \chi_q(R) \qquad (1)$$