EDUCATION DIVISION PUBLICATIONS

SYMMETRY IN CHEMISTRY

SIDNEY KETTLE

ETSG

CHEMISTRY CASSETTE

CHEMISTRY CASSETTES

General Editor:
Peter Groves
The University of Aston in Birmingham

Published 1976 by the Educational Techniques Subject Group, The Chemical Society, London.

ISBN 0 85186 729 4

USING CHEMISTRY CASSETTES

Please read this carefully before you start

This Chemistry Cassette presentation comprises two audio-cassettes with this accompanying workbook. They are designed to be used together and you should have the workbook in front of you as you listen to the cassettes. Material in the workbook is divided into numbered *frames* and Professor Kettle frequently refers to these as he speaks. Each frame contains diagrams, tables and other relevant material and you should locate and study this wherever appropriate.

During the course of the presentation you are asked, from time to time, to stop the tape and to work on some problems: you should, therefore, also have pencil and paper with you. Two of the problems ask you to make observations on a small cube and on a model of the water molecule. You should have these ready before you start. For the cube, a child's building brick would be suitable provided that all the faces are the same colour. Instructions for making a cube from a piece of card are given in frame 10. For the water molecule (which is considered at the start of the second cassette) a simple ball and stick model would be quite adequate. If this is not available, a model made from three balls of plasticine and two matchsticks would be equally suitable.

An important feature of tape recorded material is that it is 'self-pacing'. This means that you can work through it at your own pace, switching off the player whenever you wish to pause for thought, to study a diagram, to work on a problem, etc., and you can use the rewind control on the player to repeat material that you may not have fully understood on a first hearing. To gain the greatest benefit from this presentation you should make full use of these features. You should also make appropriate notes to supplement the material contained in the workbook.

Part	Side	Approximate running times	Corresponding frame numbers
1	A	20 mins.	1 – 10
	B	21 mins.	11 – 28
2	A	38 mins.	29 – 44
	B	28 mins.	45 – 58

28

<u>The ground to be covered in this presentation</u>

Symmetry elements

Symmetry operations

Multiplication of symmetry operations

Irreducible Representations of a group

Character tables

Reducible representations of a group

Example: The vibrations of the water molecule

Selection Rules

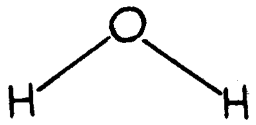
Molecular Integrals

PART 2

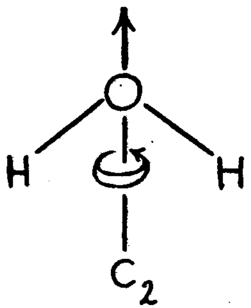
29

The four elements are

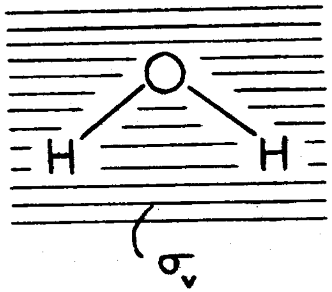
1) The identity (leave alone)



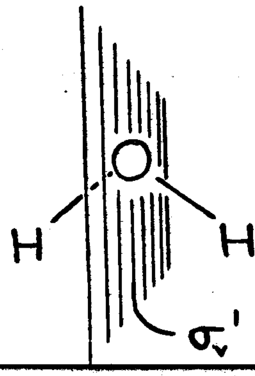
2) A C_2 rotation

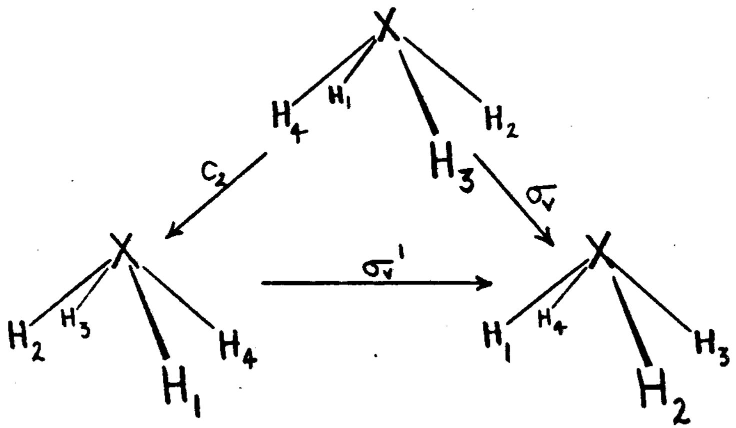


3) Reflection in a σ_v mirror plane (in the plane of the paper)



4) Reflection in a second type of σ_v mirror plane (denoted σ_v') perpendicular to the plane of the paper





Second operation

C_{2v}	E	C_2	σ_v	σ_v'
E	E			
C_2				σ_v
σ_v				
σ_v'				

