# How to Write a Paper

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*This document outlines the fundamentals of writing and the document formatting that are required in every class in Harold Hamm School of Geology and Geological Engineering.*

## Introduction

Writing a geological report, whether for publication or for a class, can be challenging. The major source of difficulty is generally deciding what information to include, and tracking down that information. However, the mechanics of writing – format, style, grammar, etc. – are also important. Any paper, no matter the content, is a bad paper if the mechanics are bad. All papers should be perfectly formatted, should contain no style or grammar errors, should look good, and should represent the best that the author can do. Fundamental mechanical errors are 100% unacceptable.

Different scientific journals, graduate schools, businesses, etc., may require that papers be formatted in different ways. The guidelines adopted below, however (based on guidelines from the Geological Society of America, GSA), are the ones you should follow when you write papers for UND geology classes. GSA guidelines are widely used in the geological literature. For more details, see the GSA instructions at
http://www.geosociety.org/pubs/bulletin/bulGuide.htm

So, below are some specifications and suggestions to guide your writing. Additionally:
- Beginning on page 11, are some examples of the kind of common mistakes that turn up in student writing – the examples are real (taken from student work)
- Starting on page 14 are a few pages from an article that Perkins and Anthony (2011) wrote a few years ago – it was accepted for publication just as it was written. Following that is part of the reference list from Perkins and Anthony – to give you an idea of what a reference list should look like.

## Basic Format

- Use 11 point Arial font
- Single line spacing
- 1" margins on all sides
- Separate paragraphs with an extra (blank) line.
- Do NOT indent the first word of a paragraph.
- All paragraphs should contain more than one sentence.
- Paragraph/section headings should be preceded by two blank lines.
- Page numbers should be in the upper right hand corner of all pages.

- Title, author, and affiliation should be at the top of the first page of the paper.

## Headings and Organization

Section and paragraph headings serve several very important purposes. First, they help the reader *navigate* a paper to find the information they want. Second, they help the reader *get ready* for what is to follow. Third, they help the author *organize thoughts* and information in a logical way.

Sometimes it is appropriate to have several different levels of headings: major headings, secondary headings, tertiary headings, etc. So, main sections of the paper have titles and each main section has parts with subtitles, etc. In general, the more different kinds of headings, the more complicated it is for the reader to follow – so, unless there is some compelling reason, keep the number of different kinds of headings to one or two.

When writing a paper – before the final draft -- it is often useful to include headings/titles for just about every paragraph. Then, you can remove all the paragraph text – just keep the headings themselves – to see if the headings are organized in a logical way. This will allow you to see quickly if the organization is good, if there are redundancies, or if some things are missing. At the end, when you get to the final version of the paper, you can go back and remove headings that are no longer needed.

Different publications have different guidelines for headings. For a standard geology class paper, do the headings as I have done them in this document:
- Put major headings in bold type with each word capitalized
- Put secondary headings in italics, unbolded.
- Do not use tertiary headings.

### *Standard Sections of a Paper*

Traditionally, scientific papers have included standard sections in a standard order (Table 1). These sections can be used as the main headings for a paper, with subheadings under some or all of them. It is not, however, necessary to include all of these sections. For example, acknowledgments and appendices may be inappropriate in many cases. Furthermore, if a paper is properly written and well explained, a discussion section near the end may be redundant, and a “conclusions” section will not be needed. In fact, some scientific journals do not allow a discussion or conclusions section!

| **Information** | **Section of Paper** |
|---|---|
| The entire paper in a nutshell | Abstract |
| What is the problem? | Introduction |
| How did I solve the problem? | Materials and Methods |
| What did I find out? | Results |

| | |
|---|---|
| What does it mean? | Discussion |
| What is/are the key outcome/s? | Conclusion |
| Who helped me out? | Acknowledgments |
| Whose work did I use for information? | References Cited |
| Extra information | Appendices |

Table 1. The Standard Sections of a Scientific Paper

## What Goes into an Abstract?

Although not necessary for class term papers, scientific abstracts are required for all manuscripts submitted to journals for publication. An abstract is NOT a summary or an introduction. It is a very short snapshot of the paper that includes all key components – its major purpose is so that other people can decide if your paper is worth reading. Abstracts should not say things like *“We investigated erionite in the Killdeer Mountain”* – because this gives no meaningful information – it is implicit that you did an investigation or you would not be writing a paper. Things to include in an abstract:

- Purpose of research – very brief description (1 sentence at most)
- Methodology – very brief description (few words to one sentence)
- Major findings/outcomes (several sentences; up to a paragraph)
- Major interpretations/implications (several sentences; up to a paragraph)

*Key Considerations*

- Abstracts should be short, generally less than 300 words and often less than 200 words.
- Use past tense or passive voice if appropriate.
- Do not include references to other papers, abbreviations readers may not understand, or any kind of table or illustration.
- Always write the abstract last!

A sample abstract is on page 11 of this document.

## The Introduction

The purpose of the introduction is to establish the context for what follows. Often, the introduction will contain a reference to some key primary literature. For example, the introduction above contains a URL for the Geological Society of America’s Guidelines to Authors.

