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THE USE OF QUANTITATIVE COLOR VALUES FOR OPAQUE-MINERAL IDENTIFICATION

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ABSTRACT

An opaque-mineral identification scheme utilizes the quantitative color values (x, y, Y, $Pe\%$ $d\lambda$) and Vickers Hardness Number (*VHN*) as determinative criteria. The color values are obtained from spectral reflectance data derived by weighted ordinates, instead of selected ordinates. Errors in reflectance measurements create problems, owing to their effect on the derivation of color values. The identification scheme operates on a desk-top computer. Checking against a file containing data on known minerals yielded only one or two possible matching minerals in 80% of samples tested, when the isotropic or anisotropic nature of the unknown mineral was also taken into account.

SOMMAIRE

Notre méthode d'identification des minéraux opaques utilise les valeurs colorimétriques quantitatives (x, y, Y, $Pe\%$, $d\lambda$) et la dureté Vickers (*VHN*) comme caractères déterminatifs. On obtient les valeurs colorimétriques à partir des données de réflectance spectrale, dérivées d'ordonnées pondérées plutôt que d'ordonnées sélectionnées. Les erreurs de mesures de réflectance exercent une répercussion sur des valeurs colorimétriques. La méthode ne requiert qu'une calculatrice de bureau. Grâce à un fichier de données sur minéraux connus préalablement établi, et en tenant compte du caractère isotrope ou anisotrope de l'échantillon, nous n'avons trouvé, dans 80% des cas, qu'une ou deux déterminations possibles.

(Traduit par la Rédaction)

INTRODUCTION

Opaque minerals have for many years been identified microscopically by measuring two physical properties, reflectance and microhardness, and comparing these in tabular or chart form with similar data for known minerals. Two comprehensive schemes for identifying opaque minerals make use of quantitative color values (Chvileva *et al.* 1977, Atkin & Harvey 1979). An improvement of the latter scheme is described here.

QUANTITATIVE COLOR MEASUREMENT

Color is potentially the most diagnostic property of ore minerals when viewed in reflected light. Unfortunately, it is difficult to describe a color accurately, as is shown by the numerous different colors quoted in the literature for the same mineral, *e.g.*, pyrrhotite: "yellow", "brownish-yellow", "yellow-brown", "light-pink-brown" and so on. This is due to the fact that most ore minerals in polished section are weakly colored and have a wide range of brightness. The color described for ore minerals depends in many cases upon what other colors are present for comparison in the field of view, as in Uytenbogaardt & Burke (1971).

In 1931, La Commission Internationale d'Eclairage (CIE) devised a system for the quantitative description of color, but only since the development of suitable apparatus (especially photomultipliers) has it been possible to apply this system to ore minerals in reflected light.

It is not the intention of this paper to describe the apparatus required for color measurement except to say that a photometric device on a reflecting-light microscope capable of measuring in monochromatic light throughout the visible spectrum is necessary (see Bowie & Henry 1964, Galopin & Henry 1972 for details). Such apparatus is now readily available from several manufacturers.

Neither are we going to elaborate on the principles of the CIE (1931) system, as these are readily available in several publications (*e.g.*, Judd & Wyszecki 1963, 1975; Wyszecki & Stiles 1967). The CIE (1931) system uses three parameters to describe color quantitatively; two are the trichromatic coefficients (x, y) and the third is the luminance (Y). These values are defined with respect to a particular light source.

For ore minerals in polished section we can obtain these values from spectral reflectance data in the region 400–700 nm. A spectral reflectance curve can be defined adequately for most ore minerals by taking sixteen reflectance readings at 20 nm intervals from 400 to 700 nm. For strongly colored minerals better definition will be obtained if 31 readings are taken, *i.e.*, at 10 nm intervals from 400 to 700 nm, but this has not been found necessary for routine identification work.

Having obtained the spectral reflectance data, we calculate the color values (x, y, Y) by first obtaining the tristimulus values X, Y, Z, which are defined by the integrals:

$$X = \frac{1}{K}\int_{\lambda = 400}^{\lambda = 700} (\bar{x}\lambda \cdot S\lambda) \cdot R\lambda \cdot d\lambda$$

$$Y = \frac{1}{K}\int_{\lambda = 400}^{\lambda = 700} (\bar{y}\lambda \cdot S\lambda) \cdot R\lambda \cdot d\lambda$$

$$Z = \frac{1}{K}\int_{\lambda = 400}^{\lambda = 700} (\bar{z}\lambda \cdot S\lambda) \cdot R\lambda \cdot d\lambda$$

where $\bar{x}\lambda$, $\bar{y}\lambda$ and $\bar{z}\lambda$ are the tristimulus values for the spectral colors red, green and blue, respectively, $S\lambda$ is the relative spectral energy for the particular light source used, $R\lambda$ is the reflectance, and K is a normalizing constant.