First operation

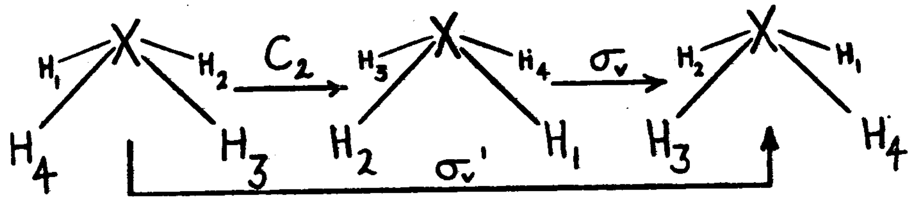
Second operation

C_{2v}	E	C_2	σ_v	σ_v'
E	E	C_2	σ_v	σ_v'
C_2	C_2	E	σ_v'	σ_v
σ_v	σ_v	σ_v'	E	C_2
σ_v'	σ_v'	σ_v	C_2	E

First operation

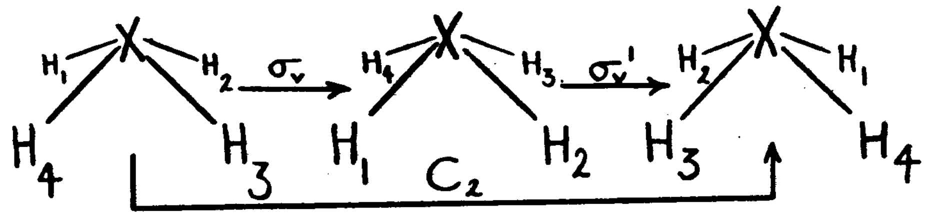
The symmetry seen in the entries in this table across the leading diagonal (shown dotted) is a characteristic of Abelian groups.

Example 1; C_2 followed by σ_v

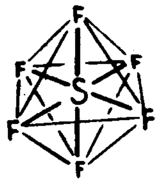


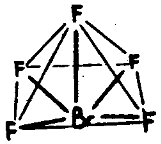
So, C_2 followed by σ_v is equivalent to σ_v'

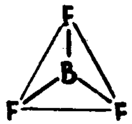
Example 2; σ_v followed by σ_v'

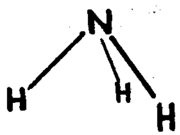


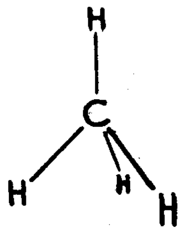
So, σ_v followed by σ_v' is equivalent to C_2











Point Group	Symmetry Operations
C_1	E
C_s	E, σ_h (There is no unique axis of highest symmetry but the axis perpendicular to the mirror plane is unique so σ_h is used)
C_i	E, i
C_2	E, C_2
C_3	E, C_3, C_3^2 (Note C_3^2 means C_3 carried out twice; C_4^3 means C_4 carried out thrice etc.
C_4	E, C_4, C_2, C_4^3
C_5	E, C_5, C_5^2, C_5^3, C_5^4
C_6	E, C_6, C_3, C_2, C_3^2, C_6^5
D_2	E, C_2, C_2', C_2''
D_3	E, $2C_3$, $3C_2$
D_4	E, $2C_4$, C_2, $2C_2'$, $2C_2''$
D_5	E, $2C_5$, $2C_5^2$, $5C_2$
D_6	E, $2C_6$, $2C_3$, C_2, $3C_2'$, $3C_2''$
C_{2v}	E, C_2, σ_v, σ_v'
C_{3v}	E, $2C_3$, $3\sigma_v$
C_{4v}	E, $2C_4$, C_2, $2\sigma_v$, $2\sigma_v'$
C_{5v}	E, $2C_5$, $2C_5^2$, $5\sigma_v$
C_{6v}	E, $2C_6$, $2C_3$, C_2, $3\sigma_v$, $3\sigma_v'$
C_{2h}	E, C_2, i, σ_h
C_{3h}	E, C_3, C_3^2, σ_h, S_3, S_3^5
C_{4h}	E, C_4, C_2, C_4^3, i, S_4^3, σ_h, S_4
C_{5h}	E, C_5, C_5^2, C_5^3, C_5^4, σ_h, S_5, S_5^3, S_5^7, S_5^9
C_{6h}	E, C_6, C_3, C_2, C_3^2, C_6^5, i, S_3^5, S_6^5, σ_h, S_6, S_3

