MATHCHAPTER A

Complex Numbers

Throughout chemistry, we frequently use complex numbers. In this MathChapter, we review some of the properties of complex numbers. Recall that complex numbers involve the imaginary unit, i, which is defined to be the square root of -1:

$$i = \sqrt{-1} \tag{A.1}$$

or

$$i^2 = -1 \tag{A.2}$$

Complex numbers arise naturally when solving certain quadratic equations. For example, the two solutions to

$$z^2 - 2z + 5 = 0$$

are given by

$$z = 1 \pm \sqrt{-4}$$

or

$$z = 1 \pm 2i$$

where 1 is said to be the real part and ± 2 the imaginary part of the complex number z. Generally, we write a complex number as

$$z = x + iy \tag{A.3}$$

with

$$x = \mathrm{Re}(z) \qquad y = \mathrm{Im}(z) \tag{A.4}$$

We add or subtract complex numbers by adding or subtracting their real and imaginary parts separately. For example, if $z_1 = 2 + 3i$ and $z_2 = 1 - 4i$, then

$$z_1 - z_2 = (2 - 1) + [3 - (-4)]i = 1 + 7i$$

Furthermore, we can write

$$2z_1 + 3z_2 = 2(2 + 3i) + 3(1 - 4i) = 4 + 6i + 3 - 12i = 7 - 6i$$

To multiply complex numbers together, we simply multiply the two quantities as binomials and use the fact that $i^2 = -1$. For example,

$$\begin{aligned}(2 - i)(-3 + 2i) &= -6 + 3i + 4i - 2i^2 \\ &= -4 + 7i\end{aligned}$$

To divide complex numbers, it is convenient to introduce the complex conjugate of z, which we denote by z^* and form by replacing i by $-i$. For example, if $z = x + iy$, then $z^* = x - iy$. Note that a complex number multiplied by its complex conjugate is a real quantity:

$$zz^* = (x + iy)(x - iy) = x^2 - i^2y^2 = x^2 + y^2 \tag{A.5}$$

The square root of zz^* is called the magnitude or the absolute value of z, and is denoted by $|z|$.

Consider now the quotient of two complex numbers:

$$z = \frac{2 + i}{1 + 2i}$$

This ratio can be written in the form $x + iy$ if we multiply both the numerator and the denominator by $1 - 2i$, the complex conjugate of the denominator:

$$z = \frac{2 + i}{1 + 2i}\left(\frac{1 - 2i}{1 - 2i}\right) = \frac{4 - 3i}{5} = \frac{4}{5} - \frac{3}{5}i$$

EXAMPLE A–1

Show that

$$z^{-1} = \frac{x}{x^2 + y^2} - \frac{iy}{x^2 + y^2}$$

SOLUTION:

$$z^{-1} = \frac{1}{z} = \frac{1}{x+iy} = \frac{1}{x+iy}\left(\frac{x-iy}{x-iy}\right) = \frac{x-iy}{x^2+y^2}$$
$$= \frac{x}{x^2+y^2} - \frac{iy}{x^2+y^2}$$

Because complex numbers consist of two parts, a real part and an imaginary part, we can represent a complex number by a point in a two-dimensional coordinate system where the real part is plotted along the horizontal (x) axis and the imaginary part is plotted along the vertical (y) axis, as in Figure A.1. The plane of such a figure is called the complex plane. If we draw a vector **r** from the origin of this figure to the point $z = (x, y)$, then the length of the vector, $r = (x^2 + y^2)^{\frac{1}{2}}$, is the magnitude or the absolute value of z. The angle θ that the vector **r** makes with the x axis is the phase angle of z.

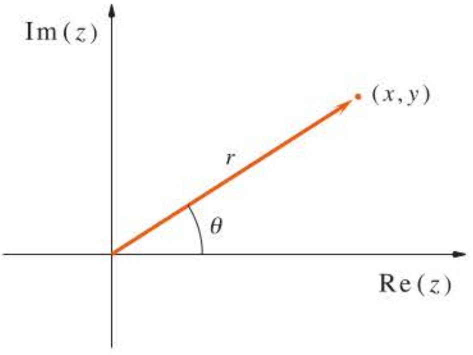

FIGURE A.1
Representation of a complex number $z = x + iy$ as a point in a two-dimensional coordinate system. The plane of this figure is called the complex plane.

EXAMPLE A–2
Given $z = 1 + i$, determine the magnitude, $|z|$, and the phase angle θ of z.