Good approximations for X, Y and Z may be obtained from the summations:

$$X = \frac{1}{K}\sum_{\lambda = 400}^{\lambda = 700} (\bar{x}\lambda \cdot S\lambda) \cdot R\lambda \cdot \Delta\lambda$$

$$Y = \frac{1}{K}\sum_{\lambda = 400}^{\lambda = 700} (\bar{y}\lambda \cdot S\lambda) \cdot R\lambda \cdot \Delta\lambda$$

$$Z = \frac{1}{K}\sum_{\lambda = 400}^{\lambda = 700} (\bar{z}\lambda \cdot S\lambda) \cdot R\lambda \cdot \Delta\lambda$$

TABLE 1. TRISTIMULUS WEIGHTS FOR SIXTEEN ORDINATES* BASED ON THE 1931 'STANDARD OBSERVER' FOR C-SOURCE ILLUMINANT

λ	S.$\bar{x}$	S.$\bar{y}$	S.$\bar{z}$
400	0.1699	0.0040	0.8076
420	2.5862	0.0738	12.2914
440	7.9457	0.5237	39.8545
460	6.7204	1.3873	38.5772
480	2.2228	3.2343	18.9118
500	0.1039	6.7983	5.7249
520	1.1514	12.9170	1.4232
540	5.5670	18.2881	0.3898
560	11.7537	19.6714	0.0780
580	16.8249	15.9754	0.0320
600	17.8883	10.6263	0.0140
620	14.1324	6.3026	0.0040
640	7.3820	2.8645	0.0002
660	2.7205	1.0075	0.0000
680	0.7376	0.2678	0.0000
700	0.1639	0.0580	0.0000
TOTAL	98.0706	100.0000	118.1086

*Calculated for 20nm intervals by reweighting the values at 5nm intervals given in Wyszecki & Stiles (1967).

If $\Delta\lambda$ is constant, it can be omitted from the above summations and ($x\lambda.S\lambda$), ($y\lambda.S\lambda$), and ($z\lambda.S\lambda$) can be tabulated so that the calculation of the tristimulus values becomes a simple computation that can be readily performed on a calculator in about ten minutes or a computer in a fraction of that time. The tristimulus weights ($\bar{x}\lambda.S\lambda$), ($\bar{y}\lambda.S\lambda$) and ($\bar{z}\lambda.S\lambda$) for a $\Delta\lambda$ interval of 20 nm and C-source light are given in Table 1. For these weights, $K = 100$ for each of the tristimulus values X, Y and Z.

The trichromatic coefficients (or chromaticity coordinates) x and y are then calculated from the tristimulus values, using:

$$x = \frac{X}{X+Y+Z} \qquad y = \frac{Y}{X+Y+Z}$$

The third trichromatic coefficient z could be calculated in a similar manner, but as $x + y + z$ must total 1 this is not necessary. The luminance (brightness) is the tristimulus value Y. If reflectance values used in the calculation of the tristimulus values are in percent form, then luminance becomes Y divided by 100.

The above method of calculating tristimulus values is known as the weighted-ordinate meth-

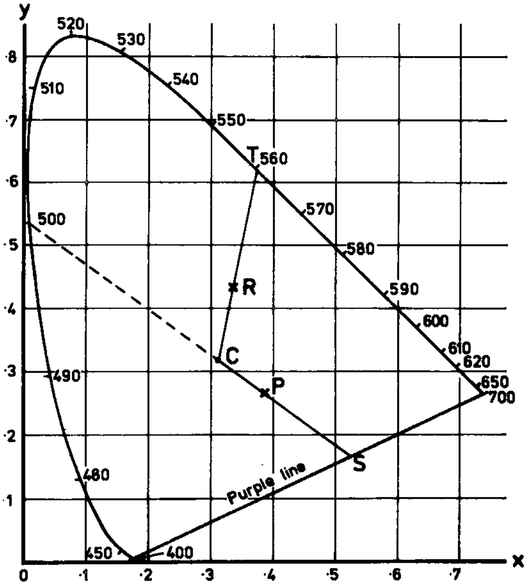


FIG. 1. CIE (1931) chromaticity diagrams showing the derivation of Helmholtz coordinates.

od and, with the ready availability of calculators and computers, is easier to apply than the "selected-ordinate method" described by Piller (1966).

The chromaticity coordinates are plotted on a 2-dimensional diagram known as a chromaticity diagram; the CIE (1931) chromaticity diagram is shown in Figure 1. For details of the construction of the diagram the reader is referred to Piller (1966) or the texts on color mentioned above.

We now have a system of describing color quantitatively, but it takes considerable experience before a mineralogist is able to appreciate immediately the color of a mineral from its chromaticity coordinates. In lieu of experience one can convert these coordinates into two other values, the Helmholtz (or polar) coordinates. These are dominant wavelengths ($d\lambda$) and excitation purity ($Pe\%$), which together with luminance also fully describe the color of an object. These coordinates are obtained either graphically or by computer from the CIE (1931) chromaticity diagram as follows: if the chromaticity coordinates of an object plot at point R in Figure 1, then 560 is the value given to $d\lambda$, *i.e.*, the point of intersection on the spectral locus of a line drawn from the light source, point (C), through R. The excitation purity is the distance C–R expressed as a percentage of C–T. If the object falls in the purple region as at point P on Figure 1, then the dominant wavelength becomes the negative value of the complementary wavelength (–500 in this case), and the excitation purity becomes the distance C–P expressed as a percentage of C–S.