FRAME CONTINUED ON NEXT PAGE

33
CONTD.

Point Group	Symmetry Operations
D_{2h}	$E, C_2, C_2', C_2'', i, \sigma_v, \sigma_v', \sigma_v''$ (The labels on the mirror planes are somewhat arbitrary - one might be labelled σ_h)
D_{3h}	$E, 2C_3, 3C_2, \sigma_h, 2S_3, 3\sigma_d$
D_{4h}	$E, 2C_4, C_2, 2C_2', 2C_2'', i, 2S_4, \sigma_h, 2\sigma_d, 2\sigma_d'$
D_{5h}	$E, 2C_5, 2C_5^2, 5C_2, \sigma_h, 2S_5, 2S_5^3, 5\sigma_d$
D_{6h}	$E, 2C_6, 2C_3, C_2, 2C_2', 3C_2'', i, 2S_3, 2S_6, \sigma_h, 3\sigma_d, 3\sigma_d'$
D_{2d}	$E, 2S_4, C_2, 2C_2', 2\sigma_d$
D_{3d}	$E, 2C_3, 2C_2, i, 2S_6, 3\sigma_d$
D_{4d}	$E, 2S_8, 2C_4, 2S_8^3, C_2, 4C_2', 4\sigma_d$
D_{5d}	$E, 2C_5, 2C_5^2, 5C_2, i, 2S_{10}^3, 2S_{10}, 5\sigma_d$
D_{6d}	$E, 2S_{12}, 2C_6, 2S_4, 2C_3, 2S_{12}^5, C_2, 6C_2', 6\sigma_d$
S_4	E, S_4, C_2, S_4^3
S_6	$E, C_3, C_3^2, i, S_6, S_6^5$
T	$E, 4C_3, 4C_3^2, 3C_2$
T_d	$E, 8C_3, 3C_2, 6S_4, 6\sigma_d$
T_h	$E, 4C_3, 4C_3^2, 3C_2, i, 4S_6, 4S_6^5, 3\sigma_h$
O	$E, 8C_3, 6C_2, 6C_4, 2C_2'$
O_h	$E, 8C_3, 6C_2, 6C_4, 3C_2', i, 8S_6, 6\sigma_d, 6S_4, 3\sigma_h$
I	$E, 12C_5, 12C_5^2, 20C_3, 15C_2$
I_h	$E, 12C_5, 12C_5^2, 20C_3, 15C_2, i, 12S_{10}, 12S_{10}^3, 20S_6, 15\sigma_v$

34

The multiplication table is

C_{2v}	E	C_2	σ_v	σ_v'
E	E	C_2	σ_v	σ_v'
C_2	C_2	E	σ_v'	σ_v
σ_v	σ_v	σ_v'	E	C_2
σ_v'	σ_v'	σ_v	C_2	E

so that substitution gives

	1	1	-1	-1
1	1	1	-1	-1
1	1	1	-1	-1
-1	-1	-1	1	1
-1	-1	-1	1	1

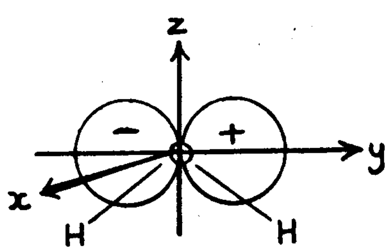
35

	1	1	1	1
1	1	1	1	1
1	1	1	1	1
1	1	1	1	1
1	1	1	1	1

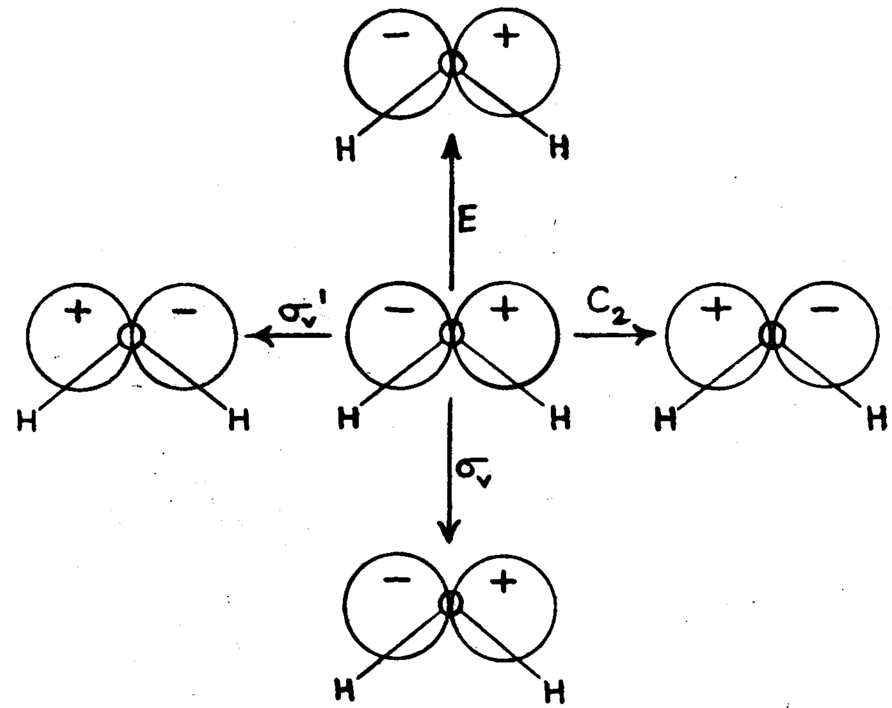
	1	-1	1	-1
1	1	-1	1	-1
-1	-1	1	-1	1
1	1	-1	1	-1
-1	-1	1	-1	1

