GEOL3010 Course Web Site: http://ruby.colorado.edu/~smyth/syl3010.html

My Mineral _____

GEOL3010 Mineralogy

Adopt-a-Mineral

This course requires a brief research paper on a pure mineral end-member. Each person will have a different mineral. One purpose is to familiarize you with the mineralogical and geological literature and procedures for searching for and extracting information. Another is to link the various laboratory exercises and focus them on making measurements to test or confirm literature observations. Another is to familiarize you with proper writing, report, and citation procedures. A sample research paper on quartz will be on reserve in the library.

Your literature search will begin with an Internet search. Most citable references are now available on line.

In addition, you may want to begin with a quick search through *Glossary of Mineral Species* (Fleischer) if you have any question about the composition of your mineral. You should also check *Georef*. You may also check *Mineralogical Abstracts*, *Chemical Abstracts*, MSA's *Reviews in Mineralogy*, and/or *Science Citation Index* <http://isi1.med.iacnet.com/ISI/CIW.cgi>

In order to make your drawing and calculated X-ray powder pattern, you will need to find a paper or source that contains the space group and atom positional coordinates. Most of the files included with XTALDRAW contain a reference to the original structure study. You will need to the original paper and cite it properly. In addition to online resources, a reference to original crystallographic data the common minerals may be found in Smyth and McCormick (1995) [*Crystallographic data for minerals. Mineral Physics and Crystallography A Handbook of Physical Constants, Vol.2, AGU, 1-17*.]

The paper should consist of the following sections in correct prose with proper citation procedure.

I.(10) Introduction:

You need a paragraph introducing general information on your mineral such as the origin of the name, formula, and chemical and structural affinities.

II.(15) Physical and Optical Properties

This section will include reference to the following tabulated data (Tables 1).

Table 1. General and Physical Properties (Tabulated)

a) Chemical Formula
b) Optical Properties
c) Cleavage common crystal forms
d) Color, Opacity and Luster
e) Hardness

III. (15)Chemistry

This section will cover the principal chemical variations and substitutions in the mineral species and will include a table (Table 2) of chemical analyses as weight percent oxides and as atoms per formula unit.

Table 2. Three typical chemical analyses (Tabulated). These may be imported from Excel with calculations of cation ratios as done in your homework. You need to give at least three weight percent analyses. These will be in oxide weigh percents for oxygen-bearing minerals or elemental weight percents for sulfides and halides. If you have an F-bearing silicate or phosphate get help recalculating the analyses.

IV. Structure

This section will include a paragraph briefly describing the structure of the mineral. This section will include reference to data in Table 3 and Figures 1, 2, and 3.

Table 3. Crystallographic Information (Tabulated)

a) Crystal System
b) Point Group
c) Space Group
d) Unit Cell Parameters
e) Z (No. of Formula Units per Cell)
f) Density (Literature values and your calculation)
g) Fractional Coordinates for each unique atom (This may be a separate table for complex structures)

Figure 1. A Drawing of the Crystal Structure from XTALDRAW

V. X-ray Diffraction

Give a brief description of the X-ray powder diffraction experiment you did and the powder pattern you calculated using XPOW.

Figure 2. Your raw pattern. These come out as .emf files which are graphics files that can be imported directly into word. If you have difficulty, you can convert them to .jpg files in Photoshop.

Figure 3. Your processed X-ray powder diffraction pattern with peaks and the standard pattern.

Figure 4. A Calculated X-ray Powder Diffraction pattern for your mineral.

Table 4. X-ray powder diffraction data for your mineral. Tabulate and compare the observed and calculated peaks for your pattern. This will be a merge of your XPOW and observed patterns presented as a single table with the peaks indexed (Miller indices).

VI. Occurrences

Give in correct prose a description of the general occurrences of you mineral. You should give the type of mineral environment and/or description of one or two type localities if it is a rare mineral. This should be approximately one page of double-spaced word-processed text (~250 words).

VII. Raman spectrum

You will need to find a Raman spectrum online for your mineral. Just search with Raman and your mineral name and you should fine a Raman spectrum.

VI. References

Use the reference format of the *American Mineralogist*.
http://www.minsocam.org/MSA/AmMin/instructions.html
You MUST follow the format exactly!!!
Each item in tables 1-3 must be referenced (or be your own measurement).

