

Project Introduction

Acid Mine Drainage: Measuring Metal Release Rate of Arsenopyrite

For this project experience, you'll be exploring the chemistry surrounding the dissolution of metal sulfide miners. More specifically, you will design and conduct experiments to test the importance of a particular experimental variable (which you choose) in controlling the overall mineral release rate from a sample of arsenopyrite, FeAsS . Our goals for this project are:

- For you to learn quantitative analysis in the context of a real-life environmental problem.
- For you to learn how to apply the scientific method as you develop hypotheses, design your experiments, and develop your own interpretation – in short, how to be a scientist!
- For you to understand some of the complexities and uncertainties associated with scientific measurement, especially when working with complex systems and the natural environment.
- For you to learn how to effectively communicate your scientific results, both orally and in writing.

You will investigate the dissolution rate of arsenopyrite under acidic conditions using a variety of analytical chemistry measurement techniques. In the early stages of the project you will use spectrophotometry to measure the concentration of dissolved iron as a function of time in solutions that contain arsenopyrite. In the latter part of the project, many of you will use the technique of inductively coupled plasma (ICP) atomic emission spectroscopy to measure arsenic and sulfur in addition to iron. Some of you may choose to use an alternative technique in an effort to better understand the chemistry of arsenopyrite dissolution. Throughout the project, you will design, test, and refine your experimental procedures so that you can obtain meaningful results from which you can learn something about the chemistry of arsenopyrite in the environment.

Why do we care about the dissolution rate of arsenopyrite? Many naturally occurring minerals contain metals (for example, arsenic, lead or mercury) that can be toxic if released into the environment. Human activities such as mining or construction of wells for water can lead to the inadvertent release of these metals into the atmosphere or our waterways. In order to prevent potentially serious environmental consequences, it is important to understand the conditions under which these minerals dissolve and release toxic metals. As you will see in the discussion that follows, the chemistry is quite complex and in many cases not well understood.

BACKGROUND

Wisconsin is loaded with metal sulfide minerals. Native Americans mined the southwestern region of Wisconsin as early as the 1700s, and the first European settlers in Wisconsin, in the early 1800s, were trappers and miners. In fact the term “badgers” was originally applied to the miners, who dug shallow “badger-holes” to mine the minerals that were located just beneath the surface. In the early 1800s the miners were primarily after galena (PbS), since it can easily be smelted to lead, which was used for bullets, cannonballs, and a variety of metal utensils. Galena is actually the official state mineral of Wisconsin, and the galena miner, his pickaxe, and a stack of lead are featured prominently on the right side of the Wisconsin state flag (see Figure 1).



Figure 1. Picture of emblem on Wisconsin state flag.

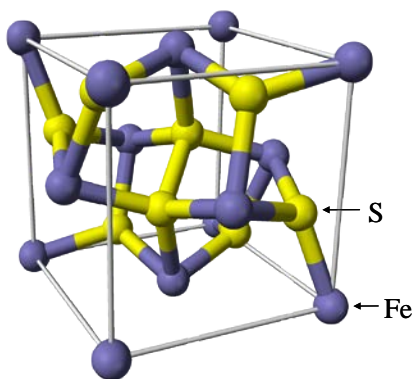


Figure 2. Structure of pyrite.¹

The most common sulfide mineral, pyrite (FeS_2) is a very hard, heavy, shiny, yellow mineral, sometimes referred to as “fool’s gold”. Chemically, it is primarily composed of iron and pairs of sulfur atoms in the form of S_2^{2-} dumbbells. The crystal structure can be viewed as a face-centered cubic lattice of Fe^{2+} ions with 8 sulfur atoms within the unit cell. Each sulfur atom has three Fe^{2+} ions and one sulfur atom as nearest neighbors. (See Figure 2).¹ Other ions such as arsenic can substitute for sulfur in the crystal lattice forming a “solid solution” with up to ~6% arsenic concentration, so that “pyrite” also has other potentially hazardous metals locked into its crystal structure. At higher concentrations, a different mineral known as arsenopyrite, FeAsS , exists. A number of other sulfide minerals (based on lead, gold, silver, mercury, or copper, for instance) exist naturally in the environment. Examples include galena (PbS), argentite (Ag_2S),

