

**Table 13-1**

The 65 space groups allowed for molecules with no mirror or inversion symmetry

| Crystal system            | Number of independent parameters | Lattice         | Minimum symmetry of unit cell             | Unit cell edges and angles <sup>§</sup>                                    | Diffraction pattern symmetry <sup>#</sup> | Space groups <sup>†</sup>   |
|---------------------------|----------------------------------|-----------------|---|--|---|---|
| Triclinic                 | 6                                | P               | None                                      | $a \neq b \neq c$<br>$\alpha \neq \beta \neq \gamma$                       | $\bar{1}$                                 | P1  |
| Monoclinic                | 4                                | P               | Twofold axis parallel to <b>b</b>         | $a \neq b \neq c$<br>$\alpha = \gamma = 90^\circ$<br>$\beta \neq 90^\circ$ | 2/m                                       | P2, P2 <sub>1</sub><br>C2   |
| Orthorhombic              | 3                                | P               | Three mutually perpendicular twofold axes | $a \neq b \neq c$<br>$\alpha = \beta = \gamma = 90^\circ$                  | mmm                                       | P222, P2 <sub>1</sub> -2 <sub>1</sub> , P222 <sub>1</sub> , P2 <sub>1</sub> -2 <sub>1</sub> -2  |
|                           |                                  | C               |   |  |   | C222, C222 <sub>1</sub>   |
|                           |                                  | I               |   |  |   | [I222, I2 <sub>1</sub> -2 <sub>1</sub> -2 <sub>1</sub> ]  |
| Tetragonal                | 2                                | P               | Fourfold axis parallel to <b>c</b>        | $a = b \neq c$<br>$\alpha = \beta = \gamma = 90^\circ$                     | 4/m                                       | P4, (P4 <sub>1</sub> , P4 <sub>3</sub> ), P4 <sub>2</sub><br>I4, I4 <sub>1</sub>  |
|                           |                                  | I               |   |  |   | P422, (P4 <sub>1</sub> 22, P4 <sub>3</sub> 22), P4 <sub>2</sub> 22,<br>P4 <sub>2</sub> 12, (P4 <sub>1</sub> 2 <sub>1</sub> 2, P4 <sub>3</sub> 2 <sub>1</sub> 2), P4 <sub>2</sub> 2 <sub>1</sub> 2<br>I422, I4 <sub>1</sub> 22 |
| Trigonal/<br>rhombohedral | 2                                | R <sup>§§</sup> | Threefold axis parallel to <b>c</b>       | $a = b = c$<br>$\alpha = \beta = \gamma \neq 90^\circ$                     | $\bar{3}$                                 | R3  |
|                           |                                  | P <sup>§§</sup> |   |  |   | P3, (P3 <sub>1</sub> , P3 <sub>2</sub> )<br>R32<br>[P321, P312],<br>[(P3 <sub>1</sub> 21, P3 <sub>2</sub> 21), (P3 <sub>1</sub> 12, P3 <sub>2</sub> 12)]  |
| Hexagonal                 | 2                                | P               | Sixfold axis parallel to <b>c</b>         | $a = b \neq c$<br>$\alpha = \beta = 90^\circ$<br>$\gamma = 120^\circ$      | 6/m<br>6/mmm                              | P6, (P6 <sub>1</sub> , P6 <sub>5</sub> ), P6 <sub>3</sub> , (P6 <sub>2</sub> , P6 <sub>4</sub> )<br>P622, (P6 <sub>1</sub> 22, P6 <sub>5</sub> 22), P6 <sub>3</sub> 22,<br>(P6 <sub>2</sub> 22, P6 <sub>4</sub> 22)           |
|                           |                                  | P               | Threefold axes along cube diagonals       | $a = b = c$<br>$\alpha = \beta = \gamma = 90^\circ$                        | m3  | P23, P2 <sub>1</sub> 3<br>[I23, I2 <sub>1</sub> 3]<br>F23   |
| Cubic                     | 1                                | I<br>F          |   |  | m3m                                       | P432, (P4 <sub>1</sub> 32, P4 <sub>3</sub> 32), P4 <sub>2</sub> 22<br>I432, I4 <sub>1</sub> 43<br>F432, F4 <sub>1</sub> 32  |

§ See Figure 13-16 for definitions of edge and angle symbols.

# A number with an overbar indicates a rotary inversion axis;  $2/m$  = a mirror plane;  $2/m$  = a mirror plane perpendicular to a twofold axis;  $6/m$  indicates a mirror plane perpendicular to a sixfold axis.

† Pairs of space groups in parentheses differ from each other only in that they are enantiomorphs. Space groups enclosed in brackets (and also those in parentheses) cannot be distinguished from one another by systematic extinctions of reflections in the diffraction pattern. All other space groups can be assigned on the basis of the diffraction pattern.

§§ The rhombohedral system often is regarded as a subdivision of the hexagonal system, and unit cells in this system may be chosen on either hexagonal or rhombohedral axes. SOURCE: After D. Eisenberg, in *The Enzymes*, 3d ed., vol. 1, P. D. Boyer (New York: Academic Press, 1970).