Members of your team \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

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A transition metal ion has \_\_\_\_\_\_ valence atomic orbitals:[[1]](#footnote-1)†

\_\_\_\_\_\_\_ d and \_\_\_\_\_\_\_ s and \_\_\_\_\_\_\_p orbitals.

* Would the pz orbital of a metal be able to form a bond with a ligand approaching on an axis?
* py?
* Draw the s and the px orbitals on the empty axes.

{{insert figure of empty axes}}

* Decide if either of these orbitals can form a bond with a ligand approaching along the x, y, or z axes.

Repeat the same analysis with each of the d orbitals.

{{insert figure of d orbitals and empty axes}}

* Which d orbitals have good overlap with ligands (can form bonds)?
* Which d orbitals remain non-bonding?
* Explain why these orbitals do not make sigma bonds with ligands in octahedral complexes.

{{insert figure of octahedral crystal field splitting derivation}}

* On the diagram above, name the two d orbitals that have gone up in energy and also the three d orbitals that have gone down in energy.
* The set that goes down in energy is called the “t2g” set, while the set that goes up in energy is called the “eg” set.
* Show, in units of ∆o, that the total energy of the orbitals that go up in energy is equal to the total energy of the orbitals that go down in energy.
* How many valence electrons would a Cr(III) metal ion have? Populate the energy splitting diagram with these electrons.
* For a d1 metal ion (a metal ion with 1 electron in the d orbital set) in an octahedral complex, draw the ground state (the lowest energy way to arrange the electron in the set of five d orbitals).
* When the complex absorbs light with an energy corresponding to the ligand field splitting, an electron is promoted from the lower energy orbitals to the higher energy orbitals. Redraw the five orbitals and show the new electron position.
* As wavelength of absorbance increases, the energy \_\_\_\_\_\_\_\_\_\_\_\_\_\_ (increases/decreases).
* If a solution appears yellow, what wavelength of light does it absorb?
* The visible region of the spectrum runs from approximately 400 nm to 700 nm. What are these limits in cm-1?
* The color that a compound *appears* is on the opposite side of the artists’ color wheel (see below) from the color of light it *absorbs*. [Ti(H2O)6]3+ absorbs light around 520 nm. What color is it?
* consider a square planar complex in the x-y plane.
* Predict which orbitals may be able to overlap with ligands.
* Predict a splitting diagram for square planar complexes. Note, with less interaction along the z-axis, there will be less repulsion between ligands and the metal orbitals along the z-axis. It might be easier to consider what would happen if you “pulled” the ligands on the z-axis outwards from an octahedral complex.
* Using this picture of a tetrahedral complex, predict which orbitals overlap best with ligands.

{{insert figure of a tetrahedral geometry inscribed in a cube}}

* Predict a splitting diagram for tetrahedral.
* Predict the size of ∆t relative to ∆o assuming metal ion and ligands are the same. Hint: What causes the ∆? How are they different for tetrahedral and octahedral?

**UV Practice Problems**

1. If a solution of an octahedral metal complex appears yellow,
   * What wavelength of light is it absorbing?
   * What is the ligand field splitting ∆ for the complex in cm-1?
2. An octahedral metal complex absorbs light that is 535 nm.
   * What color is it?
   * What is the ligand field splitting ∆ for the complex in cm-1?
3. [Cu(NH3)4]+ is completely colorless while [Cu(NH3)4]2+ is intensely blue.

* Draw the splitting diagrams to explain this observation.

1. For each cobalt complex below, draw a d-orbital splitting diagram and fill with electrons (hint: think about geometries and type of ligand). Note, ∆o is larger for NH3 ligands and smaller for H2O ligands.

[Co(NH3)6]2+

[Co(H2O)6]2+

[CoCl4]2-

* The colors of these complexes are red, yellow and blue. Assign the correct color to each.

1. † All of these questions come from the guided inquiry exercise “A Guided Inquiry Activity for teaching Ligand Field Theory,” Johnson, B. J., and Graham, K. J., *J. Chem. Educ.*, **2015**, *92*, 1369-1372. I have listed the subset of questions I took from this reference to guide adapters of this learning object. There are many more topics, details, and questions in the original reference. [↑](#footnote-ref-1)