

# Classification of Energy Dispersion X-ray Spectra of Mineralogical Samples by Artificial Neural Networks<sup>†</sup>

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Automatic classification of different mineralogical samples into 12 prespecified classes using Kohonen artificial neural networks (ANNs) is studied in comparison with standard chemometric techniques: hierarchical clustering and principal component analysis. The mineral types into one of which the unknown samples should be classified are pyrrhotite, pyrite, chalcopyrite, pentlandite, magnetite, biotite, albite, talc, chlorite, lizardite, dolomite, and amphibole. The basis for classification are 15-dimensional EDX spectra of individual grains taken from large matrices of compositions each containing a variety of grains belonging either to the same or to different minerals. The discussed classification procedure is based on the 15–15–15 Kohonen neural network cube. The classification results are displayed on the 15 × 15 Kohonen top-map. From the 15 weight levels of the 15–15–15 Kohonen ANN 12 logical rules that allow one to classify unknown samples into one of 12 classes are extracted. The 100% correct classification of samples using the suggested 12 logical rules is enabled by only seven of out of 15 intensity lines from each (energy-dispersive X-ray) EDX spectrum. It is shown that the Kohonen ANN allows one to draw conclusions and logical rules based on the weight patterns formed during the training in the ANN.

## INTRODUCTION

Fast and reliable classification of grain structured polycrystalline samples is one of the routine tasks in analytical laboratories for mineralogical samples. Thousand of samples brought into the analysis have to be classified, first in a qualitative way, whether they contain certain minerals or not, and second in a quantitative way, by finding the percentages of the detected minerals in given samples. Energy-dispersive X-ray spectrometry<sup>1,2</sup> (EDX) is one of the preferred ways of chemical identification of materials under scrutiny in scanning electron microscopy. It is based on the fact that a small part of electrons, that impinge on the sample, scatter inelastically. The resulting X-ray emission is characteristic for the atom that was excited during inelastic scattering. Eventually, the energy spectrum of the material observed will consist of characteristic elemental peaks on top of continuous background, due to elastic scattering.

On the basis of EDX spectra acquired it is possible to calculate quantitative data, for instance, elemental concentrations. In the case of stoichiometric materials, where the chemical composition of the candidate sample is known, the problem to solve which composition is present is less stringent: it is only necessary to decide which of possible chemical classes the unknown material falls into. In such cases a semiquantitative procedure is more adequate. For example, a mere presence or absence of a sulfur peak can help do decide whether the material in question is a sulfide or not. The advantage of such semiquantitative method are fast spectrum acquisition and short processing times, which

are considerably shorter, when compared to the case of other quantitative analyses.

In order to evaluate the artificial neural network (ANN) method proposed in the present work we have additionally explored several possibilities and performances of the standard chemometric techniques. The final goal of this research was to find a reliable and fast classification of EDX spectra of unknown samples into one of several predefined categories established by the set of EDX spectra of several standard mineralogical samples.