cinnabar (HgS), chalcocite (Cu_2S), and covellite (CuS). These metal sulfide minerals are part of a large deposit that extends through northeastern Iowa, northern Illinois, and parts of Wisconsin, especially the southwest, but including most of the state. In the southwest part of the state the sulfide minerals include large amounts of galena (PbS), which was heavily mined in the 1800s for its lead. A map of Wisconsin from the 1800s would show almost all the state’s population concentrated in the southwest part near the Mississippi, where the lead miners could mine and then ship their products down the river. When the lead ran out in the mid-1800s, the miners moved to other locations. However, their legacy is left behind in town names such as “Galena”, Illinois and “Mineral Point” just west of Madison.

Most of the sulfide minerals are located deep underground. However, several regions in central Wisconsin have significant problems with arsenic contamination arising from the natural geochemical distribution of arsenic-containing sulfide minerals, particularly pyrite and arsenopyrite. In the Fox Valley area, especially around Oshkosh and Appleton, a large amount of metal sulfide minerals containing arsenic and other metals are deposited at the boundaries of some sandstone formations. Most of these arsenic-containing metal sulfide minerals are found in a specific type of sandstone known as the St. Peter Sandstone Outcrop. The presence of these minerals has led to a large number of water quality problems in east-central Wisconsin, with naturally occurring levels of arsenic and other metals that far exceed health safety standards. One well drilled in the Green Bay area in 1977 produced water that in 1992 was measured to have a pH of 2.04 and an arsenic concentration of >4300 ppb, more than 400 times the EPA limits on arsenic concentration. Figure 3(a) on the next page shows a map with the location of private wells in Wisconsin having high arsenic concentrations (most in the outcrop in the Appleton-Oshkosh area); Figure 3(b) shows a map of the “Arsenic Advisory Area” in the Fox Valley established by the EPA.²

Recently in Wisconsin, public attention was drawn to the Crandon area, where there had been proposals to mine a sulfide ore deposit, primarily to obtain copper (found as copper sulfides) and zinc (found as zinc sulfide), along with trace amounts of silver and gold. The potential environmental problems associated with crushing and exposing large amounts of sulfide minerals, together with other environmental and economical concerns, led to a great deal of opposition to the mine and eventually resulted in the termination of the project. More information can be found on the Wisconsin Department of Natural Resources (DNR) website.³

Sulfide minerals create similar environmental problems elsewhere. The most serious problem is in Bangladesh, where more than 65 million people are exposed to high levels of arsenic due to the arsenopyrite naturally present in the sub-surface soil. In Bangladesh, the sulfide minerals were not

