MEGA MOLECULES

Name ____________________________
Date ____________________________

Coordination Complexes

Time required: 2-3 hours

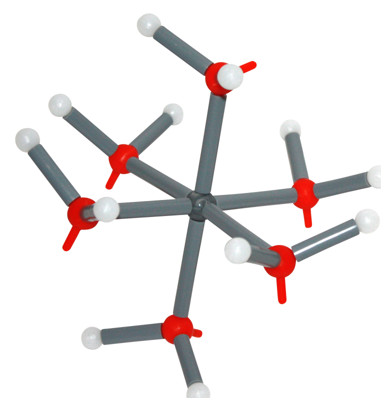
Objective: You will build coordination complexes containing monodentate and polydentate ligands and explore geometric and optical isomerism.

Introduction: Coordination complexes have a wide variety of uses including oxygen transport by hemoglobin in red blood cells, photosynthesis, water purification, pharmaceutical use, and as catalysts for many manufacturing processes. A coordination complex is the product of a Lewis acid-base reaction in which neutral molecules or anions, called ligands, bond to a central metal atom or ion by coordinate covalent bonds. Ligands may be neutral or negatively charged. Within a ligand, the atom that is directly bonded to the metal atom or ion is called the donor atom. Ligands with only one donor atom are called monodentate ligands. Ligands with more than one donor atom are called polydentate ligands.

The coordination number determines the geometry around the central metal atom or ion. The coordination number of the central metal atom or ion is the number of donor atoms bonded to it. The common geometries found in coordination complexes are tetrahedral, square planar, and octahedral. Both tetrahedral and square planar have a coordination number of four. Octahedral complexes have a coordination number of six.

A coordination sphere consists of the central metal atom or ion plus its attached ligands. Brackets in a formula enclose the coordination sphere. In the coordination sphere, $[Co(H_2O)_6]^{+2}$, cobalt(II) is the central metal ion. Six water molecules are attached as ligands by coordinate covalent bonds. The complex ion has a coordination number of 6 and an octahedral shape.

Figure 1: $[Co(H_2O)_6]^{+2}$



Use Table 1 to familiarize yourself with the atom models in your model set. The silver models may represent metal or nonmetal atoms or ions.

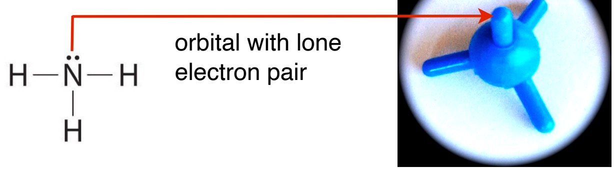
Table 1
The Atoms

Atom	Color	Atom	Color
hydrogen	white	chlorine	green
oxygen	red	fluorine	yellow
carbon	black	iodine	purple
nitrogen	blue	bromine	orange

PROCEDURE:

1. A ligand forms a coordinate covalent bond, a bond in which both of the electrons in the bond are contributed by a donor ligand. The ligand acts as an electron pair donor or Lewis base.

Figure 2: Amine Ligand



$[Ag(NH_3)_2]^{+1}$

Construct each of the ligands listed in Table 2. Identify an electron pair that may be used to form a coordinate covalent bond with a central metal atom or ion. Some of the ligands have more than one electron pair, either of which can form a coordinate covalent bond. Use the 25mm gray bonds to attach hydrogen atoms. Use two or three 51mm gray bonds to form double or triple bonds. Single bonds in monodentate ligands are 40mm gray bonds. The single bonds in polydentate ligands are black 40mm bonds which allow rotation of the ligand when attaching to multiple sites on the central atom or ion.

