5.5 SYMMETRY IN SCIENCE

5.5.1 Chemical structure

Chemists benefit greatly from a geometric understanding of the arrangement of the atoms (and ions) in chemical compounds. (For simplicity we refer to the parts of compounds as *atoms*, ignoring the distinction between atoms and ions. Similarly, we avoid discussion of electrons, orbitals, and quantum mechanics, even though symmetry plays a vital role at that level.) Chemists represent the atoms in a compound by vertices and the bonds between atoms by edges. For example, boron trifluoride (BF_3) has three fluorine atoms bonded to a boron atom (Fig. 5.33). Atoms bonded to a particular atom tend to arrange themselves as far from one another as possible, while staying the appropriate distance from that atom. The arrangement shown in Fig. 5.33 is as symmetric as possible: The six (two-dimensional) symmetries form the group $\mathbf{D}_3$. Thus symmetry frequently allows analysis of chemical structure.

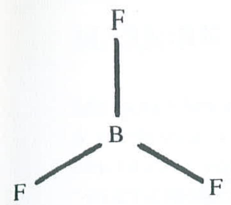

Figure 5.33 Boron trifluoride.

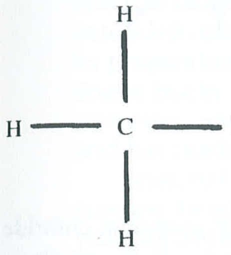

Figure 5.34 An incorrect arrangement of methane bonds.

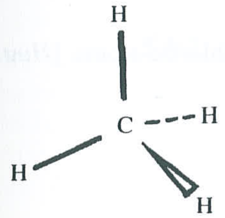

Figure 5.35 Methane (Δ denotes a bond extending from the page toward the reader, and --- denotes a bond receding into the page away from the reader.)

Carbon usually bonds with four atoms. The simplest carbon compound, the gas methane (CH_4), has just one carbon atom and four hydrogen atoms. You might first imagine that the hydrogens would arrange themselves as some chemistry textbooks display this compound for simplicity (as in Fig. 5.34, which has the symmetry group $\mathbf{D}_4$). Although this arrangement has considerable symmetry, chemistry involves three dimensions. Figure 5.35 represents the actual placement of the hydrogens as the vertices of a regular tetrahedron with the carbon at the center, which was deduced in 1874. Hence the hydrogen atoms are farther apart than depicted in Fig. 5.34. Indeed, the angle of two bonds, as shown in Fig. 5.35, is approximately 109.5°, rather than 90°, shown in Fig. 5.34. Furthermore, the tetrahedral group $\overline{\mathbf{T}}$ has 24 symmetries, or more than the 8 two-dimensional symmetries of Fig. 5.34. (As a three-dimensional shape, Fig. 5.34 has 16 symmetries, or still fewer than shown in Fig. 5.35.) An increase in symmetry corresponds to a lower, more stable energy state.

One form of pure carbon, a diamond crystal, extends the symmetry of Fig. 5.35. In a perfect diamond, each carbon atom is bonded to four other carbon atoms that form a regular tetrahedron (Fig. 5.36). To analyze a crystal, we assume that it continues in all three dimensions forever, which is a reasonable simplification. For example, a one-carat diamond has approximately 10^{22} carbon atoms, which means millions of repetitions of the pattern shown in Fig. 5.36 along any axis. The symmetries of the crystal include translations in three dimensions and the local isometries of the tetrahedral group. The variety of the directions of the bonds and their uniformity makes diamond the hardest naturally occurring substance. The angles of the bonds also determine the possible angles at which gem diamonds can be cut. For example, you will never see a diamond cut as a cube.

Carbon forms another crystal, graphite, whose very different physical and chemical properties reflect the different geometry of the crystal. The atoms of graphite form layers one atom thick with only weak bonds between layers. In each layer the carbon atoms form a pattern of hexagons (Fig. 5.37). These layers slide easily over one another, making graphite an excellent lubricant. The "lead" in pencils also contains graphite.

