Name: _____ **Date:** _____

Answer Key: Bonding Bliss: Orbital Overlaps and Molecular Mixology for College Chemists

Molecular Orbital Theory, hybridization, and lattice energy calculations — essential advanced mechanics for mastering structural inorganic chemistry and thermodynamics.

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1. In the context of Molecular Orbital (MO) theory for heteronuclear diatomic molecules like CO, which statement accurately describes the frontier orbitals?

Answer: A) The HOMO is primarily localized on the Carbon atom due to its lower electronegativity.

In CO, the Carbon atom's orbitals are higher in energy than Oxygen's. The Highest Occupied Molecular Orbital (HOMO) has a larger coefficient on the Carbon atom, explaining why CO acts as a sigma-donor through Carbon in metal carbonyls.

2. True or False: According to the Bent's Rule, central atoms with high electronegativity substituents will prefer to direct more p-character toward those substituents to decrease the bond energy.

Answer: A) True

Bent's Rule states that atomic s-character concentrates in orbitals directed toward electropositive substituents, while p-character concentrates in orbitals directed toward electronegative substituents, minimizing the energy of the system.

3. To calculate the Lattice Energy of an ionic solid without experimental data, the _____ equation accounts for the Madelung constant and the Born exponent.

Answer: B) Born-Landé

The Born-Landé equation is used to calculate the lattice energy of a crystalline ionic compound based on its electrostatic potential and the repulsive potential between ions.

4. Which transition in the Walsh diagram for an AH2 molecule explains why H2O is bent while BeH2 is linear?

Answer: C) The dramatic energy decrease of the 2a1 orbital upon bending from 180°.

In AH2 molecules, the 2a1 orbital (derived from the central atom's s and pz orbitals) significantly drops in energy as the molecule bends, making a bent structure more stable for molecules with more than 4 valence electrons.

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5. The phenomenon where a metal-ligand bond is strengthened by the synergistic transfer of electrons from a filled metal d-orbital to the ligand's empty π* orbital is called _____.

Answer: B) π-backbonding

Pi-backbonding involves the overlap of a filled metal d-orbital with an empty pi-acceptor orbital on the ligand (like CO or CN-), increasing the bond order between the metal and ligand while decreasing the bond order within the ligand.

6. True or False: In a metallic crystal, the 'Fermi Level' refers to the energy level of the highest occupied electron state at absolute zero temperature.

Answer: A) True

The Fermi level defines the top of the 'sea' of electrons in the band theory of solids, specifically representing the chemical potential of electrons at 0 Kelvin.

7. Using Fajan's Rules, which of the following compounds would you predict to have the highest degree of covalent character?

Answer: C) BeI_2

Covalent character increases with a small, highly charged cation and a large, easily polarizable anion. Beryllium (Be^{2+}) is smaller and more polarizing than Mg^{2+}, and Iodide (I^-) is larger and more polarizable than chloride or fluoride.

8. In Valence Bond Theory, the mathematical process of combining atomic wavefunctions to produce new, equivalent spatial orientations is known as _____.

Answer: B) Hybridization

Hybridization is the mixing of atomic orbitals (like s, p, and d) to form new hybrid orbitals that better describe the geometry of bonding in polyatomic molecules.

9. True or False: A 'Formal Charge' of zero on all atoms in a Lewis structure always guarantees that the structure is the most accurate representation of the molecule’s actual electronic distribution.

Answer: B) False

Formal charge is a bookkeeping tool and does not account for electronegativity differences (polarization). Experimental data and MO calculations often show electron distributions that differ from what formal charge suggests.

10. Which of the following conditions is required for the formation of a 'dative' (coordinate covalent) bond?

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Answer: B) One atom must possess a lone pair while the other possesses an empty valence orbital.

A dative bond occurs when one atom (the Lewis base) provides both electrons for the bond to an electron-deficient atom (the Lewis acid).