CONFERENCE ON THE TEACHING OF CRYSTALLOGRAPHY*

The following five speakers took part in the Conference covering different phases of the teaching of crystallography: J. D. H. Donnay, D. Jerome Fisher, Samuel G. Gordon, M. A. Peacock, and George Tunell. Brief abstracts of the papers follow.

FROM THE LAW OF RATIONALITY TO THE LAW OF BRAVAIS

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The Law of Rationality is best introduced in a form that lends itself to direct experimental check—expressed in terms of *direction angles* of face normals (rather than *intercepts* of faces), since such angles are either measured on the goniometer or calculated from measured angles. Take coordinate axes Ox, Oy, Oz, parallel to the three (non-coplanar) edges between three suitable faces. Consider a fourth face, intersecting all three axes, and let ξ', η', ζ' be the angles which its normal makes with the axes Ox, Oy, Oz, respectively. Let ξ, η, ζ be the direction angles of the normal to any fifth face. The law of observation says: "quotients of corresponding direction cosines are in the ratios of small integers", or

$$\frac{\cos \xi}{\cos \xi'} : \frac{\cos \eta}{\cos \eta'} : \frac{\cos \zeta}{\cos \zeta'} = h:k:l, \tag{1}$$

where h, k, l, small integers, are the *Miller indices* of the fifth face. From (1) it appears that the indices of the fourth face are (111), hence its name "unit face."

Since the intercepts of a plane and the direction cosines of its normal are inversely proportional (a theorem easy to prove), (1) can be written as

$$a \cos \xi : b \cos \eta : c \cos \zeta = h:k:l, \tag{2}$$

where a, b, c, the unit lengths, are the intercepts of any plane parallel to the unit face. This is the "fundamental formula," the key to all crystallographic calculations, used to determine both *axial ratios* and *face indices*.

Likewise (2) becomes

$$\frac{a}{OH} : \frac{b}{OK} : \frac{c}{OL} = h:k:l,$$

where OH, OK, OL are the intercepts of any plane parallel to the fifth face. This is immediately rewritten in the familiar form

$$OH:OK:OL = \frac{a}{h} : \frac{b}{k} : \frac{c}{l} \tag{3}$$

or, reducing to the common denominator and clearing common factors, as

$$OH:OK:OL = kl\ a:lk\ b:hk\ c = ea:fb:gc, \tag{4}$$

where e, f, g, small integers, are the *Weiss coefficients* of the fifth face. In ordinary language, "any fifth face is parallel to a plane whose intercepts are either simple fractions (relation 3) or small multiples (relation 4) of the unit lengths."

Construct a lattice on a, b, c, taken as primitive translations. Let $OH = ea$, $OK = fb$, $OL = gc$. We see from (4) that the fifth face is parallel to a plane HKL passing through

three nodes, that is to say, a net plane. Moreover, since e, f, g are small, triangle HKL is small (in terms of unit lengths), and a parallelogram HKLM, whose area is twice that of triangle HKL, is also small. Points H, K, L, M, are lattice nodes, and parallelogram HKLM is either the smallest mesh or a multiple mesh of the net HKL; the smallest mesh, in either case, is thus small. Hence, the Law of Rationality can be stated in reticular terms: "any face is parallel to a net with small mesh area" or, since mesh area and interplanar distance are inversely proportional, "any face is parallel to a stratification of nets with large interplanar distance."

The Classical Law of Bravais naturally follows as an additional law of observation: "usually the faces actually observed are parallel to nets with largest interplanar distances; the larger the interplanar distance, the more frequent (and the larger) the face." (The Generalized Law cannot be introduced at this point, of course, since it requires some knowledge of space-group symmetry.)

CHANGES IN THE OBJECTIVES IN THE TEACHING OF MINERALOGICAL CRYSTALLOGRAPHY

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An attempt is made to outline a beginning course covering the basic crystallography needed by the modern mineralogist. Assumed prerequisites are one year's college work of good calibre in each of the following subjects mathematics, physics, and chemistry. The total time required by the average well-prepared student is taken as 175 hours, subdivided as shown in Table 1.

Table 1. A Basic Course in Mineralogical Crystallography

Subject	Time in hours				Per Cent of total time
	Class[1]	Supervised laboratory	Remainder[2]	Total	
Morphology	6	6	18	30	17
Crystal Physics[3]	21	21	63	105	60
Fracture[4]	1	1	3	5	3
Isotropics	5	5	15	25	14
Uniaxials	8	8	24	40	23
Biaxials	7	7	21	35	20
Crystal Chemistry	7	3	25	35	20
X-ray diffraction[5]	3	3	9	15	8½
Chemical crystallography	4	—	16	20	11½
Final examination	3	2	—	5	3
Total	37	32	106	175	100

[1] Lecture, discussion, quiz and examination.

