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Eigenvector and principal components Analysis of Granitic Rocks from the Bergell Alps

by *Olav H. J. Christie**

Abstract

Geological samples may be considered as points in an observation space that has as many orthogonal axes as there are variables. Conventional petrologic diagrams represent projections from this observation space, and by the projection significant information may be lost. The optimum retained information is obtained by projection into eigenvector spaces. This is exemplified by projection of sample points of granitic rocks from the Bergell Alps from an eighteen-dimensional observation space into a three-dimensional eigenvector space. A disjoint principal components analysis in the direct observation space quantifies the degree of relation between the studied rocks, and confirms the cluster pattern observed in the eigenvector space.

Introduction

In a recent paper WENK et al. (1977) studied relations in chemical composition between migmatites, granites, tonalites and amphibolites in the Bergell Alps. They suggested that Bergell megacrystic granite may have formed by partial melting of the Gruf migmatites, and Bergell tonalite by a mixture of the Bergell megacrystic granite and amphibolite. Furthermore, they demonstrated by aid of discriminant analysis that there is no continuous transition from tonalites to granites, thus revising the viewpoint of RICHARDSON et al. (1974).

WENK et al. have not studied the petrogenetic relations between Bergell microgranites and aplites. In their Figure 2, displaying plots in conventional petrologic triangle diagrams, the granites, microgranites and aplites are not resolved, but the pairwise discriminant analysis presented in their paper indicates that there is information in the data about differences between the granitic rocks that may clarify petrogenetic relations. The goal of the present work is to study in more detail the interrelations of the granitic rocks of the Bergell Alps.

METHODS

All the data for the present work has been taken from WENK et al. (1977). The variables used are given in Table 1. It is worth noting that these variables are not independent. The first twelve of them are the conventional "main chemical

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Table 1. *List of variables*

1	SiO_2	10	K_2O
2	TiO_2	11	P_2O_5
3	$Al2O_3$	12	H_2O
4	Fe_2O_3	13	Qtz
5	FeO	14	Cor
6	MnO	15	Or
7	MgO	16	Ab
8	CaO	17	An
9	Na_2O	18	Bi

constituents" and constitute a numerically closed system. With the exception of K_2O they are all negatively correlated with the main constituent SiO_2. Furthermore, the values of the normative minerals are calculated from the chemical constituents, and reflect interrelations between them in a manner different from the correlation coefficients.

The data have been subjected to a Karhunen-Loéwe based eigenvector analysis, using autoscaled data, as described by KOWALSKI and BENDER (1974). The calculations have been made by the program ARTHUR, written by B. R. KOWALSKI of the University of Washington, Seattle. The result of this analysis is displayed in a stereoscopic first-to-second-to-third eigenvector plot made by aid of a Calcomp plotter and the program OR-TEP, written by JOHNSON (1964). The grouping of the studied rocks has been studied in more detail by aid of the disjoint principal components analysis by WOLD (1976), and the calculations have been made by the program SIMCA, written by him.

RESULTS

Eigenvector Analysis

The stereoscopic plot of Bergell megacrystic granites, inclusions of megacrystic granite in migmatite, equigranular Bergell granites, Gruf migmatites, Cameraccio granodiorites, augengneisses of the Tambo nappe, micrograniteset and aplites is given in Figure 1. It is a typical feature of the plot that different groups of the studied rocks tend to spread out from the center of the diagram in particular directions. Thus, each of these directions in the eigenvector space characterises its rock group.

The old granitic augengneisses of the Tambo nappe are, as a group, well separated from the migmatites.

The Bergell megacrystic granite and Gruf migmatites are closely related by their chemical and normative composition, as already pointed out by WENK et al. It is, furthermore, evident that micrograniteset form a cluster with an orientation in the eigenvector space different from that of the Gruf migmatites and the

