## **Review of Matrices and Vectors**

Matrices and vectors are used quite often to describe transformations or symmetry operations of molecules. It is important to remember that matrices are merely a very compact means of notation; the is nothing that absolutely requires the use of a matrix. However, matrices and vectors are so convenient that those of you comfortable with them may choose to use them instead of the graphical method. This handout should help you refamiliarize with some of the basic rules and properties of matrices and vectors.

An  $\underline{m \ x \ n \ matrix}$  is an ordered rectangular array of elements containing m rows and n columns. Each matrix element is given two indices, the first identifying the row and the second identifying the column:

$$\underline{\underline{A}} = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & & \vdots \\ a_{m1} & a_{m2} & & a_{mn} \end{bmatrix}$$

A <u>square matrix</u> is one in which the number of rows equals the number of columns. A <u>column</u> <u>vector</u> (or just a plain <u>vector</u>) has only one column, and a <u>row vector</u> has only one row. For the purposes of this course, we will only be concerned with square matrices and column vectors. A column vector has m rows and one column, and can be thought of as an m x 1 matrix.

Two matrices,  $\underline{A}$  and  $\underline{B}$  are equal if, and only if, all of their elements are equal:

$$\underline{\mathbf{A}} = \underline{\mathbf{B}}$$
 if  $\mathbf{a}_{ij} = \mathbf{b}_{ij}$  for all i and j

Adding two matrices is straightfoward and is achieved through the addition of each element:

If 
$$\underline{C} = \underline{A} + \underline{B}$$
, then  $c_{ii} = a_{ii} + b_{ii}$  for all i and j

Two matrices, <u>A</u> and <u>B</u>, can only be added if they have the same dimensions (same number or rows and columns).

The most important way in which matrices differ from numbers is in they way in which they are multiplied. The product of <u>A</u> and <u>B</u> is defined only if the number of column is <u>A</u> equals the number of rows in <u>B</u>. The resulting product will be a matrix with the same number of rows as <u>A</u> and the same number of columns as <u>B</u>.

An easy way of looking at matrix multiplication is to write down the dimensions of the two matrices, in the order they are being multiplied. The "middle" dimensions must match, and the "outer" dimensions become those of the product matrix. For example, if  $\underline{A}$  is an m x n matrix and  $\underline{B}$  is an n x m matrix, then the product,  $\underline{C}$  will be an m x m matrix:



Note that if  $\underline{D} = \underline{B} \bullet \underline{A}$ , then  $\underline{D}$  is an n x n matrix. Thus, matrix multiplication is not commutative, since  $\underline{C}$  and  $\underline{D}$  do not even have the same dimensions. However, the multiplication of square matrices may or may not be commutative. Because the order of multiplication is important, if we refer to the product of  $\underline{A}$  and  $\underline{B}$ , we mean that  $\underline{A}$  is on the left and  $\underline{B}$  is on the right ( $\underline{A} \bullet \underline{B}$ ). The product of  $\underline{B}$  and  $\underline{A}$  would refer to the reverse order,  $\underline{B} \bullet \underline{A}$ .

You should convince yourself that the following statements are true:

- (1) The product of two square matrices is a square matrix of the same dimension.
- (2) The product of an n x n matrix and an n x 1 column vector is another n x 1 column vector.
- (3) The product of an n x 1 vector and an n x n matrix is not defined.
- (4) The product of a 1 x n row vector and an n x 1 column vector is a single number, called a <u>scalar</u>.
- (5) Reversing the order of (4) will produce an  $n \ge n$  matrix.

If  $\underline{C} = \underline{A} \cdot \underline{B}$ , the element of  $\underline{C}$  are **not** simply the direct product of the elements of  $\underline{A}$  and  $\underline{B}$ . The element in the i<sup>th</sup> row and j<sup>th</sup> column of  $\underline{C}$ ,  $c_{ij}$ , is obtained by matching the ith row of  $\underline{A}$  with jth row of  $\underline{B}$ , multiplying the corresponding elements and summing up all of these products. Because it is hard to put into words, let us consider the following 2 x 2 matrices,  $\underline{A}$  and  $\underline{B}$ , and their product,  $\underline{C} = \underline{A} \cdot \underline{B}$ :



such that the element  $c_{11} = (a_{11} \bullet b_{11}) + (a_{12} \bullet b_{21}), c_{12} = (a_{11} \bullet b_{12}) + (a_{12} \bullet b_{22}), c_{21} = (a_{21} \bullet b_{11}) + (a_{22} \bullet b_{21}),$ and  $c_{22} = (a_{21} \bullet b_{12}) + (a_{22} \bullet b_{22})$ . Using numbers,

1 2	]	5	6		19	22
3 4	•	7	8	=	43	50

Here, to get c11 (19), we match up the first row of <u>A</u> with the first column of <u>B</u>, take the products of these (1 • 5 = 5 and 2 • 7 = 14), and sum up the products (5 + 14 = 19). You should verify that you can also obtain the other elements in matrix <u>C</u> on your own.

In general, matrix multiplication can be expressed compactly as the algebraic statement:

$$c_{ij} = \sum_{k} a_{ik} b_{kj}$$

Below are the matrices that define the operations that we will be using in this course.

$$\begin{split} \mathbf{E} &= \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \qquad \mathbf{i} = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \\ \sigma_{x} &= \sigma_{yz} &= \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \qquad \sigma_{y} = \sigma_{xz} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \qquad \sigma_{z} = \sigma_{xy} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \\ \mathbf{C}_{n}^{z} &= \begin{bmatrix} \cos(2\pi/n) & -\sin(2\pi/n) & 0 \\ \sin(2\pi/n) & \cos(2\pi/n) & 0 \\ 0 & 0 & 1 \end{bmatrix} \qquad \mathbf{S}_{n}^{z} = \begin{bmatrix} \cos(2\pi/n) & -\sin(2\pi/n) & 0 \\ \sin(2\pi/n) & \cos(2\pi/n) & 0 \\ 0 & 0 & -1 \end{bmatrix} \\ \mathbf{C}_{n}^{x} &= \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos(2\pi/n) & -\sin(2\pi/n) \\ 0 & \sin(2\pi/n) & \cos(2\pi/n) \end{bmatrix} \qquad \mathbf{S}_{n}^{x} = \begin{bmatrix} -1 & 0 & 0 \\ 0 & \cos(2\pi/n) & -\sin(2\pi/n) \\ 0 & \sin(2\pi/n) & \cos(2\pi/n) \end{bmatrix} \\ \mathbf{C}_{n}^{y} &= \begin{bmatrix} \cos(2\pi/n) & 0 & \sin(2\pi/n) \\ 0 & \sin(2\pi/n) & \cos(2\pi/n) \end{bmatrix} \qquad \mathbf{S}_{n}^{y} = \begin{bmatrix} \cos(2\pi/n) & 0 & \sin(2\pi/n) \\ 0 & \sin(2\pi/n) & \cos(2\pi/n) \\ 0 & -1 & 0 \\ -\sin(2\pi/n) & 0 & \cos(2\pi/n) \end{bmatrix} \\ \sigma_{x=y} &= \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \qquad \sigma_{x=-y} = \begin{bmatrix} 0 & -1 & 0 \\ -\sin(2\pi/n) & 0 & \cos(2\pi/n) \\ 0 & 0 & 1 \end{bmatrix}$$