

Appendix 3. Six worked examples to illustrate the procedure to identify a garnet

OUTLINE OF RECOMMENDED PROCEDURE

Step 1. Calculate a formula on the basis of 12 anions and 8 cations (e.g., Appendix Table 1).

Step 2. Allocate cations (see section **Site allocation of cations**, e.g., Appendix Table 2).

Step 3. Identify dominant valences at each site, and dominant cation for each valence, being mindful of valency-imposed double site-occupancy (e.g., Appendix Table 3). This will identify the garnet by group and species.

Step 4. Write an empirical formula, ordering the cations first by valence and then by abundance.

Step 5. Calculate the maximum proportions of generalized components using the spreadsheet in Appendix 4 (e.g., Appendix Table 4).

Step 6. It may be necessary to factor in the results from step 4 before finalizing species identification (see notes).

Step 7. In some cases the maximum proportions of generalized components total 100% (examples 2, 6), in which case the components are all independent variables and can be used for plotting in Figures 6-9, 11. In most cases, the maximum proportions will total above 100%, and a subset of independent generalized components must be selected and recalculated to 100% for plotting, which is done for the other four examples.

Note: Discrepancies in the last decimal place are the result of rounding of tabulated values.

EXAMPLE 1. URANIAN DZHULUITE FROM THE NORTHERN CAUCASUS (GALUSKINA AND GALUSKIN, UNPUBLISHED DATA)

Appendix Table 1. Electron microprobe analysis with calculated $\text{Fe}^{2+}/\text{Fe}^{3+}$ ratio

	wt. %	apfu per	
12 O			
UO ₃	11.15	U ⁶⁺	0.282
Nb ₂ O ₅	0.87	Nb ⁵⁺	0.047
Sb ₂ O ₅	14.79	Sb ⁵⁺	0.661
SiO ₂	0.15	Si	0.018
TiO ₂	1.32	Ti	0.120
ZrO ₂	3.48	Zr	0.204
SnO ₂	16.20	Sn	0.777
Al ₂ O ₃	4.26	Al	0.604
Sc ₂ O ₃	0.13	Sc	0.014
Fe ₂ O ₃	20.96	Fe ³⁺	1.897

MgO	0.03	Mg	0.005
CaO	22.79	Ca	2.936
FeO	4.35	Fe ²⁺	0.437
Sum	100.48		8.000

Appendix Table 2. Site Allocation

	Z	
Fe ²⁺	0.437	0.379
Al ³⁺	0.604	0.604
Fe ³⁺	1.897	1.897
Si ⁴⁺	0.018	0.018
Ti ⁴⁺	0.044	0.103
Sum	3.000	3.000
charge	8.625	8.793

	Y	
Sc ³⁺	0.014	0.014
Ti ⁴⁺	0.075	0.016
Sn ⁴⁺	0.777	0.777
Zr ⁴⁺	0.204	0.204
Nb ⁵⁺	0.047	0.047
Sb ⁵⁺	0.661	0.661
U ⁶⁺	0.282	0.282
Sum	2.060	2.000

	X	
Ca	2.936	2.936
Mg	0.005	0.005
Fe ²⁺	0.000	0.059
Sum	2.941	3.000

1. Si, Al, Fe³⁺, Fe²⁺ and sufficient Ti to fill Z
2. Sc, remaining Ti, Sn, Nb, Sb and U to Y.
3. Ca and Mg to X

Column 1 gives allocation from Appendix 4. Because of the assignment of Fe²⁺ to the Z site in advance of Ti, calculated Y site occupancy exceeds 2 apfu, and X site occupancy is less than 3 apfu. Column 2 allocation with distribution of Fe²⁺ to achieve stoichiometry.

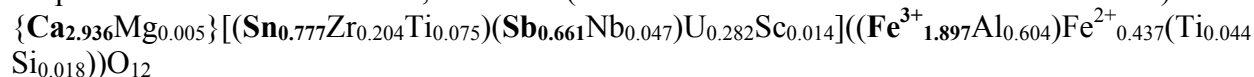
Appendix Table 3. Dominant valences, constituents and percent of homovalent cations (from column 1 of Table 1)

Site	Valence	Constituent	%	
Identification				
Z	+3	Fe	76	Bitikleite
group				
Y	+5	Sb	93	Dzhuluite
Y	+4	Sn	74	Dzhuluite

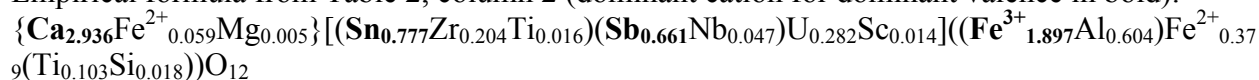
X +2 Ca 99.8 Dzhuluite

Note: Y is constrained to have two occupants because of valency-imposed double site-occupancy.