Table 2: Common Ligands

Monodentate Ligands		Polydentate Ligands	
Neutral	**Anions**	**Neutral**	**Anions**
NH_3 amine	Cl^{-1} chloro	$NH_3—CH_2—CH_2—NH_3$ ethylene diamine, (en)	$[O—C(=O)—C(=O)—O]^{-2}$ oxalato
H_2O aqua	$C{\equiv}N^{-1}$ cyano		

Distinguish between a monodentate and a polydentate ligand. ____________________

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2. The silver models represent the central atom or ion which is bonded to one or more ligands. The central metal atom or ion is commonly a transition metal or inner transition metal, although main group elements can also form coordination complexes. The central metal atom or ion has orbitals that can accept one or more electron pairs and act as a Lewis acid. Examine the molecular model of $[Ag(NH_3)_2]^{+1}$ in Figure 2. Notice that Ag^{+1} is represented by a silver model with two orbitals available to accept electron pairs from two amine ligands. Select the appropriate silver model and build each of the coordination spheres in Table 3.

Table 3: Coordination Spheres

Formula	Coordination Number (CN)	Geometry
$[Ag(NH_3)_2]^{+1}$	2	linear
$[Cu(CN)_3]^{-2}$	3	trigonal planar
$[CuCl_4]^{-2}$ or $[Zn(CN)_4]^{-2}$	4	tetrahedral
$[Pt(NH_3)_2Cl_2]$	4	square planar
$[CoCl_5]^{-2}$	5	trigonal bipyramidal
$[Co(H_2O)_6]^{+2}$	6	octahedral

Write a general statement relating the number of orbitals of the central atom or ion that can accept electron pairs and the coordination number.

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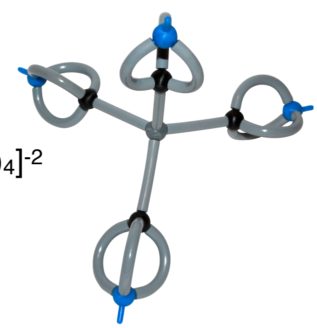
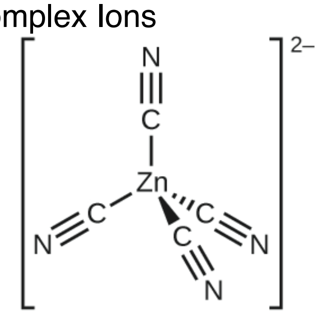
3. Neutral compounds that contain a coordination sphere are called coordination compounds. If the coordination sphere carries a net charge, it is called a complex ion. The complex ion, $[Zn(CN)_4]^{-2}$, is shown as an example in Figure 3. Label each coordination sphere as either a coordination compound or a complex ion. Use Table 3 to determine the coordination number and identify the geometry.

Figure 3: Coordination Compounds vs. Complex Ions

$[Zn(CN)_4]^{-2}$

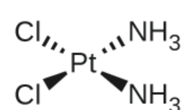




complex ion

CN = 4, tetrahedral

$[Pt(NH_3)_2Cl_2]$



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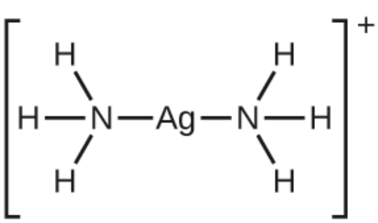

$[Ag(NH_3)_2]^{+1}$

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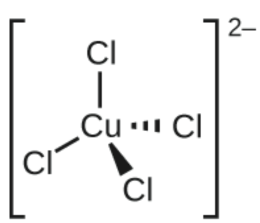

$[CuCl_4]^{-2}$

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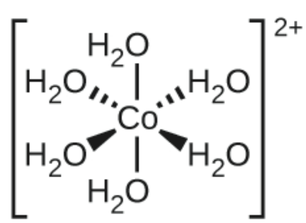

$[Co(H_2O)_6]^{+2}$

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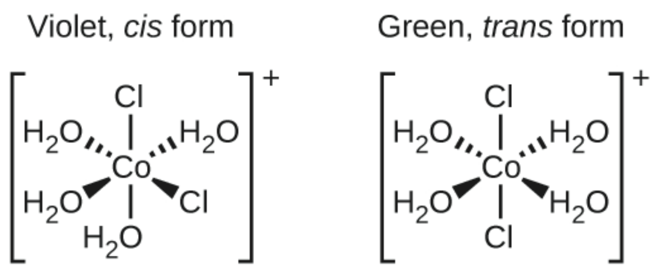
ISOMERISM

