CHEMISTRY 413

Test 1, Thursday, February 19, 1998, 9:30 am - 10:45 am

(1.) (a) Please draw a Lewis structure for the species $TeOF_4^-$; please consider the formal negative charge to be residing on the Te atom.

(b) What is the predicted shape of this species? Please draw your answer, and give the occupancy and hybridization at each atom.

(c) By the valence-bond description, please show the bonding σ hybrid orbitals, and unhybridized π orbitals, if necessary, on the $TeOF_4^-$ species.

(d) Do you anticipate a dipole moment for this species? Please draw the polarity in the bonds of the species, and the direction of overall dipole, if any.

(e) Please assign oxidation numbers for each element in the species.

(f) The Te-O internuclear separation is found to be 1.93 Å; is this consistent with π bonding here, or not? If consistent, what kind of π bonding is it (*p-p*, *p-d*, *d-d*)? Please explain your choice. (Covalent radii: O, 0.66 Å; Te, 1.37 Å).

(2.) (a) Please draw the molecular orbital (M.O.) diagrams, alongside each other, for the hypothetical species BO^- and OF^+.

(b) Please write the electronic configuration for each species.

(c) What is the bond order for each species?

(d) Please draw a Lewis structure for each consistent with the bond order you obtained in part (c).

(e) Is the boron atom coordinatively-saturated in BO^-? Please explain.

(3.) (a) Please consider the carbocation CH_3^+. Please report the shape of this molecular ion and assign its point group.

(b) Based on the symmetry of the point group, please show how the available atomic orbitals will combine to generate molecular orbitals, and please label their "symmetry types."

(c) Please show how the electrons occupy the molecular orbitals in an M.O. diagram.

(d) Please explain the difference in bonding between the valence-bond description of CH_3^+ and the M.O. description.

(e) What is the point group of CH_3^-? Which atomic orbitals combine to form the non-bonding M.O. of a_1 symmetry in this species?

(f) Please write the wave function ψ of the a_1 molecular orbital in part (e).

(g) Using the character table, please explain why CH_3^- does not form any molecular orbitals of a_2 symmetry.

(4.) (a) Please write the short-hand electronic configurations of the *4d* and *5d* transition-metals of Group 4. Please explain why the atomic radii of these two elements are virtually identical.

(b) Please write the short-hand electronic configurations of Sn and Pb. Which group in the Periodic Table are these elements in? Does the lanthanide contraction operate here? Will the occupation of *6p* orbitals in Pb make the atomic radius larger or smaller than the *5d* transition-metals? Please explain.