Exercise 1 Classify the wallpaper pattern of a layer of graphite.

Salt (NaCl) exhibits a third crystalline structure (Fig. 5.38). The cubic arrangement at the atomic level ensures that salt grains always have rectangular faces. Potassium chloride (KCl) has the same crystalline form as salt and is extremely close chemically to salt. Indeed, KCl is a salt substitute for those restricting their intake of sodium (Na).

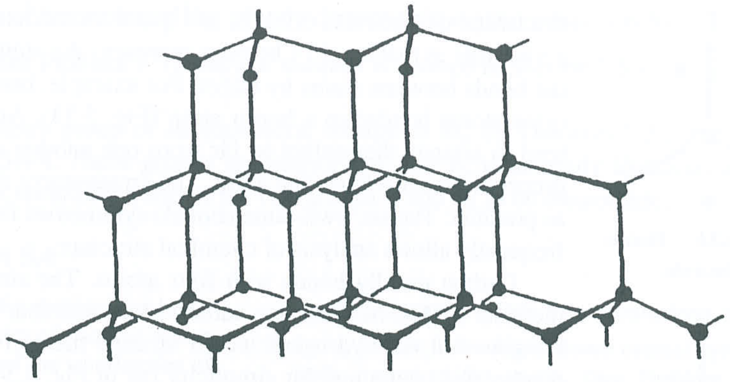

Figure 5.36 The crystal structure of diamond.

The presence of two different kinds of atoms in either salt or potassium chloride affects the group of symmetries. For example, a translation of one bond's length along the *x*-, *y*-, or *z*-axis switches the sodium and chlorine atoms. This switch corresponds to the color symmetries discussed in Section 5.3. The crystal sphalerite, made of zinc and sulfur, is a two-color version of the diamond crystal, with each zinc atom bonded to four sulfur atoms and conversely. (See Senechal [17] for more on crystals.)

Exercise 2 Describe a rotation of the salt crystal that switches sodium and chlorine atoms. [*Hint:* the axis isn't one of the lines for the bonds.]

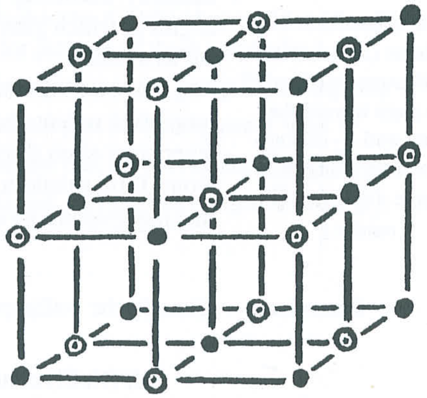

Figure 5.37 The crystal structure of graphite. Each layer consists of a pattern of regular hexagons.

Figure 5.38 The crystal structure of salt.

MARJORIE SENECHAL

Marjorie Senechal (1939–) is a leading researcher in mathematical crystallography and a professor at Smith College, a distinguished college for women. Although she was fascinated with patterns from a young age, not until much later did she realize that "mathematics is the science of patterns." She believes visual thinking to be vital for all mathematics and particularly crystallography.

After completing her Ph.D. in number theory in 1965, Senechal shifted her focus on patterns to mathematical crystallography and, more generally, to discrete geometry. She has taught and conducted research at Smith College since 1966, interspersed with extended research stays in seven countries. Senechal has published six books (with several in preparation) and dozens of articles, and has contributed chapters in more than a dozen books. In addition, she has organized numerous conferences, given many featured addresses, and served several professional organizations as a committee or board member, and has made many other less visible contributions to modern mathematical research.

Senechal eagerly responded to the discovery of quasicrystals in 1984 and the ensuing heightened activity in mathematics, chemistry, and physics. In addition to traditional research in this area, Senechal has worked with the advanced computing facilities at the Geometry Center of the University of Minnesota. Powerful computers are beginning to provide needed visual and analytic insight into the mathematical structure of quasicrystals, which lack the well-understood repetitions of crystals.

