

# **EPSC 501 Crystal Chemistry**

## **Week 2**

### **The garnet structure as an example**

## Indicator minerals selected

Mathieu: garnet and **zircon**

Kristal: **spinel**, garnet

Myriam: **chalcopyrite**, **fluorite**

Cedrick: Cr-pyrope, Cr-**diopside**

Killian: **cinnabar**, Cr-spinel

Fahimeh: Cr-garnet, **priderite**

Philippe: **magnetite**, **tourmaline**

Lynn: to be announced

Yumi: to be announced

By the end of today/this week, you should:

Know the structural formula for your two mineral species.

Know which system/crystal class matches its space group.

Examine a structural model of your model to recognize its coordination polyhedra (number of anions around each cationic site).

Do the coordination polyhedra share corners, edges or faces?

Look up the Dana chemical classification for your two minerals.

Know if your mineral is an end-member, belongs within a series or to which broader group.

How do we *define* a mineral?

Mineral names:

What is the distinction between a mineral species and a broader *series* or *group*?

Is a “Cr-garnet” or “Cr-diopside” a valid mineral species?

(The nomenclature of minerals continues to be revised periodically...)

# How do we describe a mineral?

- structure: atomic pattern
  - determined or verified by X-ray diffraction (or, possibly, by optical properties)
- composition
  - chemical analysis (major, minor elements)
- shape of actual grains:
  - monocrystalline or polycrystalline?
  - if euhedral or subhedral
    - morphology (forms)
    - habit (general as-grown aspect)
  - fragmented: shape may reflect cleavage

**Table 1**

Cation site occupancies for garnet end-members

End-members <sup>a</sup>	Dodecahedral	Octahedral	Tetrahedral	Anion
Henritermierite	Ca <sub>3</sub>	Mn <sub>2</sub> <sup>3+</sup>	Si <sub>2</sub> (H <sub>4</sub> )	O <sub>12</sub>
<i>Blythite</i>	Mn <sub>3</sub> <sup>2+</sup>	Mn <sub>2</sub> <sup>3+</sup>	Si <sub>3</sub>	O <sub>12</sub>
Katoite	Ca <sub>3</sub>	Al <sub>2</sub>	(H <sub>4</sub> ) <sub>3</sub>	O <sub>12</sub>
<i>FCa garnet</i>	Ca <sub>3</sub>	Al <sub>2</sub>	( ) <sub>3</sub>	F <sub>12</sub>
<i>FMn garnet</i>	Mn <sub>3</sub>	Al <sub>2</sub>	( ) <sub>3</sub>	F <sub>12</sub>
<i>Yttrogarnet (YAG)</i>	Y <sub>3</sub>	Al <sub>2</sub>	Al <sub>3</sub>	O <sub>12</sub>
Kimzeyite	Ca <sub>3</sub>	Zr <sub>2</sub>	SiAl <sub>2</sub>	O <sub>12</sub>
<i>Kimzeyite-Fe</i>	Ca <sub>3</sub>	Zr <sub>2</sub>	SiFe <sub>2</sub> <sup>3+</sup>	O <sub>12</sub>
<i>Tin garnet</i>	Ca <sub>3</sub>	SnFe <sup>2+</sup>	Si <sub>3</sub>	O <sub>12</sub>
Schorlomite	Ca <sub>3</sub>	Ti <sub>2</sub>	SiFe <sub>2</sub> <sup>3+</sup>	O <sub>12</sub>
<i>Schorlomite-Al</i>	Ca <sub>3</sub>	Ti <sub>2</sub>	SiAl <sub>2</sub>	O <sub>12</sub>
Morimotoite	Ca <sub>3</sub>	TiFe <sup>2+</sup>	Si <sub>3</sub>	O <sub>12</sub>
<i>NaTi garnet</i>	Na <sub>2</sub> Ca	Ti <sub>2</sub>	Si <sub>3</sub>	O <sub>12</sub>
<i>Morimotoite-Mg</i>	Ca <sub>3</sub>	TiMg	Si <sub>3</sub>	O <sub>12</sub>
<i>Morimotoite-Fe</i>	Fe <sub>3</sub> <sup>2+</sup>	TiFe <sup>2+</sup>	Si <sub>3</sub>	O <sub>12</sub>
Majorite	Mg <sub>3</sub>	MgSi	Si <sub>3</sub>	O <sub>12</sub>
<i>Sc garnet</i>	Ca <sub>3</sub>	Sc <sub>2</sub>	Si <sub>3</sub>	O <sub>12</sub>
Goldmanite	Ca <sub>3</sub>	V <sub>2</sub>	Si <sub>3</sub>	O <sub>12</sub>
<i>Yamatoite</i>	Mn <sub>3</sub> <sup>2+</sup>	V <sub>2</sub>	Si <sub>3</sub>	O <sub>12</sub>
Uvarovite	Ca <sub>3</sub>	Cr <sub>2</sub>	Si <sub>3</sub>	O <sub>12</sub>
Knorringite	Mg <sub>3</sub>	Cr <sub>2</sub>	Si <sub>3</sub>	O <sub>12</sub>
Spessartine	Mn <sub>3</sub> <sup>2+</sup>	Al <sub>2</sub>	Si <sub>3</sub>	O <sub>12</sub>
Pyrope	Mg <sub>3</sub>	Al <sub>2</sub>	Si <sub>3</sub>	O <sub>12</sub>
Almandine	Fe <sub>3</sub> <sup>2+</sup>	Al <sub>2</sub>	Si <sub>3</sub>	O <sub>12</sub>
Grossular	Ca <sub>3</sub>	Al <sub>2</sub>	Si <sub>3</sub>	O <sub>12</sub>
Andradite	Ca <sub>3</sub>	Fe <sub>3</sub> <sup>3+</sup>	Si <sub>3</sub>	O <sub>12</sub>
Calderite	Mn <sub>3</sub> <sup>2+</sup>	Fe <sub>2</sub> <sup>3+</sup>	Si <sub>3</sub>	O <sub>12</sub>
<i>Skiagite</i>	Fe <sub>3</sub> <sup>2+</sup>	Fe <sub>2</sub> <sup>3+</sup>	Si <sub>3</sub>	O <sub>12</sub>
<i>Khoharite</i>	Mg <sub>3</sub>	Fe <sub>2</sub> <sup>3+</sup>	Si <sub>3</sub>	O <sub>12</sub>

