

HW #7 Answers

1. You were not given enough information to determine $J_{g,og}$. You were given the total $(E_{el} + E_{nu})$ ground state energy. You need E_{el} alone to extract this particular J value. Thus you need to know the bond length. I actually expected that you would extract only $J_{g,ou}$, $K_{g,ou}$ from the information on the excited states.

$$\Delta E_T = E_{ou} - E_{og} - J_{g,ou}$$

$$21.5 = 40.2 - J \Rightarrow J = 18.7 \text{ eV.}$$

$$\Delta E_S = E_{ou} - E_{og} - J_{g,ou} + 2K_{g,ou}$$

$$31.0 = 21.5 + 2K \Rightarrow K = 4.75 \text{ eV}$$

2. • single excitations are excluded by Brillouin's theorem.

• triple excitations do not occur as we have only two electrons

• Since there are only two electrons, we would not expect quadruple excitations to occur. However, there is a subtlety here due to what are called exclusion-principle violating diagrams.