The introduction should state the purpose of the work in the form of a hypotheses, question, or problem. The introduction often outlines a gap in scientific knowledge that you are filling. It may also explain the rationale for the approach used and the potential value of your completed investigation. Introductions may be quite brief or quite long, depending on how much background information is presented.

Like the abstract, the introduction should be written after the rest of the paper is completed. This way you will know what information needs to be in the introduction and what does not.

### Notes to the Reader and References to the Author

Introductions – and other parts of your paper – should NOT contain chatty comments, personal notes or fatuous commentary. If a paper is properly organized, with good headings, there is no reason to tell the reader what you are about to say, or will say later on. Do not, for instance, ever have a sentence that begins *"In this paper, I will explain . . ."* Do not say things like *"You may wonder what this means?"* Do not say *"I investigated Finnish beer and found it to be skunky."* Just say what you have to say without the conversational distractions. Explain the purpose without referring to yourself or to the reader.

### Grammar, Syntax, Spelling, etc.

Today, we have spell checkers. We also have grammar checkers. We also have the UND Writing Center and instructors who are willing to help you with your writing. Consequently, your papers should include zero grammar, syntax, or spelling errors. Yes, an occasional homonym will slip in, and there may be other oddball mistakes – but the rule is that zero mechanical errors are allowed.

One key tool – you should always use it – is *Grammatik*. Grammatik is a fantastic grammar and style checker. Unfortunately, it is only available with WordPerfect. The good news is that WordPerfect can open and read Word files (and also some other formats). So, we have installed WordPerfect on the computers in the lounge in the Leonard Hall basement. You should get in the habit of using Grammatik for everything you write. Be sure to set Grammatik to be "super strict" before you use it. It may flag some things that you don't want to change – you can ignore those – but it won't miss anything.

### Abbreviations and Symbols

Only use abbreviations if they are standard – unless you define them the first time you use them. Most major publications have a list of allowable abbreviation in their instructions for authors. Also, don't be lazy. Your computer and word processor can put symbols in your paper. Don't cheat and say "degree" because you don't know where the symbol is – find the symbol. Similarly, subscripts and superscripts must be subscripts and superscripts.

### Figures and Tables

If you write a paper that you plan to submit to a journal, you will put all figures (including photos) and tables at the end, and you will have separate pages with a list of the figure captions. However, for term papers and class reports, it is best if possible, to embed the figures in the manuscript where they are referenced. The reference to a figure or table has to precede the figure/table itself. Also, every figure and table has to be referenced in the text. It is also usually best to center them on the page without text wrapping around. If this leads to too many formatting or spacing problems, you can put figures/tables at the end of your paper – but try to put them in the text if you can.

All figures <u>must</u> have captions and they must be numbered. The first figure is Figure 1 and they are numbered sequentially. Similarly, all tables must have titles, and the first table is Table 1, etc.

Any figures in your papers must be sharp and NOT pixelated. If they are fuzzy, do not use them (Figure 1). If you swipe them from the internet or some other source, you MUST tell where they came from in the figure caption. Furthermore, if the original image was in color, and your paper is going to be read in black and white, you must make sure the contrast is OK (Figure 1).

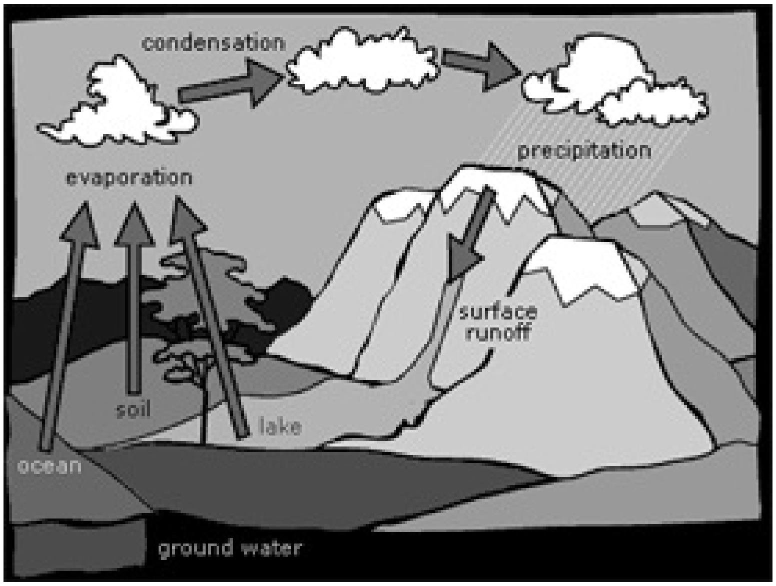

**Figure 1**. The water cycle. This figure was originally in color but the contrast is OK in black and white. However, the figure is too fuzzy/pixilated and so should be redrafted if you are going to use it. This drawing from http://www.cotf.edu/ete/modules/msese/earthsysflr/water.html

If you write a paper for publication, and if you use somebody else's figure, you must get permission. Alternatively, although it seems a bit arbitrary, if you redraft and change slightly what somebody else created, you can pretend it is yours and not have any copyright issues. However, in the figure caption you must say something like *"This figure modified from Figure X in . . . "* and give the original source.