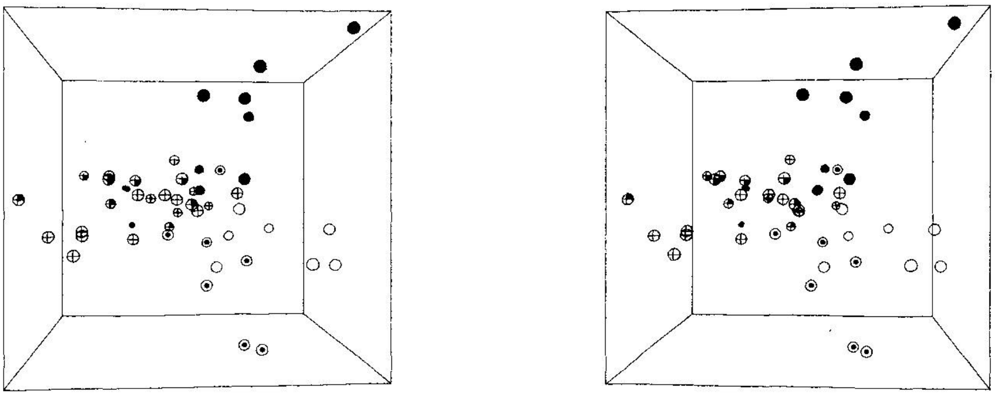

Figure 1. Stereoscopic plots of sample points in the first-to-second-to-third eigenvector space. Projection from the eighteen-dimensional observation space with 75.3 per cent of the total information about point spread retained. The first, second and third eigenvector fall along the x, y and z direction respectively, and for clarity of display they have been made equally long. Point marking: Bergell megacrystic and equigranular granite—cross, inclusions in migmatite—cross and central dot, Gruf migmatite—cross and shade, microgranite—central dot, aplite—open spheres, Cameraccio granite—small black spheres, augengneiss of the Tambo nappe—large black spheres.

Bergell granite. This indicates that there is no significant petrogenetic relation between the microgranites and the group Bergell granite and Gruf migmatites.

Aplites, however, could conceivably be considered as a cluster oriented in continuation of the Bergell-Gruf cluster. The Cameraccio granodiorites are located near the center of the Bergell granite point cluster.

From Table 2 it is evident that the data for SiO_2, TiO_2, FeO, MgO and CaO give important contributions to sample point spread along the first eigenvector, Na_2O along the second eigenvector, and Al_2O_3 and Fe_2O_3 along the third eigenvector. The interrelations between the constituents are also reflected in the contribution of Or, An an Bi to the first eigenvector, Ab to the second eigenvector and Cor to the third eigenvector.

Consequently, a plot of Or + An + Bi versus Ab would be the most efficient two-dimensional cartesian system to distinguish between the sample points, as

Table 2. *Elements (loadings), retained and cumulative information of the three first eigenvectors.*

	1	2	3
SiO_2	+0.309	+0.007	+0.220
TiO_2	−0.283	+0.214	+0.042
Al_2O_3	−0.203	−0.083	−0.514
Fe_2O_3	−0.193	+0.144	−0.410
FeO	−0.278	+0.179	−0.165
MnO	−0.106	+0.022	+0.116
MgO	−0.298	+0.004	+0.152
CaO	−0.320	+0.035	+0.056
Na_2O	−0.086	−0.591	+0.009
K_2O	+0.250	+0.087	−0.025
P_2O_5	−0.243	+0.240	+0.176
H_2O	−0.087	+0.104	−0.213

	1	2	3
Qtz	+0.228	+0.291	+0.155
Cor	+0.028	+0.218	−0.524
Or	+0.287	+0.058	−0.093
Ab	−0.112	−0.570	+0.008
An	−0.310	−0.016	+0.026
Bi	−0.293	+0.084	+0.254
% Ret. info	49.5	14.3	11.5
% Cum. info.	49.5	63.8	75.3

long as untreated data are concerned. This plot is, however, inferior to the first-to-second eigenvector plot, that accounts for 63.8 per cent of the total information about sample point spread. The three-dimensional first-to-second-to-third eigenvector diagram of Figure 1 accounts for 75.3 per cent of the total information.

This makes it clear that it is neccessary to use rather sophisticated methods in data analysis if one wishes to investigate subtle differences between groups of rocks in terms of their chemical and normative composition. As a first approach eigenvector analysis may give valuable information about clusters among the sample points.

Disjoint principal components analysis

The diagram of Figure 1 is a projection from an eighteen-dimensional observation space into a three-dimensional eigenvector space. Even though it contains 75.3 per cent of the total information, it is desirable to extract the optimum of information from the observation space, and to quantify the interrelations between the clusters of sample points.