## EXPERIMENTAL SECTION

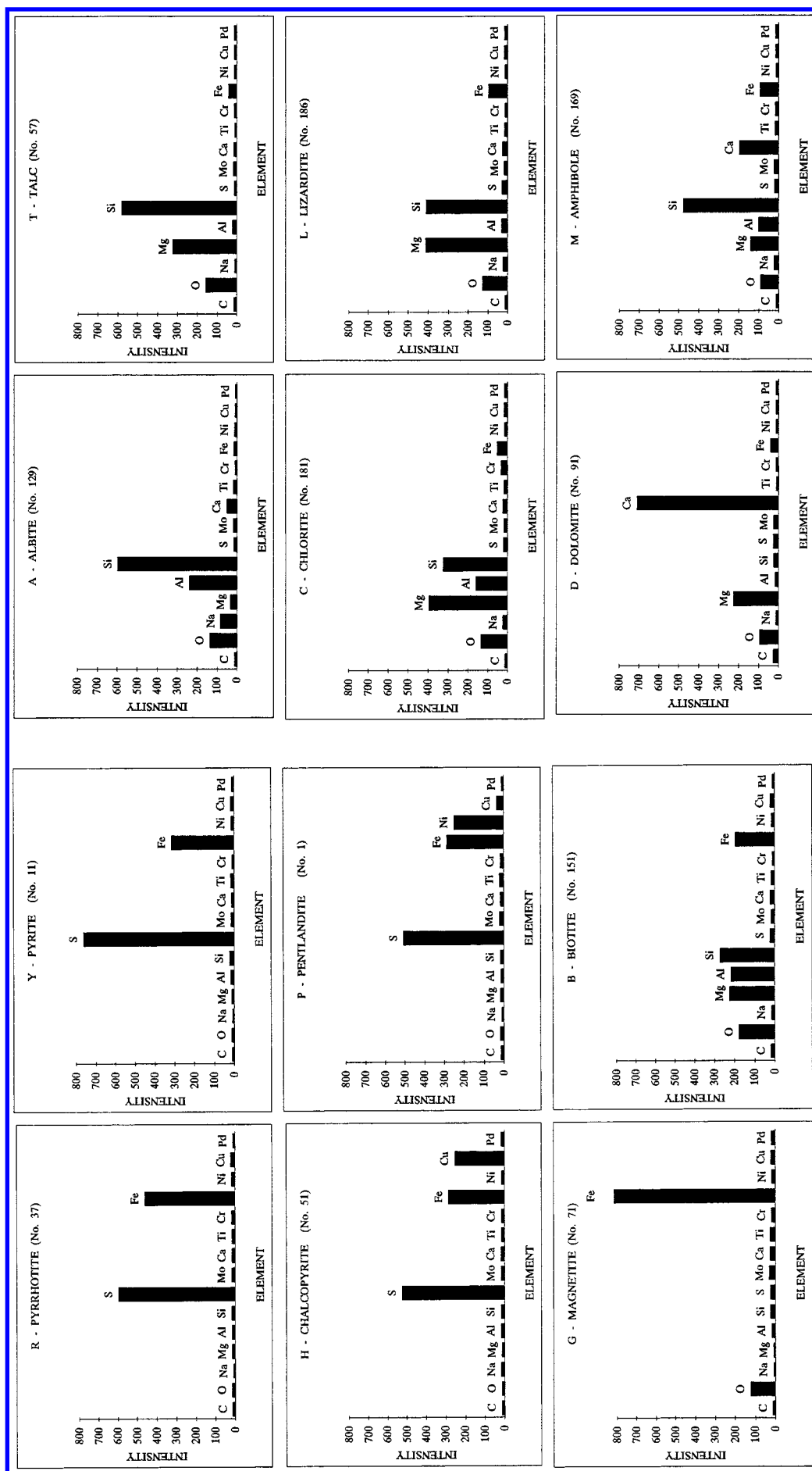
In the present study, a sample containing a complex case on Nickel-bearing ore has been analyzed using Philips XL-40 scanning electron microscope (SEM), EDAX DX4 energy dispersion X-ray (EDX) instrument and Kontron Elektronik SEM-IPS scanning electron microscope image analyzer. The SEM-IPS instrument was used as the integrating part of the complete system. Its flexible design allows remote control of both SEM and EDX instrument and design, implementation, and testing of new algorithms at the customer's site.

The samples were provided in a form of crushed ore—grain sizes in order of up to 200 micrometers—embedded and coated in the usual way. For the observation of the sample back-scattered detector was used. In order to test the mineral identification software developed only the unavoidable grey image processing steps (noise suppression for example) for the discrimination of grains were used. Small particles and small holes were deleted. The essential command was actively steering the electronic beam over the discriminated grains on a one-by-one basis. During this time the EDX instrument is actively accumulating the spectrum (passing the X-ray signals to SEM processor). After the prespecified period of time (typically 100 ms) a profile of total counts for the chosen elements has been generated and stored as an

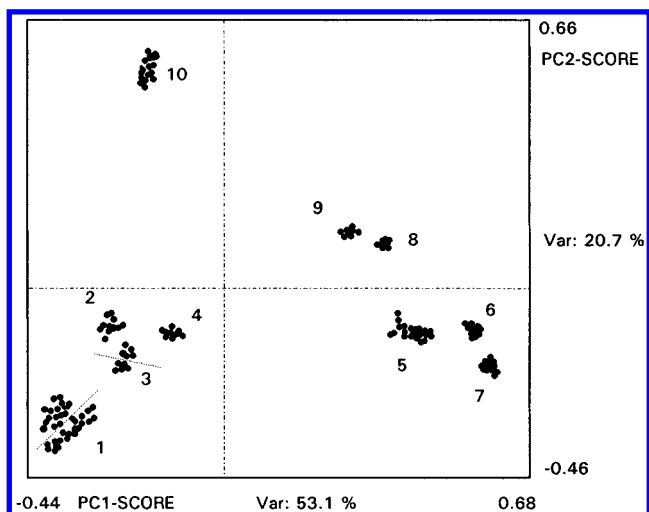
<sup>†</sup> This paper is dedicated to the 70th birthday of Prof. Shin-ichi Sasaki, a scientist, a mentor, and a good friend for his contribution to the spread of the chemometric ideas throughout the world.