### References in the Text

Any facts, ideas, or quotations in your text must have a reference telling where you found the information. The exception is for something that is clearly common knowledge. For some examples of the proper way to give references, see the manuscript beginning on page 11 of this document.

To identify the source of the quote/information: If there is a single author, use the author's last name. If there are two authors, list both last names. If there are more than two, use "et al."

If you are directly quoting from an author, you need to include the author, year of publication, and the page number. For example:

> *According to Jones (1998), "Students often had difficulty using APA style, especially when it was their first time" (p. 199).*
>
> *They stated, "Students often had difficulty using APA style" (Jones and Brown, 1998, p. 23), but she did not offer an explanation as to why.*

If you summarize something that somebody said, you can do it like this (with or without the page number depending on how unique or unusual the information is):

> *According to Smith and Gosnold (1998), GSA style is a difficult citation format for first-time learners.*
>
> *APA style is a difficult citation format for first-time learners (Smith and Gosnold, 1998, p. 199).*

In a similar way, you reference the source of facts or ideas. If the information comes from more than one source, list the multiple sources (second example below):

> *Research by Perkins and Putkonen (2009) supports the idea that frog populations are declining.*
>
> *The world is getting warmer at the fastest rate in modern time (Perkins et al., 1912; Harlow and Jones, 2011).*
>
> *According to the American Geophysical Union (2014), the world is warming at a rate faster than any time since the Pleistocene.*

Typically you put the reference at the end of the sentence that contains the quote or fact. Sometimes, however, you will have a bunch of facts in a single paragraph. If they all come from the same source, you can simply put the reference at the end of the paragraph – it is implicit that all the information came from the same place.

If you have an indirect source of information, don't cheat and pretend you read the original paper. Do it like this:

> *Hartman argued that clams are too important to eat (as cited in Smith, 2003, p. 102).*

Generally you will only use an indirect reference for impossible to obtain original publications or, perhaps, for things originally published in a foreign language.

## Footnotes and Endnotes

Don't use them in scientific writing.

## Sources of Information

For scientific research and writing, you must get (most of) your information from books, journals, and other print literature, or from copies of print literature that you download form the internet. To get started, you can use GeoRef or Scopus – they are both good search engines that are available on line. Ask your instructor, another student, or Darin Buri (the Geology librarian) how to use them. Or, you can start with references that you find in a textbook.

Once you find a single key article, you can look in the reference list at the end of that article – pick out some other articles that look good and track them down. Look at them and pick out some others. In this way, you will soon find a bunch of sources to use. Unfortunately, they will all be older than the first one you find. So, when you do your initial search, you want to find the most recent publication you can, even if it is not exactly on the topic you are investigating.

Note: We have a good geology library but we don't have every publication. Often, some key articles need to be ordered through Interlibrary Loan. The process is easy but may take days or longer. So, it is important to get started early.

### *What about Google and the Internet?*

The internet is the number one source of information today. It is also very unreliable. For science research and writing, you <u>cannot</u> use sources such as Wikipedia. You also cannot use somebody's lecture notes or class web page. The reason is that such sources have not been peer reviewed and may contain incorrect information. Basically, you cannot use information from the internet at all – with a few key exceptions. (Of course, it is often convenient to use Wikipedia or some similar source to get some ideas about what is important – but, you must find other legitimate sources if you wish to include facts, etc., in your paper.)

If you find a copy of an article on the internet, and the article has been peer reviewed and published in a journal (print or electronic), then you may use it as a source of information. Cite it, and in the reference list at the end of the paper, list the *original* print/electronic source. You must know the title, author, journal, volume, page number, and year of publication.

You may also use the internet as a source of raw data from some reputable government or other agency source, but only if it is 100% assured that the source is reliable. For example, see the two example references on page 10 of this document: Margins (1999) and Johnson (2001).

## References Listed in the References Cited Section

In the References Cited section, all references should be in alphabetical order by author. If you have more than one article by the same author(s) list them chronologically. Below are examples of common reference types, formatted properly. For a paper, you will not separate them by type of source (as has been done below), and you will not, of course, include the section headers (Abstract, Book, Journal, etc.) below. See page 16 of this document for an example of a partial reference list form a paper that was accepted for publication.

All references must be referred to somewhere in your text, and every citation in your text must have a matching reference in the References Cited section. Note: In the References Cited section you list all authors – do not use “et al.”

### *Format for Listing an Abstract*

Fitzgerald, P.G., 1989, Uplift and formation of Transantarctic Mountains: Applications of apatite fission track analysis to tectonic problems: International Geological Congress, 28th, Washington, D.C., Abstracts, v. 1, p. 491.

LeMasurier, W.E., and Landis, C.A., 1991, Plume related uplift measured by fault displacement of the West Antarctic erosion surface, Marie Byrd Land [abs.]: Eos (Transactions, American Geophysical Union), v. 72, p. 501.