This has been done by aid of the disjoint principal components analysis by WOLD (1976). Emphasis has been put on investigation of the clusters, called classes below, describing them in terms of a principal components equation, finding the least number of terms that adequately describes the classes and the distance between them, and to what extent each variable contributes to the discrimination between them.

As a first approach it was assumed that the rocks could be assigned to classes corresponding to the classification made by Wenk et al. in their Table 2, ignoring the information about similarities and differences given in their text. This is a "blind" approach, in so far that no emphasis is put on this important information, but it is also a test to see if the petrographic classification based upon thin section work and field experience is reflected in the chemical parameters.

Thus seven classes were assumed to be present: megacrystic Bergell granite, equigranular Bergell granite, Cameraccio granodiorite, microgranite, aplite dikes, Gruf migmatites and related rocks, and granitic augengneisses of the Tambo nappe. Following the results of the crossvalidation of the principal components analysis, this initial step was based on describing each class with a two-term principal components equation.

The cluster distance matrix, variable relevance, and discrimination power for each variable are given in the Table 2. From this table it is evident that there is a small cluster distance between the megacrystic and the equigranular Bergell granite, whereas there is a large cluster distance between the equigranular and the megacrystic Bergell granite. This is not a contradictory statement, but expresses that the megacrystic class is much larger than the equigranular class, which consists only of two samples.

The Cameraccio granodiorite is reasonably well separated from all the other classes. The microgranite cluster is close to the equigranular Bergell granite cluster, the Gruf migmatite is close to both the latter classes, and the augengneisses of the Tambo nappe are poorly separated from the equigranular Bergell granite and the aplite dikes.

The distance between sample points in the Gruf migmatite as a whole is somewhat larger than the sample point distance between the Gruf migmatite model and samples of the Bergell granite and the Cameraccio granodiorite.

Furthermore, it is worth of note that with the exception of the data for MnO, all variables contribute to the separation of classes.

The data of Table 3 indicate that some clusters are very closely situated, and actually should be classified as one class. Therefore, a selection of samples were used for definition of a reduced number of classes. The class defining samples are given in Table 4. The reason why a selection of samples was used for the class definition rather than all samples of each class is that by this approach it is

Table 3: *Cluster distance matrix, normalised values, for the original seven classes of rocks from the Bergell Alps: 1 megacrystic Bergell granite, 2 equigranular Bergell granite, 3 Cameraccio granite, 4 microgranite, 5 aplite dikes, 6 Gruf migmatites and 7 old granitic augengneisses of the Tambo nappe.*

1	2	3	4	5	6	7	
1	1.000	2.266	1.952	2.150	2.297	0.968	1.872
2	1.039	1.000	2.394	1.168	1.392	0.983	1.105
3	1.518	2.366	1.000	1.913	2.396	0.996	2.003
4	1.757	1.841	2.800	1.000	1.440	1.223	1.690
5	1.762	1.881	3.420	1.686	1.000	1.120	1.456
6	1.738	2.664	2.153	2.454	2.238	1.000	2.081
7	1.844	2.048	3.320	2.292	2.099	1.414	1.000

Variable Variable	Discr. relevance	power	Variable Variable	Discr. relevance	power
SiO_2	0.832	5.4	Qtz	0.580	4.1
TiO_2	0.847	3.6	Cor	0.702	3.6
Al_2O_3	0.527	2.1	Or	0.993	6.1
Fe_2O_3	0.529	2.2	Ab	0.964	6.4
FeO	0.886	3.7	An	0.924	11.5
MnO	0.175	1.3	Bi	0.953	4.6
MgO	1.000	9.9			
CaO	0.963	12.7			
Na_2O	0.941	6.0			
K_2O	0.947	4.9			
P_2O_5	0.917	4.3			
H_2O	0.724	3.2			

Table 4: *Class defining samples for reduced number of classes*

Bergell granites		Microgranite		Old granitic rocks of the Tambo nappe	
579	Sciora	1086	Sissone	62	Promontogno
667	Albigna	1098	Forno	328	Marlun
954	Badile	1101	Forno	740	Castasegna
1102a	Rosso	1108	Rossi	801	Soglio
Gruf migmatites		**Aplite dikes**			
531b	Borgonovo	665	Albigna		
1112a	Lera	1103	Rosso		
1438	Gruf	1105	Rosso		
1554	Torrone	1107c	Forno		

possible to test the "goodness" of each approach by observing how well the class defining samples (training set) and the unclassified samples (test set) are assigned to proper classes.