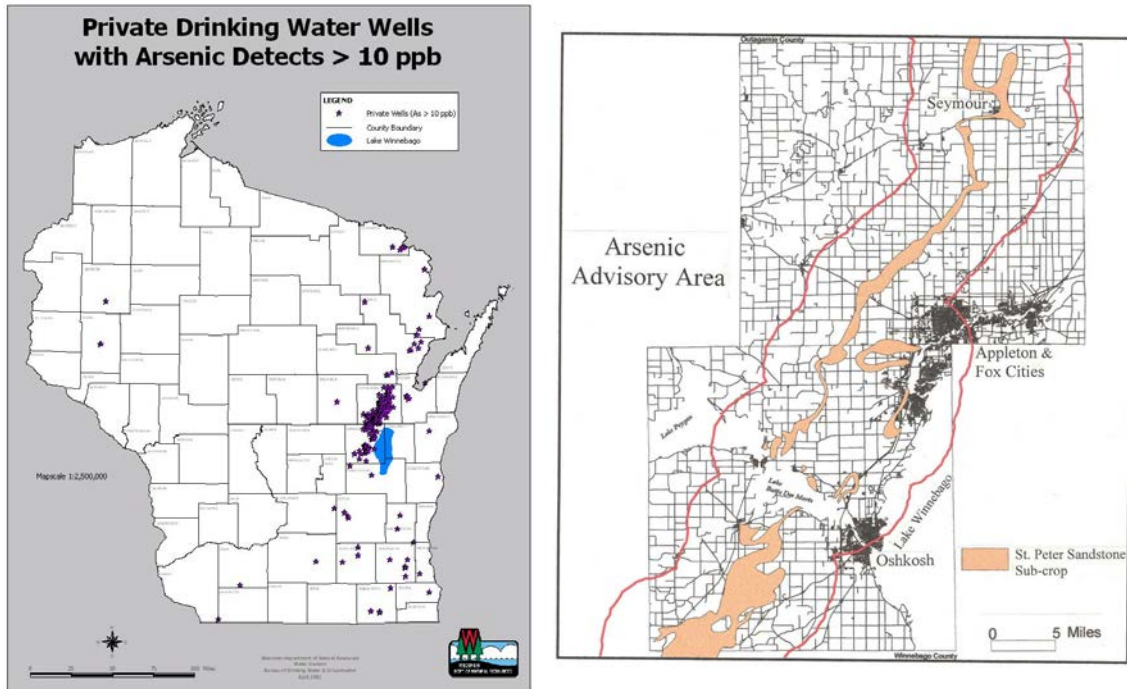


Figure 3. (a) Map showing private wells with arsenic levels greater than the 10 ppb. (b) Map showing the arsenic advisory area near Appleton and Oshkosh.²

considered a problem until the 1970s. An exploding population and poor sanitation led to contamination of the surface water, such as lakes and rivers. When the UN encouraged use of wells instead of surface water as a well-intentioned attempt to improve water quality in Bangladesh, the water quality improved temporarily, but eventually the heavy use of wells caused a drop in the level of the water table. Arsenic-bearing pyrite minerals that were previously completely under water (and therefore protected from oxygen and other oxidizers such as ferric ion) were now repeatedly exposed to oxygen and then water, leading to rapid release of arsenic into the underwater aquifers. While millions of people were exposed to very high levels of arsenic, it has only been in the last few years that the source of the contamination has been identified as sub-surface arsenopyrite and related arsenic-bearing minerals. Even today, the population of Bangladesh continues to use this contaminated water. You can find more information about this problem from numerous sources.^{4, 5}

The problems associated with metal sulfide minerals often go by the name of “acid mine drainage”, or “AMD”. This term refers to the fact that the oxidation of sulfide minerals ultimately produces sulfuric acid, as described in more detail below. Water trickling through a mining area, for example, will react with the sulfide minerals, releasing sulfuric acid and lowering the pH. This highly acidic runoff flows to rivers and streams, where it impacts fish and other plant and animal life. Despite the term “AMD”, however, the most serious environmental consequences of sulfide minerals arises from the release of metals such as arsenic, lead, silver, and copper into the water system. Many metals are toxic even at very small concentrations. For instance, the EPA standard for the maximum allowable amount of arsenic in drinking water is 10 ppb. The “AMD” term is often used to denote both the acid generation and the

release of high concentrations of metals into the environment. More information on the problems of arsenic in drinking water can be found on the EPA and the Wisconsin Water Library websites.^{6,7}

Although the sulfide minerals are present naturally and slowly react under ambient conditions, mining activities accelerate their reactions and have the potential to create very significant, long-lasting environmental problems. Assessing the risk versus benefit of these activities is difficult in part because the underlying science is actually quite complex, making it difficult to quantitatively predict the environmental impact of these activities in the real environment. Additionally, it must be remembered that many of the raw materials must be obtained from somewhere, and mining operations not conducted in the United States may be conducted in other locations, such as the “Minas Gerais” region of Brazil, with much poorer controls on discharges into the environment. Thus, while opposition to the Crandon mine, for example, helps to protect the environment in Wisconsin, it may have a secondary effect of leading to much worse environmental contamination elsewhere, particularly in developing countries such as Brazil and China.

