# CHEM 260

## Assignment 11

Due 2nd April 2003

35. Calculate the normalization factor *N* for the hybrid orbital

$$\Psi = N\left\{\psi_{2s} + \tfrac{1}{\sqrt{2}}\psi_{2px} + \sqrt{\tfrac{3}{2}}\,\psi_{2py}\right\}.$$

and show that this orbital is orthogonal to

$$\Psi = N\left\{\psi_{2s} - \sqrt{2}\psi_{2px}\right\}$$

and $$\Psi = N\left\{\psi_{2s} + \tfrac{1}{\sqrt{2}}\psi_{2px} - \sqrt{\tfrac{3}{2}}\,\psi_{2py}\right\}.$$

36. Suggest an electron configuration for the cyanide ion, $CN^-$ [Write it in the form $(1s\sigma)^2(1s\sigma^*)^2\ldots$]. Is the ion diamagnetic or paramagnetic? What about the $CN^+$ cation and the CN radical? Which of these three forms has the strongest bond? Explain.

37. Carry out a Hückel calculation for the π electron system of the allyl radical $[CH_2\text{-}CH\text{-}CH_2]^\bullet$ and thence calculate the molecular orbital energies in terms of the Hückel parameters α and β. Sketch and label an energy level diagram to show which molecular orbitals are occupied.

38. The atomic orbital coefficients from a Hückel calculation for the allyl radical are given below. Use this data to calculate (i) the unpaired spin distribution in the allyl radical; (ii) the charge distribution in the allyl cation.

| | $\phi_1$ | $\phi_2$ | $\phi_3$ |
|---|---|---|---|
| $\psi_1$ | 0.500 | 0.707 | 0.500 |
| $\psi_2$ | 0.707 | 0.000 | 0.707 |
| $\psi_3$ | 0.500 | -0.707 | 0.500 |