	1	-1	-1	1
1	1	-1	-1	1
-1	-1	1	1	-1
-1	-1	1	1	-1
1	1	-1	-1	1

36

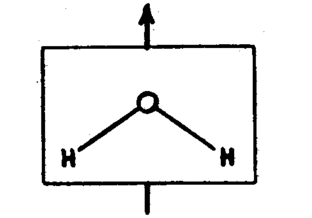


37

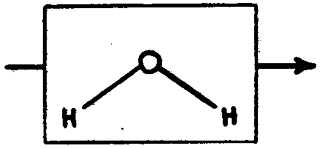


38

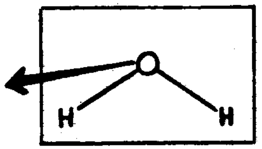
a



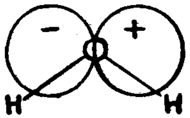
b



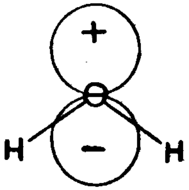
c



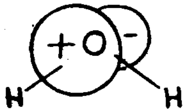
d



e



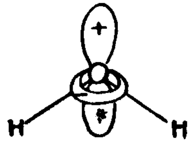
f



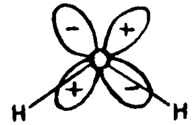
FRAME CONTINUED ON NEXT PAGE

38
CONTD.

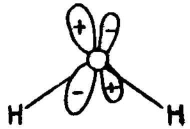
g



h



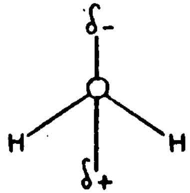
i



j

k

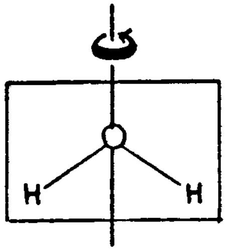
ℓ



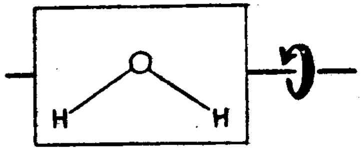
FRAME CONTINUED ON NEXT PAGE

38
CONTD.

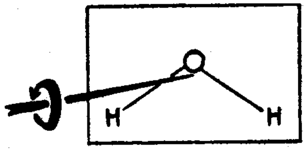
m



n



o



39

A <u>representation</u> of a group is a set with the property that the members of the set multiply (using an appropriate law of multiplication - which may be ordinary multiplication, matrix multiplication or some other form of combination) in a way which is isomorphous to the multiplication (i.e. one followed by the other) of the operations of the group.

In the applications with which we are concerned such representations are matrices; in this tape we largely concentrate on 1 x 1 matrices - these are ordinary numbers. Further, it is usually possible to work with the sum of those elements of the matrix which fall along the leading diagonal - the <u>character</u> of the matrix rather than the whole matrix.

When such a set of matrices may simultaneously be reduced to a block-diagonal form we have a <u>reducible representation</u> of the group, when they cannot be so reduced we have an <u>irreducible representation</u>. The characters of the matrices of the irreducible representations are listed in the <u>character table</u> of a group.

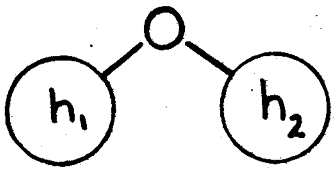
The <u>totally symmetric irreducible representation</u> of a group has a character of 1 for all operations of the group. It describes the symmetry properties of something which is turned into itself by every one of the operations of the group.

40

a)

C_{2v}	E	C_2	σ_v	σ_v'
A_1	1	1	1	1
A_2	1	1	-1	-1
B_1	1	-1	1	-1
B_2	1	-1	-1	1

b)



41

C_{3v}	E	$2C_3$	$3\sigma_v$
A_1	1	1	1
A_2	1	1	-1
E	2	-1	0

C_{2h}	E	C_2	i	σ_h
A_g	1	1	1	1
B_g	1	-1	1	-1
A_u	1	1	-1	-1
B_u	1	-1	-1	1

D_{2h}	E	$C_2(z)$	$C_2(x)$	$C_2(y)$	i	$\sigma(xy)$	$\sigma(yz)$	$\sigma(zx)$
A_g	1	1	1	1	1	1	1	1
B_{1g}	1	1	-1	-1	1	1	-1	-1
B_{2g}	1	-1	1	-1	1	-1	1	-1
B_{3g}	1	-1	-1	1	1	-1	-1	1
A_u	1	1	1	1	-1	-1	-1	-1
B_{1u}	1	1	-1	-1	-1	-1	1	1
B_{2u}	1	-1	1	-1	-1	1	-1	1
B_{3u}	1	-1	-1	1	-1	1	1	-1