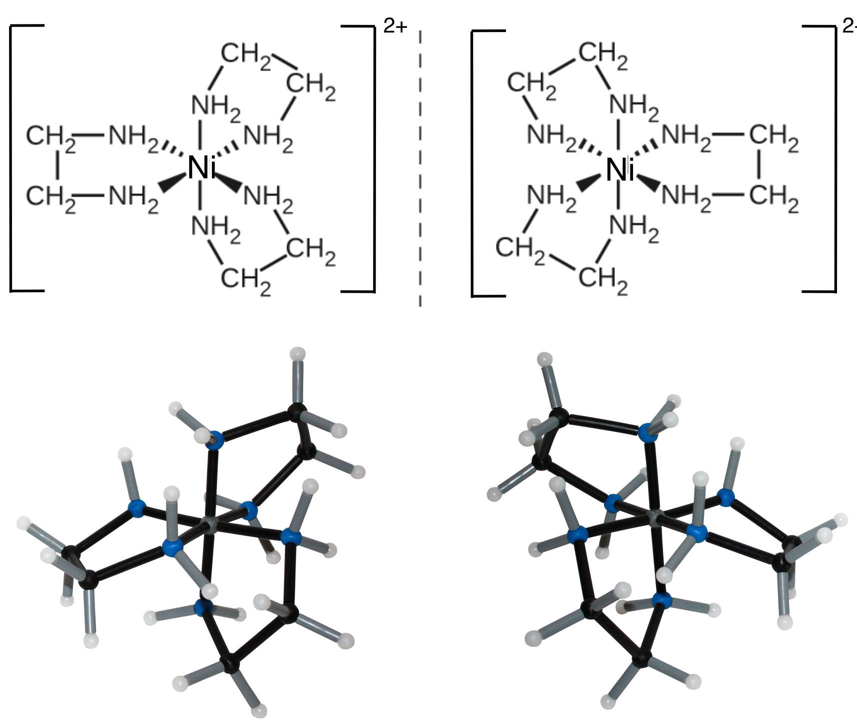
Cis and trans configurations are geometric isomers that are possible in some octahedral and square planar complexes. For example, the octahedral $[Co(H_2O)_4Cl_2]^{+2}$ ion has two isomers. In the cis configuration, the two chloride ligands are adjacent to each other. The other isomer, the trans configuration, has the two chloride ligands directly across from one another. As shown in Figure 4, the cis and trans isomers of $[Co(H_2O)_4Cl_2]^{+2}$ contain the same ligands attached to the same metal ion, but the spatial arrangement causes these two compounds to have very different properties.

Figure 4: Cis and Trans Isomers of $[Co(H_2O)_4Cl_2]^{+1}$



Another important type of isomers is optical isomers, or enantiomers. Optical isomers are molecules or ions that are mirror images and are non-superimposable. Although similar in appearance, these isomers differ from each other in the same way that your left hand differs from your right hand. Like your left and right hands, optical isomers are non-superimposable. Compounds containing a central metal atom or ion with four different attached ligands display optical isomerism.

Figure 5: Optical Isomers of $[Ni(en)_3]^{+2}$ (Note: en = ethylenediamine)



PROCEDURE (continued):

4. Construct a tetrahedral model of [Co(H_2O)$_2$ClBr].

   Does [Co(H_2O)$_2$ClBr] have isomers? ______________________________

   What are the requirements for a tetrahedral structure to exhibit isomerism? ________

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5. Construct the cis and trans isomers of the square planar compound, [Pt(NH_3)$_2$$Cl_2$]

