Answers to Exercise 3.3
Bonding, Antibonding and Nonbonding Molecular Orbitals

1. When theoretical calculations and experimental data conflict (and you are sure that no errors were made when conducting or interpreting the experimental data), the experimental data is always correct. As such, you should be most confident in the bond order given by the PES spectrum; however, you should ensure that you are correctly interpreting the PES spectrum.

   It's also possible that the MO is "partially bonding" or "partially antibonding" (since not all MOs are 100% bonding, 100% antibonding or 100% nonbonding). This can be difficult for a beginner to interpret from a PES spectrum, so they would want to consult an expert.

2.

(a)	antibonding π-symmetric	(b)	nonbonding π-symmetric	(c)	bonding π-symmetric
(d)	bonding σ-symmetric	(e)	antibonding σ-symmetric	(f)	antibonding σ-symmetric

3.

(a)	bonding π-symmetric	(b)	bonding π-symmetric	(c)	bonding σ-symmetric
(d)	bonding π-symmetric	(e)	antibonding σ-symmetric	(f)	antibonding π-symmetric
(g)	bonding σ-symmetric	(h)	antibonding π-symmetric	(i)	bonding σ-symmetric

For the less obvious cases, the easiest approach is to look at each pair of adjacent atoms and classify that interaction as bonding (the orbital has a lobe connecting the two atoms), antibonding (there is a node perpendicular to the bond between the two atoms) or nonbonding (neither bonding nor antibonding). If there are more bonding interactions, the MO is bonding. If there are more antibonding interactions, the MO is antibonding. If the number of bonding and antibonding interactions is equal, the MO is nonbonding.

e.g.