FRAME CONTINUED ON NEXT PAGE

D_{4h}	E	$2C_4$	C_2	$2C_2'$	$2C_2''$	i	$2S_4$	σ_h	$2\sigma_d$	$2\sigma_d'$
A_{1g}	1	1	1	1	1	1	1	1	1	1
A_{2g}	1	1	1	-1	-1	1	1	1	-1	-1
B_{1g}	1	-1	1	-1	1	1	-1	1	-1	1
B_{2g}	1	-1	1	1	-1	1	-1	1	1	-1
E_g	2	0	-2	0	0	2	0	-2	0	0
A_{1u}	1	1	1	1	1	-1	-1	-1	-1	-1
A_{2u}	1	1	1	-1	-1	-1	-1	-1	1	1
B_{1u}	1	-1	1	-1	1	-1	1	-1	1	-1
B_{2u}	1	-1	1	1	-1	-1	1	-1	-1	1
E_u	2	0	-2	0	0	-2	0	2	0	0

T_d	E	$8C_3$	$6\sigma_d$	$6S_4$	$3C_2$
A_1	1	1	1	1	1
A_2	1	1	-1	-1	1
E	2	-1	0	0	2
T_1	3	0	-1	1	-1
T_2	3	0	1	-1	-1

FRAME CONTINUED ON NEXT PAGE

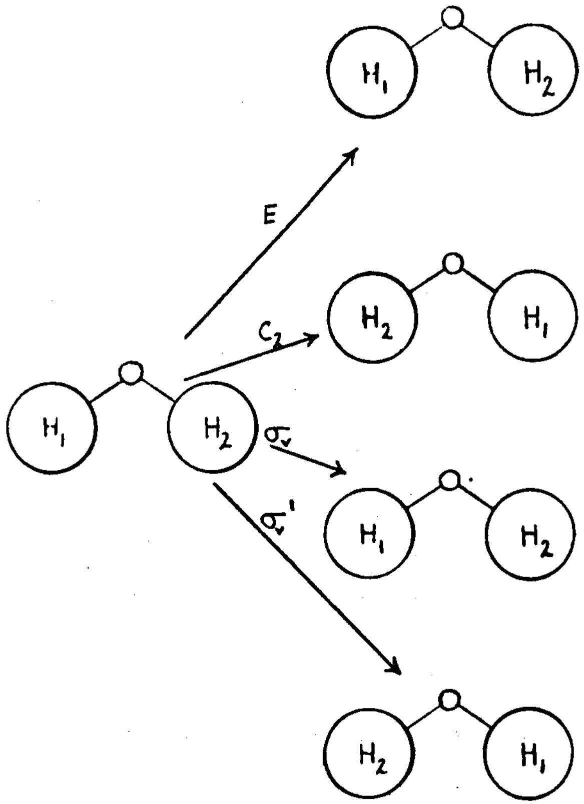
41
CONTD.

O_h	E	$8C_3$	$6C_4$	$3C_2$	$6C_2'$	i	$8S_6$	$6S_4$	$3\sigma_h$	$6\sigma_d$
A_{1g}	1	1	1	1	1	1	1	1	1	1
A_{2g}	1	1	-1	1	-1	1	1	-1	1	-1
E_g	2	-1	0	2	0	2	-1	0	2	0
T_{1g}	3	0	1	-1	-1	3	0	1	-1	-1
T_{2g}	3	0	-1	-1	1	3	0	-1	-1	1
A_{1u}	1	1	1	1	1	-1	-1	-1	-1	-1
A_{2u}	1	1	-1	1	-1	-1	-1	1	-1	1
E_u	2	-1	0	2	0	-2	1	0	-2	0
T_{1u}	3	0	1	-1	-1	-3	0	-1	1	1
T_{2u}	3	0	-1	-1	1	-3	0	1	1	-1

(O_h is the symmetry group of the cube and of the regular octahedron)

Note that for those point groups given above in which i is a symmetry operation the character table blocks into four, the corresponding characters in each block bearing a very simple relationship to each other. This arises from a relationship between the operators listed at the top of the table. Thus, in the O_h table, i is equivalent to E followed by i, S_6 is equivalent to C_3 followed by i etc. (see Frame 14).

