Problem 6, Chemistry 301X-2006

Construct the molecular orbitals (MOs) for linear BeH_2 from H_2 and the AOs for Be. We suggest the following protocol:

(a) how many MOs will there be?

(b) show the orbitals of H_2 and Be that you will use in your construction.

(c) order these building block orbitals in energy. Remember that at this level of "theory" you will only have to interact the orbitals closest in energy. You might stop right here and ask a TA if you are right.

(d) construct the proper MOs for linear BeH_2.

(e) order the bonding and nonbonding MOs in energy.

There is a machine, called an EPR spectrometer, that can detect ("see") unpaired electron spin. Would the EPR spectrometer see unpaired spin in: neutral BeH_2? $^{+}BeH_2$? $^{-}BeH_2$? Explain.