Notice that none of the references in the sample paper is a website. Websites are not citable references because they are not refereed and can disappear or change at any time. You need to find the original published source of the information you use. Often the original citation is given in a website or other source such as in the input files to XPOW or XTALDRAW. You must follow this up and cite the original. Acceptable references are published books or journal articles. Many journal articles are available on-line and have a proper citation. Websites are NOT acceptable references!!

Following is an annotated sample paper for quartz with more specific instructions for each section.

Quartz

Joseph R. Smyth

Adopt-a-Mineral Project
Example Paper

Your paper is done individually, no collaborations. In blue font below, please specific instructions for the various sections of the paper. In red are the point percentages assigned to each section.

I. Introduction (10)

Quartz, or α-quartz, is the mineral form of SiO_2 stable at low temperatures and pressures. The English word derives from the Saxon word querkluftertz (cross-vein ore) (Gaines et al., 1997). It occurs in igneous, sedimentary, metamorphic, and hydrothermal mineral environments, particularly in continental regions. It is, however, rare in oceanic rocks. As the structure is acentric, it occurs in both left and right-handed varieties and is both piezoelectric and pyroelectric. It is usually nearly pure and accepts only very limited amounts of other elements in substitution. Polymorphs include β-quartz, tridymite, cristobalite, coesite, stishovite, and keatite.

This is a brief introductory paragraph. Mineral names are **not** capitalized. They are common nouns. Tell what the mineral is, its formula, the name and origin of the name and a brief summary of outstanding properties and occurrences. Use citations in standard journal format. Please use the subscript in MSWord for chemical formulas.

II. Physical Properties (10)

The physical and optical properties of quartz are outlined in Table 1. It is generally colorless, but many colored varieties have been described, including rose quartz (pink), amethyst (purple), citrine (yellow) and smoky quartz (gray). The luster is vitreous, and there is no cleavage so it exhibits conchoidal fracture. The hardness is seven, and the density is 2.67 g/cm^3. Optically, it is uniaxial, positive with a maximal birefringence of 0.0095.

Table 1. General and Physical Properties of Quartz (Deer et al., 1963)

Chemical Formula	SiO_2
Optical Properties	Uniaxial positive
	Nω = 1.5443
	Nε = 1.5538
Cleavage	None
Common crystal forms	Prism {1010}
	Pyramids {1011} and {0111}
Luster	Vitreous
Color, Opacity	Transparent, colorless
	Also gray (smoky quartz), blue, purple (amethyst), yellow (citrine), pink (rose quartz)
Hardness	7

This section has a brief paragraph describing the outstanding physical properties. The table lists optical properties, (note there will be three indices for biaxial, two for uniaxial, and one for isotropic), luster, density, color, pleochroism and hardness.

III. Chemistry (15)

Quartz is always nearly pure silica with less than 0.2 percent of total impurities. Typical chemical analyses are given in Table 2.

Table 2. Typical chemical analyses of quartz (Deer et al., 1963).

	1	2	3	4
SiO2	99.97	99.98	99.53	99
TiO2	0.048	0.015	0	0
Al2O3	0.042	0	0.02	0
Cr2O3	0	0	0	0
Fe2O3	0.007	0.07	0.05	0
FeO	0	0.04	0.05	0
MnO	0.009	0	0	0.02
MgO	0.008	0.09	0	0
CaO	0.01	0	0	0
Na2O	0	0	0	0
K2O	0	0	0	0
H2O	0	0	0	0
Total	100.094	100.195	99.65	99.02
	3.330549	3.3315	3.314516	3.295559
Oxygens /formula unit	4	4	4	4
Si	1.998208	1.997837	1.999036	1.999829
Ti	0.000722	0.000225	0	0
Al	0.000989	0	0.000473	0
Cr	0	0	0	0
Fe3+	0.000105	0.001053	0.000756	0
Fe2+	0	0.000668	0.00084	0
Mn	0.000152	0	0	0.000342
Mg	0.000238	0.002681	0	0
Ca	0.000214	0	0	0
Na	0	0	0	0
K	0	0	0	0
H	0	0	0	0
	2.000629	2.002464	2.001105	2.000171

This section has a brief paragraph describing the composition and principal substitutions. If your mineral is an oxygen mineral, list by oxide weight percents. If it is a halide, sulfide, or native element, just give the atomic weight percents. You must then recalculate the analysis to mole ratios. You need to find at least three chemical analyses of your mineral in the literature. And you must cite the source.