42



43

a)

C_{2v}	E	C_2	σ_v	σ_v'
A_1	1	1	1	1
A_2	1	1	-1	-1
B_1	1	-1	1	-1
B_2	1	-1	-1	1

and the reducible representation

b)

C_{2v}	E	C_2	σ_v	σ_v'
	2	0	2	0

c) Select the A_1 irreducible representation; multiply the characters of the reducible representation by those of the A_1 irreducible representation and add the products together,

$$(1 \times 2) + (1 \times 0) + (1 \times 2) + (1 \times 0) = 4$$

d) Divide the result by the order of the group

$$4/4 = 1.$$

The answer, in this case 1, is the number of A_1 irreducible components in the reducible representation (2,0,2,0).

e) This is repeated for all the irreducible representations. Thus for the A_2 irreducible representation

$$(1 \times 2) + (1 \times 0) + (-1 \times 2) + (-1 \times 0) = 0.$$

$$0/4 = 0$$

and we conclude that there are no A_2 irreducible representations in the reducible representation (2,0,2,0).

FRAME CONTINUED ON NEXT PAGE

f) For the B_1 irreducible representation

$$(1 \times 2) + (1 \times 0) + (1 + 2) + (-1 \times 0) = 4$$

$$4/4 = 1$$

we have found that there is a B_1 component in the reducible representation (2,0,2,0).

g) For the B_2 irreducible representation

$$(1 \times 2) + (-1 \times 0) + (-1 \times 2) + (1 \times 0) = 0$$

$$0/4 = 0.$$

That is, there is no B_2 component in the reducible representation (2,0,2,0). Thus, in summary, we have the result that the the irreducible components of the reducible representation (2,0,2,0) are $A_1 + B_1$.

h) Consider the C_{3v} character table

C_{3v}	E	$2C_3$	$3\sigma_v$
A_1	1	1	1
A_2	1	1	-1
E	2	-1	0

and the reducible representation

i) 4 1 0

First multiply these characters by the number of elements in the corresponding classes. Thus

	4 x 1	1 x 2	0 x 3
gives	4	2	0

Now proceed as for the C_{2v} case:-

FRAME CONTINUED ON NEXT PAGE

Test for A_1: $(4 \times 1) + (2 \times 1) + (0 \times 1) = 6$

The order of the group is 6, so, $\frac{6}{6} = 1$ (A_1 component).

Test for A_2: $(4 \times 1) + (2 \times 1) + (0 \times -1) = 6$

$\frac{6}{6} = 1$ so there is one A_2 component

Test for E: $(4 \times 2) + (2 \times -1) + (0 \times 0) = 6$

$\frac{6}{6}$ = - so there is one E component.

Thus, the reducible representation (4, 1, 0) has irreducible components $A_1 + A_2 + E$.

C_{2v}	E	C_2	σ_v	σ_v'
A_1	1	1	1	1
A_2	1	1	-1	-1
B_1	1	-1	1	-1
B_2	1	-1	-1	1

C_{3v}	E	$2C_3$	$3\sigma_v$
A_1	1	1	1
A_2	1	1	-1
E	2	-1	0

D_{2d}	E	$2S_4$	C_2	$2C_2'$	$2\sigma_d$
A_1	1	1	1	1	1
A_2	1	1	1	-1	-1
B_1	1	-1	1	1	-1
B_2	1	-1	1	-1	1
E	2	0	-2	0	0

FRAME CONTINUED ON NEXT PAGE

44

1.

C_{2v}	E	C_2	σ_v	σ_v'
	4	2	0	2

2.

C_{2v}	E	C_2	σ_v	σ_v'
	7	-1	1	-3

3.

C_{3v}	E	$2C_3$	$3\sigma_v$
	7	1	-1

4.

C_{3v}	E	$2C_3$	$3\sigma_v$
	3	0	1

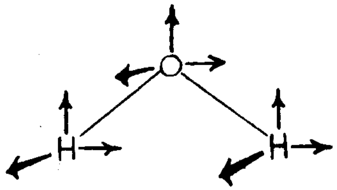
5.

D_{2d}	E	$2S_4$	C_2	$2C_2'$	$2\sigma_d$
	4	0	0	-2	0

6.