Empirical formula from Table 2, column 1 (dominant cation for dominant valence in bold):



Empirical formula from Table 2, column 2 (dominant cation for dominant valence in bold):



Appendix Table 4. Proportions of generalized components

Component	Maximum Proportion*	Proportion as independent variable [#]	Group or formula type
$\{R^{2+}_3\}[R^{6+}_2](R^{2+}_3)\text{O}_{12}$	14.08%	12.62%	yafsoanite-type
$\{R^{2+}_3\}[R^{4+}_{1.5}R^{6+}_{0.5}](R^{3+}_3)\text{O}_{12}$	56.32%	5.85%	Bitikleite: elbrusite-type
$\{R^{2+}_3\}[R^{5+}R^{4+}](R^{3+}_3)\text{O}_{12}$	70.78%	70.78%	Bitikleite: dzhuluite-type
$\{R^{2+}_3\}[R^{4+}_2](R^{4+}R^{3+}_2)\text{O}_{12}$	6.24%	10.07%	Schorlomite
$\{R^{2+}_3\}[R^{3+}_2](R^{4+}_3)\text{O}_{12}$	0.68%	0.68%	Garnet: eringaite-type
Total	141.11%	100.00%	

Note: *From column 1. [#]From column 2. The five generalized components are independent variables, but proportions as independent variables can only be calculated from a formula for ideal stoichiometry.

Comment: Uranium is split between two components (bitikleite and yafsoanite-type), both of which are subordinate, and thus Table 4 (either column 2 or column 3) and the empirical formulae give the same identification, dzhuluite, which has the generalized formula, $\{R^{2+}_3\}[R^{5+}R^{4+}](R^{3+}_3)\text{O}_{12}$.

EXAMPLE 2. GARNET MCO₄, HIGH TI, SCHORLOMITE FROM MAGNET COVE, ARKANSAS (CHAKHMOURADIAN AND MCCAMMON 2005)

Appendix Table 5. Electron microprobe analysis with calculated Fe²⁺/Fe³⁺ ratio

	Wt%		apfu per 12 O
SiO ₂	26.16	Si	2.250
TiO ₂	16.52	Ti	1.069
ZrO ₂	1.31	Zr	0.055
Al ₂ O ₃	1.60	Al	0.162
Fe ₂ O ₃	17.07	Fe ³⁺	1.105

FeO	3.44	Fe ²⁺	0.247
MnO	0.48	Mn	0.035
MgO	1.21	Mg	0.155
CaO	31.54	Ca	2.907
Na ₂ O	0.09	Na	0.015
Sum	99.42	Sum	8.000

Appendix Table 6. Site Allocation

<i>Z</i>	
Si	2.250
Al	0.162
Fe ³⁺	0.588
Sum	3.000
Charge	11.250
<i>Y</i>	
Ti	1.069
Zr	0.055
Fe ³⁺	0.517
Mg	0.155
Fe ²⁺	0.204
Sum	2.000
<i>X</i>	
Fe ²⁺	0.043
Ca	2.907
Mn	0.035
Na	0.015
Sum	3.000

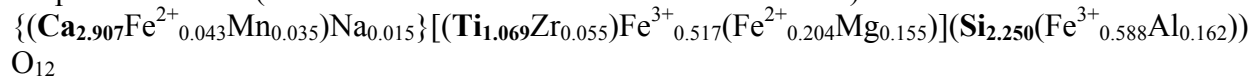
1. Si to *Z*
2. Al to *Z*
3. Fe³⁺ to *Z* to bring total to 3 apfu, then *Y*
4. Ca and Na to *X*
5. Ti⁴⁺, remaining Fe³⁺, and Zr to *Y*.
6. Mg: First to *Y*
7. Fe²⁺ First to *Y* to bring total to 2 apfu, then to *X*
8. Mn²⁺ to *X*, which brings total *X* to 3 apfu

Appendix Table 7. Dominant valences, constituents and percent of homovalent cations

