Quantum Chemistry Supplementary Subject
GROUP THEORY PROBLEMS 1

1. Do the following sets of elements form a group under the specified operation? If they do not, which of the group axioms are not obeyed?
   (a) The integers 0, ±1, ±2 … under multiplication.
   (b) The positive integers 1, 2, 3, …, taking the group operation to be addition.
   (c) Matrices of form
   $$\begin{pmatrix} 1 & x \\ 0 & 1 \end{pmatrix}$$
   where x is real, under matrix multiplication.

2. (a) If a and b are elements of a group, show that the inverse of ab is $b^{-1}a^{-1}$.
   (b) Hence, or otherwise, show that if p is conjugate to q, and q is conjugate to r, then p is conjugate to r. (This allows us to say that p, q and r form a *class* of conjugate elements.)

   [Hint: elements p and q are conjugate if they can be related by $p = a^{-1}qa$ using some element a of the group.]

3. (a) Show that the identity element E is always in a class by itself.
   (b) Show that *every* element of an abelian group is in a class by itself.

4. The numbers 1, i, -1 and $-i$ form a group under multiplication.
   (a) What is the order of the group?
   (b) Is the group abelian?
   (c) Construct the group multiplication table. Which is the identity element?
   Which elements are inverses of each other?
   (d) What are the subgroups of the group? What are their orders?

5. Show that if $ab = ac$ for elements a, b and c of a group, then $b = c$. Hence explain why each row and each column of a group multiplication table must contain every element of the group once and once only.

6. Write down the Hamiltonian for the water molecule. Show that this is left unchanged following the permutation (interchange) of the two protons. Also demonstrate that the Hamiltonian is unaffected by the inversion of all particles about the origin.

7. (More challenging.) The Hamiltonian for the hydrogen atom is invariant to rotations of the coordinate axes by any angle. By considering certain specific rotations, show that the three $2p$ orbitals, described by the following wavefunctions, are degenerate.
   $$\psi_x = xf(r) \quad \psi_y = yf(r) \quad \psi_z = zf(r)$$
   where $f(r) = Ne^{-r/2}$, N is a normalization constant, and $r^2 = x^2 + y^2 + z^2$.