McKinnon, W.B., and Schenk, P.M., 2000, Chaos on Io: A model for formation of mountain blocks by crustal heating, melting, and tilting: Houston, Texas, Lunar and Planetary Institute, Lunar and Planetary Science XXXI, CD-ROM, abstract 2079.

Sammis, C.G., 1993, Relating fault stability to fault zone structure: Geological Society of America Abstracts with Programs, v. 25, no. 6, p. A115–A116.

### *Format for Listing a Book*

Burchfiel, B.C., Chen Zhiliang, Hodges, K.V., Liu Yuping, Royden, L.H., Deng Changrong, and Xu Jiene, 1992, The South Tibetan detachment system, Himalayan orogen: Extension contemporaneous with and parallel to shortening in a collisional mountain belt: Boulder, Colorado, Geological Society of America Special Paper 269, 41 p.

Coffin, M.F., Frey, F.A., Wallace, P.J., et al., 2000, Proceedings of the Ocean Drilling Program, Initial reports, Volume 183: College Station, Texas, Ocean Drilling Program, CD-ROM.

France-Lanord, C., Derry, L., and Michard, A., 1993, Evolution of the Himalaya since Miocene time: Isotopic and sedimentologic evidence from the Bengal Fan, *in* Treloar, P.J., and Searle, M., eds., Himalayan tectonics: London, Geological Society [London] Special Publication 74, p. 603–621.

Shipboard Scientific Party, 1987, Site 612, *in* Poag, C.W., Watts, A.B., et al., Initial reports of the Deep Sea Drilling Project, Volume 95: Washington, D.C., U.S. Government Printing Office, p. 31–153.

Vogt, P., and Tucholke, B., editors, 1986, The western North Atlantic region: Boulder, Colorado, Geological Society of America, Geology of North America, v. M, 696 p.

*Format for Listing a Journal Article*

Arias, O., and Denyer, P., 1991, Estructura geológica de la región comprendida en las hojas topográficas Abras, Caraigres, Candelaria y Río Grande, Costa Rica: Revista Geológica de América Central, no. 12, p. 61–74.

Bernardin, T., Cowgill, E., Gold, R.D., Hamann, B., Kreylos, O., and Schmitt, A., 2006, Interactive mapping on 3-D terrain models: Geochemistry Geophysics Geosystems, v. 7, no. 10, Q10013, doi: 10.1029/2006GC001335.

Brown, M., 1993 *P-T-t* evolution of orogenic belts and the causes of regional metamorphism: Journal of the Geological Society [London], v. 150, p. 227–241.

Doglioni, C., 1994, Foredeeps versus subduction zones: Geology, v. 22, p. 271–274.

Drygant, D.M., 1986, Novye konodonty roda Polygnathus Hinde, 1879 iz srednego I verkhnego devona L’vovskogo progiba (New conodonts of the genus Polygnathus Hinde, 1879, from the Middle and Upper Devonian of the L’vov Depression): Paleontologiche-skiy sbornik (L’vovskiy gosudarstvennyy universiteit), no. 23, p. 47–52.

Walter, L.M., Bischof, S.A., Patterson, W.P., and Lyons, T.L., 1993, Dissolution and recrystallization in modern shelf carbonates: Evidence from pore water and solid phase chemistry: Royal Society of London Philosophical Transactions, ser. A, v. 344, p. 27–36.

*Format for an article from an online version of a print article*

Fricke, David. "Forty Years of Beatlemania: A look back at the Beatles' debut on 'The Ed Sullivan Show.'" Geology of Popular Music, v. 34, p. 345-349. Downloaded from Rolling Stone, 19 Sept. 2009. Web. 8 Oct. 2009.

*Format for a Paper in a Government or University Serial Publication*

Hay, R.L., 1963, Stratigraphy and zeolitic diagenesis of the John Day Formation of Oregon: University of California Publications in Geological Sciences, v. 42, p. 199–262.

Smith, D.C., Fox, C., Craig, B., and Bridges, A.E., 1989, A contribution to the earthquake history of Maine, *in* Anderson, W.A., and Borns, H.W., Jr., eds., Neotectonics of Maine: Maine Geological Survey Bulletin 40, p. 139–148.

Yager, R.M., 1993, Estimation of hydraulic conductivity of a riverbed and aquifer system on the Susquehanna River in Broome County, New York: U.S. Geological Survey Water-Supply Paper 2387, 49 p.

*Format for a Paper in a Multiauthor Volume*

Carpenter, F.M., 1992, Superclass Hexapoda, *in* Kaesler, R.L., ed., Treatise on invertebrate paleontology, Part R, Arthropoda 4, Volume 3: Boulder, Colorado, Geological Society of America (and University of Kansas Press), 277 p.

Kane, J.S., and Neuzil, S.G., 1993, Geochemical and analytical implications of extensive sulfur retention in ash from Indonesian peats, *in* Cobb, J.C., and Cecil, C.B., eds., Modern and ancient coal-forming environments: Boulder, Colorado, Geological Society of America Special Paper 286, p. 97–106.

Keller, G., 1992, Paleoecologic response of Tethyan benthic foraminifera to the Cretaceous-Tertiary transition, *in* Takayanagi, Y., and Saito, T., eds., Studies in benthic foraminifera: Tokyo, Tokai University Press, p. 77–91.