Site	Valence	Constituent	%	
Identification				
<i>Z</i>	+4	Si	100	Garnet group *
<i>Y</i>	+4	Ti	95	Schorlomite
<i>X</i>	+2	Ca	97	
Schorlomite				

Note: * Cf. Appendix Table 8, which gives schorlomite group

Empirical formula (dominant cation for dominant valence in bold):



Appendix Table 8. Maximum proportions of generalized components

Component	Proportion	Group and type
$\{R^{2+}_3\}[R^{4+}_2](R^{4+}R^{3+}_2)\text{O}_{12}$	37.5%	Schorlomite
$\{R^{2+}_3\}[R^{3+}_2](R^{4+}_3)\text{O}_{12}$	25.9%	Garnet: andradite-type
$\{R^{2+}_3\}[R^{4+}R^{2+}](R^{4+}_3)\text{O}_{12}$	35.9%	Garnet: morimotoite-type
$\{R^{2+}_2R^{2+}\}[R^{4+}_2](R^{4+}_3)\text{O}_{12}$	0.8%	Garnet: $\{\text{Na}_2\text{Ca}\}[\text{Ti}_2](\text{Si}_3)\text{O}_{12}$ -type
Total	100.00%	

Note: The four generalized components are independent variables.

Comment: The empirical formula gives R^{4+} the dominant valence at Z and Y , but the identification is clear only from Table 8, which gives, $\{R^{2+}_3\}[R^{4+}_2](R^{4+}R^{3+}_2)\text{O}_{12}$, schorlomite, as the dominant component. The contradiction results from garnet-group components together being dominant, whereas schorlomite is more abundant than any one of the garnet components.

EXAMPLE 3. HOLOTYPE MENZERITE, PARRY SOUND, ONTARIO, CANADA-(Y) (GRAIN NO. 1-5, GREW ET AL. 2010)

Appendix Table 9. Electron microprobe analysis with calculated $\text{Fe}^{2+}/\text{Fe}^{3+}$ ratio

	Wt%		apfu per 12 O
SiO_2	30.64	Si	2.820
TiO_2	1.10	Ti	0.076
Al_2O_3	4.87	Al	0.528
Sc_2O_3	0.17	Sc	0.014
V_2O_3	0.17	V	0.013
Cr_2O_3	0.04	Cr	0.003
Fe_2O_3	8.36	Fe^{3+}	0.579
Y_2O_3	16.93	Y	0.829
La_2O_3	0.00	La	0.000
Ce_2O_3	0.01	Ce	0.000
Pr_2O_3	0.00	Pr	0.000
Nd_2O_3	0.12	Nd	0.004
Sm_2O_3	0.15	Sm	0.005
Eu_2O_3	0.01	Eu	0.000
Gd_2O_3	0.36	Gd	0.011
Tb_2O_3	0.11	Tb	0.003
Dy_2O_3	1.52	Dy	0.045
Ho_2O_3	0.63	Ho	0.018

Er ₂ O ₃	2.40	Er	0.069
Tm ₂ O ₃	0.38	Tm	0.011
Yb ₂ O ₃	2.03	Yb	0.057
Lu ₂ O ₃	0.68	Lu	0.019
MgO	3.98	Mg	0.546
CaO	13.92	Ca	1.372
MnO	0.85	Mn	0.066
FeO	11.84	Fe ²⁺	0.911
Sum	101.26	Sum	8.000

Appendix Table 10. Site Allocation

<i>Z</i>	
Si	2.820
Al	0.180
Sum	3.000
Charge	11.820
<i>Y</i>	
Ti	0.076
Al	0.348
Sc	0.014
V	0.013
Cr	0.003
Fe ³⁺	0.580
Mg	0.546
Fe ²⁺	0.422
Sum	2.000
<i>X</i>	
Y + REE	1.072
Ca	1.372
Mn	0.066
Fe ²⁺	0.489
Sum	3.000

1. Si: First to *Z*
2. Al to *Z* to bring total to 3 apfu, then *Y*
3. Fe³⁺ to *Y*
4. Ca, Y, REE to *X*
5. Al (after deducting Al at *Z*), Sc³⁺, Ti⁴⁺, V³⁺, Cr³⁺, Fe³⁺ to *Y*.
6. Mg: First to *Y*
7. Fe²⁺ First to *Y* to bring total to 2 apfu, then to *X*
8. Mn²⁺ to *X*, which brings total *X* to 3 apfu