<sup>a</sup> Mineral names listed in regular font, hypothetical end-members in italics.

# Garnet group

Do these share:

- a single structural formula? Yes
- the same atomic pattern? Similar polyhedra but their content differs
- the same symmetry (described by a space group)?

These end-members are listed, and many are discussed in Locock (2008), now posted at [www.eps.mcgill.ca/~courses/c186-501](http://www.eps.mcgill.ca/~courses/c186-501)

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<sup>a</sup> Mineral names listed in regular font, hypothetical end-members in italics.

# Garnet group

What is the definition of an “end member”?

Names in italics are hypothetical (they do not exist as a mineral species) but are used to describe compositional variation.

Fahimeh and Mathieu: are all Cr-garnets either uvarovite or knorringite?

Cedric: what, exactly, is Cr-pyrope?

A useful reference (in general):

Nickel and Grice, 1998. The IMA commission on new minerals and mineral names: procedures and guidelines on mineral nomenclature, 1998. *Canadian Mineralogist*, vol. 36, pp. 913-926.

(IMA: International Mineralogical Association)

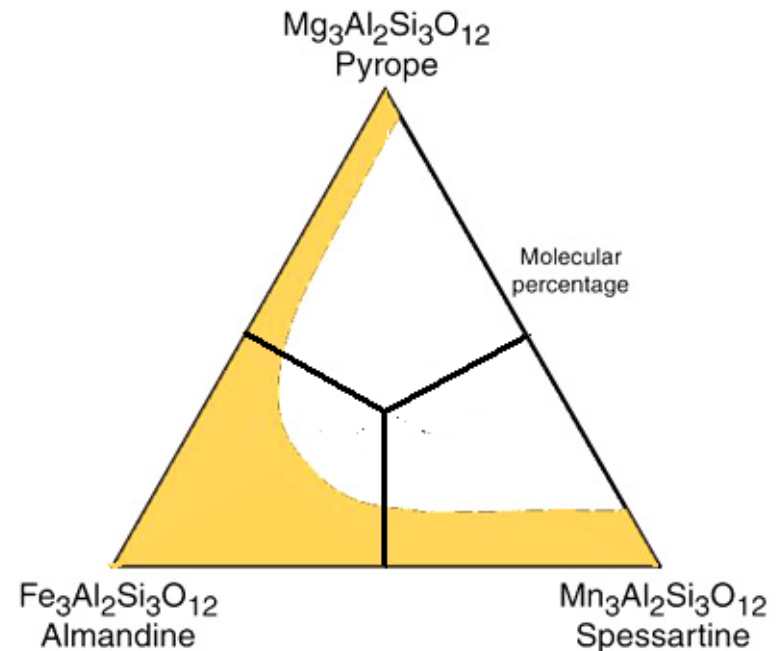
A tool for garnet crystal chemistry:

Locock, A.J. (2008). An Excel spreadsheet to recast analyses of garnet into end-member components, and a synopsis of the crystal chemistry of natural silicate garnets. *Computer & Geosciences*, vol. 34, pp. 1769-1780.



Naming minerals: mineralogical nomenclature in solid-solution series follows a system called “the 50% rule” (in binary solid solution series, defined by two end-member mineral species).

In a ternary solid solution (i.e. 3 end-member species), it is more correct to call this the 100%/n rule or the dominant-constituent rule, in which the constituents are atoms (cations or anions), molecular groups, or vacancies.