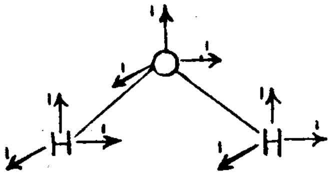
D_{2d}	E	$2S_4$	C_2	$2C_2'$	$2\sigma_d$
	6	0	2	-2	-2

45



46

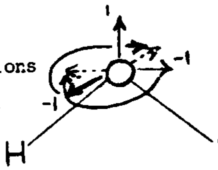
The E operation



Character = 9

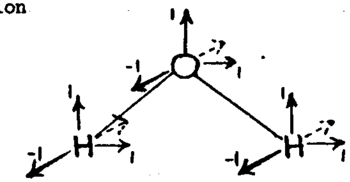
The C_2 operation

the 'after' positions of the arrows are shown dotted



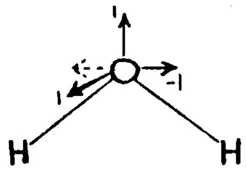
Character = -1

The σ_v operation



Character = 3

The σ_v' operation



Character = 1

47

C_{2v}	E	C_2	σ_v	σ_v'
A_1	1	1	1	1
A_2	1	1	-1	-1
B_1	1	-1	1	-1
B_2	1	-1	-1	1

The reducible representation is

	E	C_2	σ_v	σ_v'	
Γ_{red}	9	-1	3	1	
Test for A_1					
A_1	1	1	1	1	
$\Gamma_{red} \times A_1$	9	-1	3	1	sum = 12; divide by the order of the group (4) ➡ 3. Hence Γ_{red} contains $3A_1$
Test for A_2					
A_2	1	1	-1	-1	
$\Gamma_{red} \times A_2$	9	-1	-3	-1	sum = 4; hence Γ_{red} contains A_2
Test for B_1					
B_1	1	-1	1	-1	
$\Gamma_{red} \times B_1$	9	1	3	-1	sum = 12; hence Γ_{red} contains $3B_1$
Test for B_2					
B_2	1	-1	-1	1	
$\Gamma_{red} \times B_2$	9	1	-3	1	sum = 8; hence Γ_{red} contains $2B_2$

FRAME CONTINUED ON NEXT PAGE

47 CONTD.

Hence Γ_{red} contains $3A_1 + A_2 + 3B_1 + 2B_2$

From the solution to problems a, b, c and m, n and o of Frame 38 (given in Frame 57) we conclude that:-

a) The translations of H_2O transform as $A_1 + B_1 + B_2$

b) The rotation of H_2O transform as $A_2 + B_1 + B_2$

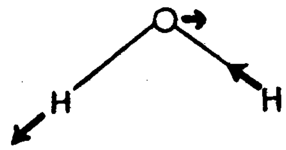
Subtract these from the components of Γ_{red} to obtain the symmetry species of the vibrations of H_2O. These are $2A_1 + B_1$

48

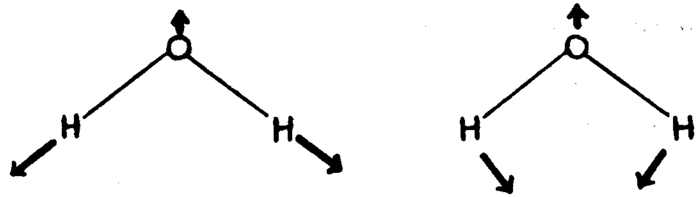
C_{2v}	E	C_2	σ_v	σ_v'		
A_1	1	1	1	1	z , T_z	x^2, y^2, z^2
A_2	1	1	-1	-1	R_z	xy
B_1	1	-1	1	-1	y, T_y, R_x	yz
B_2	1	-1	-1	1	x, T_x, R_y	xz

49

The B_1 mode (schematic)



The A_1 modes (schematic)



Because the molecule must not rotate (rotations have been factored out) the H atom motions must lie in the yz plane for both of the A_1 modes. Further, their motions in the two A_1 modes must be quite different (the two A_1 modes must be quite different - they must be orthogonal). It makes chemical sense that one mode should be, essentially, an O-H stretching mode. It follows that the second A_1 mode must have the general form shown.

The A_2 irreducible representation of the C_{2v} point group is

	E	C_2	σ_v	σ_v'
A_2	1	1	-1	-1

The B_1 irreducible representation is

B_1	1	-1	1	-1

Form the direct product by multiplying pairs of characters together

$A_2 x B_1$	(1x1)	(1x-1)	(-1x1)	(-1x-1)	
	1	-1	-1	1	= B_2

We conclude that the direct product $A_2 x B_1$ is B_2.

The direct product of two representations is the representation obtained when pairs of corresponding characters are multplied together

The direct product table of the C_{2v} point group

C_{2v}	A_1	A_2	B_1	B_2
A_1	A_1	A_2	B_1	B_2
A_2	A_2	A_1	B_2	B_1
B_1	B_1	B_2	A_1	A_2
B_2	B_2	B_1	A_2	A_1

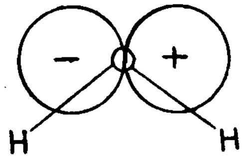
The direct product table of the C_{3v} point group

C_{3v}	A_1	A_2	E
A_1	A_1	A_2	E
A_2	A_2	A_1	E
E	E	E	A_1+A_2+E

Note that the totally symmetric irreducible representation (A_1 in both of the above tables) only appears on the leading diagonal of these tables. This is invariably the case for all direct product tables. We conclude that it is always true that:-

> The totally symmetric irreducible representation is only generated when an irreducible representation is multiplied by itself.

