# 2H43 InTRODUCTORY THEORETICAL CHEMISTRY <br> <br> Molecular symmetry and Group Theory 

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## 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

$$
H_{i j}=\int \phi_{i}^{*} \hat{H} \phi_{j} d \tau
$$

is zero when $\phi_{i}$ and $\phi_{j}$ 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.