Sawyer, D.S., Buffler, R.T., and Pilger, R.H., 1991, The crust under the Gulf of Mexico basin, *in* Salvador, A., ed., The Gulf of Mexico Basin: Boulder, Colorado, Geological Society of America, Geology of North America, v. J, p. 53–72.

Taylor, J.C.M., 1990, Upper Permian—Zechstein, *in* Glennie, K.W., ed., Introduction to the petroleum geology of the North Sea (third edition): Oxford, UK, Blackwell, p. 153–190.

*Format for Reference to a Web Site*

Note: Month and year in parentheses at end denote date author accessed site.

MARGINS, 1999, The Seismogenic Zone Experiment (SEIZE): Science plan: http://www.soest.hawaii.edu/margins/SEIZE_sci_plan.html (July 2001).

Johnson, A.B., 2001, Raw data for relay stations AB1–AB15 in the Mojave desert: http://www.seismo.berkeley.edu/mojave (December 2001).

## Appendix 1: Some common problems with student papers

(Some of the things listed below deal with content, organization or style. Others deal with grammar and syntax.)

big stuff
Organization lacking – ideas seem to dangle or do not fit together
Superficial ideas
Nothing new
Basic grammar problems
Poor wording or syntax
Spell check
All sentences must have verbs and nouns
Overly large font or spacing
Poor looking figures or photos

technical
Facts in the text must have citations.
Must give source for all figures, photos, tables of information if you get them from somebody/somewhere else
Punctuation goes inside quote marks.
    "This is it." not "This is it".

passive voice
Avoid passive voice. Do not start sentences with "There is . . . " or "There are . . . "
    Start with the subject instead.
Any sentence that begins with "It is" or "It was" can be rewritten to improve.

extra words
Watch out for extra words.
"Martinique is located in the Caribbean . . ." => "Martinique is in the Caribbean . . ."
". . . whether or not . . ." => "whether"
"oftentimes" => often
"goes clear back to" => "goes back to"
". . . in order to . . ." => "to"
"I obviously agree with . . . " => "I agree with . . ."
"I agree with a great deal of what he says." => "I agree with much of what he says."

wrong words
Alright is incorrect.
"All ready" is not the same as "already"
Spell check may introduce problems such as:
    from/from
    for/fro
    eat/ate
    causal/casual
don't use words that are not words:
    legit

stats
LOL

antecedents

It is usually best not to begin a sentence with “it” – because it may be unclear what you are talking about.
Watch out when using “this” or “these” – antecedent must be clear.
“Many people were killed by the eruption of Mt. ST. Helens, Mt. Pelee, and Tambora. This could have been avoided.” [What does “this” refer to?]

use of “or”

It is best not to use “or” unless there is a choice. Not “Chimichangas, or chimis, are Mexican food . . .”
“Sedimentary rocks, or clastic rocks . . .” => “Sedimentary rocks, also called clastic rocks . . .”

vague sentences, terms and modifiers

Avoid vague modifiers and phrases such as “pretty interesting.”
“Mt. St. Helens might be the greatest disaster . . .” – too vague, don’t be wishy-washy.
Avoid “may,” “might,” “could,” “would,” “seem,” “possibly,” “probably,” etc., unless there is good reason to use them.
“The eruptions was incredible.” – what does this mean?
“Researching will help give you background.” –what does this sentence mean?

choppy sentences such as:

“Small sentences are boring to read. Many of them strung together look bad. They appear simple. Your thoughts look simple, too. It's like you can't sustain an idea for more than a few words. You can think in only trivial, simplistic ways. Small thoughts seem to come from small minds. You will leave your reader with the impression of simplemindedness. Is that what you want? “

run-on sentences

“The disaster was the greatest in the 21st century because it killed so many people due not only to the eruption but also to the tidal wave that followed”

cliches

Avoid rotten/cheap cliches. e.g.,
“at this time in history”
“in the poor house”
“wiped out”
“will be hurting”
“last but not least”
“left their mark”
“mind blowing”
“over the top”
“out there”
“springboard”
“aka”

sarcasm

Don't use it.

introduction

Do not include an introduction that tells what you are going to do. Introductions should be about the topic, not about your paper.
Do not say, "In this next part I will discuss . . . ."
Avoid personal asides . . .
Do not say "I believe . . ." or refer to the reader as "you."

numbers

It is usually best to put commas in numbers, e.g., 30,000.
However you do it, be consistent.

personal comments

"You have to ask yourself if . . ."
You don't need to use "I" in an opinion paper.
Avoid "I believe . . ." or "I will discuss . . . " etc. Just say what you have to say.
And, it is generally inappropriate to address the reader as "you."
Don't say "You will have to use less gasoline . . ." – use "people" or some other impersonal noun as a subject.
Don't say "Bear in mind . . ." or "Take for example . . ." – too personal.

quotes

When you quote someone, or even give a paraphrase of their ideas, you must cite the source of your material.

agreement

Subject of a sentence must agree with the verb – if one is plural the other must be, etc.
wrong: "If a person eats an apple, they will get sick."
If you start a sentence with "you" don't switch to "one."
bad: "If you eat bananas, one will fart."
For that matter, avoid "one" as a subject.