SOLUTION: The magnitude of z is given by the square root of

$$zz^* = (1+i)(1-i) = 2$$

or $|z| = 2^{\frac{1}{2}}$. Figure A.1 shows that the tangent of the phase angle is given by

$$\tan\theta = \frac{y}{x} = 1$$

or $\theta = 45°$, or $\pi/4$ radians. (Recall that 1 radian $= 180°/\pi$, or $1° = \pi/180$ radian.)

We can always express $z = x + iy$ in terms of r and θ by using Euler's formula,

$$e^{i\theta} = \cos\theta + i\sin\theta \tag{A.6}$$

which is derived in Problem A–10. Referring to Figure A.1, we see that

$$x = r\cos\theta \qquad \text{and} \qquad y = r\sin\theta$$

and so

$$\begin{aligned} z &= x + iy = r\cos\theta + ir\sin\theta \\ &= r(\cos\theta + i\sin\theta) = re^{i\theta} \end{aligned} \tag{A.7}$$

where

$$r = \left(x^2 + y^2\right)^{\frac{1}{2}} \tag{A.8}$$

and

$$\tan\theta = \frac{y}{x} \tag{A.9}$$

Equation A.7, the polar representation of z, is often more convenient to use than Equation A.3, the cartesian representation of z.

Note that

$$z^* = re^{-i\theta} \tag{A.10}$$

and that

$$zz^* = \left(re^{-i\theta}\right)\left(re^{-i\theta}\right) = r^2 \tag{A.11}$$

or $r = (zz^*)^{\frac{1}{2}}$. Also note that $z = e^{i\theta}$ is a unit vector in the complex plane because $r^2 = (e^{i\theta})(e^{-i\theta}) = 1$. The following example proves this result in another way.

EXAMPLE A–3

Show that $e^{-i\theta} = \cos\theta - i\sin\theta$ and use this result and the polar representation of z to show that $|e^{i\theta}| = 1$.

SOLUTION: To prove that $e^{-i\theta} = \cos\theta - i\sin\theta$, we use Equation A.6 and the fact that $\cos\theta$ is an even function of θ [$\cos(-\theta) = \cos\theta$] and that $\sin\theta$ is an odd function of θ [$\sin(-\theta) = -\sin\theta$]. Therefore,

$$e^{-i\theta} = \cos\theta + i\sin(-\theta) = \cos\theta - i\sin\theta$$

Furthermore,

$$\begin{aligned}|e^{i\theta}| &= [(\cos\theta + i\sin\theta)(\cos\theta - i\sin\theta)]^{1/2} \\ &= (\cos^2\theta + \sin^2\theta)^{1/2} = 1\end{aligned}$$

Problems

A–1. Find the real and imaginary parts of the following quantities:

(a) $(2-i)^3$ (b) $e^{\pi i/2}$

(c) $e^{-2+i\pi/2}$ (d) $(\sqrt{2}+2i)e^{-i\pi/2}$

A–2. If $z = x + 2iy$, then find

(a) $\mathrm{Re}(z^*)$ (b) $\mathrm{Re}(z^2)$

(c) $\mathrm{Im}(z^2)$ (d) $\mathrm{Re}(zz^*)$

(e) $\mathrm{Im}(zz^*)$

A–3. Express the following complex numbers in the form $re^{i\theta}$:

(a) $6i$ (b) $4-\sqrt{2}i$

(c) $-1-2i$ (d) $\pi + ei$

A–4. Express the following complex numbers in the form $x + iy$:

(a) $e^{\pi/4i}$ (b) $6e^{2\pi i/3}$

(c) $e^{-(\pi/4)i+\ln 2}$ (d) $e^{-2\pi i} + e^{4\pi i}$

A–5. Prove that $e^{i\pi} = -1$. Comment on the nature of the numbers in this relation.

A–6. Show that

$$\cos\theta = \frac{e^{i\theta} + e^{-i\theta}}{2}$$

and that

$$\sin\theta = \frac{e^{i\theta} - e^{-i\theta}}{2i}$$

A–7. Use Equation A.6 to derive

$$z^n = r^n(\cos\theta + i\sin\theta)^n = r^n(\cos n\theta + i\sin n\theta)$$

and from this, the formula of de Moivre:

$$(\cos\theta + i\sin\theta)^n = \cos n\theta + i\sin n\theta$$

A–8. Use the formula of de Moivre, which is given in Problem A–7, to derive the trigonometric identities

$$\begin{aligned}\cos 2\theta &= \cos^2\theta - \sin^2\theta \\ \sin 2\theta &= 2\sin\theta\cos\theta \\ \cos 3\theta &= \cos^3\theta - 3\cos\theta\sin^2\theta \\ &= 4\cos^3\theta - 3\cos\theta \\ \sin 3\theta &= 3\cos^2\theta\sin\theta - \sin^3\theta \\ &= 3\sin\theta - 4\sin^3\theta\end{aligned}$$