5.5.2 Quasicrystals

In Section 5.3 we proved Theorem 5.3.3, the crystallographic restriction, describing the angles of rotation compatible with translations in two or more dimensions. This mathematical result matched chemists' experimental data on x-ray diffraction patterns perfectly until 1984. That year a team of chemists found a compound that gave sharp diffraction patterns with the angle of 72°, which was inconsistent with Theorem 5.3.3. Sharp patterns had previously only been seen with crystals, so these new compounds were called *quasicrystals*. Mathematicians, chemists, and others have explored the rapidly growing field of quasicrystals. Chemists found that, as the crystallographic restriction assures us, the arrangement of atoms in these quasicrystals is not periodic.

Ten years before quasicrystals were discovered, Roger Penrose devised patterns, which he showed could cover the plane but had no translational symmetry. (See Project 15.) By the early 1980s, Penrose and others had generalized these tilings to three dimensions. Some of these three-dimensional tilings corresponded mathematically to the diffraction patterns of quasicrystals, providing one approach to the mathematical analysis of quasicrystals.

Another mathematical insight of the 1970s brought symmetry into the study of quasicrystals. Mathematicians showed that a six-dimensional "hypercrystal" could be sliced into a three-dimensional cross section that would look like a quasicrystal. The symmetries (including translations) of the six-dimensional model and the angle of the cut determine the properties of the three-dimensional cross section. We still don't know the chemical relevance of six mathematical dimensions, but researchers Bak and Goldman "emphasize that thinking of [a quasicrystal] as a periodic structure in six dimensions is not merely an amusing mathematical abstraction." (Jaric [10, 146]) (See Peterson [13, 200–212] and Senechal [17] for more information on quasicrystals.)

5.5.3 Symmetry and relativity

Albert Einstein's theory of relativity transformed physics. In geometric language, the special theory corresponds to a four-dimensional group of symmetries that preserve physical properties. Although physicists had already used time as a fourth dimension, Einstein (1879–1955) realized that space and time interacted. The simpler concept of Galilean relativity is helpful both to illustrate the role of symmetry and to clarify Einstein's contribution.

Galileo Galilei (1564–1642) explained why we don't feel the motion of the earth as it travels through space. The motion of everything on the earth includes the speed of the earth, so our measurements (and senses) detect only the relative differences in the speeds of objects, not their absolute speeds. That is, the laws of physics remain the same at different velocities. In other words, this principle of relativity holds that constant velocities in any direction are symmetries for the laws of physics.

Sir Isaac Newton (1642–1727) and physicists following him added another principle: The measurement of time and distance is absolute. That is, clocks record the same amount of time passing and rulers measure the same lengths, regardless of the speed and direction they are traveling relative to one another. This absolute measurement of space and time leads to the additivity of velocities. For example, suppose that an observer on the ground measures a train moving 20 m/sec and an observer in the train observes someone else in the train walking in the direction of the train at 1.5 m/sec. For the observer on the ground, the walker would be moving at 21.5 m/sec. At modest speeds, the additivity of velocities matches our experience.

The Mickelson–Morley experiments conducted at the end of the nineteenth century revealed a problem with Newton's assumption. These experiments sought to measure the influence of the motion of the earth on the velocity of light. Relative to the sun the earth is moving approximately 18 mi/sec, a tiny part of light's velocity of approximately 186,000 mi/sec. However, Mickelson and Morley devised an experiment accurate enough to detect the small difference between 186,000 and 186,018 mi/sec. Regardless of the direction the light was sent, they found its velocity always to be the same, contradicting the additivity of velocities. Later experiments have confirmed that the speed of light in a vacuum is constant. In 1906, Einstein showed how to combine the constancy of the speed of light and Galileo's principle of relativity by dropping the absolute measurement of space and time and so the additivity of velocities. Surprisingly, Eq. (5.1), the formula for combining velocities, corresponds to composing hyperbolic translations, which we discuss in Section 6.5. For ease, we write velocities as fractions of the speed of light, so 1 is the speed of light. For the simple case of velocities along a line, we replace the addition of velocities, $x + y$, with

