

Student name: _____ (1 pt)

(1) a) Construct molecular orbital schemes to describe the bonding in the following diatomic species. Fill the electrons in the appropriate molecular orbitals and label the HOMO and LUMO. (18 pts)

O₂

LiF

NO

b) Determine the bond order, spin multiplicity, and magnetism (paramagnetic or diamagnetic) for each molecule. (9 pts)

O₂ : Bond order Spin multiplicity Magnetism

LiF :

NO :

c) Explain whether you expect the bond in each molecule to become *stronger*, *weaker*, or *unchanged* upon 1-electron oxidation and 1-electron reduction. (6 pts)

O₂ : 1-e oxidation 1-e reduction

LiF :

NO :

(2) Use group theory to construct a reasonable molecular orbital scheme to describe the σ -bonding in the polyatomic ions tetrahydroborate and nitrate. Fill the electrons in the molecular orbitals and label the HOMO and LUMO.

(24 pts)

BH_4^-

NO_3^-

(3) a) Give the predicted basicity order of NH_3 , CH_3NH_2 , $(\text{CH}_3)_2\text{NH}$, and $(\text{CH}_3)_3\text{N}$ in the gas phase. **Explain.** (8 pts)

b) Why does the basicity order change when the same compounds act as Lewis bases with the Lewis acid $\text{B}(t\text{-Bu})_3$? (4 pts)

c) Why does the basicity order change in aqueous solutions of the same compounds? (4 pts)

(4) Answer parts a) and b) below in regard to the two following observations:

i) The Lewis acid AlF_3 becomes soluble in hydrofluoric acid if NaF is present.

ii) When the other Lewis acid BF_3 is subsequently added to the resulting solution in i), AlF_3 precipitates.

a) Explain these two observations by writing the two chemical equations responsible for each observation. (6 pts)

i)

ii)

b) Explain why your equations above occur in the forward instead of the reverse direction. (4 pts)

i)

ii)

(5) Refer to the figure shown on the overhead showing the HOMO and LUMO for various species and then predict the role of water when it reacts with the following species. You do **not** have to write chemical equations; just indicate how you expect water to behave (*e.g.*, as an acid, base, oxidant, reductant, no reaction, etc.) **and explain your answer.** (16 pts)

a) Calcium metal

b) Cl^-

c) Mg^{2+}

d) F_2