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**Figure 1.** Representative EDX spectra of 12 standard minerals. Each spectrum consists of 15 intensities of the 15 elements. The set and order of elements is the same for all EDX spectra in our study. For each standard mineral between eight and twelve different spectra were recorded.



**Figure 2.** Principal component projection into the PC1/PC2 plane of all 198 objects (15-dimensional EDX spectra). The first two principal axes PC1 and PC2 contain 73.8% of all information. Group No. 1 is composed of talc and albite, group No. 3 of chlorite and lizardite, and group No. 5 of pentlandite and chalcopyrite minerals. Magnetite samples form two separate groups No. 8 and No. 9. Groups No. 2, No. 4, No. 6, No. 7, and No. 10 belong to the minerals amphibole, biotite, pyrrhotite, pyrite, and dolomite, respectively.

EDX spectrum of an individual grain.

Each EDX spectrum recorded for our analysis was composed of 15 intensities for 15 different atomic lines of carbon, oxygen, sodium, magnesium, aluminium, silicon, sulfur, molybdenum, calcium, titanium, chromium, iron, nickel, copper, and palladium, respectively. The intensities were all normalized across the whole spectrum, i.e., the integral of each spectrum was kept constant to 1200 counts. First, several EDX spectra of each well-defined mineral sample (pyrrhotite, pyrite, chalcopyrite, pentlandite, magnetite, biotite, albite, talc, chlorite, lizardite, dolomite, and amphibole) were recorded. In this way all 189 EDX spectra of above 12 standard minerals have been collected. Next, the collection was divided into two sets of approximately the same size: into a training set of 94 for finding the proper method and a test set of 95 EDX spectra for testing. Due to the fact that the samples were acquired from the real lot of specimens we did not have enough different samples to form the subsets with equal number of samples for each of minerals in this study. In Figure 1 selected EDX spectra one for each of the 12 studied minerals are shown.<sup>3</sup>

#### STANDARD CHEMOMETRIC METHODS

**Principal Component Analysis (PCA).** The projection of the EDX spectra onto the first two principal components<sup>4,5</sup> (Figure 2) shows ten different groups of samples, but only four of them coinciding with one of the mineralogical defined ones. As it can be deduced from Figure 2, the PCA method shows the samples forming the following ten clusters: cluster No. 1 is composed of talc (T) and albite (A) minerals, clusters No. 2 amphibole (M) and No. 3 are partially overlapped, additionally, cluster No. 3 is composed of lizardite (L) and chlorite (C) samples, clusters No. 4, No. 6, No. 7, and No. 10 contain only one type of minerals: biotite (B), pyrrhotite (R), pyrite (Y), and dolomite (D), respectively, cluster No. 5 is composed of pentlandite (P) and chalcopyrite (H), while clusters No. 8 and No. 9 both contain samples of magnetite (G).

In the view of relatively poor separation ability, it should be said that in the PC1/PC2 plot, only 73.8% of the total

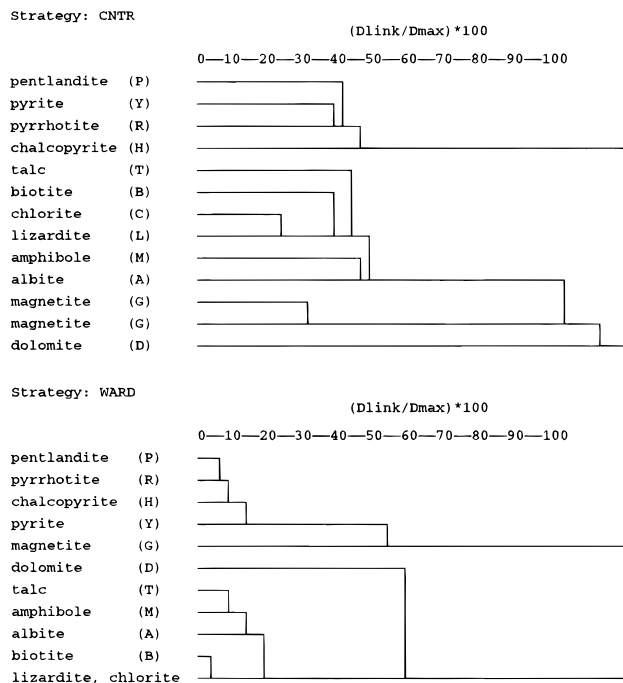
variance of the original data is considered. A “zoom” inspection (blow-up of the PC1/PC2 plot) of the cluster No. 1 shows that talc (T) and albite (A) samples, although grouped together can still be linearly separated one from the other. However, a linear separation cannot be made between the pentlandite (P) and chalcopyrite (H) within the cluster No. 5. From Figure 1, it can be seen that both have high (approximately the same) intensities values for sulfur and iron, while they differ when intensities of nickel and copper are considered. Magnetite samples are grouped in two different areas in the PC1/PC2 space, the smallest one contains six samples. The same group of this six samples appear as a subgroup in all dendrograms obtained by the different methods of clustering, with the exception of Ward’s clustering method. Finally, chlorite and lizardite samples appear in the same group No. 3. Inspecting the variables values (Figure 1), both the chlorites (C) and lizardites (L) have high values of oxygen, aluminium, and sodium intensities, the only difference is that chlorites have higher values of the silicon intensities compared to those of lizardite samples.