IV. Structure (20)

The structure of quartz consists of corner-sharing SiO_4 tetrahedra so that each Si is bonded to four oxygens, and each oxygen is bonded to two silicon atoms. The resulting structure forms an open three-dimensional framework, so that quartz is classified as a tektosilicate or framework silicate. Quartz is the stable form of SiO_2 at atmospheric temperature and pressure. It is denser than tridymite and cristobalite, the high temperature forms, but less dense than the high pressure forms, coesite and stishovite. At 573 ºC, trigonal low quartz transforms reversibly to hexagonal high quartz.

The crystallographic data for quartz are outlined in Table 3. The structure is acentric, so exists in right- and left-handed enantiomorphs. The space groups are $P3_121$ (right handed) or $P3_221$ (left-handed). The structure is illustrated in Fig. 1.

Table 3. Crystallographic Information

Crystal System	Trigonal
Point Group	32
Space Group	$P3_121$ or $P3_221$
Unit Cell Parameters	
a	4.1937Å
c	5.4047Å
Z (No. of Formula Units per Cell)	3
Density (calculated)	2.648 g/cm^3
Density (measured)	2.65 g/cm^3

Table 4. Atom coordinates for quartz at 298K (Kihara et al., 1990)

Atom	*x/a*	*y/b*	*z/c*
Si	0.4697	0	0
O	0.4133	0.2672	0.1188

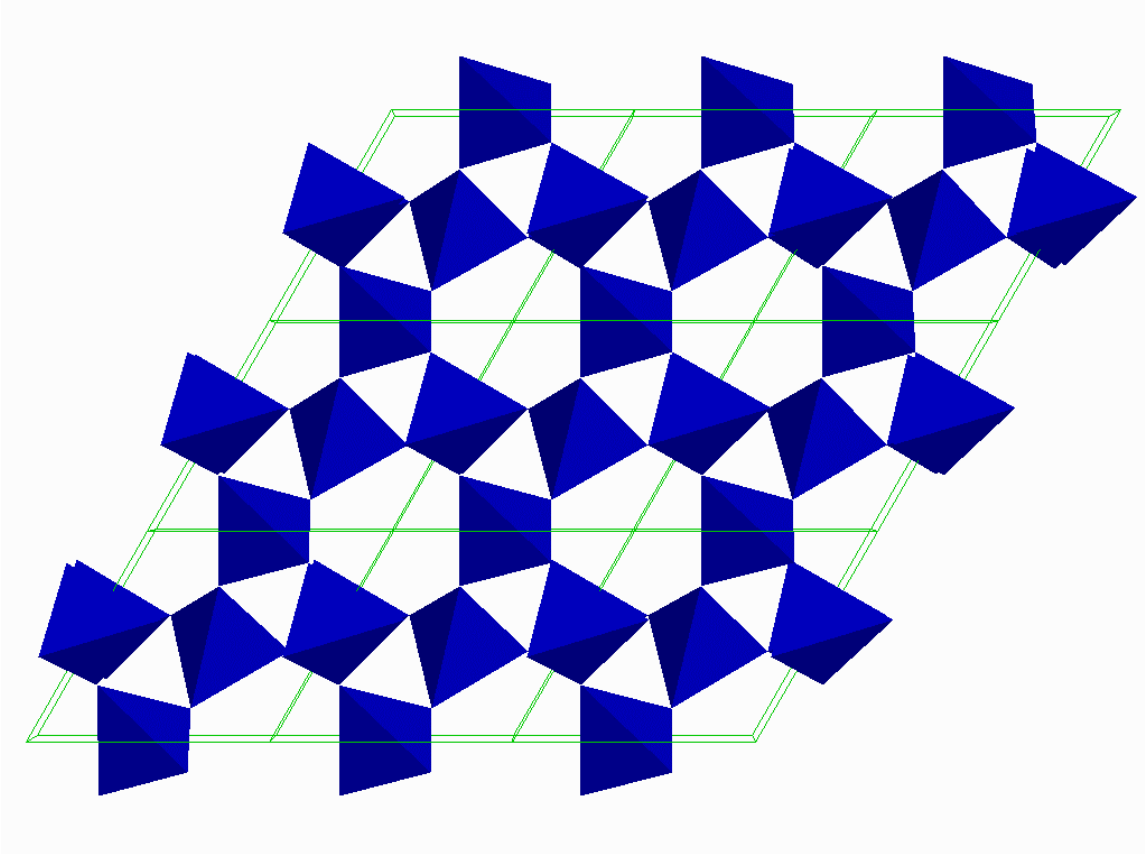

Figure 1. The crystal structure of quartz (*c*-axis projection).

Table 5. Selected interatomic distances and coordination parameters of the Si atoms in quartz.

Atoms	Distance (Å)
Si – O (2)	1.6052
Si – O (2)	1.6134
<Si – O>	1.6093
Polyhedral Volume	2.138Å^3
Tet. Quadratic Elong.	1.0002

In this section you must start with a brief paragraph describing the structure and the coordination of the various cations. You will need a table listing the main structural features as above including the unit cell parameters a, b, c, α, β, γ. For cubic you only need a, for hexagonal, tetragonal and trigonal you need a and c. You must cite the source of the information. You need to find a measured density and you need to calculate the density from your cell parameters and chemical analysis. You need a table with the atom coordinates with citation to the source. You need a drawing form XTALDRAW that you have prepared. You will need a table of nearest neighbor coordination for each cation from XTALDRAW geometry file.

V. X-ray diffraction (20)

An X-ray powder diffraction pattern was obtained for a sample of pure quartz and is shown in Figure 2. The background and alpha-2radiation were subtracted and peaks were located using the program package DSMNT (Scintag Inc, 1998). The processed pattern, derived peaks are shown in Figure 2 compared to the standard pattern number 46-1045 (JCPDS, 2000). A powder pattern was calculated from the structure data of Kihara et al. (1990) and is presented in Figure 4. The observed and calculated diffraction peaks are given in Table 5.

