

OLLSCOIL NA hÉIREANN, GAILLIMH  
THE NATIONAL UNIVERSITY OF IRELAND, GALWAY

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WINTER EXAMINATIONS 2002

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Second Year Mathematics

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**MA206 - Mathematics for Molecular Science**

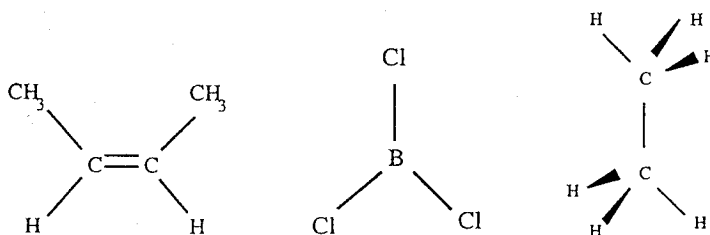
Dr Dave Johnson  
Professor T. Hurley  
Dr J. Burns  
Dr G. Ellis

Time allowed: *two* hours  
Attempt *three* questions

1. (a) Find the  $3 \times 3$  matrix representing rotation through  $180^\circ$  about the  $z$ -axis followed by reflection in the  $xy$ -plane.
- (b) Decide which one of the following two matrices represents a symmetry, and then decide whether this symmetry is a rotation or an improper rotation.

$$A = \begin{pmatrix} 1/3 & 2/3 & 2/3 \\ 2/3 & 2/3 & 1/3 \\ 2/3 & 1/3 & 2/3 \end{pmatrix}, B = \begin{pmatrix} 1/3 & 2/3 & 2/3 \\ 2/3 & -2/3 & 1/3 \\ 2/3 & 1/3 & -2/3 \end{pmatrix}.$$

- (c) The water molecule has four symmetries:  $E$  = identity,  $C_2$  = rotation through  $180^\circ$  about the  $z$ -axis,  $\sigma_{xz}$  = reflection in the  $xz$ -plane,  $\sigma_{yz}$  = reflection in the  $yz$ -plane. Determine the multiplication table of its symmetry group.
2. (a) Use the algorithm in the Appendix to determine the point groups of the following three molecules. Give full details of how you arrive at your answers.



- (b) Find a 1-dimensional representation of the group  $C_{2v} = \{E, C_2, \sigma_{xz}, \sigma_{yz}\}$  to which a  $p_x$  orbital belongs. Also find a 1-dimensional representation of  $C_{2v}$  to which a  $d_{xy}$  orbital belongs.

# APPENDIX

## Systematic classification of molecules into point groups

$C$  = rotation axis

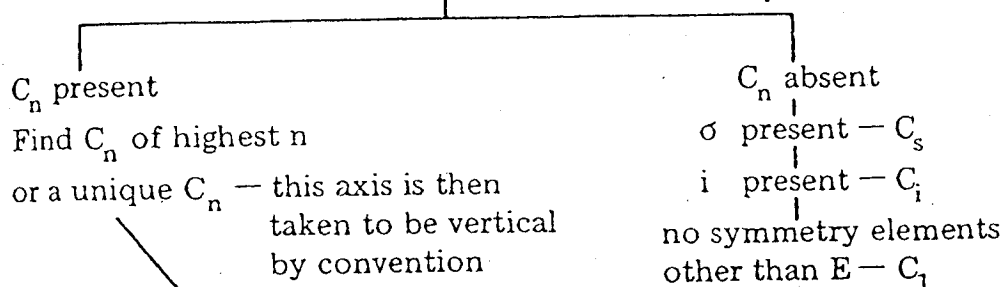
$i$  = inversion centre

$S$  = improper axis (alternating axis)  $\sigma$  = plane of symmetry

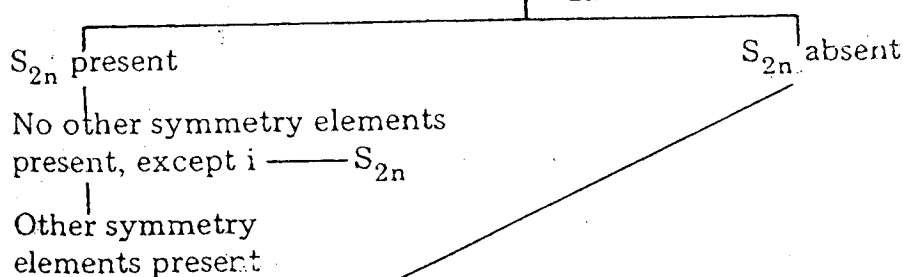
### 1. Examine for special groups

- Linear, no  $\sigma$  perpendicular to molecular axis —  $C_{\infty v}$
- Linear,  $\sigma$  perpendicular to molecular axis —  $D_{\infty h}$
- Tetrahedral —  $T_d$
- Octahedral —  $O_h$
- Dodecahedral or icosahedral —  $I_h$

### 2. Examine for a $C_n$ axis



### 3. Examine for $S_{2n}$ colinear with $C_n$



### 4. Examine for $n$ horizontal $C_2$ axes

