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EDITORIAL POLICY FOR THE SECOND ISSUE OF THE IMA/COM QUANTITATIVE DATA FILE

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General Introduction

In 1970 the Commission on Ore Microscopy (COM) of the International Mineralogical Association (IMA) published a provisional issue of *International Tables for the Microscopic Determination of Crystalline Substances Absorbing in Visible Light*. The level of acceptance was data for the four standard wavelengths of the COM, and 118 cards were included. The success of this encouraged the COM to publish in 1977 the first issue of the IMA/COM Quantitative Data File (QDF) consisting of 204 cards containing data for 155 ore minerals; the data were in varying states of completeness. This was envisaged as the first stage in what would eventually include data for all ore minerals to a high state of completeness. Although reflectance data measured at an interval of 20 nm between 400 and 700 nm were aimed at, cards containing reflectances at only the four standard wavelengths of the COM were accepted. A card format was chosen to provide the flexibility required for a publication that was to grow. The success of this first issue has exceeded expectations in the number of citations in the literature and has encouraged the COM to proceed with the second issue. In addition to the application of the cards in mineral identification, the Data File has been made the base for computerized schemes for this purpose. Further, the ease of access to such data has encouraged an interest in the possibility of deriving optical constants from reflectances in two media. These provide data for the study of atomic bonding in mineral substances. This application requires the measurements to be made in oil as well as in air, and the first issue did not insist on this. Also, the first issue accepted cards that were lacking a quantitative chemical analysis, X-ray powder data or microindentation hardness measurements. In formulating the editorial policy for the second issue, the ready availability of improved instrumentation and the advances that have been made in recent years in the technical and theoretical aspects of opaque mineral identification were taken into account. The user of the Data File was considered also, and it was concluded that the main data base should be as comprehensive as is practicable. Compositional and X-ray data will be required and, wherever possible, the reflectance data supplied (in air and in oil) should cover the visible spectrum at intervals of 20 nm. At the same time it was appreciated that, whereas many workers have access to X-ray and electron-microprobe equipment, they may not be as well equipped for microscope photometry. Thus, provision will be made in the second issue for workers who can contribute reflectance data at only the four wavelengths recommended by the COM.

Contributions, which should conform to the editorial requirements for the second issue, are now cordially invited. Many of the cards in the first issue will meet the requirements of the second; others would do so with the addition of a few data. If contributors wish to resubmit their data to meet the new requirements, and in the new format, such data will be included in the new issue.

Publication of the second edition will be serial, with each part consisting of not less than two hundred cards. Early submission should ensure inclusion in part one of the second issue.

Introduction

The second issue of the QDF will consist of cards of the same size as those in the first issue, and there will be the same five types. The format has been altered from that of the first issue in order to accommodate more information; a sample form (Fig. 1) and a blank form (Fig. 2) illustrate the new format. The recommendations in the 1980 IMA/COM Report

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Number 2.6200

Name & Chemical Formula
Nukundamite $Cu_{5.5}Fe\ S_{6.5}$

Symmetry
Hexagonal

Provenance
Undu Mine, Nukundamu, Fiji
16° 4' 12" S, 179° 33' 0" W

Standard
SiC (Zeiss, 055)
Monochromator Δλ ≈ 12nm
Line interference filter
Photomultiplier
S 20, Hamamatsu type R 446
Effective N.A.
Air 0.35, 0.3 Oil 0.4, 0.3

Polishing Method
800 & 600 grade carborundum; 1200 alumina on glass. Diamond (14, 6, & 3μm) on cloth. Water lubricated throughout.

VHN: 103 - 110 *Load(gf)* 20 sf,cc

Reference & Further Information:
Rice(C.M.), Atkin(D), Bowles (J.F.W.) & Criddle(A.J.) 1979, Mineral Mag. 43, 192-200.

The R-data are for a single grain.

nm	Air R_o	Air R'_e	Zeiss Oil at 20°C R_o	Zeiss Oil at 20°C R'_e
470	14.0	23.6	5.4	11.8
546	16.2	23.7	8.4	11.9
589	19.6	24.0	11.6	12.1
650	25.0	26.8	15.7	15.0
400	15.4	23.8	5.5	11.4
420	14.9	23.8	5.2	11.4
440	14.3	23.8	5.2	11.6
460	14.1	23.6	5.4	11.8
480	14.0	23.7	5.5	11.8
500	14.1	23.7	6.1	11.9
520	14.7	23.7	7.0	11.9
540	15.8	23.7	8.1	11.9
560	17.1	23.8	9.3	11.9
580	18.7	23.9	10.8	12.0
600	20.4	24.0	12.1	12.2
620	22.1	24.7	13.7	12.9
640	24.0	26.1	15.0	14.1
660	25.7	27.9	16.4	16.0
680	27.3	30.0	17.5	17.4
700	28.7	30.2	18.6	18.5