Who/Whom/That/Which

Who and whom refer to people
That and which refer to things
"That" is usually better to use than "which."
"The volcano which erupted in 1902 . . ." => "The volcano that erupted in 1902 . . ."

overstatement

"Missing the meeting was a tragedy" – is probably overstated.
"His eloquence could split rocks" - yuck
"Volcanoes always kill people."
"It was the greatest disaster . . ." – probably not.
"The author bombarded the reader . . ." – not.

## Appendix 2: Writing Example (the first few pages, and part of the reference list, of an article by Perkins and Anthony, 2011)

# The Evolution of Olivine-orthopyroxene-clinopyroxene-spinel Lherzolites and Application to Xenoliths from Kilbourne Hole, New Mexico

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## Abstract

In peridotites, olivine, clinopyroxene, and orthopyroxene are complex solid solutions with wide stability fields. Depending mostly on bulk composition and pressure, these minerals may be accompanied by plagioclase (low pressure), spinel (moderate pressure), or garnet (high pressure), resulting in 4-phase (most commonly) and 5-phase (rarely) assemblages. Although a particular mineral assemblage is stable over a range of P-T, the compositions of the individual minerals vary with changing P-T conditions.

Application of standard geothermobarometers to olivine-clinopyroxene-orthopyroxene-spinel peridotites is problematic. An alternative approach is to use a bulk rock composition to calculate equilibrium phase diagrams to determine the conditions under which a particular 4-phase assemblage is stable. This requires consideration of the 7-component system $SiO_2$-$Al_2O_3$-$Cr_2O_3$-FeO-MgO-CaO-$Na_2O$, internally consistent thermodynamic data for end members, and reliable mixing models for all mineral solutions. Experimental studies in simpler systems, and solution models from the literature, permit derivation of multicomponent thermodynamic mixing models for the four minerals. The models, when applied to xenoliths from Kilbourne Hole, constrain P and T of equilibration and are less sensitive to mineral compositional variations, or uncertainty in activity models, than standard thermobarometry.

Our modeling provides the first tightly constrained pressure estimates for Kilbourne Hole, placing the xenoliths in the spinel stability field at depths (30-45 km) that correspond to the uppermost mantle beneath the Rio Grande rift. The fine-grained equigranular lherzolite, porphyroclastic lherzolite, and some harzburgite-dunite specimens equilibrated at average conditions of 11.5 Kbar-930 °C, 12 Kbar-990 °C, and 13 Kbar-1080 °C, respectively. The mantle beneath the Rio Grande Rift is layered; the fine-grained equigranular lherzolite derives from relatively shallow depth (35 km average), and the porphyroclastic lherzolite from slightly deeper levels. Lying 5-10 km beneath both lherzolites, the harzburgite-dunite represents a depth where melt extraction has significantly altered mantle chemistry, and where local thermodynamic equilibrium has not been maintained. Sub-Moho seismic velocities require the temperatures of 930 to 1100 °C to be a regional phenomenon rather than restricted simply to the vertical column sampled by Kilbourne Hole. These temperatures are probably greater than a steady state conductive geotherm.

## Introduction

Mantle xenoliths provide the only way for us to look directly at the rocks that comprise Earth's mantle, so they provide information that otherwise would be unavailable. Although the xenoliths vary somewhat in composition, most are olivine rich peridotites (lherzolites) containing orthopyroxene and clinopyroxene, or (clino)pyroxenites (Carter, 1970; Wilshire and Shervais, 1975; Frey and Prinz, 1978; Irving, 1980; Bussod and Irving, 1981; Bussod and Williams, 1991; Smith, 1999; Kil and Wendlandt, 2004). Partial melting of primary mantle lherzolite selectively removes clinopyroxene, so lherzolite xenoliths generally contain more orthopyroxene than clinopyroxene, and some evolve to become clinopyroxene-poor harzburgites, dunitic-harzburgite, or dunites. In these ultramafic rocks, olivine (ol), clinopyroxene (cpx), and orthopyroxene (opx) are complex solid solutions with wide stability fields. Depending mostly on bulk composition and pressure, the three minerals may be accompanied by small amounts of plagioclase (plag), spinel (sp), or garnet (gt).

In this paper, we present multi-component mixing models for olivine, clinopyroxene, plagioclase, spinel and garnet which can be used to calculate equilibrium phase diagrams. We then use the models to calculate the conditions of formation for xenoliths from Kilbourne Hole, New Mexico. The Kilbourne Hole samples are excellent for testing our models because they include a variety of compositions, minerals in most samples are homogeneous and have equilibrium textures, and complications due to high chrome content are absent. The results of our calculations provide new, previously unavailable, information about the uppermost mantle beneath the Rio Grande rift in southern New Mexico.