   Describe the differences in the two isomers. ______________________________

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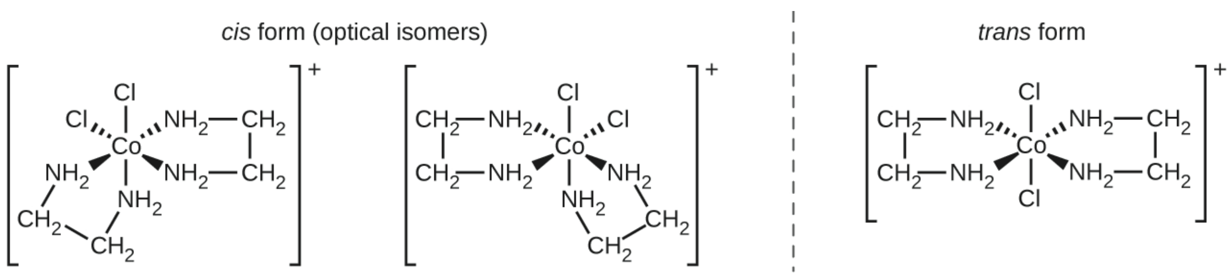
6. The [Co(en)$_2$$Cl_2$]$^{+1}$ ion exhibits geometric isomerism (cis/trans), and its cis isomer exists as a pair of optical isomers. Build the three structures shown in Figure 6 to demonstrate cis/trans and optical isomers.

Figure 6: The Isomers of [Co(en)$_2$$Cl_2$]$^{+1}$



   Explain why a trans structure cannot form optical isomers. ____________________

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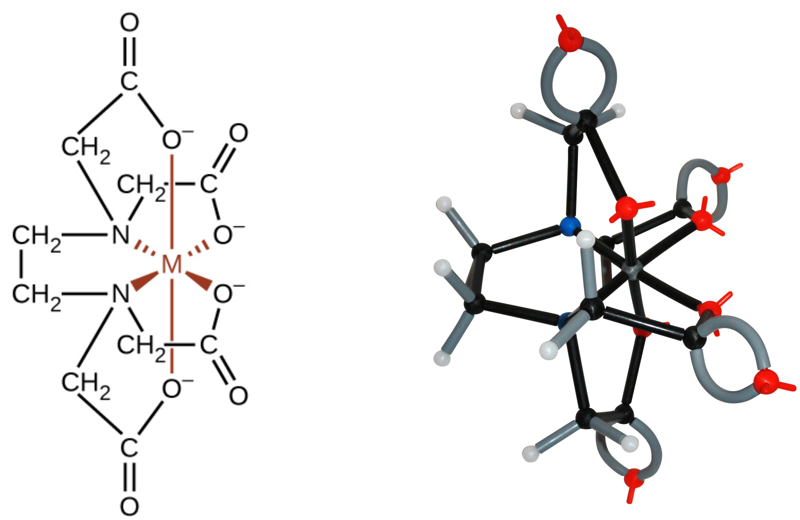
7. Build all of the possible stereoisomers of [Cr(NH_3)$_2$(C_2O_4)$_2$]$^{-1}$. How many isomers can be constructed for [Cr(NH_3)$_2$(C_2O_4)$_2$]$^{-1}$? ______________________________

USES OF COORDINATION COMPLEXES

Coordination complexes are often used for water softening because they tie up such ions as Ca^{2+}, Mg^{2+}, and Fe^{2+}, which make water hard. In addition, many metal ions are undesirable in food products because these ions can catalyze reactions that change the color of food. EDTA, ethylenediaminetetraacetic acid, is a food additive that is generally recognized as safe by the U.S. Food and Drug Administration. EDTA coordinates to metal ions through six donor atoms and prevents the metals from reacting. EDTA, shown in Figure 7, is also used to bind metal ions in paper production, textiles, detergents, and has pharmaceutical uses.

Figure 7: The EDTA Complex



Chelation therapy is a treatment that involves repeated intravenous administration of a chemical solution of ethylenediaminetetraacetic acid, or EDTA. It is used to treat acute and chronic lead poisoning by pulling toxins, including heavy metals such as lead, cadmium, and mercury, from the bloodstream. The word "chelate" comes from the Greek root chele, which means "to claw." EDTA has a claw-like molecular structure that binds to heavy metals and other toxins.

8. What is the coordination number of EDTA and the geometry around the central metal ion?

   coordination number = ______________ geometry = ______________________________

9. Name the six atoms in the EDTA complex shown in Figure 7 that act as Lewis bases and form coordinate covalent bonds with the central metal atom or ion?

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10. Why is EDTA used in chelation therapy? ______________________________________

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