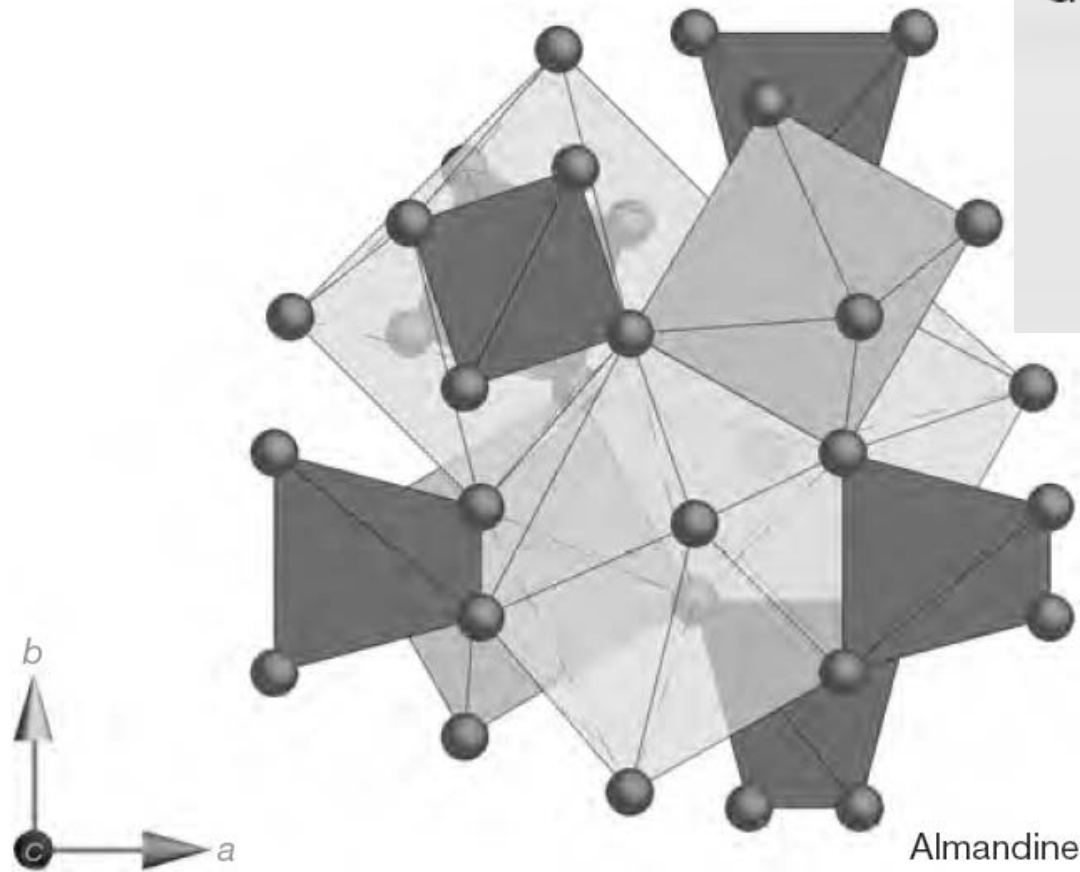
Garnets:  $A_3B_2Si_4O_{12}$

where,

$A > B$ , and

$A = Ca^{2+}, Mg^{2+}, Fe^{2+}, Mn^{2+}$

$B = Al^{3+}, Fe^{3+}, Cr^{3+}$



**Figure 10.6.** A portion of the crystal structure of a garnet, showing its three coordination polyhedra. From largest to smallest these are: a distorted CN = 8 site (translucent gray), an octahedron CN = 6 (light gray), and a tetrahedron CN = 4 (dark gray). Large cations like  $Ca^{2+}$  would enter the CN = 8 site, intermediate cations like  $Fe^{2+}$  would enter the CN = 6 site, while small cations like  $Si^{4+}$  would reside in the CN = 4 site. The oxygen anions defining the corners of each polyhedron are shown as small spheres.

All species of garnet share the same structural formula, based on three distinct coordination polyhedra.

# Dana's chemical classification

(51) Nesosilicate **Insular**  $\text{SiO}_4$  Groups Only

(51.04) with cations in [6] and  $>[6]$  coordination

A chemical classification that takes into account the coordination of ions.

A **group** is broader than a **series**.

(51.04.03b) Garnet **group** (Ugrandite **series**)

51.04.03b.01 Andradite  $\text{Ca}_3\text{Fe}_2(\text{SiO}_4)_3$  | a3d 4/m -3 2/m

51.04.03b.02 Grossular  $\text{Ca}_3\text{Al}_2(\text{SiO}_4)_3$  | a3d 4/m -3 2/m

51.04.03b.03 Uvarovite  $\text{Ca}_3\text{Cr}_2(\text{SiO}_4)_3$  | a3d 4/m -3 2/m

51.04.03b.04 Goldmanite  $\text{Ca}_3(\text{V,Al,Fe})_2(\text{SiO}_4)_3$  | a3d 4/m 3 2/m

51.04.03b.05 Yamatoite?  $(\text{Mn,Ca})_3(\text{V,Al})_2(\text{SiO}_4)_3$  | a3d 4/m 3 2/m

(51.04.03a) Garnet group (Pyrospite **series**)

51.04.03a.01 Pyrope  $\text{Mg}_3\text{Al}_2(\text{SiO}_4)_3$  | a3d 4/m -3 2/m

51.04.03a.02 Almandine  $\text{Fe}_3\text{Al}_2(\text{SiO}_4)_3$  | a3d 4/m -3 2/m

51.04.03a.03 Spessartine  $\text{Mn}_3\text{Al}_2(\text{SiO}_4)_3$  | a3d 4/m -3 2/m

51.04.03a.04 Knorringite  $\text{Mg}_3\text{Cr}_2(\text{SiO}_4)_3$  | a3d 4/m -3 2/m

51.04.03a.05 Majorite  $\text{Mg}_3(\text{Fe,Al,Si})_2(\text{SiO}_4)_3$  | a3d 4/m -3 2/m

51.04.03a.06 Calderite  $(\text{Mn,Ca})_3(\text{Fe,Al})_2(\text{SiO}_4)_3$  | a3d 4/m -3 2/m

Are all “garnets” necessarily silicate minerals?

Consider schafherite:  $\text{Ca}_2\text{NaMg}_2\text{V}_3\text{O}_{12}$

*Garnets:*  $\text{A}_3\text{B}_2\text{Si}_4\text{O}_{12}$

where,

$\text{A} > \text{B}$ , and

$\text{A} = \text{Ca}^{2+}, \text{Mg}^{2+}, \text{Fe}^{2+}, \text{Mn}^{2+}$

$\text{B} = \text{Al}^{3+}, \text{Fe}^{3+}, \text{Cr}^{3+}$

What element(s) fill the A site?

What element(s) fill the B site?

What element fill the tetrahedral site?

Why is it said to have the “garnet structure”?

Mineral names are sometimes used to refer to (and “personalize”) certain types of crystalline structures.