As it was found in the subsequent studies with other methods, several mineralogical classes require from each a different specific variable (element) to be distinguished from the rest. This means that several variables are independent from each other with respect to the classification of specific minerals. Such independence of variables makes the PCA method less usable for separation of objects (mineralogical samples represented as 15-dimensional EDX spectra in our case) into different classes (different minerals).

**Clustering Analysis.** Seven different hierarchical clustering methods (single and complete linkage, unweighted and weighted pair-group average, unweighted and weighted pair-group centroid and Ward’s methods<sup>6,7</sup>) were applied to all 189 EDX samples of which the identification was known. With the exception of the Ward’s method which does not distinguish the lizardite from chlorite samples, all other six clustering methods have clearly distinguished all 12 groups. Effectively, in dendrograms obtained by these six clustering methods always 13 clusters can be distinguished. This is caused by the fact that the magnetite group is split into two clusters long before the lizardite and chlorite groups were separated. Due to much larger separation between two subgroups of magnetite materials compared to the distance between the chlorites and lizardites, all 12 prespecified mineralogical groups were not possible to separate with **one** threshold distance level only (Figure 3). If the threshold limit which would separate the dendrogram into exactly 12 required groups is sought the distinction between the lizardite and chlorite vanishes in all seven dendrograms long before the magnetites are joined into one single group.

With the exception of the Ward’s dendrogram, chlorites and lizardites can always be distinguish as two separate groups. Due to the fact that the first six clustering methods yield practically the same clustering schemes, only the dendrogram obtained by the centroid<sup>6,7</sup> clustering strategy is shown on Figure 3a. The dendrogram obtained with the Ward’s<sup>6,7</sup> clustering method (Figure 3b) is the only one in which the samples of chlorites and lizardites appear together.

In spite of the fact that clustering methods are quite well performing in separation of mineralogical classes, they are, unfortunately, rather inconvenient for the use in automatic and continuously running classification procedures. This is true especially if high speed and large amount of classifica-



**Figure 3.** Clusters of 94 EDX spectra. Because all spectra from each class of minerals have been linked to a single cluster, only the branches leading to these clusters are shown. The centroid (CNTR) clustering (above) was chosen for the comparison with the Ward's clustering (below) just because it shows most clearly the properties all other five standard clustering methods. The dendrograms obtained by these other five clustering methods show virtually identical clustering schemes with only slight differences among the corresponding linking distances of the same clusters.

tions are need during the process. The bottleneck of any standard clustering procedure in the continuous process is the calculation of the distance matrix  $D$  of order  $N + 1$  ( $N$  standard samples plus the unknown one) and than the  $N - 1$  reductions of matrix  $D$  to obtain the matrix  $D$  of order 2. For the classification of each unknown sample  $X$  all these steps have to be performed anew.

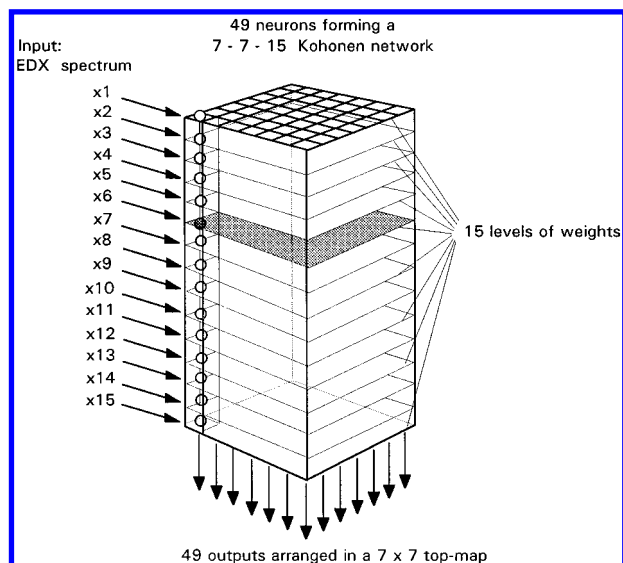
**Kohonen ANNs.** In order to solve the problem of fast classification of large amount of analyses and to avoid the tedious clustering procedure we have tried the ANN approach. For this purpose the Kohonen ANN<sup>8-12</sup> was applied. As the representation of objects (mineralogical samples) we took exactly the same form of 15-dimensional normalized EDX spectra as it was used in the PCA and clustering procedures. The training of the Kohonen ANN was performed using the eqs 1 and 2<sup>13</sup> for the selection of the central neuron  $c$  and the correction of weights  $\Delta w_{ji}$ , respectively.