$$x \oplus y = \frac{x + y}{1 + xy}. \tag{5.1}$$

Example 1 Suppose that observer A is moving at a velocity of 0.4 with respect to observer B and that an object is moving in the same direction at a velocity of 0.5 with respect to A. Then the object is moving at a velocity of $0.4 \oplus 0.5 = 0.75$ with respect to observer B, or less than $0.4 + 0.5 = 0.9$. The velocities of a spacecraft and the earth are much smaller, or approximately 0.00003 and 0.0001. For these velocities, $0.00003 \oplus 0.0001 = 0.0001299999996$, which for all practical purposes is $0.00003 + 0.0001$, or 0.00013. Thus NASA doesn't need to use relativity theory to plan space missions. ●

Exercise 3 Verify that two observers find the same speed of light ($y = 1$ in Eq. 5.1) regardless of their relative velocities, x.

Example 2 Suppose that two people A and B each find the coordinates of two points C and D by using different axes, as illustrated in Fig. 5.40. The Pythagorean theorem in Euclidean geometry guarantees that they will obtain $\Delta x_{\mathrm{A}}^2 + \Delta y_{\mathrm{A}}^2 = \Delta x_{\mathrm{B}}^2 + \Delta y_{\mathrm{B}}^2$ for the square of the distance between two points. ●

In the theory of relativity the measurements of elapsed time and distance by different observers are related much as distances are in Example 2. Suppose that two observers each record two events taking place using suitable units. Observer A finds the difference in time between the events to be Δt_{A} and the differences in the x-, y-, and z-directions to be Δx_{A}, Δy_{A} and Δz_{A}. Similarly, Δt_{B}, Δx_{B}, Δy_3, and Δz_{B} are observer B's measurements. The theory of relativity guarantees that

$$\Delta x_{\mathrm{A}}^2 + \Delta y_{\mathrm{A}}^2 + \Delta z_{\mathrm{A}}^2 - \Delta t_{\mathrm{A}}^2 = \Delta x_{\mathrm{B}}^2 + \Delta y_{\mathrm{B}}^2 + \Delta z_{\mathrm{B}}^2 - \Delta t_{\mathrm{B}}^2. \tag{5.2}$$

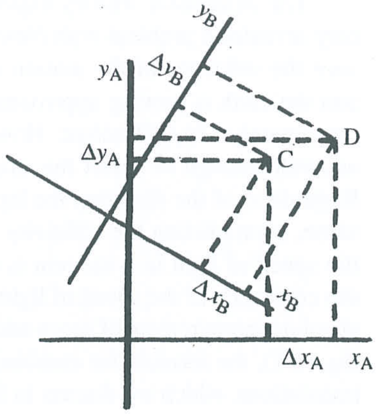

Figure 5.40

Hermann Minkowski developed a four-dimensional geometry by using Eq. 5.2 as a "distance" formula. The Lorentz transformations preserve Eq. 5.2 and so are the symmetries for the special theory of relativity. (In Section 6.6 we discuss these transformations. See Taylor and Wheeler [19] for more on the theory of relativity.)

Example 3 Suppose that person A flashes a light twice, 1 s apart according to A's measurement. If person B is traveling in the x-direction at some velocity with respect to A and observes these light flashes, Δx_B and Δt_B will differ from $\Delta x_A = 0$ and $\Delta t_A = 1$, but $\Delta x_B^2 - \Delta t_B^2 = \Delta x_A^2 - \Delta t_A^2 = 0 - 1 = -1$. The faster B is traveling with respect to A, the larger both Δx_B and Δt_B will be. Note that if B flashes the light twice, the situation is reversed. Thus, although A and B think that their clocks are running at different rates, it doesn't make sense to say whose clock "actually" is slower. Similarly, we can't say that one has a shorter unit of x-distances than the other. ●

The use of symmetry in quantum mechanics, although important, goes beyond the level of this text. See Project 19.