Garnet: in the *chemical classification* of minerals, “garnet” are silicates from the subclass of orthosilicates (or nesosilicates).

Schaferite is from a *different chemical class* (Dana class 38): which includes phosphates, vanadates and arsenates with the general formula  $(A^+ B^{2+})_5 (XO_4)_3$

“Garnet structure” refers to the similar proportions of their coordination polyhedra. Schaferite is *isostructural* with the garnet group.

# From the American Mineralogist crystal structure database

## □ Uvarovite



Novak G A, Gibbs G V



American Mineralogist 56 (1971) 791-823

The crystal chemistry of the silicate garnets

sample Uv

11.988 11.988 11.988 90 90 90 Ia-3d

atom	x	y	z	occ	Biso	B(1,1)	B(2,2)	B(3,3)	B(1,2)	B(1,3)	B(2,3)
Si	.375	0	.25		.253						
Cr	0	0	0	.865		.00046	.00046	.00046	-.00018	-.00018	-.00018
Al	0	0	0	.105		.00046	.00046	.00046	-.00018	-.00018	-.00018
Fe	0	0	0	.025		.00046	.00046	.00046	-.00018	-.00018	-.00018
Ti	0	0	0	.005		.00046	.00046	.00046	-.00018	-.00018	-.00018
Ca	.125	0	.25	.997		.00049	.00074	.00074	0	0	.00015
Mn	.125	0	.25	.003		.00049	.00074	.00074	0	0	.00015
O	.03991	.04737	.65354			.00102	.00076	.00058	0.00002	-.00018	-.00009

[Download AMC data \(View Text File\)](#)

[Download CIF data \(View Text File\)](#)

[Download diffraction data \(View Text File\)](#)

[View Jmol 3-D Structure](#)

You can display the model:  
a) save the data in the AMC format, and b) open it with XtalDraw.

Which site of the general formula of garnet are Cr, Al, Fe and Ti filling? They have the same x,y, z coordinates....

□ Uvarovite



Novak G A, Gibbs G V



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The crystal chemistry of the silicate garnets  
sample Uv

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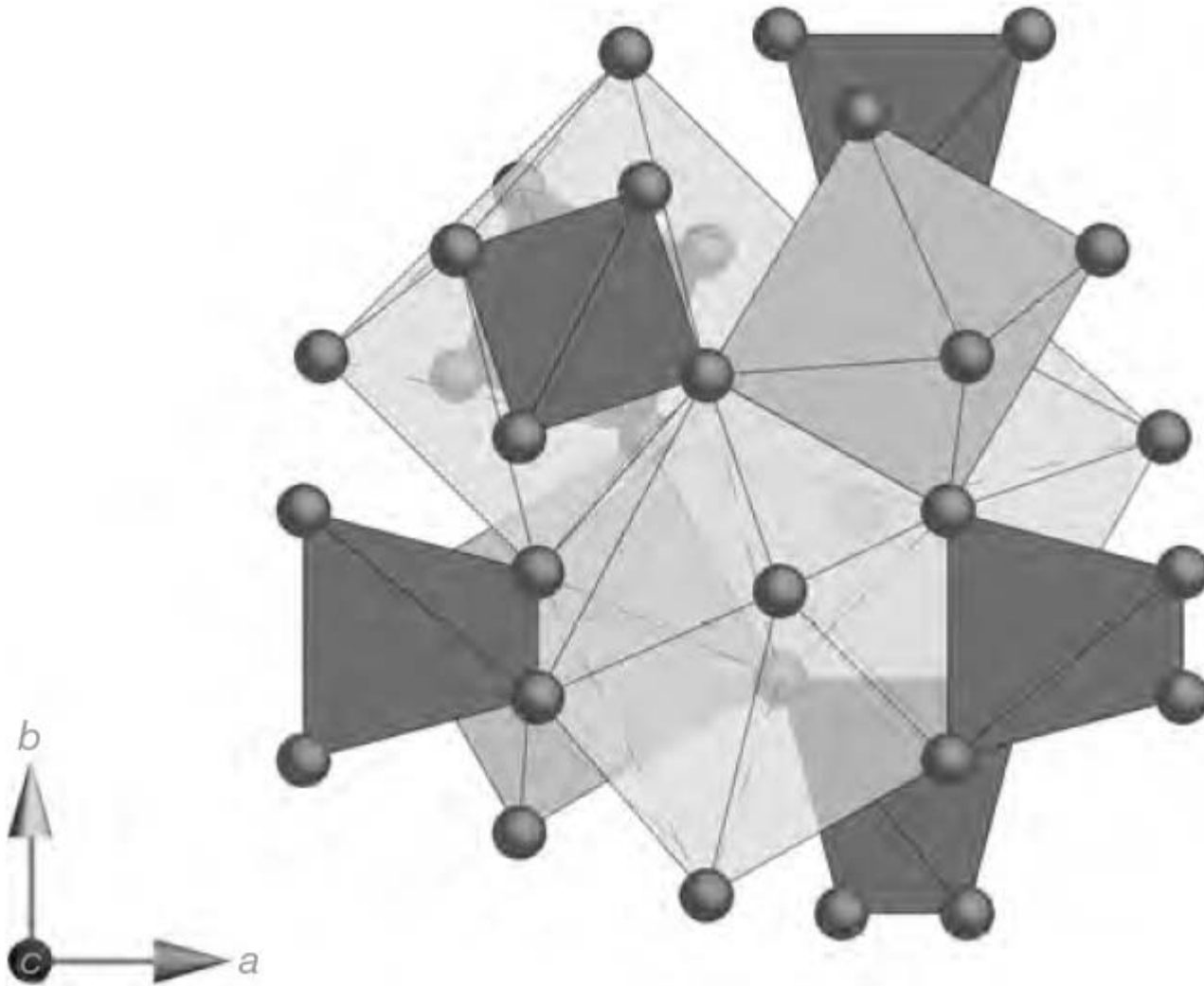
Look for similar  
phenomena in files for  
your other mineral.