There exists a great deal of rhetoric regarding surrounding the environmental science of mining run-off. Opponents of mining and other activities with potential for damaging the environment often overstate the problems and point to worse-case scenarios, while mine operators/owners underestimate the likely environmental damage. What is nominally a scientific issue rapidly becomes politicized, and the public is left trying to figure out who (if anyone) to believe. As scientists, one of our roles is to provide unbiased scientific data and models that can be used to provide a rational, scientific basis for understanding and predicting the potential effects of human activities on the environment. A second, and often underutilized, responsibility is to communicate this information to the general public. Most people do not have sufficient scientific background to understand the detailed science. However, especially because environmental issues are rarely black-and-white, in order to make informed decisions the public needs to be able to discern between fact and political hyperbole.

METAL SULFIDE REACTIONS

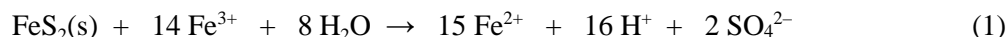
At the very outset it is important for you to know that relatively little is understood about the fundamental reactions of metal sulfide minerals. As you will see below, the reactions can be rather complex because there are many possible intermediate products. The dissolution of pyrite (FeS_2) and arsenopyrite (FeAsS) involves a series of oxidation reactions. Pyrite has been studied more intensely, and some aspects of its chemistry are well understood.^{8, 9, 10, 11} Arsenopyrite is much more reactive than pyrite and while there is much evidence that the mechanism of its oxidation is different from that of pyrite, the exact mechanism is not known. However, since pyrite is the most common and most widely studied metal sulfide, it is useful to review the chemistry of pyrite as a starting point for understanding arsenopyrite and other metal sulfides.

In both pyrite and arsenopyrite, the oxidation states of the elements in the minerals are Fe^{2+} , S^{1-} and As^{1-} . The iron is released in the +2 oxidation state (as ferrous ion), which is the same oxidation state that it has in the solid mineral. Because the -1 oxidation states for S and As are not stable in solution, the mineral reactions always involve oxidation of the S and As to some higher oxidation state in order to be released into solution. Consequently, most of the mechanistic chemistry of these metal sulfides is associated with *oxidation* of the sulfur species, and we refer to the reactions as “*oxidative dissolution*” to emphasize that oxidation *must* occur in order to dissolve at an appreciable rate. Because sulfur can be present in a number of different forms (sulfur, sulfite, sulfate, thiosulfate, and several other forms), measuring the sulfur species is not a good way of determining the overall rate of metal release. Arsenic is also very difficult to measure directly at the low concentrations needed. Consequently, in the first part of

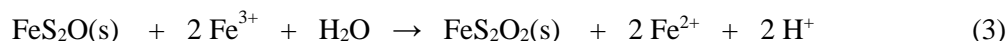
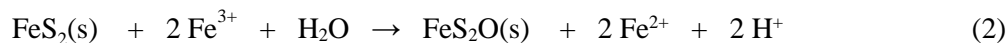
the design project you will be focusing on measuring the *iron* that is released when metal sulfides are exposed to aqueous solutions.

Oxidation of sulfur

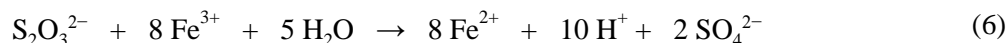
The process of arsenopyrite oxidation can occur via several mechanisms, depending on what one assumes is the oxidizing agent and what oxidation state one assumes the products are in. In the environment, Fe^{3+} and O_2 are the two main oxidizing agents. Ferric ion is the one of greatest interest. Because sulfur and arsenic both have several different stable oxidation states, one can write a number of different reactions depending on whether one is interested in the forms that are released from the mineral, or if one also includes subsequent reactions occurring in the water. For pyrite, the overall reaction is usually written:



Looking at this equation, you should notice that in order to balance the equation you need 23 moles of reactants! Clearly, this reaction does not occur by having 14 ferric ions and 8 water molecules simultaneously converge onto one spot on the FeS_2 crystal lattice. Instead, it is generally believed that oxidation of pyrite occurs by sequential oxidation of the sulfur atoms at the surface to produce the thiosulfate anion, which is then released from the mineral surface into the aqueous phase, where it is later converted to sulfate.

