THE CHEMIST'S TOOLKIT 22 The manipulation of vectors

In three dimensions, the vectors $\boldsymbol{u}$ (with components u_x, u_y, and u_z) and $\boldsymbol{v}$ (with components v_x, v_y, and v_z) have the general form:

$$\boldsymbol{u} = u_x\boldsymbol{i} + u_y\boldsymbol{j} + u_z\boldsymbol{k} \qquad \boldsymbol{v} = v_x\boldsymbol{i} + v_y\boldsymbol{j} + v_z\boldsymbol{k} \tag{22.1}$$

where $\boldsymbol{i}$, $\boldsymbol{j}$, and $\boldsymbol{k}$ are **unit vectors**, vectors of magnitude 1, pointing along the positive directions on the x, y, and z axes. The operations of addition, subtraction, and multiplication are as follows:

1. *Addition*:

$$\boldsymbol{v} + \boldsymbol{u} = (v_x + u_x)\boldsymbol{i} + (v_y + u_y)\boldsymbol{j} + (v_z + u_z)\boldsymbol{k} \tag{22.2}$$

2. *Subtraction*:

$$\boldsymbol{v} - \boldsymbol{u} = (v_x - u_x)\boldsymbol{i} + (v_y - u_y)\boldsymbol{j} + (v_z - u_z)\boldsymbol{k} \tag{22.3}$$

Brief illustration 22.1: Addition and subtraction

Consider the vectors $\boldsymbol{u} = \boldsymbol{i} - 4\boldsymbol{j} + \boldsymbol{k}$ (of magnitude 4.24) and $\boldsymbol{v} = -4\boldsymbol{i} + 2\boldsymbol{j} + 3\boldsymbol{k}$ (of magnitude 5.39) Their sum is

$$\boldsymbol{u} + \boldsymbol{v} = (1 - 4)\boldsymbol{i} + (-4 + 2)\boldsymbol{j} + (1 + 3)\boldsymbol{k} = -3\boldsymbol{i} - 2\boldsymbol{j} + 4\boldsymbol{k}$$

The magnitude of the resultant vector is $29^{1/2} = 5.39$. The difference of the two vectors is

$$\boldsymbol{u} - \boldsymbol{v} = (1 + 4)\boldsymbol{i} + (-4 - 2)\boldsymbol{j} + (1 - 3)\boldsymbol{k} = 5\boldsymbol{i} - 6\boldsymbol{j} - 2\boldsymbol{k}$$

The magnitude of this resultant is 8.06. Note that in this case the difference is longer than either individual vector.

3. *Multiplication*:
   (a) The **scalar product**, or *dot product*, of the two vectors $\boldsymbol{u}$ and $\boldsymbol{v}$ is

$$\boldsymbol{u}\cdot\boldsymbol{v} = u_x v_x + u_y v_y + u_z v_z \tag{22.4}$$

The scalar product of a vector with itself gives the square magnitude of the vector:

$$\boldsymbol{u}\cdot\boldsymbol{u} = u_x^2 + u_y^2 + u_z^2 = u^2 \tag{22.5}$$

   (b) The **vector product,** or *cross product,* of two vectors is

$$\boldsymbol{u}\times\boldsymbol{v} = \begin{vmatrix} \boldsymbol{i} & \boldsymbol{j} & \boldsymbol{k} \\ u_x & u_y & u_z \\ v_x & v_y & v_z \end{vmatrix}$$

$$= (u_y v_z - u_z v_y)\boldsymbol{i} - (u_x v_z - u_z v_x)\boldsymbol{j} + (u_x v_y - u_y v_x)\boldsymbol{k} \tag{22.6}$$

(Determinants are discussed in *The chemist's toolkit* 23.) If the two vectors lie in the plane defined by the unit vectors $\boldsymbol{i}$ and $\boldsymbol{j}$, their vector product lies parallel to the unit vector $\boldsymbol{k}$.

Brief illustration 22.2: Scalar and vector products

The scalar and vector products of the two vectors in *Brief illustration* 22.1, $\boldsymbol{u} = \boldsymbol{i} - 4\boldsymbol{j} + \boldsymbol{k}$ (of magnitude 4.24) and $\boldsymbol{v} = -4\boldsymbol{i} + 2\boldsymbol{j} + 3\boldsymbol{k}$ (of magnitude 5.39) are

$$\boldsymbol{u}\cdot\boldsymbol{v} = \{1 \times (-4)\} + \{(-4) \times 2\} + \{1 \times 3\} = -9$$

$$\boldsymbol{u}\times\boldsymbol{v} = \begin{vmatrix} \boldsymbol{i} & \boldsymbol{j} & \boldsymbol{k} \\ 1 & -4 & 1 \\ -4 & 2 & 3 \end{vmatrix}$$

$$= \{(-4)(3) - (1)(2)\}\boldsymbol{i} - \{(1)(3) - (1)(-4)\}\boldsymbol{j} + \{(1)(2) - (-4)(-4)\}\boldsymbol{k}$$

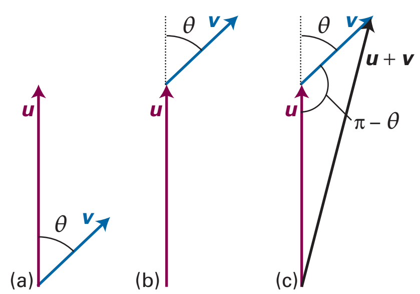
$$= -14\boldsymbol{i} - 7\boldsymbol{j} - 14\boldsymbol{k}$$

The vector product is a vector of magnitude 21.00 pointing in a direction perpendicular to the plane defined by the two individual vectors.