Again, the crossvalidation indicated that the principal components equation with two terms most adequately describes the classes, and, consequently, this was chosen for the following data analysis. The cluster distance matrix, the variable relevance and the discrimination power for each variable are given in Table 5. Now all the variables contribute to the separation of the classes, and it is evident that the Bergell granite and the Gruf migmatites are poorly separated,

Forno Table 5: *Cluster distance matrix, normalised values, variable relevance, and the discrimination power for each variable. 1 Bergell granites, 2 Gruf migmatites, 3 microgranite, 4 aplite dikes, 5 old granitic gneisses of the Tambo nappe.*

	1	2	3	4	5
1	1.000	1.612	3.380	2.917	3.311
2	1.185	1.000	3.548	1.956	3.156
3	2.377	2.057	1.000	1.891	3.044
4	2.321	1.990	2.682	1.000	2.356
5	1.924	2.277	3.967	2.477	1.000

Variable Variable	Discr. relevance	power	Variable Variable	Discr. relevance	power
SiO_2	0.738	6.4	Qtz	0.628	10.0
TiO_2	0.657	6.6	Cor	0.833	17.0
Al_2O_3	0.873	7.5	Or	0.851	13.1
Fe_2O_3	0.660	5.5	Ab	0.937	25.0
FeO	0.461	7.8	An	0.711	9.6
MnO	0.432	3.2	Bi	0.527	9.0
MgO	0.569	8.9			
CaO	0.744	10.1			
Na_2O	0.921	25.0			
K_2O	1.000	14.8			
P_2O_5	0.529	11.5			
H_2O	0.252	2.9			

Table 6: *Cluster distance matrix, normalised values, variable relevance, and the discrimination power for each variable. 1 Bergell granites and Gruf migmatites, 2 microgranite, 3 aplite, 4 old granitic gneisses of the Tambo nappe.*

	1	2	3	4
1	1.000	3.520	3.296	3.333
2	1.793	1.000	2.034	3.133
3	1.430	2.989	1.000	2.470
4	1.614	4.106	2.489	1.000

Variable Variable	Discr. relevance	power	Variable Variable	Discr. relevance	power
SiO_2	0.715	34.6	Qtz	0.681	33.2
TiO_2	0.640	5.2	Cor	0.854	10.5
Al_2O_3	0.834	6.9	Or	0.821	16.8
Fe_2O_3	0.639	7.8	Ab	0.969	23.2
FeO	0.428	8.8	An	0.711	12.7
MnO	0.510	4.0	Bi	0.434	7.6
MgO	0.493	8.1			
CaO	0.725	12.9			
Na_2O	0.954	22.4			
K_2O	1.000	16.6			
P_2O_5	0.504	9.9			
H_2O	0.165	1.4			

whereas the other classes are more well defined. This indicates that the Gruf migmatites and the Bergell granite may be considered as being one class with respect to their content of main constituents and normative minerals.

Consequently, the final disjoint principal components analysis was based upon the assumption that there are four distinct classes, and that the Gruf migmatites and the Bergell granite make up one single class. The crossvalidation demonstrated that the Bergell-Gruf class was best described by a principal equation with three terms, the other classes with two terms, as earlier. It also turned out that the class defining sample 1105, Rosso, of the class 3 should be considered as an outlier of the class, and consequently it was exchanged with sample 932, Pr. Rossa.

The result of this data analysis is given in Table 6. From the cluster distance matrix it is seen that all classes are reasonably well separated, and the variable relevance and the discrimination power for each variable shows that all variables except H_2O contribute to the separation of the classes.

It was stated above that in the three-dimensional first-to-second-to-third eigenvector plot, the aplites could be considered as a continuation of the Gruf migmatite-Bergell granite cluster. From the cluster distance matrix of Table 6 it is evident that the aplite class is closer to the Gruf-Bergell class than any of the other classes according to the values of the first column of the cluster distance matrix.