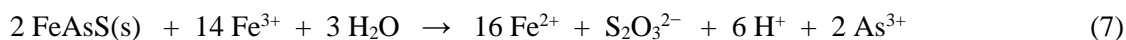


Once released into water, the thiosulfate can be further oxidized to sulfate:



Adding Equations 2 through 6 gives the overall reaction in Equation 1.

In the case of arsenopyrite, you can write a similar balanced equation, although in this case the arsenic only needs to be oxidized to the +3 oxidation state (As^{3+}).

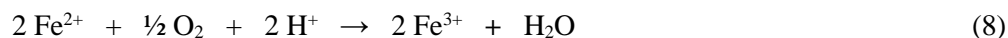


The thiosulfate anion in solution *might* then be oxidized to sulfate, completing the formation of sulfuric acid. *Remember, that while some aspects of the pyrite reaction are understood, much less is known about the overall mechanism of reaction for arsenopyrite.* In particular, it is worthwhile noting that in pyrite the crystal structure has two sulfur atoms already closely bonded together in the S_2 subunit, while in arsenopyrite the structure is more complicated. Thus, in arsenopyrite and most other sulfide-containing minerals it is not clear whether thiosulfate is important, or whether other pathways involving sulfite or other anions are most important.

Understanding the fate of the sulfur-containing species is important because they control the overall reaction rate. Although the overall reaction should eventually produce sulfate (SO_4^{2-}), there are many possible intermediates and reaction pathways. One particularly important intermediate is elemental sulfur. It is possible for the oxidation to stop at S^0 , leaving elemental sulfur (S_8) as a product. Since sulfur is not very soluble in water, it remains on the surface of the mineral. If the sulfur forms a thin even coating on the mineral it could inhibit further reaction. However, there is good evidence that the sulfur on the surface is not even, but rather it covers only parts of the surface with isolated patches, leaving considerable areas free of sulfur and exposed to the oxidative environment.^{12, 13} Quantitative measurement of the amount of elemental sulfur present have yielded some clues as to possible reaction pathways.^{14, 15}

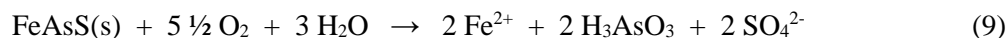
The roles of Fe^{3+} and O_2 as oxidizers

A key step in the reactions of all the sulfide minerals is that they release iron as ferrous ion (Fe^{2+}). Oxygen present in the water can then oxidize Fe^{2+} back to Fe^{3+} :



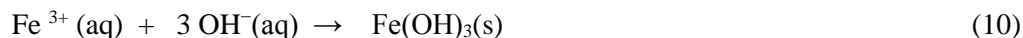
This Fe^{3+} can again react with the mineral surface. Hence, the presence of oxygen greatly accelerates the rates of reactions such as 2 to 4. However, it does so in an indirect way, rather than reacting directly with the mineral surface. Under most conditions the regeneration of Fe^{3+} from Fe^{2+} and O_2 (reaction 8) is believed to be the rate-limiting step in arsenopyrite oxidation and dissolution.

It is also theoretically possible for O_2 to react *directly* with the mineral surface, and one can write a number of different possible reactions, such as:



However, under most conditions this reaction is not as important, due in part to the fact that the solubility of O_2 in water is quite low, especially at low pH.

An additional factor that complicates the chemistry and affects the concentration of Fe^{3+} available in solution is the pH. Using Le Chatlier's principle, you might predict that the overall dissolution reaction (Reaction 7) would proceed more easily at high pH than at low pH because Reaction 7 produces H^+ , which can then react with the available OH^- . In reality, the dissolution does not occur more readily at high pH because OH^- reacts Fe^{3+} in solution to produce $\text{Fe}(\text{OH})_3$ via the precipitation reaction:



The equilibrium constant for this reaction is the inverse of the solubility product ($1/K_{\text{sp}}$) of $\text{Fe}(\text{OH})_3$ and is rather large, on the order of 10^{38} . Hence, at high pH the concentration of Fe^{3+} is very, very low. Conversely, at low pH, the solution can contain more $\text{Fe}^{3+}(\text{aq})$ and reactions 2 through 6 will occur more readily than they do at higher pH. Hence dissolution occurs more rapidly at low pH.

