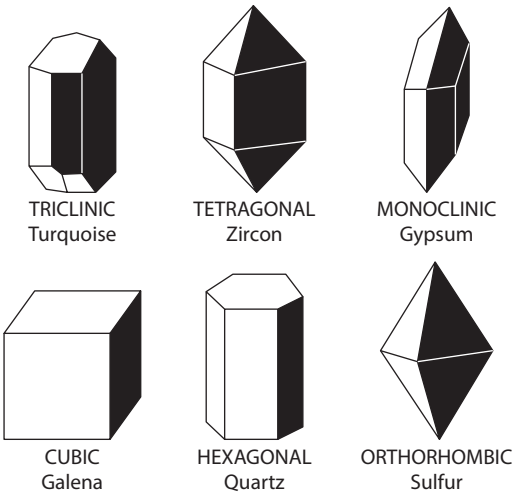

FIGURE 6.4 Common crystal habits.

crystal growth, as shown, when certain dyes or heavy metals are mixed with solutions. If an impurity can adsorb at the growing face, it can significantly alter the course of crystal growth and geometry. The habits bound by plane faces are termed *euhedral* and those with irregularly shaped ones are called *anhedral*. The symmetry of a crystal is generally studied by using optical goniometer that allows the measurement of the angles between the crystal faces. This technique is of use only when good crystals of size greater than 0.05 mm in each direction can be obtained, which is generally not the case.

Chemical crystallography provides accurate and precise measurements of molecular dimensions in a way that no other science can begin to approach. Historically, single crystal X-ray diffraction was used to determine the structure of what was thought of as "small molecules." Twenty years ago, it was possible to solve structures with an average of only 100 nonhydrogen atoms. However, with developments in hardware and software, the upper limit has risen to about 500, and recently, even a 1000-atom structure was solved. The APEX II line of Chemical Crystallography Solutions (1) allows single-crystal structure determination. The APEX II detector is suitable for fast processing. The Brucker SHellXTL software system works well with these systems and provides a complete characterization that is suitable for publication would include the following data:

1. Data collection
   a. Source of sample and conditions of crystallization
   b. Habit, color, and dimensions of the crystal
   c. Formula and formula weight
   d. Unit cell parameters and volume with (esds). The number of data and theta range of data used to determine the cell parameters
   e. Crystal type and space group
   f. *Z*, density, and absorption coefficient
   g. Instrument and temperature of data collection and cell parameter determination