

## Review 4

2 hour final exam. Dec. 10, Wed. 3-5 pm.

ID will be checked when the exam is turned in.

A two-page cheat sheet is allowed, but it can only contain equations and constants.

10 multiple choice questions, 5 points each, only one answer.

6 simple questions, 10 points each.

5 more complex questions, 15-20 points each.

The final is comprehensive, covering all materials in this course.

### 1. Molecular structure

Born-Oppenheimer approximation, LCAO-MO, homonuclear diatom, secular equations and secular determinant, Coulomb, resonance, and overlap integrals, bonding and antibonding MOs, quantum mechanical nature of the chemical bond,  $\sigma$  and  $\pi$  bonds, HOMO, and LUMO, bond orders, spin multiplicity, molecular orbital energy level diagram. Heteronuclear diatoms.

Hybrid orbitals and valence bond theory, Walsh diagram and the molecular structure, Hückel theory for conjugated molecules, band theory.

### 2. Electronic spectra

Molecular term symbols, Franck-Condon principle and factor, excited singlet and triplet states, chromophores, fate of excited species, internal conversion and interstate crossing, fluorescence and phosphorescence.

### 3. Symmetry and group theory

Symmetry elements and symmetry operations, definition of a group, point groups (only common ones), representations and irreducible representations, characters and character tables, basis, determining irreps in rep, projection operators, vanishing integrals, SALC-MO.