Colour Values

	x	y	Y%	λ_d	P_e	Illuminant
R_o	.350	.330	17.4	592	14.6	Air
R'_e	.314	.316	24.0	612	1.2	Air
R_o	.394	.316	9.5	586	34.8	C Oil
R'_e	.319	.318	12.1	600	2.8	C Oil
R_o	.488	.402	18.4	598	23.8	Air
R'_e	.453	.405	24.2	615	2.5	Air
R_o	.517	.406	10.4	593	47.4	A Oil
R'_e	.459	.404	12.3	607	5.7	A Oil

Chemical Composition:

		±
S	33.51	0.16
Fe	9.64	0.13
Cu	56.51*	0.14
Ag	0.09	
As	0.04	0.02
	99.79	

*Range = 0.00 to 0.34, total = mean +1σ of five analyses

X-ray Data: *a* 3.782(4), *c* 11.187 (8).

hkil	*d* Å	*I*	*hkil*	*d* Å	*I*
$10\bar{1}0$	3.273	30	$11\bar{2}0$	1.891	60
$10\bar{1}1$	3.143	100	$10\bar{1}5$	1.847	55
$10\bar{1}2$	2.826	70	$11\bar{2}4$	1.568	25
0004	2.796	45			

FIG. 1. Sample form for second issue of the IMA/COM QDF. Note that nonmetal standards used are not stated.

on Symbols and Definitions (Henry 1980) will be followed. The essentials of the present paper may be summarized here: (a) the standards used must be those approved by the COM; (b) reflectance data must be submitted for the range 400 to 700 nm at intervals of 20 nm, both in air and in a standard oil; in addition, the values at the four standard wavelengths must be supplied. The ordinary form must contain only data from a single composition (see section on Complementary Cards for ranges); (c) the quantitative chemical composition must be given; (d) X-ray powder data sufficient to identify the specimen must be given, or else the number of the corresponding card in the JCPDS powder-diffraction file (PDF) must be quoted; (e) although it is very desirable that the range of Vickers micro-indentation hardness be supplied, lack of this will not exclude a card from acceptance, and (f) data will only be accepted if typed on the official form and sent to the Editor of the COM Quantitative Data File, Department of Mineralogy, British Museum (Natural History), Cromwell Road, London SW7 5BD, England. Forms may be obtained from the Editor or else from national representatives. (The finished cards will be, as in the first issue, of A5 size, *i.e.*, half the area of the form.)

In drafting this policy we sought the opinions of several workers active in the field. It was widely agreed that, whereas more complete data were desirable and should comprise the main body of information in the second issue, we did not wish to exclude entirely a form containing only partial reflectance data (see section on Supplementary Cards). Also, although the ordinary forms must contain data for a single composition, it was agreed that we also wanted data for a range of compositions in a given mineral (see section on Complementary Cards).

Mineral Name, Symmetry and Provenance

The mineral name will be in the form recommended by the IMA; the convention of Hey