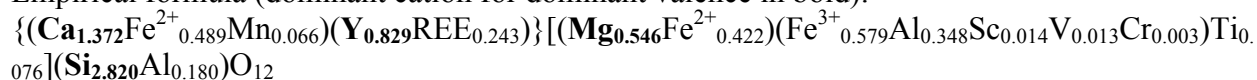
Appendix Table 11. Dominant valences, constituents and percent of homovalent cations

Site	Valence	Constituent	%
Identification			

Z	+4	Si	100	Garnet group
Y	+2	Mg	56	Menzerite-(Y)
X	+3	Y	77	Menzerite-(Y)
X	+2	Ca	71	Menzerite-
(Y)				

Note: X is constrained to have two occupants because of valency-imposed double site-occupancy.

Empirical formula (dominant cation for dominant valence in bold):



Appendix Table 12. Proportions of generalized components

Component	Maximum Proportion*	Proportion as independent variable [#]	Group and type
$\{R^{3+}_3\}[R^{3+}_2](R^{3+}_3)\text{O}_{12}$	6.02%	6.02%	$\{Y_3\}[\text{Al}_2](\text{Al}_3)\text{O}_{12}$ -type
$\{R^{2+}_3\}[R^{4+}_2](R^{4+}_2R^{3+}_2)\text{O}_{12}$	3.81%	—	Schorlomite
$\{R^{2+}_3\}[R^{4+}_2R^{2+}_2](R^{4+}_3)\text{O}_{12}$	7.61%	7.61%	Garnet: morimotoite-type
$\{R^{3+}_2R^{2+}_2\}[R^{2+}_2](R^{4+}_3)\text{O}_{12}$	48.42%	44.61%	Garnet: menzerite-(Y)-type
$\{R^{2+}_3\}[R^{3+}_2](R^{4+}_3)\text{O}_{12}$	47.77%	41.75%	Garnet: andradite-type
Total	113.64	100.00%	

Note: Y represents Y and REE. *From Appendix 4. Only four of these generalized components are independent. [#]One of two sets of independent variables

EXAMPLE 4. FLUORINE-BEARING SPESSARTINE FROM CLEAR CREEK COUNTY, COLORADO (SMYTH ET AL. 1990)

Appendix Table 13. Electron microprobe analysis with calculated $\text{Fe}^{2+}/\text{Fe}^{3+}$ ratio

	Wt%		apfu per 12 O
SiO ₂	32.55	Si	2.681
TiO ₂	0.06	Ti	0.004
Al ₂ O ₃	20.13	Al	1.954
Fe ₂ O ₃	0.33	Fe ³⁺	0.020
FeO	4.50	Fe ²⁺	0.310
MnO	37.98	Mn ²⁺	2.650
CaO	0.60	Ca	0.053
		Sum	7.672
H ₂ O+	0.64	OH	0.352
F	3.68	F	0.959
O=F	-1.55	O	10.690
Total	98.92	Sum	12.000

Note: H₂O content by IR spectroscopy.

Appendix Table 14. Site Allocation

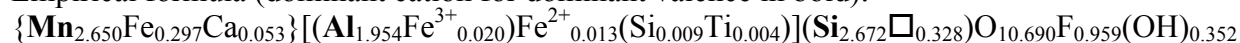
	<i>Z</i>
Si	2.672
vacancies	0.328
Sum	3.000
Charge	10.690
	<i>Y</i>
Al	1.954
Fe ³⁺	0.020
Fe ²⁺	0.013
Si	0.009
Ti	0.004
Sum	2.000
	<i>X</i>
Mn ²⁺	2.650
Fe ²⁺	0.297
Ca	0.053
Sum	3.000

1. Vacancies equal to $\frac{1}{4}$ F plus $\frac{1}{4}$ (OH) to *Z*
2. Si to *Z* to bring total of Si and vacancies to 3
3. Remaining Si to *Y*
4. Al, Ti to *Y*
5. Fe²⁺ to *Y* to bring total to 2 apfu
6. Mn, Ca and remaining Fe²⁺ to *X*

Appendix Table 15. Dominant valences, constituents and percent of homovalent cations

Site	Valence	Constituent	%	
	Identification			
<i>Z</i>	+4	Si	100	Garnet group
<i>Y</i>	+3	Al	99	Garnet group
<i>X</i>	+2	Mn	88	Spessartine