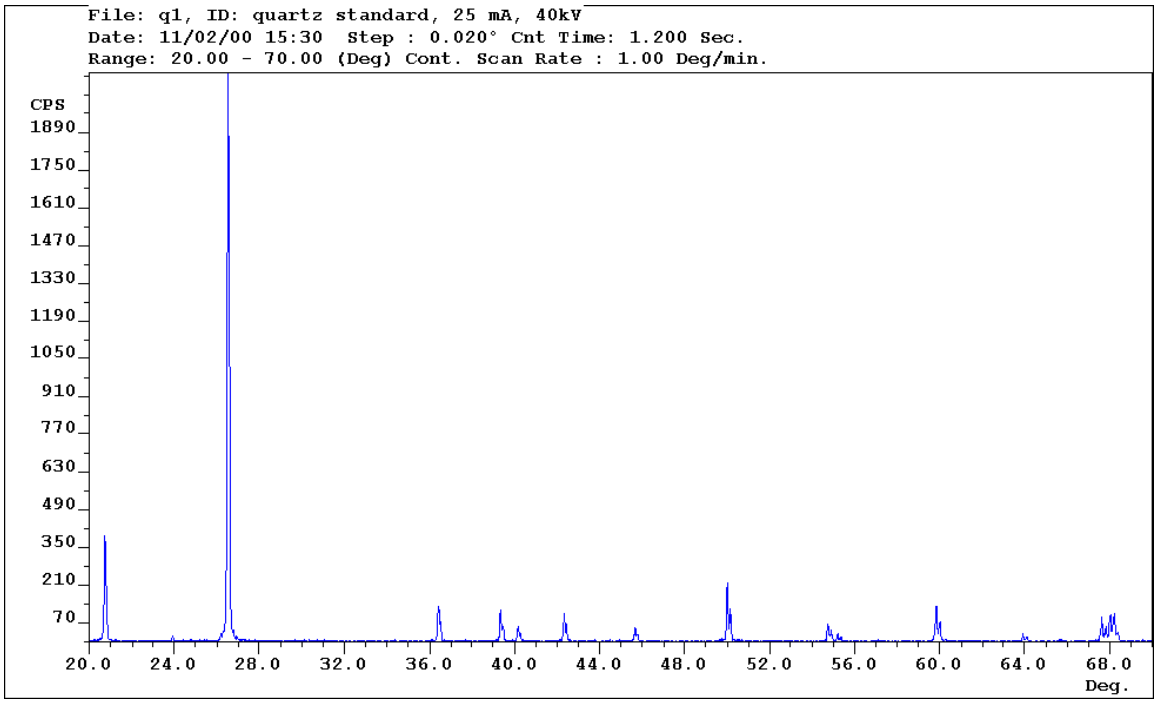

Figure 2. X-ray powder diffraction pattern of quartz.

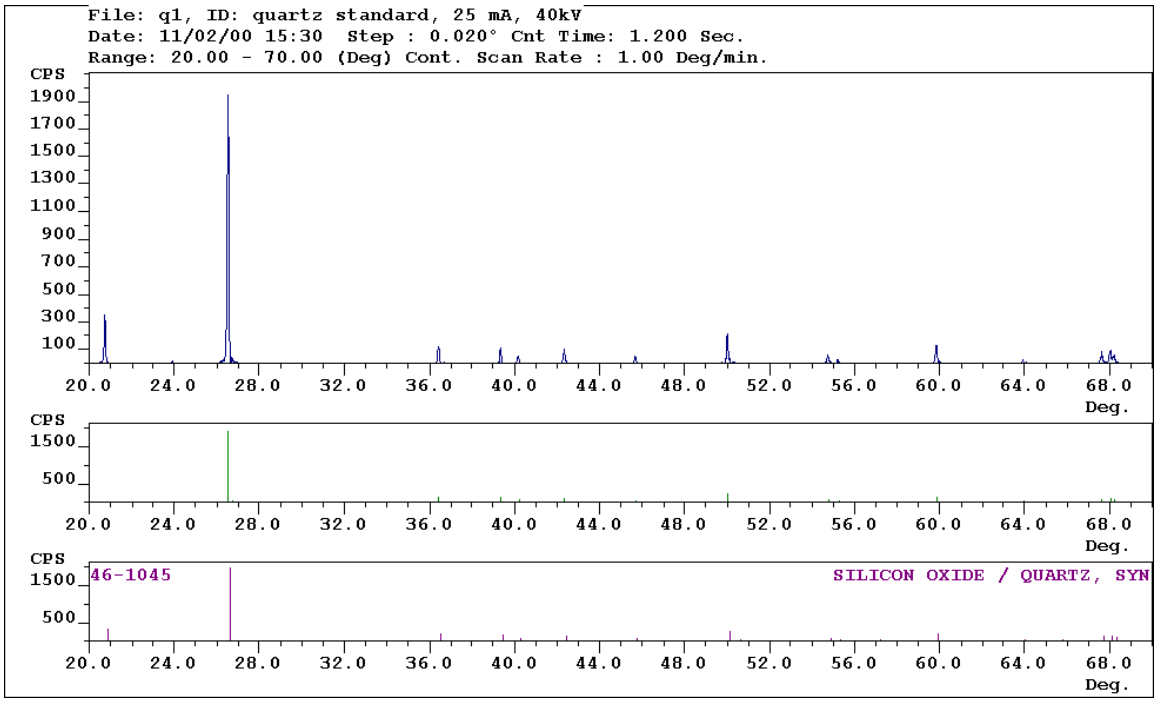

Figure 3. X-ray powder diffraction pattern of quartz showing peaks derived from the pattern compared to the JCPDS standard pattern number 46-1045.