Which site (A, B or Z) of the  
garnet formula  $A_3B_2Z_4O_{12}$  are  
Ca and Mn filling?

In which proportions are they  
present?

What is a unit cell?

How can you tell that this fragment of the garnet structure is from an incomplete unit cell?



(We would need to see the same type of ion at the eight corners of a cube-shaped unit cell...)



Full space group:  $I4_1/a \bar{3} 2/d$

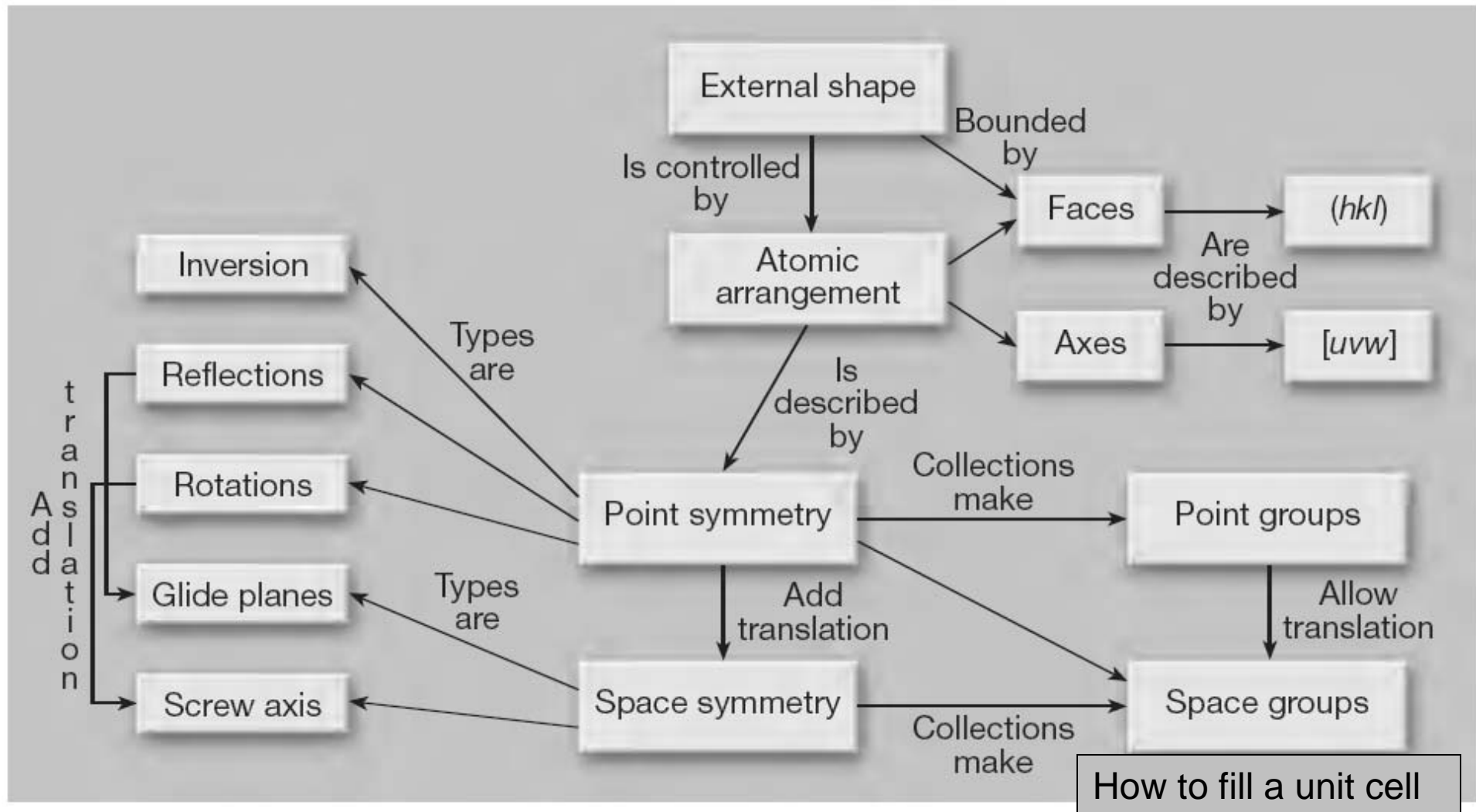
Usually abbreviated to:  $Ia3d$

Enough information was left to identify this space group as isometric (cubic).  
What gives it away?

See hand out for isogonal point groups and space groups.

Label on the hand out the different crystal systems. We will use it throughout the course.

# Symmetry operations, notations needed to describe crystal structures, shapes, cleavage (= face), twinning



**Table 12.10.**  
 The "top 20" space groups and the number  
 and percent of the minerals they contain.  
 (Data from Dana's New Mineralogy (Gaines et al., 1997)).