Empirical formula (dominant cation for dominant valence in bold):



Appendix Table 16. Proportions of generalized components

Generalized Component	Maximum proportion *	Proportion as independent variable [#]	Group or formula type
$\{R^{2+}_3\}[R^{3+}_2](\square)_3(\text{OH})_{12}$	2.93%	2.93%	katoite-type
$\{R^{2+}_3\}[R^{3+}_2](\square)_3\text{F}_{12}$	7.99%	7.99%	$\{\text{Mn}_3\}[\text{Al}_2](\square)_3\text{F}_{12}$ -type
$\{R^{2+}_3\}[R^{3+}_2](R^{4+}_2\square)(\text{OH})_4$	8.79%	—	Henritermierite-type
$\{R^{2+}_3\}[R^{4+}_2](R^{4+}R^{3+}_2)\text{O}_{12}$	0.02%	—	Schorlomite-type
$\{R^{2+}_3\}[R^{4+}R^{2+}](R^{4+}_3)\text{O}_{12}$	1.27%	1.27%	Garnet: morimotoite-type

$\{R^{2+}_3\}[R^{3+}_2](R^{4+}_3)O_{12}$	89.08%	87.81%	Garnet: spessartine-type
Total	110.06%	100.00%	

Note: *From Appendix 4.

EXAMPLE 5. GARNET JF22. „MAJORITIC“ GARNET INCLUDED IN DIAMOND, JAGERSFONTEIN KIMBERLITE, SOUTH AFRICA (TAPPERT ET AL. 2005)

Appendix Table 17. Electron microprobe analysis with calculated Fe^{2+}/Fe^{3+} ratio

	Wt%	apfu per 12
O		
P ₂ O ₅	0.09	P
	0.006	
SiO ₂	48.70	Si
	3.525	
TiO ₂	0.50	Ti
	0.027	
Al ₂ O ₃	9.65	Al
	0.823	
Cr ₂ O ₃	0.22	Cr
	0.013	
Fe ₂ O ₃	2.49	Fe ³⁺
	0.135	
MgO	21.70	Mg
	2.341	
CaO	5.73	Ca
	0.444	
MnO	0.36	Mn
	0.022	
FeO	9.46	Fe ²⁺
	0.573	
Na ₂ O	0.65	Na
	0.091	
Sum	99.55	Sum
	8.000	

Appendix Table

18. Site

Allocation

	Z
P	0.006
Si	2.994
Sum	3.000
Charge	12.006

	<i>Y</i>
Si	0.530
Ti	0.027
Al	0.823
Cr	0.013
Fe ³⁺	0.135
Mg	0.472
Sum	2.000

	<i>X</i>
Na	0.091
Ca	0.444
Mn	0.022
Fe	0.573
Mg	1.870
Sum	3.000

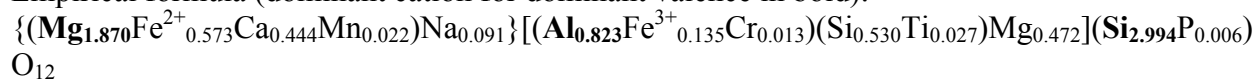
1. Si and P to Z to a maximum of 3 apfu, overflow of Si to *Y*
2. Ca and Na to *X*
3. Ti⁴⁺, Cr³⁺, Fe³⁺ to *Y*
4. Mg: First to *Y* to bring total to 2 apfu, then to *X*
5. Fe²⁺ to *X*
6. Mn²⁺ to *X*, which brings total to 3 apfu

Appendix Table 19. Dominant valences, constituents and percent of homovalent cations

Site	Valence	Constituent	%	
	Identification			
Z	+4	Si	100	Garnet group
Y	+3	Al	85	Pyrope
X	+2	Mg	64	Pyrope

Note: Because of valency-imposed double site-occupancy at *Y*, R⁴⁺Mg is considered as a unit, which is still subordinate to 2R³⁺ (Table 8).

