Semester Project

As part of the required homework for CEE 680, I'd like you to work in groups of 2 or 3 on the chemistry of a particular contaminant. Transition metals are probably the best candidates for this, but there are some ligands that could make an interesting project as well. The final product will be a report on your dissolved contaminant, including the following sections:

1. Introduction
2. General Environmental Significance
3. Acid/Base Chemistry
4. Coordination (or Complexation) Chemistry
5. Precipitation/Dissolution Chemistry
6. Review and Critique of 2 articles that concern the environmental chemistry of your chosen contaminant

I will ask to you to make a short (~ 5 min) presentation to the class at various stages. These include:

Stage	**Topic of presentation**	**Date**
Stage 1	Selection of contaminant and reason for your selection	March 13
Stage 2	Acid/base chemistry	March 25
Stage 3	Complexation chemistry	April 8
Stage 4	Precipitation & dissolution	April 22
Stage 5	Critique of 2 articles	April 29

A final written report is due on Friday May 8, 2020. See below for a bit more detail.

<u>Intro & General Significance</u>

Please begin your semester project with a discussion on why your particular contaminant would be of interest to environmental engineers or environmental chemists. Let me suggest that you include: (1) a general introduction; and (2) a section on environmental significance. This second section should summarize any environmental standards that may have been set for your contaminant. Please explain why your contaminant has been regulated and what type of hazards it presents. If it isn't a regulated substance, it is likely to be either a contaminant of importance to ecological systems or a "model contaminant" that has been used to understand the behavior of natural organic matter or humic substances. In particular, pay attention to the effects of speciation (e.g., degree of protonation, complexation with ligands) on toxicity, bioavailability or other properties such as removal in treatment.

Acid/Base and Precipitation/Dissolution Chemistry #1

Continue with a broad discussion of the acid/base and precipitation/dissolution chemistry. A good general reference is the series by Smith & Martell, Critical Stability Constants (some volumes are listed as Martell & Smith). These are available in the Marcus research labs, or in the Physical Sciences Library.

If you have chosen a **non-metal**, you will need to find its pKa's and prepare both a distribution diagram (alpha diagram) and a log concentration vs pH diagram covering the entire range from pH 0 to pH 14. Comment on the forms that are expected in natural waters. Also discuss effects of temperature and ionic strength on the acid/base speciation.

If you have chosen a **metal**, you will need to present a full discussion of its formation of metal hydroxides. You should prepare a solubility diagram (log conc vs pH) based on the presence of a metal hydroxide precipitate. If more than one hydroxide solid is listed, you may need to prepare additional solubility diagrams. You should also construct a species distribution diagram (alpha diagram) over the entire pH range. Please comment on the significance of these calculations, and on the solubility and speciation expected in natural waters. You should also discuss the effects of temperature and ionic strength. If your metal can exist in more than one oxidation state, then you will have to repeat this analysis for the oxidized or reduced forms of the metal.

Coordination (or Complexation) Chemistry and/or Precipitation/Dissolution Chemistry #2

For the last segment of the semester project, I'd like you to focus on bonding with species other than the proton or hydroxide. Specifically, you should examine two relevant Metal-ligand systems. Do not concern yourself with temperature or ionic strength effects for this section. Please comment on the significance of these calculations, and on the speciation or solubility expected for your contaminant in natural waters.

If you have chosen a **non-metal**, such as ammonia or an organic compound, you will need to choose two metals for which there exist stability constants with your chosen contaminant. Please pick something that has some environmental significance. If there is a solid phase that can form, then you should prepare a solubility diagram assuming the presence of the solid phase. If there isn't one, just assume a total contaminant concentration and present the complex speciation versus the metal concentration.

If you have chosen a **metal**, you will need to choose two ligands for which there exist stability constants (this could include either organic or inorganic ligands) with your chosen contaminant. Please pick something that has some environmental significance. If there is a solid phase that can form, then you should prepare a solubility diagram assuming the presence of the solid phase. If there isn't one, just assume a total contaminant concentration and present the complex speciation versus the ligand concentration.