Oxidation and the role of Fe^{2+}

Finally, the last unresolved question has to do with the reduced form of the oxidizer. Because the overall reactions are all energetically favorable, one would normally expect the back-reactions to not be important. However, if any of the steps involve an unusually slow step, then it is possible for the ferrous ion concentration to be significant. The most obvious way for this to happen would be if one of the steps involving an electron transfer step is close to equilibrium. The electron-donating ability of a solution is

usually described in terms of the electrochemical reduction potential. The electrochemical potential for a system containing Fe^{2+} and Fe^{3+} will be given by:

$$E = E_{\text{Fe}^{2+}/\text{Fe}^{3+}}^{\circ} - \frac{RT}{nF} \ln \left[\frac{\text{Fe}^{2+}}{\text{Fe}^{3+}} \right], \quad \text{where } n = 1. \quad (11)$$

If the slowest step in the overall reaction pathway involves a slow, nearly reversible exchange of electrons between the solid and aqueous Fe^{3+} , then we might expect the overall reaction equilibrium to depend on the *ratio* of Fe^{3+} to Fe^{2+} , rather than just the concentration of Fe^{3+} alone.

Unanswered questions

As you can see from the discussion above, the chemistry of arsenopyrite is complex and not all aspects are well understood. A scientist interested in learning how to understand, predict, and control how metal sulfide minerals affect the environment must first learn about the specific chemical interactions. Both a quantitative and qualitative study of the soil and rock samples is necessary to learn about the chemicals present, and about how these chemicals react to cause the problems discussed above. Some of the unanswered questions include:

- 1) What oxidized forms of sulfur and arsenic are present on the surface?
- 2) In what chemical forms are sulfur and arsenic released from the mineral surface?
- 3) Is elemental sulfur an intermediate in the formation of thiosulfate or sulfate, or does it form via some type of parallel reaction pathway?
- 4) Which chemical step or steps control the overall rate?
- 5) How does the reaction rate depend on variables such as pH, oxidizing agents, temperature, *etc.*?
- 6) Is the rate controlled only by the reactant Fe^{3+} , or does the product Fe^{2+} have any effect on the overall rate of reaction?

While answering all of these questions is certainly beyond the scope of what you can do in a Project Lab within a chemistry course, you should think about these questions as you are planning your project. Perhaps your experiments can yield some new information (not yet known!) that will further our understanding of the oxidative dissolution of arsenopyrite.

PROJECT DESCRIPTION

In this design project, you will be looking at the interaction of arsenopyrite with acidic solutions and some of the variables that affect the dissolution process. You will perform the experiments at low pH (typically between 1 to 4) because this will avoid precipitation of $\text{Fe}(\text{OH})_3$ and because low pH mimics the environment produced by the mineral reactions. You are expected to design an experiment to test the importance of one experimental variable in controlling the overall mineral release rate. Variables that might be of interest include the presence or absence of oxygen, presence or absence of Fe^{3+} , pH, and temperature.

The reaction rates appear to be limited by the amount of sample area that is exposed to the solution. If this is true, then you would expect that the reaction rate will be proportional to the surface area of your sample, not just its weight. Consequently, it is important to know the mass of your sample and its surface

area. The reactions we are investigating are fairly slow, and you will not see any change in the mass of your samples. To detect the arsenic/iron release on a short (about a week) time scale, you will be using samples that have been crushed to provide a higher surface area. These samples have also been placed through a sieve so that the individual particles all have roughly the same diameter. From the mass and the average particle size, you can estimate the total surface area of your sample. It is important to remember that the reactions you are looking at are occurring on the surface of the mineral samples; however, it is nearly impossible to detect what is actually on the surface. So, you are measuring what is released into solution and how this changes as a function of various control variables. You will use your results to make conclusions about what is happening on the surface.