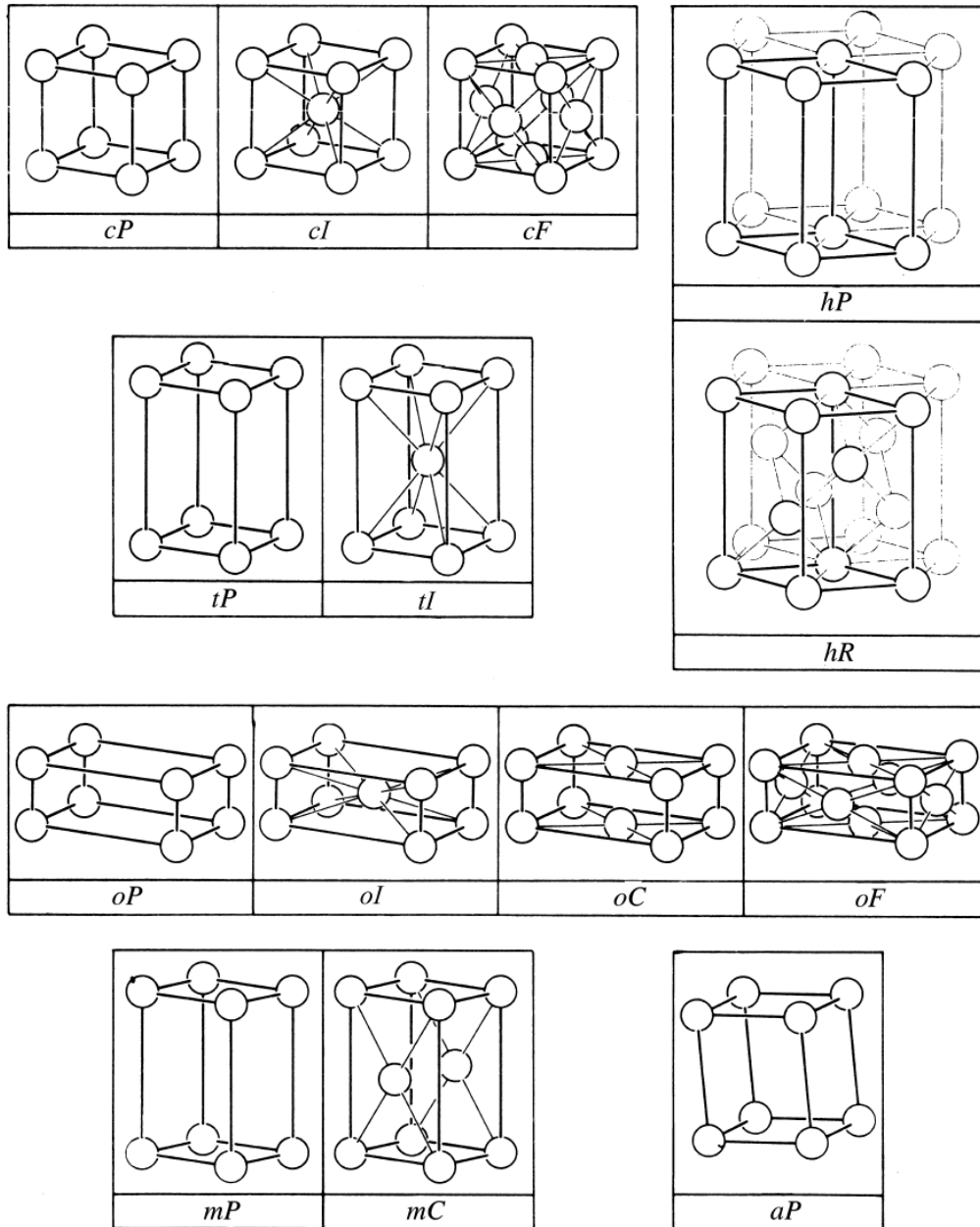
Space group	# minerals	%
$P\bar{1}$ (2)	221	6.9
$C2/m$ (12)	217	6.8
$C2/c$ (15)	138	4.3
$P2_1/c$ (14)	132	4.1
$P2_1/a$ (14)*	124	3.9
$R\bar{3} 2/m$ (166)	101	3.2
$P1$ (1)	90	2.8
$F4_1/d \bar{3} 2/m$ (227)	81	2.5
$P2_1/n$ (14)*	80	2.5
$P2_1/m$ (11)	75	2.3
$P6_3/m 2/m 2/c$ (194)	66	2.1
$F4/m \bar{3} 2/m$ (225)	58	1.8
$P2_1$ (4)	44	1.4
$P2_12_12_1$ (19)	42	1.3
$P6_3/m$ (176)	42	1.3
$P2_1/b 2_1/n 2_1/m$ (62)*	41	1.3
$R\bar{3}$ (148)	38	1.2
$R3m$ (160)	37	1.2
$P2_1/b 2_1/c 2_1/a$ (61)	32	1.0
$P2_1/a 3$ (205)	30	0.9

## Problem set #1:

Can you assign  
 each space group  
 in this list to the  
 correct crystal  
 class (point group)  
 and the correct  
 crystallographic  
 system?

## Abbreviated 32 point groups (= 32 crystal classes)

- 1,  $\bar{1}$
- 2, m,  $\frac{2}{m}$
- 222, mm2, mmm
- 4,  $\bar{4}$ ,  $\frac{4}{m}$ , 422, 4mm,  $\bar{4}2m$ ,  $\frac{4}{m}mm$
- 3,  $\bar{3}$ , 32, 3m,  $\bar{3}m$
- 6,  $\bar{6}$ ,  $\frac{6}{m}$ , 622, 6mm,  $\bar{6}2m$ ,  $\frac{6}{m}mm$
- 23,  $m\bar{3}$ , 432,  $\bar{4}3m$ ,  $m\bar{3}m$



The 14 Bravais lattices

The “spheres” are called **nodes**.

Each node represents an equivalent point in a crystal structure.

A node does not necessarily need to represent an ion or atom in a crystal structure.

