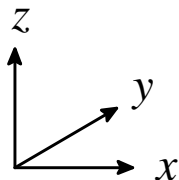


## Defining the Coordinate System

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



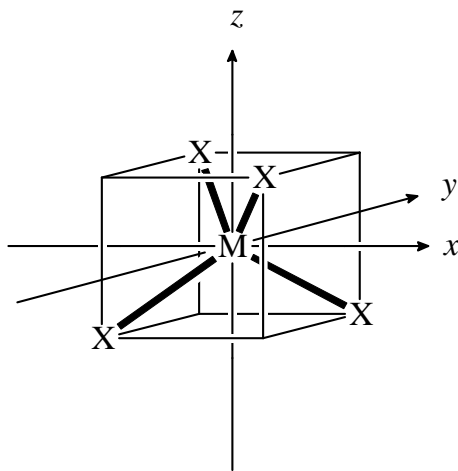
- ☞ The following conventions of axis orientation are usually observed:
  - (1) The origin of the coordinate system is located at the central atom or the center of the molecule.

## 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.

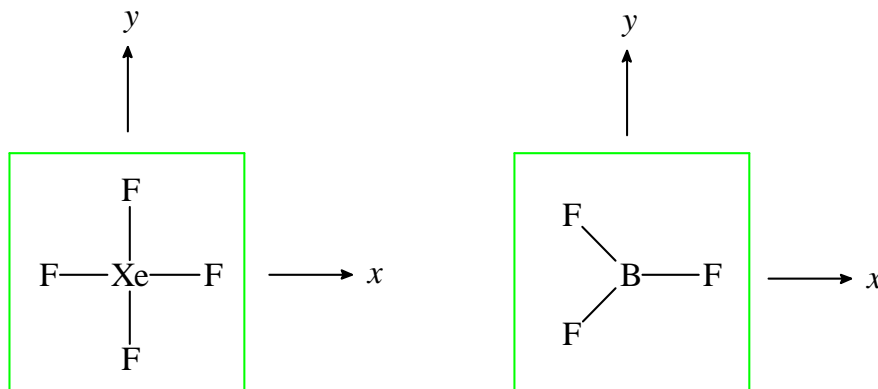


However, for a tetrahedral molecule, the  $x$ ,  $y$ , and  $z$  axes are defined as collinear with the three  $C_2$  axes (collinear with the three  $S_4$  axes).

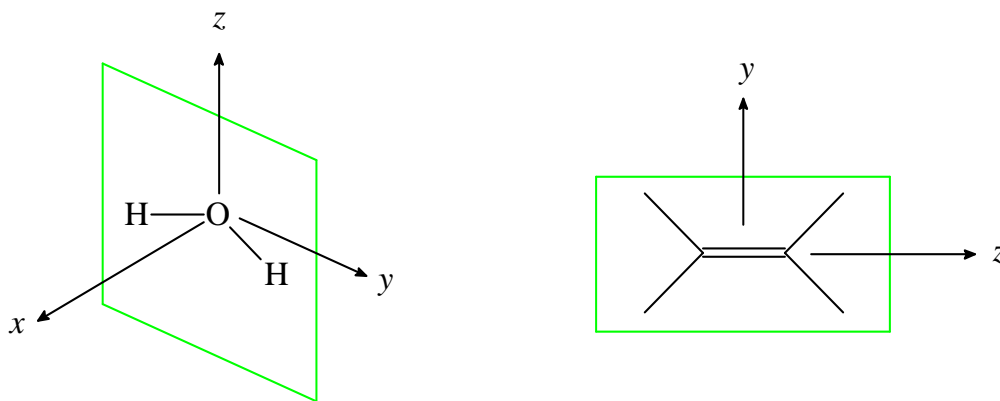


## Defining the Coordinate System

- (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.

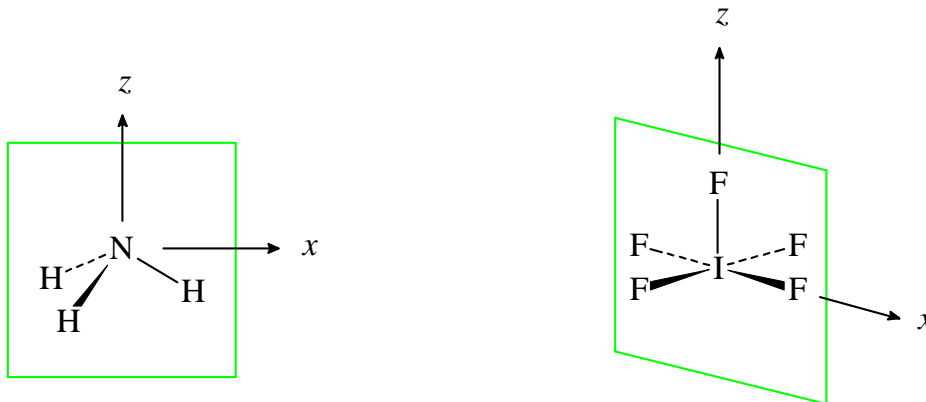


If the  $z$  axis lies in the plane of the molecule, then the  $x$  axis stands perpendicular to the plane.



## 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.