Empirical formula (dominant cation for dominant valence in bold):



Appendix Table 20. Proportions of generalized components

Component	Maximum Proportion*	Proportion as independent variable [#]	Group and type
{R ¹⁺ ₃ }[R ³⁺ ₂](R ⁵⁺ ₃)O ₁₂	0.18%	0.18%	Berzeliite: {Na ₃ }[Al ₂](P ₃)O ₁₂ -type
{R ²⁺ ₂ R ¹⁺ }[R ²⁺ ₂](R ⁵⁺ ₃)O ₁₂	0.18%	—	Berzeliite-type

$\{R^{2+}_2R^{2+}\}[R^{4+}_2](R^{4+}_3)O_{12}$	4.56%	4.28%	Garnet: $\{Na_2Ca\}[Ti_2](Si_3)O_{12}$ -type
$\{R^{2+}_3\}[R^{3+}_2](R^{4+}_3)O_{12}$	48.55%	48.37%	Garnet: pyrope-type
$\{R^{2+}_3\}[R^{4+}_2R^{2+}](R^{4+}_3)O_{12}$	47.16%	47.16%	Garnet: majorite-type
Total	100.64%	100.00%	

Note: *From Appendix 4. Only four of these generalized components are independent. * One of two sets of independent variables.

Comment: No matter which set of independent components is chosen, the generalized component, $\{R^{2+}_3\}[R^{3+}_2](Si_3)O_{12}$, pyrope, is dominant.

EXAMPLE 6. HOLOTYPE MORIMOTOITE, FUKA, OKAYAMA PREFECTURE, JAPAN (HENMI ET AL. 1995)

Appendix Table 21. Electron microprobe analysis with calculated Fe^{2+}/Fe^{3+} ratio

	Wt%		12 O
SiO ₂	26.93	Si	2.319
TiO ₂	18.51	Ti	1.199
ZrO ₂	1.48	Zr	0.062
Al ₂ O ₃	0.97	Al	0.098
Fe ₂ O ₃	11.44	Fe ³⁺	0.741
FeO	7.77	Fe ²⁺	0.559
MnO	0.23	Mn	0.017
MgO	0.87	Mg	0.112
CaO	31.35	Ca	2.893
Sum	99.54	Sum	8.000

Appendix Table 22. Site Allocation

<i>Z</i>	
Si	2.319
Al	0.098
Fe ³⁺	0.583
Sum	3.000
Charge	11.319
<i>Y</i>	
Ti	1.199
Zr	0.062
Fe ³⁺	0.158
Mg	0.112
Fe ²⁺	0.469
Sum	2.000
<i>X</i>	
Fe ²⁺	0.091
Ca	2.893
Mn	0.017

Sum 3.000

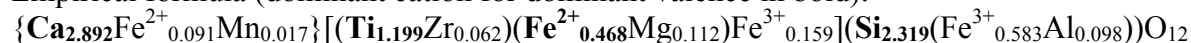
1. Si to *Z*
2. Al to *Z*
3. Fe³⁺ to *Z* to bring total to 3 apfu, then *Y*
4. Ca to *X*
5. Ti⁴⁺, remaining Fe³⁺, and Zr to *Y*.
6. Mg: to *Y*
7. Fe²⁺ First to *Y* to bring total to 2 apfu, then to *X*
8. Mn²⁺ to *X*, which brings total *X* to 3 apfu

Appendix Table 23. Dominant valences, constituents and percent of homovalent cations

Site	Valence	Constituent	%	
	Identification			
<i>Z</i>	+4	Si	100	Garnet group
<i>Y</i>	+4	Ti	95	Morimotoite
<i>Y</i>	+2	Fe	81	Morimotoite
<i>X</i>	+2	Ca	96	
	Morimotoite			

Note: *Y* is constrained to have two occupants because of valency-imposed double site-occupancy.

Empirical formula (dominant cation for dominant valence in bold):



Appendix Table 24. Maximum proportions of generalized components

Component	Proportion	Group
$\{R^{2+}_3\}[R^{4+}_2](R^{4+}R^{3+}_2)\text{O}_{12}$	34.05%	Schorlomite
$\{R^{2+}_3\}[R^{3+}_2](R^{4+}_3)\text{O}_{12}$	7.93%	Garnet: andradite-type
$\{R^{2+}_3\}[R^{4+}R^{2+}](R^{4+}_3)\text{O}_{12}$	58.01%	Garnet: morimotoite
type		
Total	100.00%	

Note: The three generalized components are independent variables.

Comment: The empirical formula gives R^{4+} the dominant valence at *Z* and *Y*, with R^{2+} second at *Y*, but the identification is clear from Table 20, which gives $\{R^{2+}_3\}[R^{4+}R^{2+}](R^{4+}_3)\text{O}_{12}$, morimotoite, as the dominant component.