The continued reference to C-source light throughout the above is due to the fact that the Commission on Ore Microscopy (C.O.M.) has standardized color values in C-source light. As this is only a component of the tristimulus weights (Table 1), it is not essential to have a microscope illuminated with C-source light as all reflectance measurements are made in monochromatic light. Details of the color temperatures and tristimulus weights of other standard light sources can be found in several texts, especially Judd & Wyszecki (1975).

ACCURACY OF COLOR MEASUREMENTS IN OPAQUE MINERALS

The above-described method for calculating color values uses spectral reflectance data as its sole determined parameter, the tristimulus weights being constant for a particular light source. The accuracy of the color values is therefore a function of the accuracy of the spectral reflectance data.

Although errors in the reflectance measurement can arise from many sources, most of these are avoidable, with the result that reflectance data can be obtained to a relative accuracy of $\pm 1\%$ (Piller 1966). Pinet *et al.* (1978) estimate that the errors in their reflectance measurements produced by the equipment are in the order of $\pm 0.2\%$ and that these errors are not significantly affected by the polish of their samples. The source of these errors and the avoidance of them have been discussed in detail by Bowie & Henry (1964), Leow (1966), Piller (1966, 1977), Galopin & Henry (1972) and others and will not be dealt with here. It is possible that a particular set of equipment may produce results from tests on the reproducibility (precision) of reflectance values more favorable than $\pm 1\%$, but allowing for fundamental errors introduced by the equipment or specimen preparation, relative accuracies of $\pm 1\%$ seem a reasonable expectation. Where these equipment and sample preparation errors are not completely eliminated a systematic bias in the reflectance measurements may result.

In addition, one may expect a random measurement error. To gain some idea of the effect that random measurement-error might have on the magnitude of the derived color-parameters, we performed a number of simulation experiments using a Monte Carlo method. In each experiment the spectral reflectance curve for a mineral, characterized by reflectances at the sixteen wavelengths, was taken and Gaussian noise added to simulate the random measurement-error. The color parameters were then computed from the curve plus its simulated error. For a given mineral this sequence was then repeated one hundred times to yield sample distributions of the five color parameters (x, y, Y, $Pe\%$ and $d\lambda$). The descriptive statistics of these distributions, themselves normal, give good estimates of the magnitude of scatter that might have been expected with real measurements. A major problem was deciding on the standard deviation to be applied to the simulated error-distribution. Despite extensive discussions about error and sources of error in photometry, there seems to have been little attempt, theoretical or practical, to determine the real magnitude of error. For this exercise we chose the 1%

TABLE 2. SUMMARY STATISTICS ON THE COLOR PARAMETERS OF SELECTED MINERALS+

	ARSENOPYRITE			PYRARGYRITE		
	μ	$\hat{\mu}$	$\hat{\sigma}$	μ	$\hat{\mu}$	$\hat{\sigma}$
x	0.3097	0.3097	0.0006	0.2875	0.2875	0.0006
y	0.3164	0.3166	0.0009	0.2944	0.2945	0.0009
Y	51.80	51.83	0.206	30.19	30.20	0.119
Pe%	0.10	*	*	10.7	10.7	0.27
dλ	495.1	*	*	477.7	477.8	0.61
	ANDORITE			EMPLECTITE		
	μ	$\hat{\mu}$	$\hat{\sigma}$	μ	$\hat{\mu}$	$\hat{\sigma}$
x	0.3047	0.3047	0.0006	0.3164	0.3165	0.0006
y	0.3132	0.3133	0.0009	0.3295	0.3300	0.0009
Y	40.79	40.81	0.162	41.80	41.85	0.167
Pe%	2.3	2.3	0.27	5.2	5.3	0.33
dλ	483.4	483.7	2.16	568.1	568.1	1.15
	UMANGITE			CUBANITE		
	μ	$\hat{\mu}$	$\hat{\sigma}$	μ	$\hat{\mu}$	$\hat{\sigma}$
x	0.3053	0.3052	0.006	0.3308	0.3308	0.0006
y	0.2732	0.2731	0.008	0.3414	0.3415	0.0009
Y	13.70	13.71	0.052	39.37	39.39	0.158
Pe%	16.5	16.5	0.30	12.3	12.4	0.32
dλ	-556.2	-556.3	0.55	574.9	574.9	0.54

+ see text for explanation
μ: 'True' value computed directly from the spectral reflectance curve
μ: arithmetic mean of parameter distribution
σ: standard deviation of parameter distribution
*: point to close to C-source for Pe% and dλ statistics to be meaningful

relative error quoted by Piller (1966) and treated this as a standard deviation for the simulated error-distribution. Because of this uncertainty, we performed only one hundred sets of simulations for each mineral, and hence obtained only moderate approximations for statistical estimates derived from the color-parameter distributions.

In Table 2 we present a summary of the simulation results on six minerals chosen to represent a reasonable range of the *x*, *y*, *Y* color space. The standard deviations on the estimation of *x* and *y* are almost constant at 0.0006 and 0.0009, respectively, values that could reasonably be applied to the whole color volume. The standard deviations on luminance (*Y*) increase with *Y* but show a near-constant coefficient of variation of 0.00392 (range: 0.00379 – 0.00400). The *Pe%* parameter shows a near-constant standard deviation of about 0.30, whereas *d*λ shows a decreasing but irregular standard deviation as *Pe%* increases. Of the Helmholtz coordinates the proportionate error about *d*λ is considerably lower than that about *Pe%* except at values of *Pe%* below about 1.5%.