PROBLEMS FOR SECTION 5.5

Two possible arrangements of the atoms for a molecule are chemically equivalent provided that a direct isometry exists that converts one arrangement to the other. If no such direct isometry exists, the possible arrangements are *isomers*.

1. a) Describe the two-dimensional symmetries of the ethene molecule (C_2H_4), which has a double bond between the carbon atoms. Find the group of symmetries of C_2H_4 (Fig. 5.41). Note that all six atoms lie in a plane.

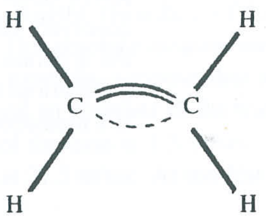

Figure 5.41 Ethene.

   b) Dichloroethene ($C_2H_2Cl_2$) replaces two of the hydrogen atoms of ethene with chlorine atoms. Draw the three isomers of this molecule and describe the symmetries of each isomer. Verify that the three groups of symmetries of these isomers are subgroups of the symmetries of ethene.

2. The six carbon atoms of benzene (C_6H_6) form a ring (Fig. 5.42). These atoms exhibit *resonance*, the nonlocalized sharing of electrons, illustrated as a circle. Thus just three atoms are directly attached to each carbon. Assume that the 12 atoms of benzene are in a plane. (Actually, the molecule is three-dimensional.)

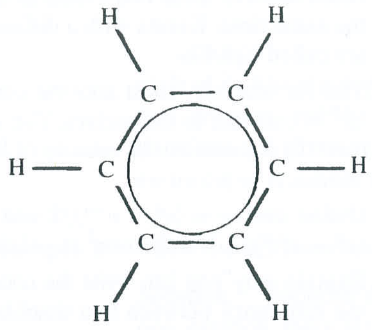

Figure 5.42 Benzene.

   a) Describe the two-dimensional symmetries of the model shown in Fig. 5.42. Find the group of symmetries of the model.
   b) Repeat Problem 1(b) for dichlorobenzene ($C_6H_4Cl_2$) which replaces two of the hydrogen atoms with chlorine atoms.
   c) Repeat Problem 1(b) for trichlorobenzene ($C_6H_3Cl_3$) which replaces three of the hydrogen atoms with chlorine atoms. Consider "color" symmetries that switch the hydrogen and chlorine atoms, as well as those that don't.

3. Draw isomers for a molecule with a central carbon atom and four different atoms (W, X, Y, and Z) attached to it. How are these isomers different geometrically? Chemically, these molecules polarize light differently.

4. Find the symmetry group of buckminsterfullerene, C_{60}, a recently found third form of pure carbon (Fig. 5.43).

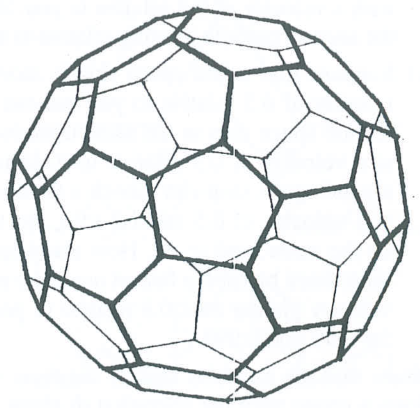

Figure 5.43 Buckminsterfullerene.

5. Each layer of carbonates (CO_3) in a crystal of calcite ($CaCO_3$) looks like the structure depicted in Fig. 5.44. Analyze the wallpaper pattern of this layer. (The calcium atoms lie in different layers not shown. Marble is one form of calcite.)

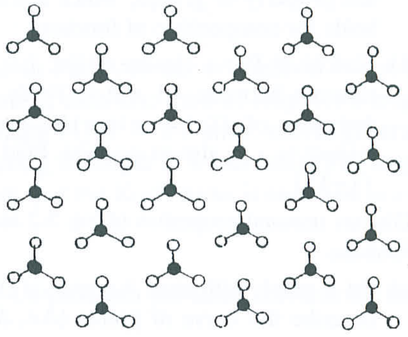

Figure 5.44 The structure of a layer of carbonates in a crystal of calcite.