$$\text{out}_c \leftarrow \min \left\{ \sum_{i=1}^m (x_{si} - w_{ji})^2 \right\} \quad J = 1, 2, \dots, N \quad (1)$$

$$\Delta w_{ji} = [(a_{\max} - a_{\min})(p/n_{\text{net}}) + a_{\min}][1 - d/(p + 1)] \times (x_{si} - w_{ji}^{\text{old}}) \quad d = 0, 1, 2, \dots, p \quad (2)$$

The part of eq 2 in front of the term  $(x_{si} - w_{ji}^{\text{old}})$  describes how the correction of the weights  $w_{ji}$  decreases with increasing learning time and increasing topological distance  $d$  between the  $j$ th and the central neuron  $c$ . The maximum distance  $d = p$  to which the correction in eq 2 is applied at each new object is evaluated during the learning procedure using the expression

$$p = (i_{\text{tot}} - i_{\text{it}})n_{\text{net}}/(i_{\text{tot}} - 1) \quad (3)$$



**Figure 4.** Architecture of the Kohonen ANN used in the present study. As shown the input data are entering the ANN as column vectors, thus allowing the same variable to be distributed on a separate horizontal level (plane) of corresponding weights. Here only the 7-7-15 ANN is drawn, while for retrieving the final results the 15-15-15 Kohonen ANN was used.

At the beginning of learning ( $i_{\text{it}} = 1$ )  $p$  covers the entire network ( $p = n_{\text{net}}$ ), while at the end of the learning iteration steps ( $i_{\text{it}} = i_{\text{tot}}$ )  $p$  is limited only to the central neuron  $c$  ( $p = 0$ ).

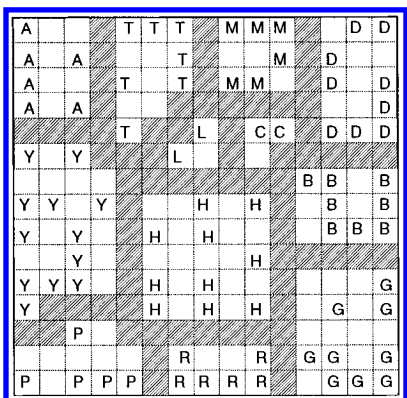
At the end of each training the 94 EDX spectra were run again through the particular ANN, and each excited neuron was labeled with one-character label according to the mineral to which it belongs (see Table 1). After trying several Kohonen ANN layouts: 7-7-15 (Figure 4), 9-9-15, 13-13-15, 15-15-15, and 17-17-15, respectively, we have obtained good separation between all 12 classes of minerals in the Kohonen ANNs having equal or larger layout than 13-13-15. In order to maintain and even improve the selectivity, i.e., to decrease the possibility of wrong classifications, we have chosen to work with the 15-15-15 ANN rather than with the 13-13-15 one.

The top  $15 \times 15$  map of one-character labels belonging to the excited neurons in the 15-15-15 is shown in Figure 5.

As it can be seen from the  $15 \times 15$  top-map of one-character labels, the separation of all 12 classes was not only good, there was between each group of minerals even a continuous separation area (shaded neurons in Figure 5) with the width of at least one nonexcited neuron. This fact has confirmed the information supplied by clustering techniques that the classes are sufficiently well described by the representation of EDX spectra.

After the 95 EDX spectra of the test set were run through the 15-15-15 network the classification was 100% correct, i.e., all 95 spectra not considered during the training were classified into the correct group of minerals.

Due to the fact that the clustering was so clear we inspected all 15 levels of the Kohonen ANN. Because each level of weights in the Kohonen ANN (see Figure 4) receives always only one type of variable, at the end of the training a particular level shows how the values of the input variable are distributed on the  $15 \times 15$  weight map. The visual effect of each map is enhanced by drawing the contour lines connecting the points (neuron positions) having the same variable value. Each of the 15 weight levels represented as



**Figure 5.** The final  $15 \times 15$  top-map of one-character labels as they are distributed according to the learning procedure in the 15–15–15 Kohonen ANN. There is a clear separation of at least one not excited neuron between each of the 12 clusters (shaded neurons).

contour maps of a particular variable was overlapped with the  $15 \times 15$  top-map containing one-character labels (Figure 6).