To illustrate the effect of adding this random error to a spectral reflectance curve we show a small set of simulated curves for cubanite in Figure 2. As determined spectral reflectance curves are generally smoother than those shown in Figure 2, we suggest that even for rapid routine measurements our choice of error bounds for the simulation experiments is probably pessimistic.

To evaluate the effect of bias (the "systematic error" of Embrey & Criddle 1978) on reflectance measurements we have computed the color parameters on the range ± 2% absolute about the spectral reflectance curve of cubanite. This simply moves the curve up or down with respect to its true position without altering its shape. A range of ± 2% should encompass any bias that might be expected. Some results from these experiments are summarized in Table 3. Because there is no change in the shape of the curves, the *d*λ parameter remains constant (574.9) in all cases. The saturation, *Pe%*, is biased in inverse proportion to the applied bias, with the rate of change being about 0.35% *per* 1% absolute bias. The variation in luminance (*Y*) is, of course, a direct additive expression of the bias.

A summary of the effects of random errors and bias as determined from these experiments is given in Table 4. Whereas the data in this table are approximations, we can reasonably expect that *x*, *y* coordinates are determined to better than ±0.002 and luminance (*Y*) to better than ±0.5%. This results in excitation

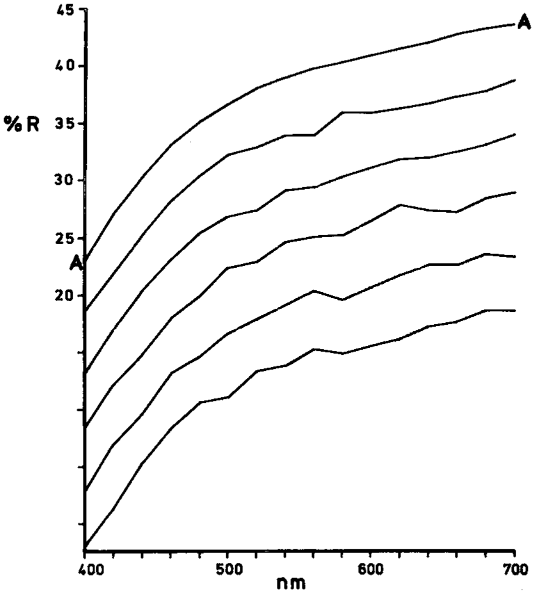


FIG. 2. Spectral reflectance curves for cubanite, showing the effect of an added random error. Curve A–A is the original spectral reflectance curve, to which the scale refers. For clarity the origin for the simulated curves is reduced by 5% *R* respectively.

TABLE 3. THE EFFECT OF BIAS ON THE MAGNITUDE OF THE COLOR PARAMETERS FOR CUBANITE

Bias	x	y	Y	Pe%
+2%	0.3297	0.3401	41.37	11.7
+1%	0.3303	0.3408	40.37	12.0
NONE	0.3308	0.3414	39.37	12.3
-1%	0.3314	0.3421	38.37	12.7
-2%	0.3320	0.3429	37.37	13.0

purity (*Pe%*) of less than ±1% and dominant wavelengths ($d\lambda$) of less than ±4 nm except at very low values of *Pe%*.

Unfortunately, there are insufficient published data to compare this level of error in color values with natural ranges encountered in many minerals. The work of Pinet *et al.* (1978) on proustite and pyrargyrites, however, suggests that the natural range in color values, of these two minerals at least, is greater than that caused by a ±2% error in reflectance measurement. This is particularly significant as Pinet *et al.* estimate that their reflectance measurements are accurate to ±0.2%.

The Distribution of the Color of Opaque Minerals in Color Space

With the publication in 1977 of the first issue of the C.O.M. Quantitative Data File, which contains color values for over one hundred minerals, it has been possible to describe the distribution of the color of opaque minerals in color space. If we first consider their distribution in the chromaticity diagram (Fig. 3), it is apparent that all the opaque minerals plot in a relatively narrow band centred on the C-source position and elongated towards 578 nm in the yellow and 475 nm in the blue region. In both the yellow and blue directions the excitation purity (*Pe%*) does not exceed 45% and is considerably less in the green and purple regions. This allows a bounding field to be drawn on the chromaticity diagram inside which all opaque minerals for which color values are available plot (Fig. 3). An enlargement of the area inside the bounding field of Figure 3 is shown in Figure 4, where a better impression can also be gained of the distribution of opaque minerals in the chromaticity diagram.

TABLE 4. SUMMARY OF SIMULATED 'ERROR' EXPERIMENTS

Parameter	Random error	Bias (β)
x	$\hat{\sigma} \simeq 0.0006$	Inversely ∝ β; 0.0006/1%β
y	$\hat{\sigma} \simeq 0.0009$	Inversely ∝ β; 0.0007/1%β
Y	$\hat{\sigma}/\hat{\mu} \simeq 0.00392$	Absolute change = % β
Pe%	$\hat{\sigma} \simeq 0.3\%$	Inversely ∝ β= 0.35%/1%β
dλ	$\hat{\sigma}<3.0$ if Pe% >1.5%	Virtually no effect

The figures quoted for the effect of bias relate to simulations based on cubanite with a luminance of about 40%. These bias effects decrease with increasing luminance, and increase slightly with decreasing luminance.