Project Design

To begin your project design, you will meet with your group and discuss your ideas. Try to get everyone in the group to participate in the discussions. It is important to build good team skills, not only for this course but also for your future. Good team skills are one of the most important qualities that employers look for and one of the keys to success. Healthy group discussions should have advocates, skeptics, cheerleaders, strategists, dreamers, etc. Sometimes individuals play one of the roles but the best groups have each person playing all the roles (at different times).

Design an experiment to measure the rate at which iron is released into solution. Each group will receive approximately 1.5 g of arsenopyrite to analyze. You should use the lab experiment “Spectrophotometric Determination of Fe”¹⁶ as a model. Instead of using bipyridyl, consider using phenanthroline as a complexing agent.¹⁷ Your experimental design must give consideration towards the following:

- a. From the suggestions below, pick a variable to investigate:
 - See how pH values (ranging from 1 – 4 pH units) affect the dissolution rate. If $\text{Fe}(\text{OH})_3$ precipitation does not occur, does $[\text{H}^+]$ affect the dissolution rate?
 - Since Fe^{3+} is proposed to act as the primary oxidant, you could investigate how adding ferric iron to solution either helps or hampers the dissolution of arsenopyrite. What is the relationship between $[\text{Fe}^{3+}]$ and the oxidation rate? Is it linear? Quadratic? Logarithmic? Exponential?
 - Does the presence of ferrous ion (Fe^{2+}) affect the rate? If so, does the rate depend on the ratio of Fe^{3+} to Fe^{2+} ?
 - Oxygen is also proposed to act as an oxidant. You could investigate the dissolution of pyrite in oxygen rich vs. oxygen deficient environments.
- b. Determine how you can estimate the exposed surface area of your sample from knowledge of the weight and the average particle size. Will this estimate result in a random or systematic error in your results? Will it affect your ability to detect trends when comparing a sample and a control? How will you make sure your samples are sufficiently homogeneous that you can get reproducible data?
- c. Will you analyze the ferric or ferrous form of the cation? How will you oxidize or reduce the iron to obtain the correct form?
- d. What range of iron concentrations will you use for your standard solutions? Your answer will depend on the iron concentration you expect to obtain from your dissolution reactions and on the iron concentrations you can measure with the spectrophotometer.

- e. What pH will you use to perform your experiment? Phenanthroline is a weak acid. The form it takes in solution depends on the pH. You should figure out which form of the complexing agent is needed to complex with the iron in solution.
- f. How will you control the pH of your solutions?
- g. What wavelength will you pick for your analysis?
- h. How will the experimental results allow you to make conclusions about how quickly the minerals will release iron and sulfuric acid into the environment?

Your group should have sound answers to all of the points above and should be able to discuss them intelligently with your instructors. It's a good idea to use library resources to find current journal articles that are related to the topic. Some articles listed in the reference section of this document may be useful. Your group will submit a written design proposal at the end of the first lab period.

Conducting your experiments

Begin collecting data. There are many interesting aspects to this experiment that could be covered if your group has the desire and time to do it. At the very least, you should take aliquots of the dissolving iron over several days time, and observe how the iron concentration changes. Does it increase linearly with time? Can you relate the buildup in iron concentration to a specific reaction rate normalized to the available surface area? The pH is another important variable. Can you predict anything about the expected influence of pH on the reaction rate, based on the overall reaction stoichiometry? Remember that research is a process that sheds light on the truth. Your group may make several attempts at getting the experiment to work before obtaining results that make sense. This may seem frustrating at first, but you will be learning analytical chemistry and the scientific method as you work through this project, and the rewards will be there in the end. Some of what you do will not have a "right" or a "wrong" answer that we are expecting – your goal is to be a scientist in the truest sense. Be patient and persistent!!

Keep in mind that your group needs to plan and organize. Every member needs to participate and be productive. Although everyone should be knowledgeable about all aspects of the project, tasks should be delegated to increase efficiency. Having one person preparing solutions and three people watching is not a good use of your resources!

Progress Report

Part way through the project your group will submit a written report where you summarize your progress. Suitable materials include: brief outlines of experimental procedures, plots of your experimental results, and brief summary of results and future plans. Exactly what you turn in is up to you, but keep in mind that you are trying to demonstrate your group's progress in a concise, scientific fashion.

