4.4: Unit 4 Practice Problems

Exercise 1

Can the following matrices be multiplied and if so what is the product matrix?

a) $\begin{bmatrix} 2 & 1 & 0 \\ 5 & 9 & 1 \\ 2 & 2 & 3 \end{bmatrix}\begin{bmatrix} 0 & 3 & 1 \\ 4 & 1 & 2 \\ -1 & -1 & 3 \end{bmatrix}$

b) $\begin{bmatrix} 3 & 1 & 0 \end{bmatrix}\begin{bmatrix} 4 \\ 2 \\ 1 \end{bmatrix}$

c) $\begin{bmatrix} 1 & 2 & 3 & 4 \\ 4 & 3 & 2 & 1 \end{bmatrix}\begin{bmatrix} 1 & 4 \\ 2 & 3 \\ 3 & 2 \\ 4 & 1 \end{bmatrix}$

d) $\begin{bmatrix} 2 & -1 \\ 1 & 1 \end{bmatrix}\begin{bmatrix} 1 & 5 & 8 \\ 2 & 2 & 4 \\ 1 & 8 & 1 \end{bmatrix}$

Answer

a) $\begin{bmatrix} 2 & 1 & 0 \\ 5 & 9 & 1 \\ 2 & 2 & 3 \end{bmatrix}\begin{bmatrix} 0 & 3 & 1 \\ 4 & 1 & 2 \\ -1 & -1 & 3 \end{bmatrix} = \begin{bmatrix} 2\times0+1\times4+0\times(-1) & 2\times3+1\times1+0\times(-1) & 2\times1+1\times2+0\times3 \\ 5\times0+9\times4+1\times(-1) & 5\times3+9\times1+1\times(-1) & 5\times1+9\times2+1\times3 \\ 2\times0+2\times4+3\times(-1) & 2\times3+2\times1+3\times(-1) & 2\times1+2\times2+3\times3 \end{bmatrix} = \begin{bmatrix} 4 & 7 & 4 \\ 35 & 23 & 26 \\ 5 & 5 & 15 \end{bmatrix}$

b) $\begin{bmatrix} 3 & 1 & 0 \end{bmatrix}\begin{bmatrix} 4 \\ 2 \\ 1 \end{bmatrix} = \begin{bmatrix} 3\times4+1\times2+0\times1 \end{bmatrix} = \begin{bmatrix} 14 \end{bmatrix}$

c) $\begin{bmatrix} 1 & 2 & 3 & 4 \\ 4 & 3 & 2 & 1 \end{bmatrix}\begin{bmatrix} 1 & 4 \\ 2 & 3 \\ 3 & 2 \\ 4 & 1 \end{bmatrix} = \begin{bmatrix} 1\times1+2\times2+3\times3+4\times4 & 1\times4+2\times3+3\times2+4\times1 \\ 4\times1+3\times2+2\times3+1\times4 & 4\times4+3\times3+2\times2+1\times1 \end{bmatrix} = \begin{bmatrix} 30 & 20 \\ 20 & 30 \end{bmatrix}$

d) $\begin{bmatrix} 2 & -1 \\ 1 & 1 \end{bmatrix}\begin{bmatrix} 1 & 5 & 8 \\ 2 & 2 & 4 \\ 1 & 8 & 1 \end{bmatrix}$

These two matrices cannot be multiplied.

Exercise 2

Determine the irreducible representations for the following orbitals in the point group D_{2h}.

The z axis is defined as the axis of the principal C_2 axis. C_2’ is defined as the axis rotating around y. σ_v is defined as the xz plane.

	E	C_2	C_2'	C_2''	i	σ_h	σ_v	σ_v'
a) 2s								
b) $2p_x$								
c) $2p_y$								
d) $2p_z$								
e) $3d_{z2}$								
f) $3d_{x2-y2}$								
g) $3d_{xy}$								
h) $3d_{yz}$								
i) $3d_{xz}$								

Answer

	E	C_2	C_2'	C_2''	i	σ_h	σ_v	σ_v'
a) 2s	1	1	1	1	1	1	1	1
b) $2p_x$	1	-1	-1	1	-1	1	1	-1
c) $2p_y$	1	-1	1	-1	-1	1	-1	1
d) $2p_z$	1	1	-1	-1	-1	-1	1	1
e) $3d_{z2}$	1	1	1	1	1	1	1	1
f) $3d_{x2-y2}$	1	1	1	1	1	1	1	1
g) $3d_{xy}$	1	1	-1	-1	1	1	-1	-1
h) $3d_{yz}$	1	-1	-1	1	1	-1	-1	1
i) $3d_{xz}$	1	-1	1	-1	1	-1	1	-1

Exercise 3

Determine the matrix representations of the symmetry elements of the following point groups:

a) D_2

Define principal C_2 axis as the axis running along z. C_2' runs along x.

b) C_3

If we define the principal C_3 axis running along the z axis:

Answer

a)

$$\begin{matrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{matrix} \qquad C_2\text{:} \begin{matrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{matrix} \qquad C_2'\text{:} \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

$$C_2''\text{:} \begin{matrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{matrix}$$

b)

$$E\text{:} \begin{matrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{matrix} \qquad C_3{}^1\text{:} \begin{matrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{matrix} \qquad C_3{}^2\text{:} \begin{matrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{matrix}$$

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