Because most minerals adhere closely to a linear relationship in x–y space, the distribution can be displayed by plotting luminance (Y) against the first principal-component scores for each point. The latter were computed from the variance–covariance relationships between x–y values and are equivalent to a "best-fit" line through the xy points, with the "points" projected normally onto the line. The projection plane is then vertical from the chromaticity base-plane. This near-orptimum spatial plot is shown in Figure 5.

From these diagrams it is apparent that the opaque phases are reasonably well-separated in color space, and hence the color values should be good discriminating parameters for identification purposes. The most clustered, and hence most difficult region, is that with a luminance between 25 and 45% and a chromaticity just to the "blue" side of the C-source.

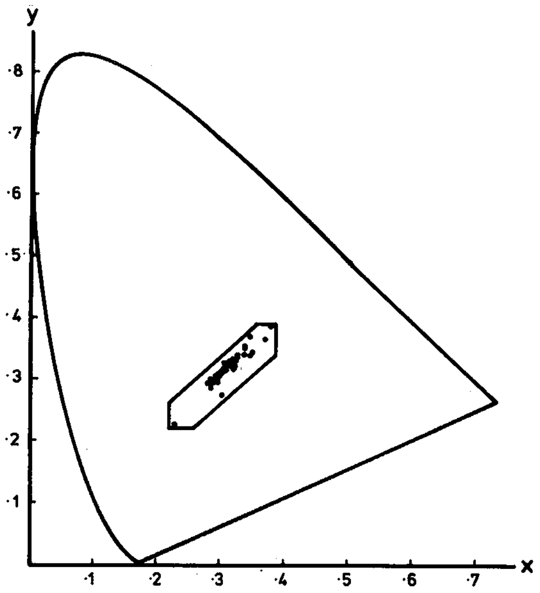


FIG. 3. CIE (1931) chromaticity diagram showing the distribution of the chromaticity of all opaque minerals represented in the first issue of the C.O.M. Quantitative Data File for which appropriate data are available.

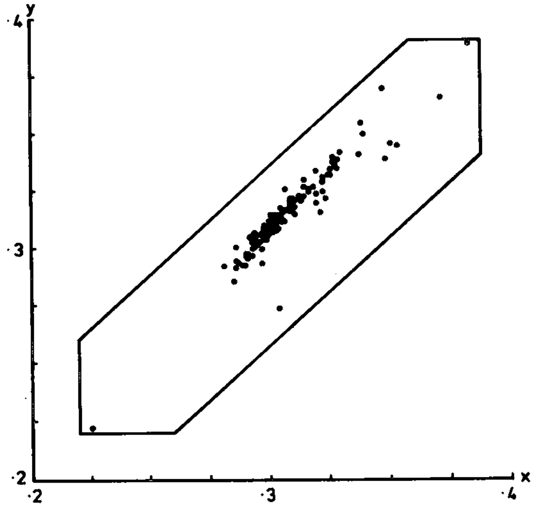


FIG. 4. Enlargement of the hexagonal area in Figure 3 that encloses all chromaticity points of opaque minerals.

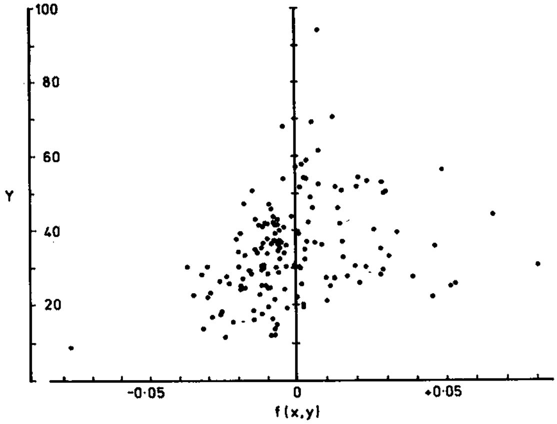


FIG. 5. Distribution, on a projection of the color space, of the mineral phases plotted in Figure 3. Vertical axis is luminance (Y) and the horizontal axis $f(x,y) = 0.71932\,(x-\bar{x}) + 0.69468\,(y-\bar{y})$, where $\bar{x}$ and $\bar{y}$ are the respective arithmetic means; $\bar{x} = 0.3089$, $\bar{y} = 0.3148$. See text for explanation.