## The Stability of Plagioclase-, Spinel-, and Garnet-Peridotites

The assemblages ol-cpx-opx±plag±sp±gt are stable under upper mantle pressure-temperature conditions. However, plagioclase peridotite reacts to produce spinel peridotite, and then garnet peridotite with increasing pressure by the reactions (Fig. 1):

plag + ol = opx + cpx + sp (reaction 1)
opx + cpx + sp = gt + ol (reaction 2)

Experimentalists have investigated reactions 1 and 2 in the model CaO-MgO-$Al_2O_3$-$SiO_2$ system. Figure 1 shows experiments summarized by Gasparik (1984). The relationships depicted are also consistent with earlier studies, including those by Kushiro and Yoder (1966), Yoder (1967), and Jenkins and Newton (1979). The thermodynamics that control these relationships are heavily influenced by the aluminum contents of the phases involved. Reaction of plagioclase to spinel to garnet with increasing pressure reflects the different densities of the minerals, in part due to different Al-coordination. The curvature of the reaction curves is caused by variable amounts of Al in orthopyroxene and clinopyroxene at different pressure-temperature conditions. Experimental results, such as those shown in Figure 1, reveal the general relationships between different kinds of peridotites. They are not, however, generally useful for constraining the pressure-temperature conditions at which spinel (or other kinds of) peridotites formed because the spinel field is very large, and because the model experimental systems do not include other chemical components that may be of significance. Consideration of other components will move reactions lines up or down, expanding or shrinking the stability fields for the different kinds of lherzolites depending on bulk-rock composition.

Although a particular lherzolite assemblage has a wide stability range, the compositions of the individual minerals vary with changing conditions. In principle, for a given assemblage, the composition of a single mineral, or compositions of several coexisting minerals, permit calculation of the pressure-temperature conditions at which the assemblage equilibrated. In practice, however, analytical uncertainties and sensitivity to small changes in composition, coupled with imprecise activity models for complex solutions, make this kind of thermobarometry problematic (Smith, 1999; Nimis and Grütter, 2010). Although equilibrium temperatures may be roughly estimated using any of a number of exchange reactions (e.g., Fe-Mg exchange between clinopyroxene and orthopyroxene), determining pressure of equilibration is especially problematic.

An alternative to conventional thermobarometry is to use a bulk rock composition to calculate equilibrium phase diagrams, also sometimes called pseudosections, to determine the conditions at which a particular assemblage is stable (Powell and Holland, 1988; Berman, 1991; Berman, 2007; de Capitani and Petrakakis, 2010). Such calculations also predict mineral modes and mineral compositions at different pressures and temperatures. This approach, a forward modeling approach that is more robust than trying to calculate pressures and temperatures from mineral analyses, constrains the pressures and temperatures of equilibration. Uncertainties in thermodynamic properties (activity models and properties of end members), translate into uncertainties in calculated equilibrium compositions of coexisting minerals. However, the stability field for a particular assemblage is much less sensitive to thermodynamic uncertainties than the conventional mineral thermometry and barometry. Unless activity models or thermodynamic values are changed greatly, calculated phase assemblage boundaries remain at about the same pressures and temperatures.

## Thermodynamic Data Base for Olivine, Orthopyroxene, Clinopyroxene, Plagioclase, Spinel, and Garnet

Calculating equilibrium phase diagrams for ultramafic rocks requires internally consistent thermodynamic data for end members and reliable mixing models for all mineral solutions. Major components in peridotites include $SiO_2$, $Al_2O_3$, FeO, MgO, and CaO. $Na_2O$ and $Cr_2O_3$, although generally present in small amounts (<1 wt%) may play a significant role because a change in the amount of either can potentially change the pressure at which the plagioclase-peridotite to spinel-peridotite, and the spinel-peridotite to garnet-peridotite, transitions occur. Other minor components include $TiO_2$ and MnO; in general neither significantly affect mineral equilibria in peridotites. So, we have considered seven components. All thermodynamic calculations reported here used the Theriak-Domino routines of de Capitani and Petrakakis (2010).

Many previous investigators have derived internally consistent thermodynamic data bases that include peridotite minerals (e.g., Berman et al., 1985; Berman, 1988; Davidson and Lindsley, 1989; Aranovich and Berman, 1996; Berman and Aranovich, 1996; Chatterjee et al., 1998; Holland and Powell, 1998). Some data bases are larger and more robust than others, but none include the multi-component pyroxene mixing models needed to calculate peridotite equilibria for natural compositions. So, as an initial step we sought to derive the thermodynamic properties of key pyroxene end members, and to develop mixing models for orthopyroxene and clinopyroxene solutions.

We conducted regressions in much the same way as has been done by others, deriving thermodynamic values for mineral end members and solutions from phase-equilibria and calorimetric studies using an approach similar to the one described by Perkins and Vielzeuf (1992). As input, we used data from many experimental studies (including most listed in Tables 2 and 3 of Berman and Aranovich, 1996). The initial regression results reproduced most experimental studies within stated uncertainties. However the derived thermodynamic values were highly correlated, had large standard deviations, and were only marginally consistent with thermodynamic values in other data bases.