From “Web Mineral” at  
<http://webmineral.com/data/Pyrope.shtml>

Pyrope

$a = 11.459$ ,  $Z = 8$ ;  $V = 1,504.67$   $\text{Den( Calc)} = 3.56$   
H-M Symbol (4/m  $\bar{3}$  2/m) Space Group: I a3d

( $Z$  = no of formula units per unit cell. An I-cell has a minimum  $Z$  of 2, but in garnets, this is multiplied by the presence of glide planes and/or screw axes that repeat the pattern elsewhere within the cell.)

You might find the same information in other sources... or not.  
Different texts, different database serve different purposes.

- Nesse “Introduction to Mineralogy”?
- Klein & Hurlbut “Mineral Sciences”?

Is any of this information included in files from the American Mineralogist Crystal Structure Database?

Indicator minerals selected

Mathieu: garnet and zircon

Kristal: spinel, garnet

Myriam: chalcopyrite, fluorite

Cedrick: Cr-pyrope, Cr-diopside

Killian: cinnabar, Cr-spinel

Fahimeh: Cr-garnet, priderite

Philippe: magnetite, tourmaline

Lynn: to be announced

For next time:

Look up the specific gravity (or density) of an end-member for your two minerals

Look up how many formula units are contained in their unit cell (the parameter  $Z$  in a crystallographic description)

Show that the density is correctly predicted by the crystal structure (use equation...)

**BREAK!** For next week, also start looking at this:  
Is one of your minerals less compositionally variable than the other?

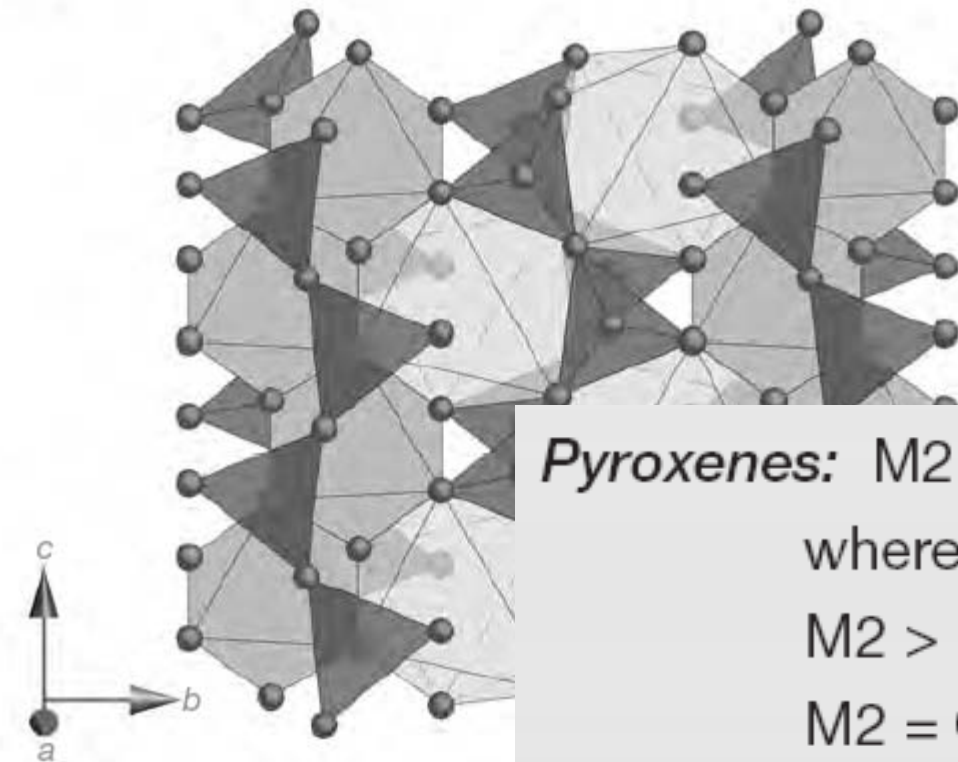
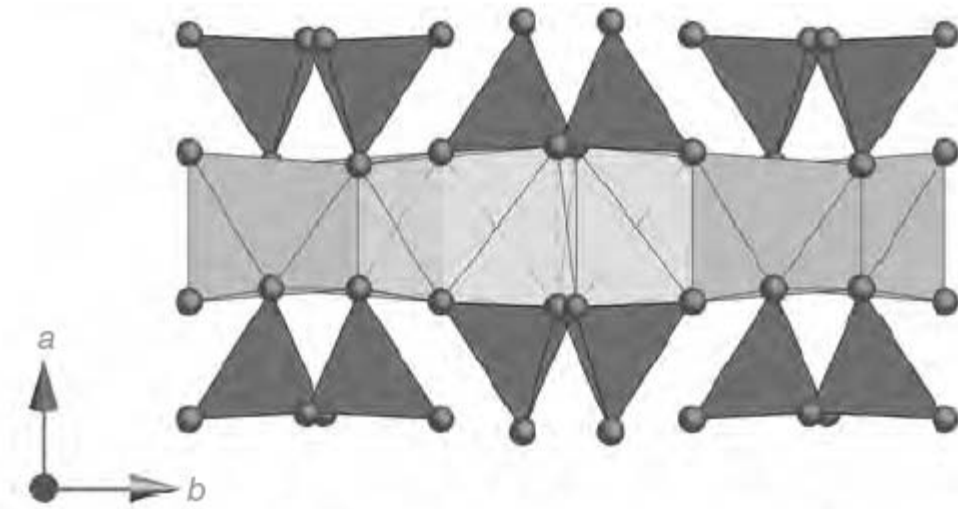
Find an article with one (or preferably) several published chemical analysis(es) of one of your minerals (ideally from a study where it is used as an indicator mineral).