THE USE OF COLOR VALUES IN THE IDENTIFICATION OF MINERALS

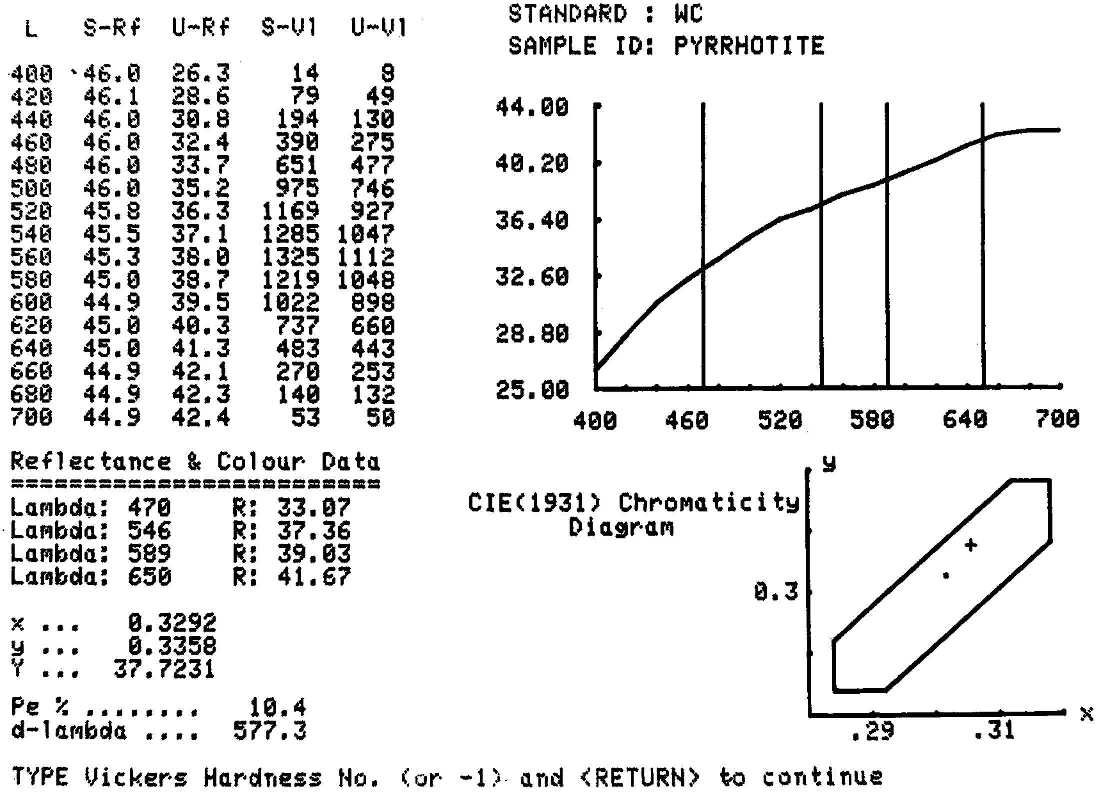
It has been shown that the use of quantitative color values is potentially a powerful tool for the identification of opaque minerals. This is also shown by the significant improvement in identification efficiency demonstrated in an earlier paper (Atkin & Harvey 1979), which described an identification system using chromaticity coordinates as discriminating parameters. This earlier system (NISOMI 1978) was developed as a natural progression from the Bowie–Simpson system (1978) which used reflectance in monochromatic light at four wavelengths across the visible spectrum and *VHN* as its discriminating parameters. Consequently, the NISOMI system used reflectance at four wavelengths, chromaticity and *VHN* as its discriminating parameters. In effect this meant that we were using the same property (the shape of the spectral reflectance curve) twice in the identification procedure. The other disadvantage with this earlier system is that it was designed to operate from a medium-sized computer (*i.e.*, a DEC PDP 11/35) rather than from a small desk-top computer.

The system to be described here uses the color values *Y*, *Pe%* and $d\lambda$ together with *VHN* as its identifying parameters and is designed to operate on a Tectronix 4051 desk-top computer. The system can be subdivided into two sections: (1) the calculation of color values from spectral reflectance data and (2) the identification routine.

The first part of this system involves the calculation of spectral reflectance data from photometer readings on both standard and specimens taken at 20 nm intervals from 400 to 700 nm. Either these photometer readings can be typed into the computer, or if a photometer is used which can be interfaced with the computer these readings may be read in directly. From the spectral reflectance data a spectral reflectance curve is plotted, the color values, x, y, Y, *Pe%* and $d\lambda$ are calculated, and the mineral's position is plotted on a chromaticity diagram. The computer then requests the *VHN* which has to be typed in (if available) *via* the keyboard.

The output from this first part of the system is shown in Figure 6 for pyrrhotite. After all the necessary data have been calculated, the system proceeds to the identification routine, which involves first comparing the color values of the unknown with similar values for minerals in the data file; only where there is a color match is a comparison made with the *VHN*. Before describing the identification routine in detail, it is necessary to describe how the color space is subdivided and how the data file is constructed.