In order to focus on the most relevant information contained in the contour maps one or two contours running **only between** the classes were selected out of all possible contours in each map. The map No. 1, No. 8, and No. 15, i.e., the maps representing the intensity lines in the EDX spectra corresponding to carbon, titanium, and palladium, respectively, do not allow for the drawing of such contours because each concentration contour splits at least one group of minerals (Figure 6—levels 1, 8, and 15). On the contrary to the three mentioned maps, the remaining 13 maps were much more informative as shown in Figure 6.

There are six maps of levels 3, 7, 10, 11, 13, and 14, representing the elements sodium, sulfur, titanium, chromium, nickel, and copper that would, at least in principle, allow separation (distinguish) of one individual class out from the rest. For instance, in the seventh map (sulfur intensities) the contour encompassing the area of higher than 0.8 (80%) sulfur intensities in the EDX spectrum overlaps exactly with the area occupied by the pyrite minerals (label Y). Here, of course, a caution should be given. In the particular case the sulfur intensity of above 0.8 can be actually used to separate pyrite from the rest of minerals. However, there are many minerals with high sulfur content, and therefore, for more general applications, the decision rule should be augmented by an additional IF statement including intensity of the iron line to be larger than 0.2 to confirm pyrite minerals.

Apart from being concentrated on single elements characteristic for classification of specific minerals, it seems to be better to concentrate on finding a minimal number of several elements for which *combinations* of different concentration intervals are characteristic for minerals in question.

By trying to overlap several among the 15 contour maps it was not too difficult to find the combination of **seven** maps that, if all were superimposed over each other, gave the possibility to separate **all 12** mineral classes completely. Figure 7 shows the overlap of seven contour maps No. 4 (magnesium), No. 5 (aluminium), No. 6 (silicium), No. 7 (sulfur), No. 9 (calcium), No. 12 (iron), and No. 14 (nickel).

The overlap of these seven contour maps as shown in Figure 7 allows the obtaining of 12 logical rules for classification of unknown mineralogical samples. Classification of the unknown mineralogical samples into one of the 12 classes is made by applying all 12 rules to only seven intensities  $I_{el}$  of the unknown sample represented as EDX

spectrum. The 12 logical rules are as follows:

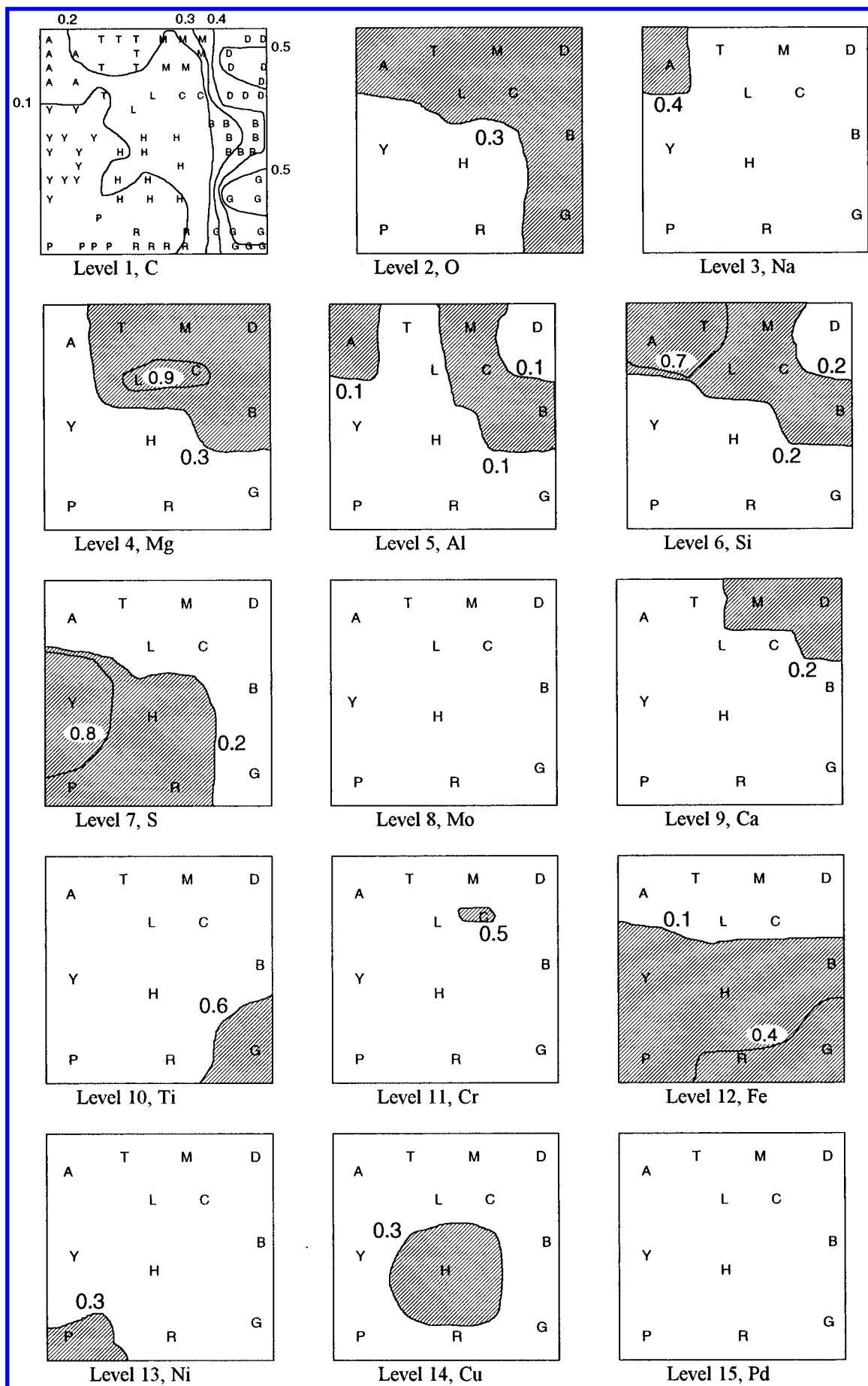
- Rule 1: if  $(0.2 < I_S < 0.8)$  AND  
if  $(I_{Fe} > 0.4)$  class = R (pyrrhotite)
- Rule 2: if  $(I_S > 0.8)$  class = Y (pyrite)
- Rule 3: if  $(0.2 < I_S < 0.8)$  AND  
if  $(0.1 < I_{Fe} < 0.4)$  AND  
if  $(I_{Ni} < 0.3)$  class = H (chalcopyrite)
- Rule 4: if  $(I_{Ni} > 0.3)$  class = P (pentlandite)
- Rule 5: if  $(I_S < 0.2)$  AND  
if  $(I_{Fe} > 0.4)$  class = G (magnetite)
- Rule 6: if  $(I_S < 0.2)$  AND  
if  $(0.1 < I_{Fe} < 0.4)$  class = B (biotite)
- Rule 7: if  $(I_{Mg} < 0.3)$  AND  
if  $(I_S < 0.2)$  class = A (albite)
- Rule 8: if  $(I_{Si} > 0.7)$  AND  
if  $(0.3 < I_{Mg} < 0.9)$  AND  
if  $(I_{Fe} < 0.1)$  class = T (talca)
- Rule 9: if  $(I_{Mg} > 0.9)$  AND  
if  $(I_{Al} > 0.1)$  class = C (chlorite)
- Rule 10: if  $(I_{Mg} > 0.9)$  AND  
if  $(I_{Al} < 0.1)$  class = L (lizardite)
- Rule 11: if  $(I_{Ca} > 0.2)$  AND  
if  $(I_{Al} < 0.1)$  class = D (dolomite)
- Rule 12: if  $(I_{Ca} > 0.2)$  AND  
if  $(I_{Al} > 0.1)$  class = M (amphibole)

In the above 12 rules the  $I_{el}$  stands for the normalized intensity of the particular element line in the EDX spectrum of the mineral to be classified. As mentioned before, the normalization of the EDX intensities  $I_{el}$  is obtained by first normalizing the entire integral of the EDX spectrum to 1200 intensity units and then expressing  $I_{el}$  in percentage of the most intensive line of this element in the entire collection (the normalization along one variable). Using the above 12 rules all remaining 95 “unknown” EDX spectra from the test set were classified correctly.

As mentioned above, the rules No. 2 and 4, employ only one element for discrimination. For the present case such rules might be sufficient, however, for a more general application, it would be wise to incorporate some additional tests. For example: the check (IF  $I_{Fe} > 0.2$ ) can be easily added to the rule No. 2. Similarly, because there are several other minerals (like violarite,  $FeNi_2S_4$ ) having high content of nickel, the check for intensities  $I_S$  and  $I_{Fe}$  should be added to rule No. 4.

The above 12 rules are, of course, not general but applicable only to the minerals from the region in question.

