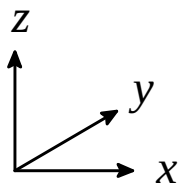


Defining the Coordinate System

- ☞ Molecules are conventionally oriented relative to a right-hand Cartesian coordinate system:



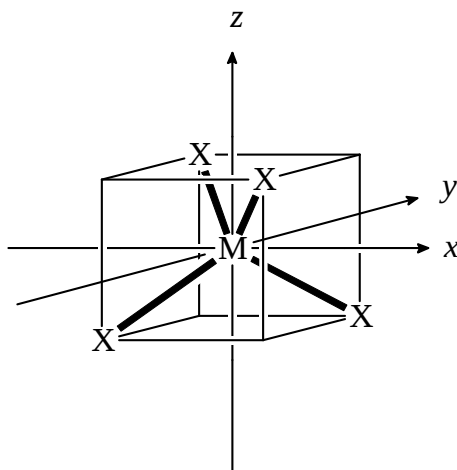
- ☞ The following conventions of axis orientation are usually observed:
 - (1) The origin of the coordinate system is located at the central atom or the center of the molecule.

Defining the Coordinate System

- (2) The z axis is collinear with the highest-order rotational axis (the principal axis). If there are several highest order rotational axes, z is usually taken as the axis passing through the greatest number of atoms.

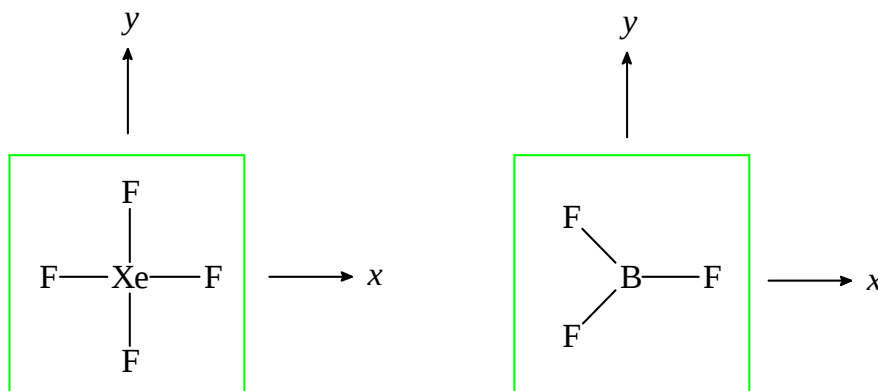


However, for a tetrahedral molecule, the x , y , and z axes are defined as collinear with the three C_2 axes (collinear with the three S_4 axes).

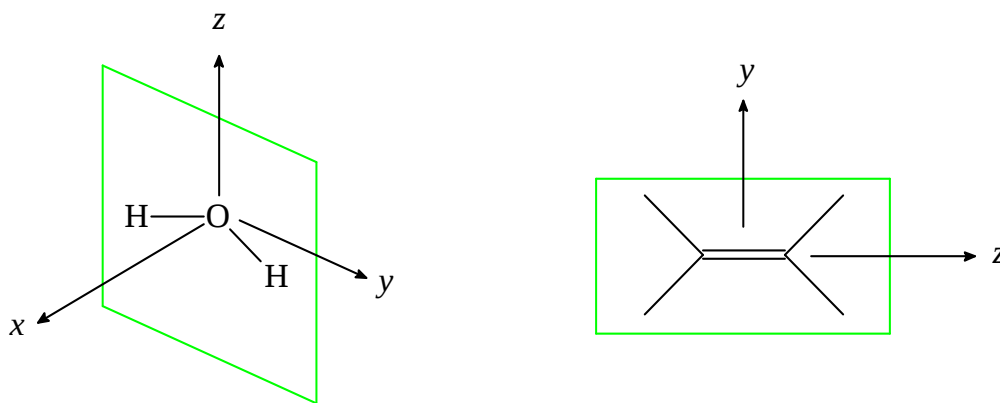


Defining the Coordinate System

- (3) For planar molecules, if the z axis as defined above is perpendicular to the molecular plane, the x axis lies in the plane of the molecule and passes through the greatest number of atoms.

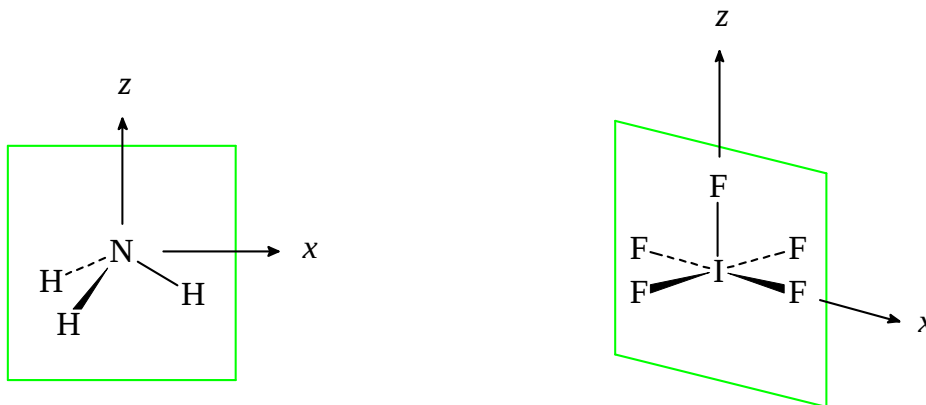


If the z axis lies in the plane of the molecule, then the x axis stands perpendicular to the plane.



Defining the Coordinate System

- (4) For nonplanar molecules, once the z axis has been defined, the x axis is usually chosen so that the xz plane contains as many atoms as possible. If there are two or more such planes containing identical sets of atoms, any one may be taken as the xz plane.



Where a decision about the orientation of the x axis cannot be made on this basis, the distinction between x and y is usually not important or is not generally fixed by convention.