The data file consists of the C.O.M. data-file number and name for each mineral followed by a range of values for luminance (Y), a range of values for *VHN*, a series of color codes (the derivation of which will be described be-



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 L    S-Rf  U-Rf  S-Vl  U-Vl

400  `46.0  26.3    14     9
420   46.1  28.6    79    49
440   46.0  30.8   194   130
460   46.0  32.4   390   275
480   46.0  33.7   651   477
500   46.0  35.2   975   746
520   45.8  36.3  1169   927
540   45.5  37.1  1285  1047
560   45.3  38.0  1325  1112
580   45.0  38.7  1219  1048
600   44.9  39.5  1022   898
620   45.0  40.3   737   660
640   45.0  41.3   483   443
660   44.9  42.1   270   253
680   44.9  42.3   140   132
700   44.9  42.4    53    50

Reflectance & Colour Data
==========================
Lambda: 470      R: 33.07
Lambda: 546      R: 37.36
Lambda: 589      R: 39.03
Lambda: 650      R: 41.67

x ...    0.3292
y ...    0.3358
Y ...   37.7231

Pe % ........   10.4
d-lambda ....  577.3

TYPE Vickers Hardness No. (or -1) and <RETURN> to continue
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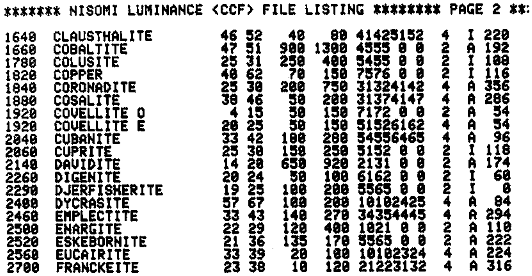
FIG. 6. Computer output for the mineral pyrrhotite (E′) showing derivation and display of color and reflectance values.

low), an indication of whether the mineral is isotropic (I) or anisotropic (A) and the page number of that mineral in Uytenbogaart & Burke (1971). The data file contains information on 135 minerals at present but will increase as new data become available. Much of the data is taken from the C.O.M. Quantitative Data File, although some is taken from other published material or has been obtained from our own laboratory. A portion of the data file is shown in Figure 7.

The color codes in the data file simply describe the position of the minerals in the chromaticity diagram. As we have insufficient data on the quantitative color of opaque minerals, we cannot yet represent the color of any mineral by a single point or even by a small area on the chromaticity diagram. To remedy this we have divided the chromaticity diagram into 43 overlapping fields based on *Pe%* and $d\lambda$ as shown in Figure 8. This means that any one point within this diagram can fall into one, two or four fields depending on where it plots in relation to the overlapping field boundaries. As the $d\lambda$ values of any point with a *Pe%* < 2 are meaningless (see section on accuracy above), all points with *Pe%* < 2 are assigned to the same field. We have coded these color fields so that any point can be reported by up to four 2-digit numbers forming the eight-column number in the data file (Fig. 7). The next column of the file gives the number of fields in which the mineral can plot (*i.e.*, 1, 2 or 4).

The identification algorithm starts by computing the color codes for the unknown mineral. The mineral file is then accessed, and the luminance (Y) of the unknown compared with the luminance range stored for each mineral in the file. If Y falls within range the color codes are compared, and again only when one or more of these match is the *VHN* of the unknown compared to the range stored on the data file. For minerals in the data file whose color and hardness match those of the unknown, the computer prints the C.O.M. number and name, the indication of isotropy, a small bar chart which shows the position of the luminance of the unknown in relation to the luminance range in



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******* NISOMI LUMINANCE <CCF> FILE LISTING ******** PAGE 2 **:

1640  CLAUSTHALITE        46 52   40   80 41425152  4  I 220
1660  COBALTITE           47 51  900 1300 4555 0 0  2  A 192
1780  COLUSITE            25 31  250  400 5455 0 0  2  I 100
1820  COPPER              40 62   70  150 7576 0 0  2  I 116
1840  CORONADITE          25 30  200  750 31324142  4  A 356
1880  COSALITE            38 46   50  200 31374147  4  A 286
1920  COVELLITE O          4 15   50  150 7172 0 0  2  A  54
1920  COVELLITE E         20 25   50  150 51526162  4  A  54
2040  CUBANITE            33 42  100  280 54556465  4  A  96
2060  CUPRITE             25 30  150  250 5152 0 0  2  I 118
2140  DAVIDITE            14 20  650  920 2131 0 0  2  A 174
2260  DIGENITE            20 24   50  100 6162 0 0  2  I  60
2290  DJERFISHERITE       19 25  100  200 5565 0 0  2  I   0
2400  DYCRASITE           57 67  100  200 10102425  4  A  84
2460  EMPLECTITE          33 43  140  270 34354445  4  A 294
2500  ENARGITE            22 29  120  400 1021 0 0  2  A 110
2520  ESKEBORNITE         21 36  135  170 5565 0 0  2  A 222
2560  EUCAIRITE           33 39   20  100 10102324  4  A 224
2700  FRANCKEITE          23 38   10  120 21223132  4  A 316
```

FIG. 7. Portion of the data file used for the identification routine. For each mineral the following data are stored in order: C.O.M. number and name, minimum and maximum acceptable values for luminance, minimum and maximum acceptable values for *VHN*, four color codes, the number of non-zero color codes, an isotropy indicator (I isotropic, A anisotropic) and finally the page number of the mineral in Uytenbogaart & Burke (1971).

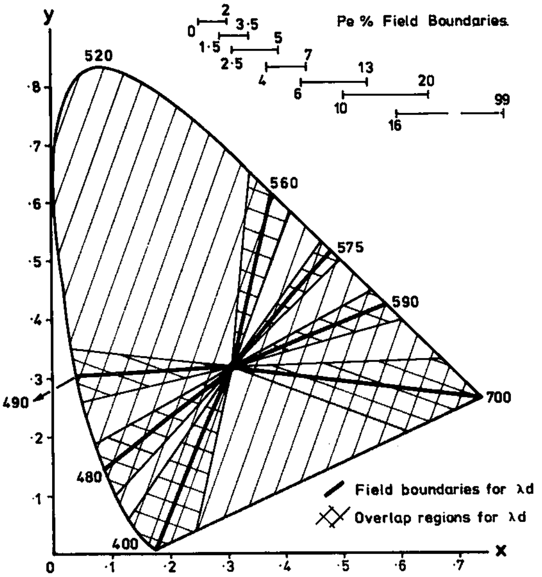
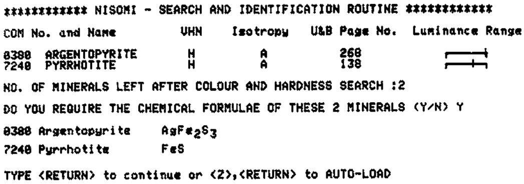


FIG. 8. CIE chromaticity diagram showing the method of subdivision as used in the identification routine.

the data file, an indication of whether or not a hardness search has been carried out, and the page number in Uytenbogaart & Burke (1971). Figure 9 shows the output from this point of the system for pyrrhotite.



