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### Lanthanides

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### Actinides

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1. (10%, 5 points each) Consider the model system for a linear butadiene C₄H₆ molecule.
   a) Construct the MO diagram of π orbitals.
   b) Consider the π bonding in butadiene: Assume the electrons in π orbitals are filled in low spin configurations. Show that the terminal C-C bonds are shorter than central C-C bond.

2. (15%, 5 points each) The structure of Ce-O phase is shown in the figure below and its unit cell parameters are listed correspondingly.

   ![Ce-O phase structure](image)

   \[ a = b = c = 5.4124 \ \text{Å} \]
   \[ \alpha = \beta = \gamma = 90^\circ \]

   Big gray circles: O
   Small light Gray circles = Ce

Answer the following questions:
   a) What is the crystal system of this compound?
   b) What is the cell content of this phase?
   c) Calculate the density of this compound.

3. (15%, 5 points each) Hydrogen azide, HN₃, is a colorless liquid and it is dangerously explosive. Answer the following questions:
   a) Draw all possible Lewis structure(s) for HN₃, including all equivalent resonance structures.
   b) Calculate the formal charges on all atoms and predict the most stable isomer.
   c) According to the experiments, the N-N bond distances in HN₃ molecule is 1.24 (central) and 1.13Å (terminal). On the other hand, the N-N distances in N₃⁻ ions is the same (1.16 Å) Try to give a rationale for these results.
4. (10%, 2 points each) Identify the point group of each of the following structures.

<table>
<thead>
<tr>
<th>a)</th>
<th>b)</th>
<th>c)</th>
<th>d)</th>
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<tbody>
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<td><img src="image-a.png" alt="Image" /></td>
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<td><img src="image-c.png" alt="Image" /></td>
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<tr>
<td>e) TeF$_4^{2-}$</td>
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</table>

5. (6%, 2 points each) Use the hard-soft acid-base concepts to determine which compound is more stable in the following pairs and give your reasons:
   a) PbO or PbS.
   b) TiO$_2$ or TiS$_2$.
   c) HgS or HgO.

6. (18%, 6 points each) (i) Determine and draw the molecular geometry (2%), (ii) sketch the $d$-orbital splittings, (3%) and (iii) show the expected electron occupancy (1%) in the orbitals for the following molecules:
   a) [Fe(phen)$_3$]$^{2+}$ (phen: phenanthroline)
   b) Pt$_6$Cl$_{12}$ (can be considered as [Cl-Pt-Cl]$_6$)
   c) Ni(CO)$_4$. 
7. (18%, 3 points each) Consider the dinitrogen complex $[(\text{H}_3\text{N})_3\text{RuN}_2\text{Ru}(\text{NH}_3)_5]^{4+}$ with point group $D_{4h}$. A set of orbital pictures describing the bonding of dinitrogen to the $\text{Ru(NH}_3)_5^{2+}$ fragments is given. Use these pictures and refer to the $D_{4h}$ point group to identify the irreducible representations ($\Gamma_1$ to $\Gamma_6$) to which the following basis sets belong.

\[
\begin{array}{cccccccccc}
\text{D}_{4h} & E & 2C_2 & C_2^* & 2C_4^* & 2S_4 & a_1 & b_1 & b_2 & b_3 & E_v \\
\hline
A_{1g} & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
A_{2g} & 1 & 1 & 1 & 1 & -1 & 1 & 1 & 1 & -1 & -1 \\
B_{1g} & 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 & 1 \\
B_{2g} & 1 & -1 & 1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 \\
E_g & 2 & 0 & -2 & 0 & 0 & 2 & 0 & -2 & 0 & 0 \\
A_{1u} & 1 & 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 & 1 \\
A_{2u} & 1 & 1 & -1 & -1 & -1 & 1 & -1 & 1 & 1 & 1 \\
B_{1u} & 1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 & 1 & 1 \\
B_{2u} & 1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 & 1 & 1 \\
E_u & 2 & 0 & -2 & 0 & 0 & -2 & 0 & 2 & 0 & 0 \\
\end{array}
\]

\[
R_y \begin{pmatrix} x^2 + y^2, z^2 \\ x^2 - y^2, xy, (x, y) \end{pmatrix} \]

\[
\Gamma_1 \quad \Gamma_4 \\
\Gamma_2 \quad \Gamma_5 \\
\Gamma_3 \quad \Gamma_6
\]
8. (8%, 2 points each) There are many synthetic methods for the synthesis of carbene complexes. The four most common ones are proposed in the followings. Complete the reactions by filling appropriate compounds in the blank.

(a) From the metal carbonyl \( \text{Cr(CO)}_6 \).

\[
\text{Cr(CO)}_6 + \text{PhLi} \rightarrow \text{OC(O)}\text{Cr} - C - \text{Ph} \quad \text{Me}_2\text{COBF}_4
\]  

(b) Activation of a neutral acyl complex.

\[
\begin{array}{c}
\text{OC(O)}\text{Ph} \quad \text{H}
\end{array}
\rightarrow \quad \text{PhCOCH}_2 \quad \text{(2)}
\]

(c) Rearrangement of coordinated ligands by tautomerization of terminal alkyne complexes to acetylides.

\[
\begin{array}{c}
\text{H} \\
\text{C} \\
\text{C} \\
\text{R}
\end{array}
\rightarrow 
\begin{array}{c}
\text{L}_4\text{M} \quad \\
\text{(3)}
\end{array}
\]

(d) From activated olefins (very strained or electron-rich).

\[
\text{Cp}_2\text{Ti(PM}_{3}\text{)}_2 + \quad \rightarrow \quad 
\]

(4)