

## HW #7 Answers

1. States from  $\pi_u^2 \pi_g$

First consider  $\pi_u^2 \rightarrow {}^1\Delta_g, {}^1\Sigma_g, {}^3\Sigma_g$

Now couple  $\pi_u$  to each of these

$${}^1\Sigma_g \times \pi_g \rightarrow {}^2\Pi_g$$

$${}^3\Sigma_g \times \pi_g \rightarrow {}^2\Pi_g, {}^4\Pi_g$$

$${}^1\Delta_g \times \pi_g \rightarrow {}^2\Phi_g, {}^2\Pi_g$$

2. acetylene ground state:  $\dots \pi_u^4 \rightarrow {}^1\Sigma_g$

acetylene excited states:  $\dots \pi_u^3 \pi_g$ . This will have the same states as  $\pi_u \pi_g$ :  ${}^1\Delta_g, {}^3\Delta_g, {}^1\Sigma_g(2), {}^3\Sigma_g(2)$

One would expect one of the triplet states to be lowest in energy.

3.  $\text{Be}_2^-$ :  $\text{Be}_2$  is  $1\sigma_g^2 1\sigma_u^2 2\sigma_g^2 2\sigma_u^2 \rightarrow {}^1\Sigma_g$

The LUMO is either  ${}^2\Pi_u$  or  $\sigma_g$ , both of which are bonding, so the anion is either  ${}^2\Sigma_g$  or  ${}^2\Pi_u$  both of which have bond order =  $1/2$ .