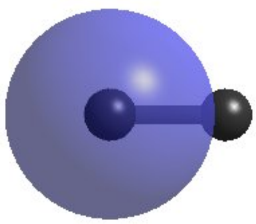
Answers to Exercise 2.1
Sigma and Pi Symmetry

The colours yellow and blue are used to show phase. You can use any pair of colours (including "coloured" and "not coloured") to show phase as long as the phases of lobes on opposite sides of a node are always opposite.

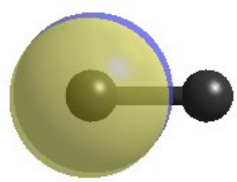
Any of these answers would be equally correct if every lobe switched colour (i.e. if all yellow lobes became blue and all blue lobes became yellow) but not if only some of the lobes switched colour.

1.

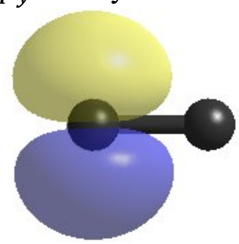
(a) s is σ-symmetric



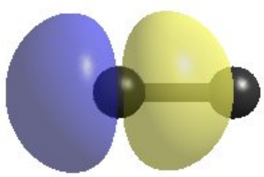
(b) p_x is π-symmetric



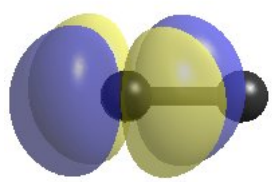
(c) p_y is π-symmetric



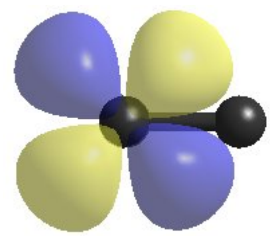
(d) p_z is σ-symmetric



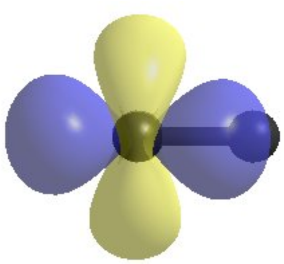
(e) d_{xz} is π-symmetric



(f) d_{yz} is π-symmetric



(g) d_{z^2} is σ-symmetric



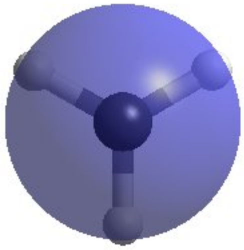
In the images above, the x axis was defined as perpendicular to the page while the y axis was defined as "up and down" along the page. It's fine if you chose to use the opposite convention. Either way, in a linear molecule, the z axis must be the axis along the bond between the two atoms.

If you're having trouble seeing the symmetry, draw in the nodes. All of the π-symmetric orbitals have a node lying along the axis of the molecule (passing through both atoms). None of the σ-symmetric orbitals have a node passing through both atoms (though they may have other nodes).

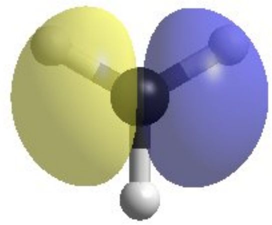
Atomic orbitals don't actually exist in molecules since they would interact with the atomic orbitals on the other atom to make molecular orbitals. The drawings here are merely tools to help you see the symmetry.

2.

(a) s is σ-symmetric

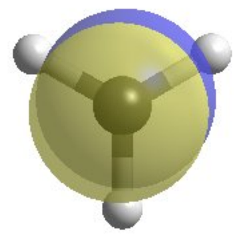


(b) p_x is σ-symmetric



(c) p_y is σ-symmetric

(d) p_z is π-symmetric



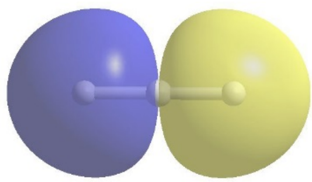
In the images above, the x axis was defined as "left and right" along the page while the y axis was defined as "up and down" along the page. It's fine if you chose to use the opposite convention. Either way, in a planar molecule, the z axis must be perpendicular to the plane of the molecule.

If you're having trouble seeing the symmetry, draw in the nodes. The π-symmetric orbital has a node lying along the plane of the molecule. None of the σ-symmetric orbitals have a node passing through all the atoms in the molecule (though they may have other nodes).

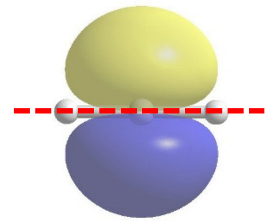
Atomic orbitals don't actually exist in molecules since they would interact with the atomic orbitals on the other atom to make molecular orbitals. The drawings here are merely tools to help you see the symmetry.

3.

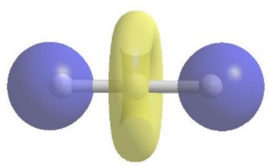
(a) σ-symmetric



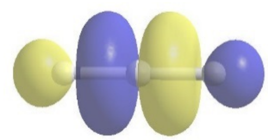
(b) π-symmetric



(c) σ-symmetric

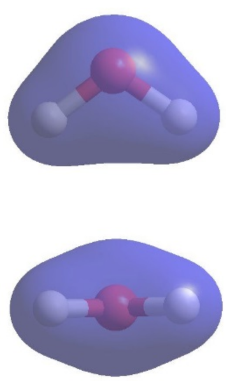


(d) σ-symmetric

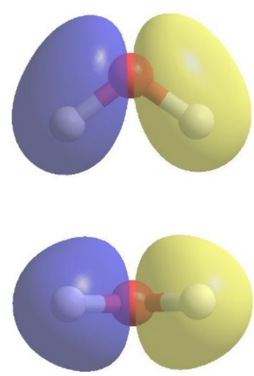


4.

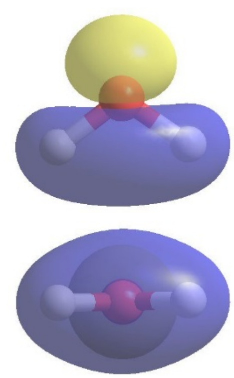
a) σ-symmetric



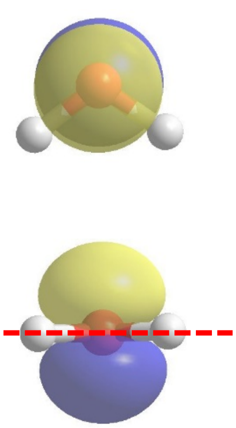
(b) σ-symmetric



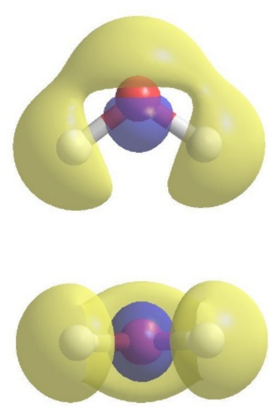
(c) σ-symmetric



(d) π-symmetric



(e) σ-symmetric



(f) σ-symmetric