Using the results of the initial regression as a starting point, we selectively assumed some values from previous studies and repeated the regressions. We tried many combinations, and found many that fit the constraining data well. We had good results using the JUN92.BS data for most end members and, to maintain consistency, adopted the values in that data base for as many end members as possible. JUN92.BS, based primarily on the data of Berman et al. (1985), is one of the two data bases distributed with the Theriak-Domino software (de Capitani and Petrakakis, 2010). We added additional pyroxene end members and derived appropriate thermodynamic values for them. We found it necessary to adjust expansivity and compressibility values for diopside and clinoenstatite in JUN92.BS or orthopyroxene became unstable at high pressure. Additionally, we changed the heat capacity of clinoenstatite to be that of high-clinoenstatite instead of low-clinoenstatite.

Thermodynamic values for most pyroxene end members, and some pyroxene mixing parameters, came from previous studies; other values were derived as part of this study (Table 1). It is important to point out that the choice of end members is arbitrary, providing a way to express compositions. There is no significance of choosing one set of end members over another except that, depending on mineral composition, some end-member mole fractions may be very small or even negative (which does not invalidate calculations) depending on choices made. Several considerations guided end member choice: (1) to reduce uncertainties due to mixing parameter uncertainty, we chose end members that are most dominant in peridotite minerals; (2) to simplify derivations of thermodynamic values from experiments, we used end members that matched those investigated in (model) experimental systems; (3) as much as possible, we chose end members for which there exists reliable thermodynamic data.

Table 1. Minerals, abbreviations, compositions, and sources of thermodynamic data

| abbreviations and formulas of minerals | | formula | source of thermodynamic data* |
|---|---|---|---|
| Clinopyroxene | Cpx | $(Ca,Mg,Fe,Na)(Mg,Fe,Al)(Si,Al)O_6$ | W values from Davidson and Lindsley (1989), Meyre et al. (1997), Benisek et al. (2007), Girnis and Brey (1999), Massone (1992) |
| diopside | Di | $CaMgSi_2O_6$ | JUN92.BS with revised $\alpha$ and $\beta$ |
| hedenbergite | Hd | $CaFeSi_2O_6$ | JUN92.BS |
| clinoenstatite | CEn | $Mg_2Si_2O_6$ | this study |
| clinoferrosilite | CFs | $Fe_2Si_2O_6$ | this study |
| Ca-Tschermaks cpx | CaTs | $CaAl_2SiO_6$ | JUN92.BS |
| jadeite | Jd | $NaAlSi_2O_6$ | JUN92.BS |
| Cr-Tschermaks cpx | CrCaTs | $CaCrAlSiO_6$ | this study; based on Onuma and Tohara (1984) and Girnis and Brey (1999) |
| Orthopyroxene | Opx | $(Ca,Mg,Fe)(Mg,Fe,Al)(Si,Al)O_6$ | W values from Davidson and Lindsley (1989) |
| enstatite | En | $Mg_2Si_2O_6$ | JUN92.BS with revised $\alpha$ and $\beta$ |
| ferrosilite | Fs | $Fe_2Si_2O_6$ | JUN92.BS |
| Mg-Tschermaks opx | MgTs | $MgAl_2SiO_6$ | this study |
| Fe-Tschermaks opx | FeTs | $FeAl_2SiO_6$ | this study |
| (ortho) diopside | ODi | $CaMgSi_2O_6$ | this study |
| (ortho) hedenbergite | OHd | $CaFeSi_2O_6$ | this study |

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|---|---|---|---|
| Garnet | Gar | $(Mg,Fe,Ca)_3Al_2Si_3\,O_{12}$ | W values from JUN92.BS |
| pyrope | Py | $Mg_3Al_2Si_3O_{12}$ | JUN92.BS |
| almandine | Al | $Fe_3Al_2Si_3O_{12}$ | JUN92.BS |
| grossular | Gr | $Ca_3Al_2Si_3O_{12}$ | JUN92.BS |
| knorringite | Kn | $Mg_3Cr_2Si_3O_{12}$ | this study; based on Girnis and Brey (1999) |
| Olivine | Oliv | $(Mg,Fe)_2SiO_4$ | W values from JUN92.BS |
| forsterite | Fo | $Mg_2SiO_4$ | JUN92.BS |
| fayalite | Fa | $Fe_2SiO_4$ | JUN92.BS |
| Spinel | Spin | $(Mg,Fe)Al_2O_4$ | W values from JUN92.BS |
| spinel | Sp | $MgAl_2O_4$ | JUN92.BS |
| hercynite | Hc | $FeAl_2O_4$ | JUN92.BS |
| picrochromite | Pc | $MgCr_2O_4$ | this study; based on Onuma and Tohara (1984) and Girnis and Brey (1999) |
| Plagioclase | Pl | $(Ca,Na)(Si,Al)_4O_8$ | W values from JUN92.BS |
| albite | Ab | $NaAlSi_3O_8$ | JUN92.BS |
| anorthite | An | $CaAl_2Si_2O_8$ | JUN92.BS |

*W-values refer to mixing parameters (Margules parameters) for minerals solutions; other references are for enthalpy, entropy, volume, heat capacity, expansivity and compressibility. More details about data sources are given in the annotated data base, available from the authors.

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*Much has been omitted here*

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