Final Written Report

After completing your experiments you will write and submit a final report. The format should be similar to a scientific paper. An overview of the format is given in the next section. More information on writing a scientific paper can be found in *The ACS Style Guide*.¹⁸

Oral Presentation

Your group will also discuss your results with the instructors in an oral presentation at the end of the semester. Your group should plan on a *brief* presentation (~5 minutes) where you highlight your

experimental method and anything of particular interest about the data. The presentation is then followed by ~15 minutes of questions. *The questions will, in general, be posed to specific individuals.* You may “handoff” the question to another group member, but remember that all group members should be aware of what was done with all aspects of the project. The primary goals of the questions are to determine your knowledge of the project itself and your analysis of your data.

FINAL WRITTEN REPORT

Title

Decide on a title after you have written the text. The title should be brief and specific but accurate and complete enough to stand on its own.

Byline

The byline contains the names of the individuals who have made substantial contributions to the work.

Abstract

The purpose of the abstract is to provide the readers the nature and scope of the information contained in the report. The readers will use the abstract to decide if the report is important to them. In the abstract you should briefly state the purpose of the project, indicate the theoretical and experimental plan used, accurately summarize the principle findings, and point out major conclusions. The abstract should be concise and self contained and should be written last to be sure that it reflects accurately the content of the report. Your abstract should be about 5 sentences and appear on the same page as the title and byline.

Introduction

A good introduction starts with a clear statement of the project and describes its importance. Give properly referenced, appropriate background material and outline the significance, scope and limits of your work.

Experimental

Give enough detail about your experimental methods and materials that other experienced workers could repeat your work and obtain comparable results.

Results (Observations)

In a scientific paper, the "Result" section focuses on your *observations* (things you directly observe or measure), along with associated graphs, etc. Some scientific publications combine the "results" and "discussion" sections, but your papers will be more objective and more clearly written if you learn how to separate them. Your results section should summarize the data collected and how it was analyzed. Use equations, figures and tables for clarity. You must provide sufficient detail to justify the conclusions you make later. The "results" section usually does *not* relate the observations to molecular-level phenomena, but focuses on what you can see and measure directly.

Discussion (includes molecular-level interpretation)

The "Discussion" section of a paper focuses on the interpretation of your result, especially what your observations (from the results section) imply at a molecular level. While experiments are typically based upon some hypothesis, it is important to discuss the results objectively – your observations may or may not support your original hypothesis, or may simply be inconclusive. The discussion section should also point out the features and any limitations of your work. If you can make specific conclusions, or if your results are supported/refuted by other experimental work, this is the place to bring it up. Suggest further study or applications if appropriate.

Conclusions

A short concise summary of the most important conclusions you can draw from your experiments.

References

Cite sources used in writing your report. Use appropriate reference format.¹⁸

Length of Report

The Introduction, Experimental section, and Results and Discussion should together be about 5 double-spaced pages. The abstract, figures, tables and references do not count toward this 5 page total.

GRADING

The project counts for a total of 90 points toward your final grade. These 90 points are broken down into the following categories:

Experimental design proposal	15 pts
Progress report	15 pts
Final report	35 pts
TA work distribution/efficiency grade	10 pts
Oral presentation	15 pts

Note that grades for the first three categories are assigned to the group as a whole. Grades for the last two categories are assigned individually.

DUE DATES (example, from a Spring 15 week semester course)

Experimental Design Proposal: Tuesday, March 2 (at end of lab)

Progress Report Wednesday, March 17 (at beginning of lecture)

Final Written Report: Wednesday, April 21 (at beginning of lecture)

Oral Presentations: Tuesday, May 4 (sections 631, 633, 635)

Thursday, May 6 (sections 632, 634)

ACKNOWLEDGEMENTS

This Chemistry Design Project was developed by Professor Robert Hamers and Dr. Pamela Doolittle, and is based on research conducted by Professor Molly McGuire (now at Bucknell University) while she was a graduate student in Professor Hamers research group.

REFERENCES

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