```
************ NISOMI - SEARCH AND IDENTIFICATION ROUTINE ************

COM No. and Name         VHN     Isotropy   U&B Page No.  Luminance Range

0380  ARGENTOPYRITE       H          A          260
7240  PYRRHOTITE          H          A          138

NO. OF MINERALS LEFT AFTER COLOUR AND HARDNESS SEARCH :2

DO YOU REQUIRE THE CHEMICAL FORMULAE OF THESE 2 MINERALS (Y/N) Y

0380 Argentopyrite     AgFe2S3

7240 Pyrrhotite        FeS

TYPE <RETURN> to continue or <Z>,<RETURN> to AUTO-LOAD
```

FIG. 9. Computer output from the identification routine for the data shown in Figure 6. The luminance range from the data file is shown as a horizontal bar. A short vertical bar shows the position within this range of the luminance value derived from the unknown. The chemical composition of the listed minerals may be added to aid final identification.

As can be seen from Figure 9 a further option exists in the search routine that enables chemical formulae of the possible minerals to be printed. This information may be of help in eliminating further minerals. The chemical formulae of the minerals are stored in a separate data file which is accessed by a separate search routine when requested.

The time taken for operation of the system varies slightly depending upon the number of possible minerals that remain after the search routine and whether or not the chemical formulae are requested for these minerals. The example used in Figures 6 and 9 took 3 minutes and 10 seconds to be produced, which included the time taken to type in the photometer readings *via* the keyboard. If the photometer were interfaced with the computer this time would be reduced to about 2 minutes.

In order to test the efficiency of this identification scheme we took data from the C.O.M. Quantitative Data File for each orientation for all the minerals where both spectral reflectance data and *VHN* data were available and passed these through the search routine. The results from these tests are summarized in Figure 10. In 80% of cases the identification routine resulted in less than three possible minerals and in only 9% of cases were more than four minerals left after filtering in color, hardness and isotropy.

These figures are more favorable than those quoted in our earlier paper describing the original NISOMI system (Atkin & Harvey 1979), mainly because of improvements in the subdivision of the CIE (1931) chromaticity diagram. In the earlier paper we compared the efficiency of the NISOMI system to other systems, especially the Bowie–Simpson system (1978), and demonstrated that the use of chromaticity coordinates as identifying parameters resulted in a better discrimination than that available in earlier systems. The improved system described here further enhances the discrimination.

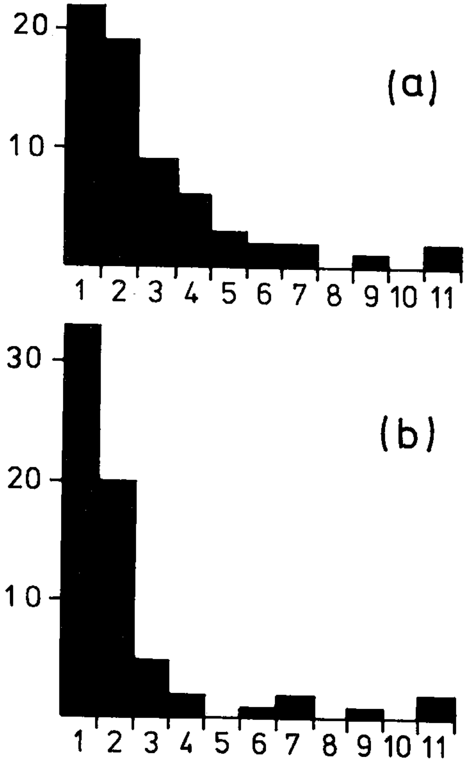


FIG. 10. Discrete histograms showing the results of efficiency tests using data from the C.O.M. Quantitative Data File. Vertical axis: frequency; horizontal axis: the number of minerals that remain as possible phases at the end of the search routine. Fig. 10 (a) is based simply on the computer output involving filtering by color and hardness; 10(b) takes into account the additional visual determination of whether the mineral is isotropic or anisotropic. Further explanation is given in the text.

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