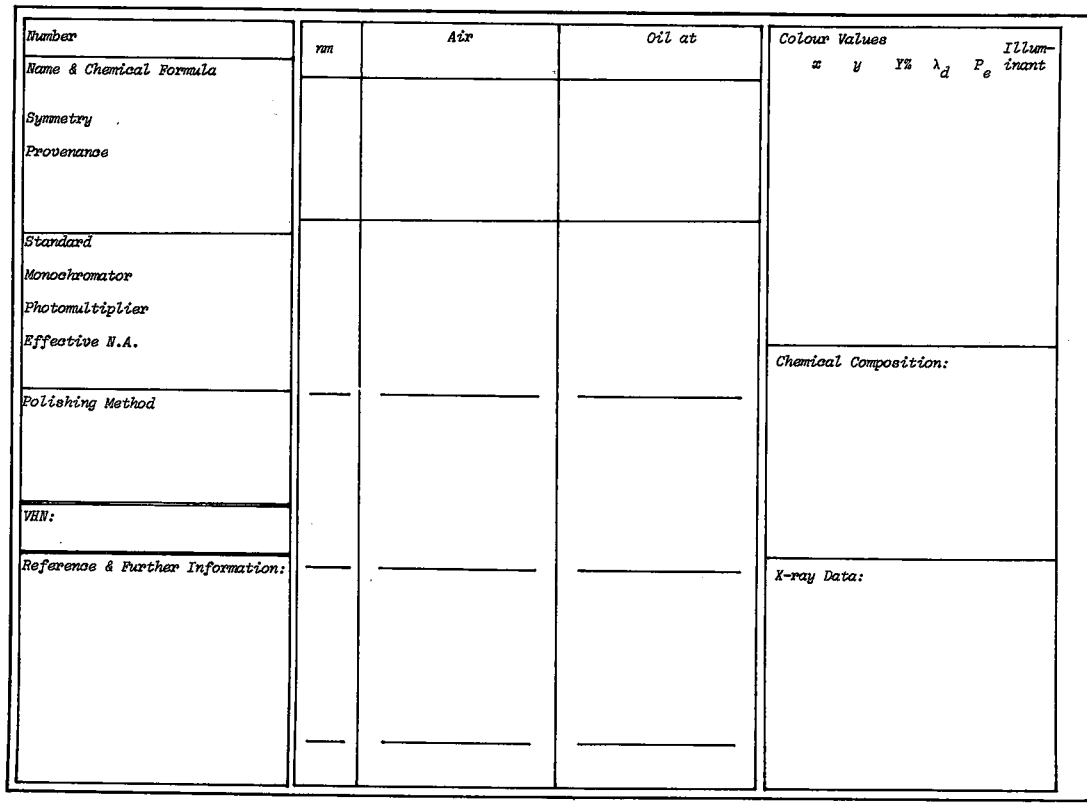

FIG. 2. Blank form for second issue of the IMA/COM QDF.

(1962, 1963) and Hey & Embrey (1974) should be used. The symmetry system will be given in the European way, using the trigonal system. For any mineral assigned to the trigonal system, mention of the lattice must be added: either "hexagonal lattice" (*hP*) or "rhombohedral lattice" (*rP* = *hR*). It is desirable that the provenance be given so that the place be located with the aid of an international gazeteer; its latitude and longitude should be given in degrees, minutes and seconds.

MONOCHROMATOR AND PHOTOMULTIPLIER

The type of monochromator should be quoted and its band width given (*e.g.*, $\Delta\lambda$ = 12–15 nm). The international code for the type of photomultiplier used should be given and also the manufacturer's name and code (*e.g.*, Fig. 1).

EFFECTIVE APERTURE ANGLE

Since different aperture angles produce different values of reflectance under certain conditions, it is desirable to provide information from which these values can be easily derived. On the image in the back focal plane of the objective, let r be the radial distance of the full aperture of the objective and r' that of the (partially closed) aperture used in the measurements (effective aperture); then the ratio (r/r') can be measured with an ocular micrometer. If the numerical aperture (N.A.) of the objective is quoted, along with the measured ratio (r/r'), then the effective aperture angle is known; these two values should be given in the appropriate space (*e.g.*, Fig. 1).

STANDARDS OF REFLECTANCE

All standards of reflectance used must be stated and must be among those approved by the COM. At present these are black glass (R~4.5%), black silicon carbide (R~20%), tungsten–titanium carbide (R~46%) and tungsten carbide (R~46%).

Reflectances in air and in oil

Reflectances must be measured with the microscope photometer at effectively normal incidence against one or more of the approved COM standards over the spectral range 400 to 700 nm at an interval of 20 nm; this must be done both in air and in an oil conforming to the German standard DIN 58.884. The manufacturer of the oil should be stated, since these oils do differ slightly among themselves; also, the temperature at which the oil measurements were made should be given. If the spectral curve of reflectance shows distinct features that have been revealed by measurement with higher spectral resolution and shorter wavelength-interval, the data needed to draw out the feature should be given, for air and for oil, under "Further Information". In addition, the reflectances at the four standard COM wavelengths (470, 546, 589 and 650 nm) must be given for air and for oil; these may be either measured specially or else obtained by graphical or calculated interpolation.

Five types of data cards are available, depending on the mineral's optical class, with an additional one for complementary cards (see below); in case of doubt, the 1980 IMA/COM Report on Symbols and Definitions (Henry 1980) should be consulted. The symbols for the five data cards are as follows:

R or R': R is used for minerals of cubic symmetry. R' is used where the substance is observed to be anisotropic, but where the reflectance measured, on rotation of the stage and at a given wavelength, is constant (*i.e.*, within measurement error); it is also used for amorphous substances.

R_o R_e: Uniaxial where the extreme values for the extraordinary vibration can be given with certainty.

R_o R'_e: Uniaxial where the extreme values cannot be given for the extraordinary vibration with certainty (Note 1).

R_1 R_2: Biaxial in general and in all cases where the vibrations cannot be otherwise named (Note 2).

R_a R_b R_c: Orthorhombic where oriented sections are used so that the three principal vibrations can be measured (Note 3); also used for monoclinic substances where the values for the vibration along the unique axis can be given (Note 4).

The form must be filled in with data as if these were from a single grain of the composition stated; thus only a single value may be given for a particular vibration at a particular wavelength (see also sections on Complementary Cards and Supplementary Cards). For additions and deletions in the headings of the reflectance columns, see Notes below.