6. Use the operation given in Eq. 5.1. Explain your answers.
   a) Two streams of protons are approaching each other head-on in a cyclotron, each with a velocity of 0.9 of the speed of light relative to an observer. How fast is one stream moving relative to the other stream?
   b) Suppose that you observe a particle moving at a velocity of 0.7 relative to you, followed by a second particle moving in the same direction

with a velocity of 0.8 relative to you. How fast is the second particle moving relative to the first?

c) Suppose that a first space ship is moving at a velocity of 0.5 relative to you and can launch a second space ship in the same direction moving at a velocity of 0.5 relative to it. In turn, the second space ship can launch a third space ship at a velocity of 0.5 relative to it, the third can do the same, and so on. How many space ships must there be for the fastest one to be moving at a velocity greater than 0.9 relative to you? Repeat for 0.99 and 0.999.

7. Show that the numbers strictly between -1 and 1 form a group with the operation $\oplus$ given in Eq. 5.1 as follows.

a) What velocity is the identity for $\oplus$? Prove your choice correct.

b) Find the inverse velocity of x. Prove your choice correct.

c) Prove that $\oplus$ is associative. That is, $a \oplus (b \oplus c) = (a \oplus b) \oplus c$. (This operation isn't necessarily a geometric transformation, so you need to verify this property of groups, which automatically holds for composition of functions.)

d) (Calculus) Prove closure. [*Hint:* Let a be any constant between -1 and 1. Verify that the derivative of $f(x) = (x+a)/(1+xa)$ with respect to x is always positive. Find $f(1)$ and $f(-1)$.]

8. Discuss unusual properties of Eq. 5.2 as a distance formula.

9. **a)** On a graph with axes Δx and Δt, draw and describe the curve of points $(\Delta x, \Delta t)$ such that $\Delta x^2 - \Delta t^2 = -1$. This curve represents the possible measurements that person B could obtain in Example 3. Events with a negative difference are called *timelike* because every observer can determine which event occurred first.

b) Repeat part (a) for $\Delta x^2 - \Delta t^2 = 1$. This difference could occur if person A flashed two different lights at the same time and at a distance of 1 apart in A's measurement. Events with a positive difference are called *spacelike*. Describe how person B could observe either light flash first.

c) Repeat part (a) for $\Delta x^2 - \Delta t^2 = 0$. Describe how person A could send two different light flashes to give this difference. Describe how person B could observe these two events as happening at the same time. Events with a difference of zero are called *lightlike*.

Symmetries for relativity must take the curves where $\Delta x^2 - \Delta t^2$ is constant to themselves. The value of b in parts (e) and (f) depends on the velocity of B with respect to A.

d) Define $\cosh a = (e^a + e^{-a})/2$ and $\sinh a = (e^a - e^{-a})/2$. Verify $\cosh^2 a - \sinh^2 a = 1$.

e) Explain why you can write the coordinates for the difference between two timelike events as $(r \sinh a, r \cosh a)$, for some a and r in $\mathbf{R}$. Verify that $f(r \sinh a, r \cosh a) = (r \sinh(a+b), r \cosh(a+b))$ preserves $\Delta x^2 - \Delta t^2$ for timelike events. Describe what f does to points on the curve of part (a).

f) Modify and repeat part (e) for spacelike events.

5.6 FRACTALS

Historically, geometry has focused on relatively simple, ideal shapes: circles, triangles, polyhedra, and the like. However, even a cursory glance at nature reveals a vast array of shapes unrelated to these traditional objects. Benoit Mandelbrot, the originator of fractals, found geometric structure underlying complicated natural shapes. In 1975 he coined the word fractal to describe the convoluted curves and surfaces that can be used to model natural shapes that had previously seemed beyond mathematical study.

Mathematicians initiated the abstract study of curves related to fractals before 1900. In 1904 Helge von Koch defined the Koch curve (Fig. 5.45) as the limit of an infinite process, illustrated in Fig. 5.46. Starting with the motif at the top of Fig. 5.46, we replace