Finally, all samples were assigned to the four classes, the assignment being based upon the distance to the three nearest classes. The result of this classifica-

Table 7: *Assignment of samples to classes, and distance to three nearest classes in terms of residual standard deviation.*

Sample		Assignm. to class	Distance to class model (no) nearest		next nearest		third nearest	
			Megacrystic Bergell granite (class 1)					
579	Sciora	1	.49	(1)	.77	(4)	.78	(2)
659	S. Martino	1	.55	(1)	1.30	(2)	1.78	(4)
667	Albigna	1	.26	(1)	.75	(2)	1.01	(4)
667a	Albigna	1	.24	(1)	.79	(2)	.98	(3)
668	Albigna	1	.56	(1)	.89	(2)	1.28	(3)
682	Casnile	1	.30	(1)	.93	(2)	1.25	(3)
687	Albigna	1	.44	(1)	.68	(2)	.75	(3)
849	Plan Canin	-	.75	(4)	.87	(2)	1.14	(3)
954	Badile	1	.54	(1)	1.61	(2)	1.98	(4)
1102a	Rosso	1	.70	(1)	1.57	(2)	1.97	(4)
1107a	Forno	1	.67	(1)	1.46	(2)	1.60	(3)
			Equigranular Bergell granite					
685	Cantone	1,3	.49	(1)	.54	(3)	.74	(2)
949	Ft. Sciora	4	.59	(4)	.71	(2)	.88	(1)
			Cameraccio granodiorite					
1537	Cameraccio	1	.33	(1)	.82	(2)	1.29	(3)
1558	A. Pioda	1	.58	(1)	.94	(2)	1.19	(4)
1559	Cas. Pioda	-	1.11	(1)	1.24	(2)	1.63	(3)
			Megacrystic granite in Gruf migmatites					
808	Tegiola	1,4	.66	(4)	.76	(1)	.78	(2)
1439	Codera	1	.53	(1)	.84	(2)	1.06	(3)
			Microgranite (class 2)					
477	Albigna	1	.70	(1)	.71	(4)	.72	(3)
1080	Laret	1	.58	(1)	.61	(2)	.94	(3)
1086	Sissone	2	.48	(2)	1.00	(3)	1.34	(1)
1098	Forno	2,1	.39	(2)	.76	(1)	.76	(3)
1101	Forno	2,1	.22	(2)	.76	(3)	.76	(1)
1107b	Forno	2,3,1	.50	(2)	.53	(3)	.76	(1)
1108	P. dei Rossi	2	.29	(2)	1.64	(3)	1.39	(1)
			Aplite dikes (class 3)					
665	Albigna	3,1	.48	(3)	.54	(1)	.70	(2)
666	Albigna	3,(1)	.43	(3)	.55	(1)	.77	(4)
932	Pr. Rossa	3	.66	(3)	.93	(4)	1.00	(2)
1102b	Rosso	3,(1)	.61	(3)	.82	(1)	.90	(2)
1103	Rosso	3	.26	(3)	.88	(1)	1.23	(4)
1105	Rosso	-	.56	(2)	.71	(3)	.87	(4)
1107c	Forno	3,(1)	.24	(3)	.85	(1)	1.16	(2)
1112b	Lera	2,3,1	.45	(2)	.60	(3)	.75	(1)

Table continued on next page

Sample		Assignm. to class	Distance to class model (no) nearest		next nearest		third nearest	
			Gruf migmatites (class 1)					
116	Codera	1	.66	(1)	1.04	(2)	1.34	(4)
531	Borgonovo	1	.58	(2)	.80	(1)	.84	(4)
531b	Borgonovo	1	.34	(1)	1.40	(3)	1.61	(4)
534	Torta	–	.90	(1)	1.82	(3)	1.95	(2)
1017	Trubinasca	1	.49	(1)	.89	(2)	1.13	(3)
1112a	Lera	1	.35	(1)	.71	(2)	81.	(3)
1438	Gruf	–	1.07	(1)	1.35	(2)	1.78	(3)
1539	Cameraccio	–	1.14	(1)	1.62	(3)	1.71	(2)
1554	Torrone	1	.44	(1)	1.01	(3)	1.27	(2)
			Old granitic rocks of the Tambo nappe (class 4)					
62	Promontogno	4	.47	(4)	.79	(3)	.84	(1)
328	Marlun	4	.31	(4)	1.20	(1)	1.50	(3)
572	Pianazzola	4,1	.69	(4)	.74	(1)	.80	(3)
677	Bondasca	1	.73	(1)	.88	(4)	1.11	(3)
723	Chiavenna	4	.70	(4)	.93	(1)	1.15	(3)
740	Castasegna	4,(1)	.61	(4)	.67	(3)	.92	(3)
801	Soglio	4	.34	(4)	1.08	(3)	1.17	(1)

tion is given in Table 7. It shows that all class defining samples have been assigned to their "own" class, but one (1105).