Determine if these examples of compositional variation represent

- 1:1 (homogeneous) ionic substitution,
- coupled ionic substitution
- interstitial ionic substitution
- omission ionic substitution



If you dig out the data, next week, we may find out what are Cr-diopside, Cr-garnet, Cr-spinel...



b. Diopside

*Pyroxenes:*  $M_2M_1Si_2O_6$

where,

$M_2 > M_1$ , and

$M_2 = Ca^{2+}, Na^{1+}, Mg^{2+}, Fe^{2+}$

$M_1 = Mg^{2+}, Fe^{2+/3+}, Mn^{2+}, Al^{3+}, Cr^{3+}, Ti^{4+}$

Whoever picked diopside should be able to interpret this description... and relate it to the formula of diopside.

**Diopside**



Cameron M, Sueno S, Prewitt C T, Papike J J



American Mineralogist 58 (1973) 594-618

High-temperature crystal chemistry of acmite, diopside, hedenbergite, jadeite, spodumene, and ureyite

T = 24 C

pyroxene

9.745 8.899 5.251 90 105.63 90 C2/c

atom	x	y	z	B(1,1)	B(2,2)	B(3,3)	B(1,2)	B(1,3)	B(2,3)
Si	.2862	.0933	.2293	.00055	.00071	.00256	-.00003	.00025	-.00010
Mg1	0	.9082	1/4	.00075	.00075	.00246	0	.00009	0
Ca2	0	.3015	1/4	.00180	.00115	.00424	0	-.00033	0
O1	.1156	.0873	.1422	.00061	.00125	.00355	.00006	.00011	.00017
O2	.3611	.25	.3180	.00151	.00095	.00497	-.00055	.00029	-.00009
O3	.3505	.0176	.9953	.00092	.00153	.00341	.00000	.00052	-.00069

[Download AMC data \(View Text File\)](#)

[Download CIF data \(View Text File\)](#)

[Download diffraction data \(View Text File\)](#)

[View JMOl 3-D Structure](#)

1) What fills the M2, M1 sites?

2) Here, no column for “occ” after the x, y, z coordinates. Why not?

Spinel	Al subgroup	spinel	$Mg[Al]_2O_4$
		galaxite	$(Mn^{2+}, Fe^{2+}, Mg)[Al, Fe^{3+}]_2O_4$
		hercynite	$Fe^{2+}[Al]_2O_4$
		gahnite	$Zn[Al]_2O_4$
	Fe subgroup	magnesioferrite	$Fe^{3+}[MgFe^{3+}]O_4$
		jacobsite	$Fe^{3+}[(Mn^{2+}, Fe^{2+}, Mg)Fe^{3+}]O_4$
		magnetite	$Fe^{3+}[Fe^{2+}Fe^{3+}]O_4$
		franklinite	$(Zn, Mn^{2+}, Fe^{2+})[Fe^{3+}, Mn^{3+}]_2O_4$
		trevorite	$Fe^{3+}[NiFe^{3+}]O_4$
		cuprospinel	$Fe^{3+}[(Cu^{2+}, Mg)Fe^{3+}]O_4$
		brunogeierite	$Ge^{2+}[Fe^{3+}]_2O_4$
	Cr subgroup	magnesiochromite	$Mg[Cr^{3+}]_2O_4$
		manganochromite	$(Mn^{2+}, Fe^{2+})[Cr^{3+}, V^{3+}]_2O_4$
		chromite	$Fe^{2+}[Cr^{3+}]_2O_4$
		nichromite	$(Ni, Co, Fe^{2+})[Cr^{3+}, Fe^{3+}, Al]_2O_4$
		cochromite	$(Co, Ni, Fe^{2+})[Cr^{3+}, Al]_2O_4$
		zincchromite	$Zn[Cr^{3+}]_2O_4$
	V subgroup	vuorelainenite	$(Mn, Fe^{2+})[V^{3+}, Cr^{3+}]_2O_4$
		coulsonite	$Fe^{2+}[V^{3+}]_2O_4$
magnesiocoulsonite		$Mg[V^{3+}]_2O_4$	
Ti subgroup	qandilite	$(Mg, Fe^{2+})_2(Ti, Fe^{3+}, Al)O_4$	
	ulvöspinel	$Fe^{2+}_2TiO_4$	

# Spinel

Next week, let's tackle examples from other groups.

If this is your mineral, be ready to speak up.

1. The mineral species **spinel**, which has a formula of  $\text{MgAl}_2\text{O}_4$ , was the first spinel structure to be described (Barth and Posnjak, 1932), and thus was given the name "normal." In **normal spinels**, the X (divalent) cations fill 8 A tetrahedral sites, and the Y (trivalent) cations occupy 16 B octahedral sites. Thus a "normal" distribution of cations in a spinel would be  $\text{X}[\text{Y}^{3+}_2]\text{O}_4$ . The tetrahedral site is listed first, and the octahedral site occupancy is given in brackets; this is reversed from the typical way formulas are written (i.e., going from the largest to smallest from left to right, respectively). Formulas in Table 23.7 are given using this nomenclature so you can figure out which ones are normal and which are inverse.
2. In **inverse spinels**, the Y (trivalent) cations occupy the tetrahedral site, and the octahedral sites contains a mixture of Y and X (divalent) cations, with a formula of  $\text{Y}^{3+}[\text{XY}^{3+}]\text{O}_4$ . Although these are more common in nature, they were described after the spinel species, and thus were given the name "inverse" to indicate that they were the opposite of what had already been described.

Magnetite is related to the spinel group.

Let's see how, next week...

Be ready to speak up.