[2] Unsupervised laboratory, problems, reading; *total* time assumed for the course is 175 hours.

[3] Microscopical crystallography in the main.

[4] Including cleavage, parting, gliding.

[5] Some might prefer to class this under crystal physics.

There is no single text-book in English which covers this ground with the distribution of space to the various topics like that here called for; see Table 2. The major objective of the course is the theory and practice of the determination of the optical constants of crushed grains in oils with the aid of the polarizing microscope.

TABLE 2. SUBDIVISIONS OF SPACE IN MINERALOGY TEXTS

Text	Subject						Total	
	Morphology		Crystal Physics		Crystal Chemistry[1]			
	Pp.	%	Pp.	%	Pp.	%	Pp.	%
Dana-Hurlbut	65	85	2	3	7	9	74	97
Kraus *et al.*	88	59	31	21	24	17	143	97
Rogers	108	55	55	28	27	14	190	97
Winchell	112	69	34	21	12	7	158	97
Dana-Ford	168	54	107	35	26	8	301	97
Bunn[2]	46	21	57	26	110	50	213	97
Average[3]......	..108..	..61..	.. 46..	..26..	....19..	..10..	...173...	...97...
D.J.F. (time)	—	17	—	60	—	20	—	97

[1] Including X-ray diffraction.

[2] Bunn, C. W., Chemical Crystallography, 1945. This is not a mineralogical text. It is relatively weak on crystal chemistry, though strong on x-ray diffraction. Chapters 7, 9, 10, and 11 are not counted in the above table.

[3] Excluding Bunn.

Some idea of the level of instruction may be judged from the final examination. This is in two parts, theory and practice. Following is a current theoretical examination (two hours).

N.B.—Notes and books may be used *except* do not look up the properties of sulfur asked for in any book. Give reasoning and show work for all answers.

Given a crystal of sulfur for which face (221) has phi$=50°53'$ and rho$=80°35\frac{1}{2}'$. $a_0=10.48$ Å. Indices of refraction are 1.96, 2.04, 2.25 with 2V of 69°. Optic plane is (010) and $a=$alpha. Density is 2.07. Assume cleavage parallel (105).

(1) Crystal System
(2) Optic Sign
(3) Axial ratio
(4) (*a*)"Picture" of interference figure 45° from extinction when lying on cleavage face (12.4 microns thick).
   (b) Show how isochromes will move if a quartz wedge (Z lengthwise) is inserted from the SE.
(5) Extinction angle (and sign) when lying on (221).
(6) (*a*) Number of atoms in unit cell.
   (*b*) Percentage "porosity."
   (*c*) What can you say of the type of packing?

THE ROLE OF THE MUSEUM IN THE TEACHING OF CRYSTALLOGRAPHY

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A distinction is made between a public museum, and a museum in a university, where it can be a useful adjunct in the teaching of crystallography. A museum exhibit must be graded to the experience level of the visitor, and a successful visual demonstration must be designed primarily for that purpose. An example is the "What is a Crystal?" exhibit in the mineral gallery of the Academy of Natural Sciences of Philadelphia. As any mineral collection is essentially an exhibit of crystals, these should be made more understandable to the visitor by the use of structure models, particularly those which will serve as a key to the classification of the minerals.

Exhibits should show the fundamental significance of crystallography to the petrographer and geologist, for much of what is called geochemistry could better be designated as geocrystallography. A mineral may be defined as a naturally occurring symmetrical structural arrangement of atoms, whose chemical composition can be expressed by an empirical formula to define a species. Mineralogy would then be defined as the study of these naturally occurring arrangements of atoms, their internal pattern and external forms; the origin of the structures; their physical and chemical properties; occurrence; and the effect upon them of physical forces and wandering ions.

THE TEACHING OF MORPHOLOGICAL CRYSTALLOGRAPHY

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Morphological crystallography—the theory underlying the description of crystal form—may be taught as an independent subject; but then it is essentially a branch of mathematics and the interest is apt to lie in mathematical elegance rather than in the forms of actual crystals, which the student may see only as represented by models and drawings. Conversely, practical crystallography can be undertaken with a minimum preparation in crystal geometry; but then the work tends to become a handicraft in which the whole interest is in the faithful description of the forms of crystals by measurements, drawings, and calculations, and little thought is given to the central problem of crystal form, namely the relation of form to other crystal properties, particularly the internal structure. Concurrent or consecutive work in theory and practice will counter these tendencies, giving the student a sound grasp of classical crystallography and a good preparation for the study of crystal structure.[1]

A course in morphological crystallography may commence with a consideration of the crystal lattice—the triperiodic array of structurally identical points in a crystal—which was firmly inferred from the Laws of Constant Angles and Simple Rational Intercepts and later demonstrated by the diffraction of x-rays. