TABLE 9. Appendix Table 1. Electron microprobe analysis with calculated Fe^{2+}/Fe^{3+} ratio

	wt%		apfu per 12 O
UO_3	11.15	U^{6+}	0.282
Nb_2O_5	0.87	Nb^{5+}	0.047
Sb_2O_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_2O_3	4.26	Al	0.604
Sc_2O_3	0.13	Sc	0.014
Fe_2O_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

TABLE 10. 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, Fe^{3+}, Fe^{2+} 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 Fe^{2+} 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 Fe^{2+} to achieve stoichiometry.

TABLE 11. 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):.

$\{\mathbf{Ca_{2.936}}Mg_{0.005}\}[(\mathbf{Sn_{0.777}}Zr_{0.204}Ti_{0.075})(\mathbf{Sb_{0.661}}Nb_{0.047})U_{0.282}Sc_{0.014}]((\mathbf{Fe^{3+}_{1.897}}Al_{0.604})Fe^{2+}_{0.437}(Ti_{0.044}Si_{0.018}))O_{12}$.

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

$\{\mathbf{Ca_{2.936}}Fe^{2+}_{0.059}Mg_{0.005}\}[(\mathbf{Sn_{0.777}}Zr_{0.204}Ti_{0.016})(\mathbf{Sb_{0.661}}Nb_{0.047})U_{0.282}Sc_{0.014}]((\mathbf{Fe^{3+}_{1.897}}Al_{0.604})Fe^{2+}_{0.379}(Ti_{0.103}Si_{0.018}))O_{12}$.

TABLE 12. Appendix Table 4. Proportions of generalized components

Component	Maximum Proportion*	Proportion as independent variable#	Group or formula type
$\{R^{2+}_3\}[R^{6+}_2](R^{2+}_3)O_{12}$	14.08%	12.62%	yafsoanite-type
$\{R^{2+}_3\}[R^{4+}_{1.5}R^{6+}_{0.5}](R^{3+}_3)O_{12}$	56.32%	5.85%	Bitikleite: elbrusite-type
$\{R^{2+}_3\}[R^{5+}R^{4+}](R^{3+}_3)O_{12}$	70.78%	70.78%	Bitikleite: dzhuluite-type
$\{R^{2+}_3\}[R^{4+}_2](R^{4+}R^{3+}_2)O_{12}$	6.24%	10.07%	Schorlomite
$\{R^{2+}_3\}[R^{3+}_2](R^{4+}_3)O_{12}$	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 formulas give the same identification, dzhuluite, which has the generalized formula, $\{R^{2+}{}_3\}[R^{5+}R^{4+}](R^{3+}{}_3)O_{12}$.

Example 2. Garnet MCO4, high Ti, schorlomite from Magnet Cove, arkansas (Chakhmouradian and McCammon 2005).

TABLE 13. Appendix Table 5. Electron microprobe analysis with calculated Fe^{2+}/Fe^{3+} 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_2O_3	1.60	Al	0.162
Fe_2O_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_2O	0.09	Na	0.015
Sum	99.42	Sum	8.000

TABLE 14. Appendix Table 6. Site Allocation

		Z
Si	2.250	
Al	0.162	
Fe^{3+}	0.588	
Sum	3.000	
Charge	11.250	
		Y
Ti	1.069	
Zr	0.055	
Fe^{3+}	0.517	
Mg	0.155	
Fe^{2+}	0.204	
Sum	2.000	
		X
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. Fe^{3+} to *Z* to bring Total to 3 apfu, then *Y*.

4. Ca and Na to *X* .

5. Ti^{4+}, remaining Fe^{3+}, and Zr to *Y*..

6. Mg: First to *Y*.

7. Fe^{2+} First to *Y* to bring Total to 2 apfu, then to *X*.

8. Mn^{2+} to *X*, which brings Total *X* to 3 apfu.

TABLE 15. Appendix Table 7. Dominant valences, constituents and percent of homovalent cations

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

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

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

$\{(\mathbf{Ca_{2.907}}Fe^{2+}_{0.043}Mn_{0.035})Na_{0.015}\}[(\mathbf{Ti_{1.069}}Zr_{0.055})Fe^{3+}_{0.517}(Fe^{2+}_{0.204}Mg_{0.155})](\mathbf{Si_{2.250}}(Fe^{3+}_{0.588}Al_{0.162}))O_{12}$.

TABLE 16. Appendix Table 8. Maximum proportions of generalized components

Component	Proportion	Group and type
$\{R^{2+}_3\}[R^{4+}_2](R^{4+}R^{3+}_2)O_{12}$	37.5%	Schorlomite
$\{R^{2+}_3\}[R^{3+}_2](R^{4+}_3)O_{12}$	25.9%	Garnet: andradite-type
$\{R^{2+}_3\}[R^{4+}R^{2+}](R^{4+}_3)O_{12}$	35.9%	Garnet: morimotoite-type
$\{R^{+}_2R^{2+}\}[R^{4+}_2](R^{4+}_3)O_{12}$	0.8%	Garnet: $\{Na_2Ca\}[Ti_2](Si_3)O_{12}$-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, $\{R^{2+}{}_3\}[R^{4+}{}_2](R^{4+}R^{3+}{}_2)O_{12}$, 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).

TABLE 17. Appendix Table 9. Electron microprobe analysis with calculated Fe^{2+}/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_2O_3	2.40	Er	0.069
Tm_2O_3	0.38	Tm	0.011
Yb_2O_3	2.03	Yb	0.057
Lu_2O_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

TABLE 18. Appendix Table 10. Site Allocation

	Z
Si	2.820
Al	0.180

Sum	3.000
Charge	11.820
	Y
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
	X
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. Fe^{3+} to *Y*.

4. Ca, Y, REE to *X* .

5. Al (after deducting Al at *Z*), Sc^{3+}, Ti^{4+}, V^{3+}, Cr^{3+}, Fe^{3+} to *Y*..

6. Mg: First to *Y*.

7. Fe^{2+} First to *Y* to bring Total to 2 apfu, then to *X*.

8. Mn^{2+} to *X*, which brings Total *X* to 3 apfu.

TABLE 19. 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):.

$\{(\mathbf{Ca_{1.372}}Fe^{2+}_{0.489}Mn_{0.066})(\mathbf{Y_{0.829}}REE_{0.243})\}[(\mathbf{Mg_{0.546}}Fe^{2+}_{0.422})(Fe^{3+}_{0.579}Al_{0.348}Sc_{0.014}V_{0.013}Cr_{0.003})Ti_{0.076}](\mathbf{Si_{2.820}}Al_{0.180})O_{12}$.

TABLE 20. Appendix Table 12. Proportions of generalized components

Component	Maximum Proportion*	Proportion as independent variable#	Group and type
$\{R^{3+}_3\}[R^{3+}_2](R^{3+}_3)O_{12}$	6.02%	6.02%	$\{Y_3\}[Al_2](Al_3)O_{12}$-type
$\{R^{2+}_3\}[R^{4+}_2](R^{4+}R^{3+}_2)O_{12}$	3.81%	–	Schorlomite
$\{R^{2+}_3\}[R^{4+}R^{2+}](R^{4+}_3)O_{12}$	7.61%	7.61%	Garnet: morimotoite-type
$\{R^{3+}_2R^{2+}\}[R^{2+}_2](R^{4+}_3)O_{12}$	48.42%	44.61%	Garnet: menzerite-(Y)-type
$\{R^{2+}_3\}[R^{3+}_2](R^{4+}_3)O_{12}$	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).

TABLE 21. Appendix Table 13. Electron microprobe analysis with calculated Fe^{2+}/Fe^{3+} ratio

	Wt%	apfu per 12 O	
SiO_2	32.55	Si	2.681
TiO_2	0.06	Ti	0.004
Al_2O_3	20.13	Al	1.954
Fe_2O_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_2O+	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: H_2O content by IR spectroscopy.

TABLE 22. Appendix Table 14. Site Allocation

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

1. Vacancies equal to ¼ F plus ¼ (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. Fe^{2+} to *Y* to bring Total to 2 apfu.

6. Mn, Ca and remaining Fe^{2+} to *X*.

TABLE 23. Appendix Table 15. Dominant valences, constituents and percent of homovalent cations

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

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

$\{\mathbf{Mn}_{2.650}Fe_{0.297}Ca_{0.053}\}[(\mathbf{Al}_{1.954}Fe^{3+}_{0.020})Fe^{2+}_{0.013}(Si_{0.009}Ti_{0.004})](\mathbf{Si}_{2.672}o_{0.328})O_{10.690}F_{0.959}(OH)_{0.352}$.

TABLE 24. Appendix Table 16. Proportions of generalized components

Generalized Component	Maximum	Proportion as Group or formula type

	proportion*	independent variable#	
$\{R^{2+}{}_3\}[R^{3+}{}_2](\text{o})_3(\text{OH})_{12}$	2.93%	2.93%	katoite-type
$\{R^{2+}{}_3\}[R^{3+}{}_2](\text{o})_3\text{F}_{12}$	7.99%	7.99%	$\{Mn_3\}[Al_2](\text{o})_3F_{12}$-type
$\{R^{2+}{}_3\}[R^{3+}{}_2](R^{4+}{}_2\text{o})(\text{OH})_4$	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
$\{R^{2+}{}_3\}[R^{3+}{}_2](R^{4+}{}_3)\text{O}_{12}$	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).

TABLE 25. Appendix Table 17. Electron microprobe analysis with calculated Fe^{2+}/Fe^{3+} ratio

	Wt%	apfu per 12 O	
P_2O_5	0.09	P	0.006
SiO_2	48.70	Si	3.525
TiO_2	0.50	Ti	0.027
Al_2O_3	9.65	Al	0.823
Cr_2O_3	0.22	Cr	0.013
Fe_2O_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_2O	0.65	Na	0.091
Sum	99.55	Sum	8.000

TABLE 26. Appendix Table 18. Site Allocation

	Z
P	0.006
Si	2.994
Sum	3.000
Charge	12.006
	Y
Si	0.530
Ti	0.027
Al	0.823
Cr	0.013

Fe^{3+}	0.135
Mg	0.472
Sum	2.000
X	
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. Ti^{4+}, Cr^{3+}, Fe^{3+} to *Y*.

4. Mg: First to *Y* to bring Total to 2 apfu, then to *X*.

5. Fe^{2+} to *X*.

6. Mn^{2+} to *X*, which brings Total to 3 apfu.

TABLE 27. 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*, R^{4+}Mg is considered as a unit, which is still subordinate to $2R^{3+}$ (Table 8).

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

$\{(\mathbf{Mg_{1.870}}Fe^{2+}_{0.573}Ca_{0.444}Mn_{0.022})Na_{0.091}\}[(\mathbf{Al_{0.823}}Fe^{3+}_{0.135}Cr_{0.013})(Si_{0.530}Ti_{0.027})Mg_{0.472}](\mathbf{Si_{2.994}}P_{0.006})\ O_{12}$.

TABLE 28. 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
$\{R^{2+}{}_2R^{1+}\}[R^{2+}{}_2](R^{5+}{}_3)O_{12}$	0.18%	–	Berzeliite-type
$\{R^{+}{}_2R^{2+}\}[R^{4+}{}_2](R^{4+}{}_3)O_{12}$	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
$\{R^{2+}{}_3\}[R^{4+}R^{2+}](R^{4+}{}_3)O_{12}$	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).

TABLE 29. 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_2O_3	0.97	Al	0.098
Fe_2O_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

TABLE 30. Appendix Table 22. Site Allocation

	Z
Si	2.319
Al	0.098
Fe^{3+}	0.583
Sum	3.000
Charge	11.319
	Y
Ti	1.199
Zr	0.062
Fe^{3+}	0.158
Mg	0.112
Fe^{2+}	0.469

Sum	2.000
	X
Fe^{2+}	0.091
Ca	2.893
Mn	0.017
Sum	3.000

1. Si to *Z*.

2. Al to *Z*.

3. Fe^{3+} to *Z* to bring Total to 3 apfu, then *Y*.

4. Ca to *X* .

5. Ti^{4+}, remaining Fe^{3+}, and Zr to *Y*..

6. Mg: to *Y*.

7. Fe^{2+} First to *Y* to bring Total to 2 apfu, then to *X*.

8. Mn^{2+} to *X*, which brings Total *X* to 3 apfu.

TABLE 31. Appendix Table 23. Dominant valences, constituents and percent of homovalent cations

Site	Valence	Constituent	%	Identification
Z	+4	Si	100	Garnet group
Y	+4	Ti	95	Morimotoite
Y	+2	Fe	81	Morimotoite
X	+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):.

$\{\mathbf{Ca_{2.892}}Fe^{2+}_{0.091}Mn_{0.017}\}[(\mathbf{Ti_{1.199}}Zr_{0.062})(\mathbf{Fe^{2+}_{0.468}}Mg_{0.112})Fe^{3+}_{0.159}](\mathbf{Si_{2.319}}(Fe^{3+}_{0.583}Al_{0.098}))O_{12}$.

TABLE 32. Appendix Table 24. Maximum proportions of generalized components

Component	Proportion	Group
$\{R^{2+}_3\}[R^{4+}_2](R^{4+}R^{3+}_2)O_{12}$	34.05%	Schorlomite
$\{R^{2+}_3\}[R^{3+}_2](R^{4+}_3)O_{12}$	7.93%	Garnet: andradite-type
$\{R^{2+}_3\}[R^{4+}R^{2+}](R^{4+}_3)O_{12}$	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 $\{R^{2+}_3\}[R^{4+}R^{2+}](R^{4+}_3)O_{12}$, morimotoite, as the dominant component.