52



53

Oxygen orbital	Symmetry species	Does integration give a non-zero result?
s	A_1	Yes
p_x	B_2	No
p_y	B_1	No
p_z	A_1	No
d_{z^2}	A_1	No
$d_{x^2-y^2}$	A_1	No
d_{xy}	A_2	No
d_{xz}	B_2	No
d_{yz}	B_1	No

54

$$\int \psi_e(A_1)\ \hat{\mu}_x\ \psi_g(A_1)\ d\tau$$

$\hat{\mu}_x$ transforms as B_2 so we have to form the triple direct product

$A_1 \times B_2 \times A_1 = A_1 \times (B_2 \times A_1) = A_1 \times B_2 = B_2$

Integration over all space of a non-totally symmetric irreducible representation gives zero so we conclude that the A_1 vibration is not active in x polarization.

$$\int \psi_e(A_1)\ \hat{\mu}_y\ \psi_g(A_1)\ d\tau$$

We have $A_1 \times B_1 \times A_1 = B_1 \rightarrow$ zero integral. The A_1 vibration is not allowed in y polarization.

$$\int \psi_e(A_1)\ \hat{\mu}_z\ \psi_g(A_1)\ d\tau$$

We have $A_1 \times A_1 \times A_1 = A_1 \rightarrow$ non-zero integral. The A_1 vibration is allowed (and may hence be identified) in z polarization.

$$\int \psi_e(B_1)\ \hat{\mu}_x\ \psi_g(A_1)\ d\tau$$

We have $B_1 \times B_2 \times A_1 = A_2 \Rightarrow$ zero integral. The B_1 vibration is not allowed in x polarization.

$$\int \psi_e(B_1)\ \hat{\mu}_y\ \psi_g(A_1)\ d\tau$$

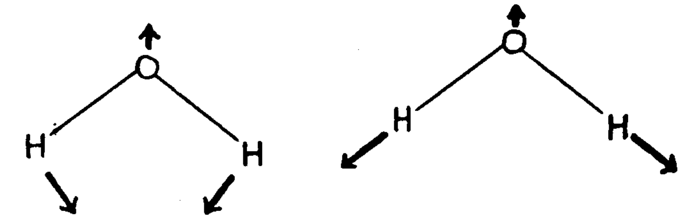
We have $B_1 \times B_1 \times A_1 = A_1 \Rightarrow$ non-zero integral. The B_1 vibration is allowed (and may hence be identified) in y polarization.

$$\int \psi_e(B_1)\ \hat{\mu}_z\ \psi_g(A_1)\ d\tau$$

We have $B_1 \times A_1 \times A_1 = B_1 \Rightarrow$ zero integral. The B_1 vibration is not allowed in z polarization.

55

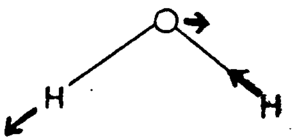
The A_1 vibrations are



In both cases the dipole moment changes along the z direction and it is only the integral

$\int \psi_e(A_1)\hat{\mu}_z \, \psi_g(A_1)d\tau$ which is non zero (direct product $A_1 \times A_1 \times A_1 = A_1$)

The B_1 vibration



The dipole moment changes along the y direction and it is only the integral

$\int \psi_e(B_1)\hat{\mu}_y \, \psi_g(A_1)d\tau$ which is non-zero (direct product $B_1 \times B_1 \times A_1 = A_1$)

56

SF_6	O_h
BrF_5	C_{4v}
BF_3	D_{3h}
NH_3	C_{3v}
CH_4	T_d

57

	E	C_2	σ_v	σ_v'
a) Translation along z	1	1	1	1
b) Translation along y	1	-1	1	-1
c) Translation along x	1	-1	-1	1
d) The oxygen p_z orbital	1	1	1	1
e) The oxygen p_y	1	-1	1	-1
f) The oxygen p_x	1	-1	-1	1
g) The oxygen d_{z^2}	1	1	1	1
h) The oxygen d_{yz}	1	-1	1	-1
i) The oxygen d_{zx}	1	-1	-1	1
j) The oxygen $d_{x^2-y^2}$	1	1	1	1
k) The oxygen d_{xy}	1	1	-1	-1
l) The dipole moment	1	1	1	1
m) Rotation about z	1	1	-1	-1
n) Rotation about y	1	-1	-1	1
o) Rotation about x	1	-1	1	-1

1. $2A_1 + A_2 + B_2$

2. $A_1 + 2A_2 + 3B_1 + B_2$

3. $A_1 + 2A_2 + 2E$

4. $A_1 + E$

5. $A_2 + B_2 + E$

6. $2A_2 + B_1 + B_2 + E$