2H43 INTRODUCTORY THEORETICAL CHEMISTRY

Molecular symmetry and Group Theory

3 Lectures by Dr S. H. Ashworth.

COURSEWORK

- 1. Determine the point group of the chair conformer of cyclohexane. How many Raman active vibrations and how many infra-red active vibrations might you expect to detect in its spectrum?
- 2. Show that the integral

$$H_{ij} = \int \phi_i^* \hat{H} \phi_j d\tau$$

is zero when ϕ_i and ϕ_i belong to different irreducible representations.

3. Use the generating operator:

$$\hat{P}_{j} = \frac{d_{j}}{h} \sum_{\hat{R}} \chi_{j}(\hat{R})\hat{R}$$

to determine symmetry adapted orbitals for the pentadienyl radical.