Note 1: In a very few uniaxial substances it has been found that different values are obtained for R_o according to whether these are measured on the basal section or on a section more or less vertical. In such a case the column headed by this symbol should be filled with the data obtained on the basal section; the other set of data is entered in a separate column headed R_o* written in at the head; (likewise, $^{im}R_o$*); an explanatory note should be added under "Further Information". This procedure should be used in all cases where one wishes to insert an additional column under Air (and one under Oil), but the data must refer to a single grain (ideally).

Note 2: The rule for the allocation of these symbols is that R_2 is the label for the set of data having the higher luminance (Y) for the C illuminant. (If desired, the data may be sent in advance to the editor for computation of the luminances.) Where the luminances cannot be obtained owing to incompleteness of the spectral reflectances, as in supplementary cards, the symbol R_2 is allocated to the set of data having the greater value of $R(546)$. This rule would also apply where the two luminances were equal. Where the two values of $R(546)$ are equal, the values of $R(589)$ would be used instead. It should be noted that there are cases in which the two rules would not agree; then the luminance rule would have priority, and a note of explanation should be inserted under "Further Information".

In uniaxial substances of very low bireflectance it may not be possible to decide with certainty which vibration is the ordinary, especially with metallic substances, because of a lack of definition of extinction positions and also because of chemical variation from grain to grain. When this difficulty is encountered, the R_1 R_2 form is used. If a guess can reasonably be made, but without certainty, the following symbols may be put under Further Information:

$R_1 \stackrel{?}{=} R_o$ or $R_2 \stackrel{?}{=} R_o$.

Note 3: In the case of oriented sections of an orthorhombic crystal, the values of the unit-cell lengths (a,b,c) must be given under X-ray data, likewise the length b in the case of a section parallel to this axis in a monoclinic crystal.

Note 4: In the case of a section parallel to the unique axis (y) in a monoclinic crystal, the

R_a R_b R_c form is used. If the set of data R_b has the higher luminance, the subscript to R_a is replaced so that the symbol becomes R_1, and R_c is deleted, its column being unused. If the set of data R_b has the lower luminance, then the first column is unused, with its heading deleted, and the last column becomes headed by the symbol R_2.

Color Values

These may be calculated by the author or else left to be calculated by the editor; the calculation should be done both for the *C* and *A* illuminants. The calculation of color values should be performed using the weighted ordinate method as recommended by the *Commission Internationale de l'Éclairage* (CIE).

Micro-indentation Hardness (Vickers)

The micro-indentation hardness range should be given, if possible, but this is not obligatory for acceptance in the second issue. Values are, preferably, given for the standard load of 100 gf (gram force). For very hard minerals this may be increased to a maximum of 200 gf. With very small grains or very soft minerals the load may be reduced to a minimum of 10 gf. Any nonstandard load should be stated. The loading speed of the indenter should be 10–20 μm/second and the duration of the indentation, 15 seconds. Measurement should be made in green light, ~546 nm, with an objective of numerical aperture ≧0.65. An indication of the quality and shape of the indentation should be given in the following symbols: *p*(perfect), *f*(fractured), *cc*(concave), *cv*(convex), *sf* (slightly fractured).

Chemical Composition and Formula

A fully quantitative analysis must be given, and the preferred method is by means of the electron microprobe. A note of the standards (excluding those of the pure metals) should also be inserted here. If there is insufficient space in this section, contributors may also use the "Further Information" section. The formula should preferably be given as the contents of the unit cell; otherwise it may be given as proportions of elements.

X-ray Data

Where the powder lines for a specimen match those on one of the cards of the powder-diffraction file (PDF) of the Joint Committee on Powder Diffraction Standards, it will suffice to quote the number of this card. If such a card has not appeared in the PDF, or where the lines differ somewhat from those on a card, the data should be supplied in sufficient detail to characterize the substance. On the $R_aR_bR_c$ card the lengths of the unit cell must be given.

Polishing Method

The author is, of course, responsible for ensuring that the polish is good, but some information on this should be given (see Fig. 1).

Reference and Further Information

Where the data have been published, the reference must be given. The remaining space can be used to provide additional information, as on the sample card (Fig. 1).

Supplementary Cards

In order to avoid the complete exclusion of a form that meets all the requirements for the second issue except that of providing reflectances for all 16 wavelengths, provision is made for supplementary cards; these will carry the letter S at the end of the card number. Reflectances, both for air and for oil, must be provided for the four standard COM wavelengths.

Complementary Cards

In order also to include data that are very useful for identification purposes, we encourage observers to enter on another copy of the form the ranges of reflectances that have been observed on different grains of the mineral studied. These will give rise to complementary cards bearing the letter C after the card number. The optimum condition, of course, is to have several ordinary cards covering the range of composition. In the meantime, however, complementary cards will be useful, and a special form is available for filling in such data.

References

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