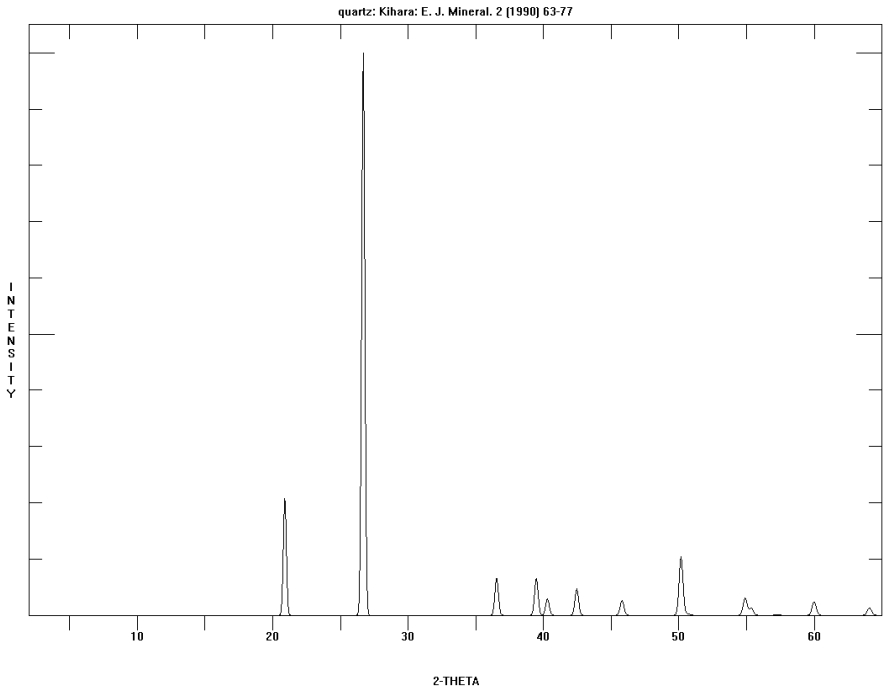

Figure 4. Calculated powder diffraction pattern for quartz using the program XPOW (Downs et al., 1993).

Table 7. Observed and Calculated X-ray Powder Diffraction Peaks (CuKα radiation)

OBSERVED			CALCULATED					
2-θ	d(Å)	REL INT	2-θ	REL INT	d(Å)	*h*	*k*	*l*
20.82	4.263	21.8	20.88	20.65	4.2554	1	0	0
26.62	3.346	100.0	26.66	69.88	3.3434	0	1	1
			26.66	30.12	3.3434	1	0	1
36.52	2.458	10.0	36.57	6.48	2.4569	1	1	0
39.44	2.283	7.9	39.50	0.60	2.2812	0	1	2
			39.50	6.10	2.2812	1	0	2
40.26	2.238	3.3	40.32	2.97	2.2366	1	1	1
42.41	2.130	4.8	42.49	5.29	2.1277	2	0	0
45.75	1.982	3.72	45.83	0.81	1.9798	0	2	1
			45.83	1.41	1.9798	2	0	1
50.10	1.819	13.1	50.18	10.29	1.8179	1	1	2
			50.67	0.40	1.8016	0	0	3
54.83	1.673	4.4	54.92	0.55	1.6717	2	0	2
			54.92	2.17	1.6717	0	2	2
			55.38	1.22	1.6590	0	1	3
			57.28	0.15	1.6084	2	1	0

This section starts with a description of the XRD experiment in the lab. You will get two eps figures from the lab and a text file of the main XRD peaks from the experiment. The text file contains a list of the strongest peaks in the pattern. You will also calculate a powder XRD pattern from XPOW. The calculated pattern should cover the same 2-theta range as the experiment. You will also get a list of the main diffraction peaks from XPOW. You need to merge these two tables to form a table that lists observed (lab) and calculated peaks (XPOW) for your mineral so that you can index the observed peaks from the calculated pattern. You must also cite the source of the structure information used for XPOW.

VI. Occurrences (15)

The occurrences of quartz have been reviewed by Gaines et al. (1997). Quartz is an abundant mineral in igneous, metamorphic, hydrothermal, and sedimentary environments. In plutonic igneous rocks, it is abundant in silicic rocks ranging in composition from quartz diorite to granite but absent in more mafic compositions. In volcanic rocks, it is common in quartz latites to rhyolites, but uncommon in vitric silicic tuffs. It is common to abundant in welded silicic tuffs. In metamorphic rocks, it is abundant in schists and gneisses of pelitic to granitic compositions. In hydrothermal rocks, it is an abundant as the principal gangue mineral; in low to high temperature vein deposits. Because of its resistance to chemical weathering, it is the principal mineral phase in sandstones and abundant in other non-marine sedimentary rocks. It is also abundant as cryptocrystalline chert in marine limestones and dolomites.