Further information

The manipulation of vectors is commonly represented graphically. Consider two vectors $\boldsymbol{v}$ and $\boldsymbol{u}$ making an angle θ (Sketch 22.1a). The first step in the addition of $\boldsymbol{u}$ to $\boldsymbol{v}$ consists of joining the tip (the 'head') of $\boldsymbol{u}$ to the starting point (the 'tail') of $\boldsymbol{v}$ (Sketch 22.1b). In the second step, draw a vector $\boldsymbol{v}_{\text{res}}$, the **resultant vector**, originating from the tail of $\boldsymbol{u}$ to the head of $\boldsymbol{v}$ (Sketch 22.1c). Reversing the order of addition leads to the same result; that is, the same $\boldsymbol{v}_{\text{res}}$ is obtained whether $\boldsymbol{u}$ is added to $\boldsymbol{v}$ or $\boldsymbol{v}$ to $\boldsymbol{u}$. To calculate the magnitude of $\boldsymbol{v}_{\text{res}}$, note that

$$v_{\text{res}}^2 = (\boldsymbol{u} + \boldsymbol{v})\cdot(\boldsymbol{u} + \boldsymbol{v}) = \boldsymbol{u}\cdot\boldsymbol{u} + \boldsymbol{v}\cdot\boldsymbol{v} + 2\boldsymbol{u}\cdot\boldsymbol{v}$$
$$= u^2 + v^2 + 2uv\cos\theta' \tag{22.7a}$$

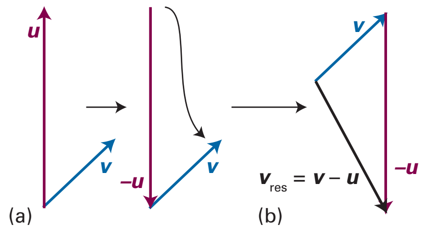


Sketch 22.1

where θ' is the angle between $\boldsymbol{u}$ and $\boldsymbol{v}$. In terms of the angle $\theta = \pi - \theta'$ shown in the Sketch, and $\cos(\pi - \theta) = -\cos\theta$,

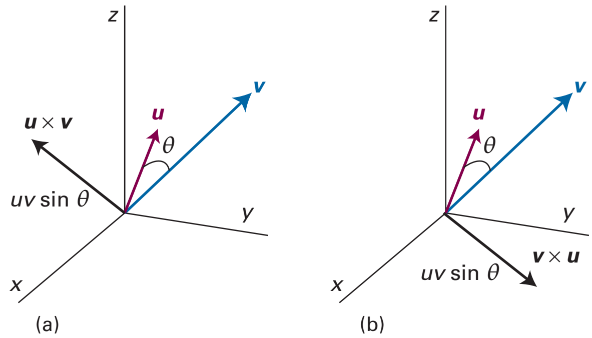
$$v_{\rm res}^2 = u^2 + v^2 - 2uv\cos\theta \qquad \text{Law of cosines} \qquad (22.7b)$$

which is the **law of cosines** for the relation between the lengths of the sides of a triangle.



Sketch 22.2

Subtraction of $\boldsymbol{u}$ from $\boldsymbol{v}$ amounts to addition of $-\boldsymbol{u}$ to $\boldsymbol{v}$. It follows that in the first step of subtraction $-\boldsymbol{u}$ is drawn by reversing the direction of $\boldsymbol{u}$ (Sketch 22.2a). Then, the second step consists of adding $-\boldsymbol{u}$ to $\boldsymbol{v}$ by using the strategy shown in the Sketch; a resultant vector $\boldsymbol{v}_{\rm res}$ is drawn by joining the tail of $-\boldsymbol{u}$ to the head of $\boldsymbol{v}$ (Sketch 22.2b).



Sketch 22.3

Vector multiplication is represented graphically by drawing a vector (using the right–hand rule) perpendicular to the plane defined by the vectors $\boldsymbol{u}$ and $\boldsymbol{v}$, as shown in Sketch 22.3. Its length is equal to $uv\sin\theta$, where θ is the angle between $\boldsymbol{u}$ and $\boldsymbol{v}$. Note that $\boldsymbol{u}\times\boldsymbol{v}$ (Sketch 22.3a) is opposite in direction to $\boldsymbol{v}\times\boldsymbol{u}$ (Sketch 22.3b).