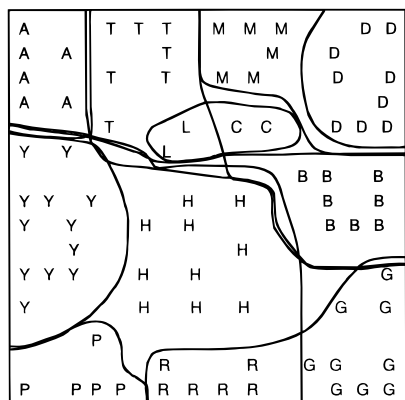




**Figure 6.** Fifteen weight maps corresponding to 15 input variables, each overlapped with the 15 × 15 top-map of labels and with one or two contour line(s) that run(s) only between the groups of labels. On map No. 1, No. 8, and No. 15 such contours cannot be detected (for example: in map No. 1 each contour line crosses at least one group of minerals). For the sake of clarity, the areas belonging to each mineral are assigned with only one character instead with as many labels as there are actually present in the top map shown in Figure 5.

**Table 1.** List of Minerals and Their One-Character Labels in the Study

no.	mineral	abbrev	no.	mineral	abbrev
1	pyrrhotite	R	7	albite	A
2	pyrite	Y	8	talc	T
3	chalcopryite	H	9	chlorite	C
4	pentlandite	P	10	lizardite	L
5	magnetite	G	11	dolomite	D
6	biotite	B	12	amphibole	M

**Figure 7.** Overlap of maps No. 4, No. 5, No. 6, No. 7, No. 9, No. 12, and No. 14 (compare with corresponding contour lines in Figure 6) showing that these seven variables can separate all 12 minerals.

If more general applicability of **this specific** rules would be sought, additional sampling and analyses should be made.

### CONCLUSION

The goal of the study was to set up a fast and reliable classification tool which can be implemented as an automatic and continuously working procedure for classification of mineralogical samples from a specific geographic region. By extracting 12 extremely simple rules involving only seven elements out of which in a single decision only one or two different elements are used we have achieved this task. The goal was achieved using 15 contour maps from the final 15–15–15 Kohonen ANN obtained and tested on the standard set of 189 spectra. To repeat again: the goal was not discrimination of minerals in a small set of 189 EDX but for a given set of samples from the same geographical area as represented with the standard set. We sought to generate a robust and reliable procedure to be used in fast automatic system requiring thousands of decisions in a short period of time. We consider checking of 12 simple *if-then-rules* the fastest possible procedure to solve the problem.

It is obvious that the implementation of the obtained 12 rules on a computer is quite straightforward allowing the instrument to perform the classification much faster than by any of the other three methods tried before: be PCA, clustering, or the Kohonen ANN. On the contrary the use of ANN which are normally employed as a blackbox, the explained method of extracting logical rules from the network's weight layers offers the user the explanation why the unknown mineral is classified into a given class.

It should be noted that in the view of very simple mathematics used in Kohonen ANN, i.e., Euclidean distance calculations, comparison of distances (eq 1), and linear interpolation for ANN weight corrections (eq 2), the described method is mathematically much simpler compared to other statistical methods, especially if compared with methods like PCA or SIMCA<sup>14</sup> (which includes principal component calculations), where diagonalization of the cor-

relation matrix has to be carried out for each projection. In terms of its simplicity the Kohonen ANNs are much easier to understand and to carry out than the methods involving PCA calculations.

Besides the fact that the 15 logical rules were obtained from the Kohonen ANN trained with a set of 94 complete 15-dimensional EDX spectra, there is another experimental advantage of this method. It was shown that by combinations and inspection of several overlapped weight maps the required information can be extracted from less than a half of initially employed variables (elements in the EDX spectra). The final rules are based on only seven variables (elements: aluminum, calcium, iron, magnesium, nickel, silicon, and sulfur). Further, it was shown that three (carbon, molybdenum, and palladium) of the 15 elements employed do not contribute significantly to the classification of minerals and that the rest of elements (copper, chromium, oxygen, sodium, and titanium), apart from the seven ones used in the 12 rules, although being very significant for the classification of specific minerals add only redundant information already contained in other elements. Again, the obtained rules can be used only for the classification of minerals from the same geographical site from which the standard samples were prepared. For more general classification broader standard set of samples should be explored.

Hence, the advice of measuring only seven element intensity lines instead of 15 initially suggested ones represents a considerable improvement of the complete analytical procedure. Such reduction of analytical requirements and experimental efforts turns out to be more effective and desired than mere reduction in the computation time.

### ACKNOWLEDGMENT

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