Numerous varieties have been described, and defined mainly on color. Quartz is most commonly colorless and transparent. Rose quartz is pink and contains minor Mn impurities, recently identified as dumortrierite. Citrine is yellow, and amethyst is purple.

You need a paragraph or two summarizing the major occurrences and varieties of your mineral. You must cite the sources of the information.

VII. Raman Spectrum (5 extra credit points for 2013)

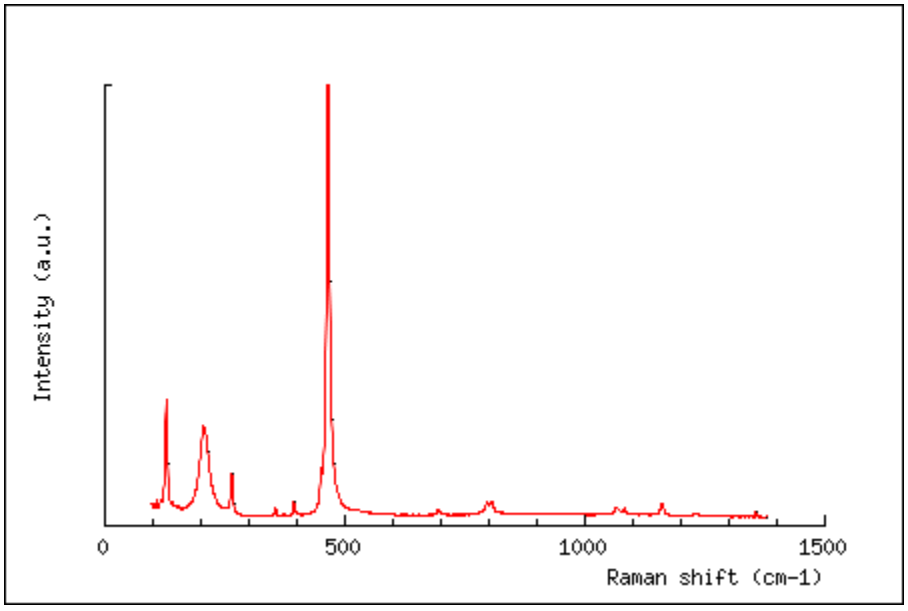

Figure 5. Raman Spectrum of quartz (Hemley, 1987).

VIII. References (10)

Deer, W.A., R. A. Howie, and J. Zussman (1963) *Rock-Forming Minerals* Vol 4. Longmans, London, 435pp.

Downs, R.T., K.L. Bartelmehs, G. V. Gibbs, and M. B. Boysen, Jr. (1993) Interactive software for calculating and displaying X-ray or neutron powder diffractometer patterns of crystalline materials. *American Mineralogist* 78, 1104-1107.

Gaines, R.V., H.C.W. Skinner, E.E. Foord, B. Mason, A. Rosenzweig, V.T. King and E. Dowty (1997*) Dana's New Mineralogy*, Eighth Edition, New York, John Wiley & Sons, 1819 pp.

ICDD, (2001) Powder Diffraction File. International Center for Diffraction Data, Newtown Square, PA, USA.

R. J. Hemley, (1987) Pressure dependence of Raman spectra of SiO_2 polymorphs: alpha-quartz, coesite and stishovite. *High-pressure research in mineral physics*, M. H. Manghnani and Y. Syono (Eds), Terra Scientific Publishing Company and AGU, Tokyo/Washington D.C., pp. 347-360

Kihara, K. (1990) An X-ray study of the temperature dependence of the quartz structure. *European Journal of Mineralogy* 2, 63-77.

LePage, Y., L. D. Calvert, and E. J. Gabe (1980) Parameter variation in low quartz between 94 and 298K. *Journal of Physical Chemistry of Solids*, 41, 721-725.

All references in the text and tables of the paper are to be listed here. The list is alphabetical by first author's last name. YOU MAY NOT USE WEBSITES as they are not refereed. You must use the Instructions to Authors for American Mineralogist for format of each type of reference.
YOU MUST FOLLOW THE FORMAT EXACTLY!!!!!!!!!!!!!!!