A–9. Consider the set of functions

$$\Phi_m(\phi) = \frac{1}{\sqrt{2\pi}}e^{im\phi} \qquad \begin{cases} m = 0, \pm 1, \pm 2, \ldots \\ 0 \le \phi \le 2\pi \end{cases}$$

First show that

$$\int_0^{2\pi} d\phi\Phi_m(\phi) = \begin{cases} 0 & \text{for all values of } m \neq 0 \\ \sqrt{2\pi} & m = 0 \end{cases}$$

Now show that

$$\int_0^{2\pi} d\phi\Phi_m^*(\phi)\Phi_n(\phi) = \begin{cases} 0 & m \neq n \\ 1 & m = n \end{cases}$$

A–10. This problem offers a derivation of Euler's formula. Start with

$$f(\theta) = \ln(\cos\theta + i\sin\theta) \tag{1}$$

Show that

$$\frac{df}{d\theta} = i \tag{2}$$

Now integrate both sides of equation 2 to obtain

$$f(\theta) = \ln(\cos\theta + i\sin\theta) = i\theta + c \tag{3}$$

where c is a constant of integration. Show that $c = 0$ and then exponentiate equation 3 to obtain Euler's formula.

A–11. Using Euler's formula and assuming that x represents a real number, show that $\cos ix$ and $-i\sin ix$ are equivalent to real functions of the real variable x. These functions are defined as the hyperbolic cosine and hyperbolic sine functions, $\cosh x$ and $\sinh x$, respectively. Sketch these functions. Do they oscillate like $\sin x$ and $\cos x$?

A–12. Show that $\sinh ix = i \sin x$ and that $\cosh ix = \cos x$. (See the previous problem.)

A–13. Evaluate i^i.

A–14. The equation $x^2 = 1$ has two distinct roots, $x = \pm 1$. The equation $x^N = 1$ has N distinct roots, called the N roots of unity. This problem shows how to find the N roots of unity. We shall see that some of the roots turn out to be complex, so let's write the equation as $z^N = 1$. Now let $z = e^{i\theta}$ and obtain $e^{iN\theta} = 1$. Show that this must be equivalent to $e^{iN\theta} = 1$, or

$$\cos N\theta + i \sin N\theta = 1$$

Now argue that $N\theta = 2\pi n$, where n has the N distinct values $0, 1, 2, \ldots, N-1$ or that the N roots of unity are given by

$$z = e^{2\pi i n/N} \qquad n = 0, 1, 2, \ldots, N-1$$

Show that we obtain $z = 1$ and $z = \pm 1$, for $N = 1$ and $N = 2$, respectively. Now show that

$$z = 1, \; -\frac{1}{2} + i\frac{\sqrt{3}}{2}, \text{ and } -\frac{1}{2} - i\frac{\sqrt{3}}{2}$$

for $N = 3$. Show that each of these roots is of unit magnitude. Plot these three roots in the complex plane. Now show that $z = 1, i, -1$, and $-i$ for $N = 4$ and that

$$z = 1, \; -1, \; \frac{1}{2} \pm i\frac{\sqrt{3}}{2}, \text{ and } -\frac{1}{2} \pm i\frac{\sqrt{3}}{2}$$

for $N = 6$. Plot the four roots for $N = 4$ and the six roots for $N = 6$ in the complex plane. Compare the plots for $N = 3$, $N = 4$, and $N = 6$. Do you see a pattern?

A–15. Using the results of Problem A–14, find the three distinct roots of $x^3 = 8$.

A–16. The *Schwartz inequality* says that if $z_1 = x_1 + iy_1$ and $z_2 = x_2 + iy_2$, then $x_1x_2 + y_1y_2 \le |z_1| \cdot |z_2|$. To prove this inequality, start with its square

$$(x_1x_2 + y_1y_2)^2 \le |z_1|^2\, |z_2|^2 = (x_1^2 + y_1^2)(x_2^2 + y_2^2)$$

Now use the fact that $(x_1y_2 - x_2y_1)^2 \ge 0$ to prove the inequality.

A–17. The *triangle inequality* says that if z_1 and z_2 are complex numbers, then $|z_1 + z_2| \le |z_1| + |z_2|$. To prove this inequality, start with

$$|z_1 + z_2|^2 = (x_1 + x_2)^2 + (y_1 + y_2)^2 = x_1^2 + y_1^2 + x_2^2 + y_2^2 + 2x_1x_2 + 2y_1y_2$$

Now use the Schwartz inequality (previous problem) to prove the inequality. Why do you think this is called the triangle inequality?