All the unclassified samples of the megacrystic Bergell granite have been assigned to the Bergell-Gruf class, except for the sample 849, Plan Canin, that is listed by Wenk et al. as an outlying sample. Among the three samples of the Cameraccio granodiorite two have been assigned to the Bergell-Gruf class, and the third sample (1559, Cas. Pioda) somehow mid-way between this class and the microgranite class.

The unclassified Gruf migmatite samples are also assigned to the Bergell-Gruf class, with the exception of the samples 534, Torta, and 1539, Cameraccio, that are listed as outliers.

The microgranite was considered to be a separate class, and all the class defining samples were assigned to it. However, two of the three unclassified samples (477, V. Largh, and 1080, Laret) were assigned to the Bergell-Gruf class, and the third microgranite sample (1107b, Forno) was assigned to all of the three classes Bergell-Gruf, microgranite and aplite.

This may be a result of unfortuitous choice of class defining samples, but there is no indication in the data for a "better" choice of class defining samples. Thus, the disagreement is in itself no justification for choosing other class defining samples. It may also be that the microgranites have been derived from different sources in such a fashion that even though four of them form a well separated class in the principal components analysis, the whole group is not geochemically homogeneous. The distribution in the diagram of Figure 1 may support this assumption.

Among the four unclassified aplites, two of them are assigned to both the aplite class and the Bergell-Gruf class, although they are closest to the aplite class (666, Albigna, and 1102, Rosso). One of the aplites has been assigned to all of the classes Bergell-Gruf, microgranite and aplite, and the sample 1105, Rosso, is an outlier that is not assigned to any class.

Two of the three unclassified augengneiss samples of the Tambo nappe are assigned to the Tambo class. The third sample (677, Bondasca) is assigned to the Bergell-Gruf class, but the next closest class is Tambo. It is interestingly the sample closest to the Bergell granite contact.

The condition for assignment of a sample to a class is that the distance from the sample to the class model shall not exceed 1.2 times the standard deviation (epsilon of the class model).

The distance to class models, therefore, should always be compared to the epsilon value of Table 8.

Table 8: *Number of terms in principal components and standard deviation (epsilon of class model) for each class describing it's size*

Class	Number of terms	epsilon
1	3	.722
2	2	.469
3	2	.584
4	2	.589

The assignment criterion is very strict, and this is the reason why the class defining sample 1438, Gruf migmatite, is not assigned to its own class. From the table it is evident, however, that it is closer to its own class than to any other class and within the distance range 1.5 times epsilon. This sample could, of course, have been ommitted from the list of class defining samples, thus reducing the epsilon value for class 1. However, it is better to tolerate some discrepancies from expected results than to hamper with the choice of class defining samples until the situation looks better than is actually true.

CONCLUSIONS

There is agreement between the assignment of samples to classes made through the data analysis of the present work and through the detailed observations reported by WENK et al. (1977). The misclassified samples are all odd "transitional" samples (WENK, personal comm. 1978).

Among the studied granatic rocks of the Bergell Alps the megacrystic Bergell granite and the Gruf migmatites are closely related in terms of concentrations of main constituents and normative composition. They are distinctively different from the augengneisses of the Tambo nappe, and from the microgranites of the Bergell Alps. The microgranites seem to be a more inhomogeneous group in terms of variations in main constituents and normative composition than the above-mentioned groups. Since they are obviously younger (crosscutting Bergell granite and in some places migmatites) they may have been derived from different sources, this explaining why their chemical composition is erratic.

Aplites seem to be more closely related to the Bergell granite and Gruf migmatite group, but they make up a distinct class in the principal component analysis. There may possibly be a petrogenic connection between the aplites and the formation of the Bergell megacryst granite. Furthermore, the aplites are distinctly different from the microgranites and the old augengneisses of the Tambo nappe.

The equigranular Bergell granites are poorly separated from the megacrystic Bergell granites, the Gruf migmatites and the old augengneiss granites of the Tambo nappe.

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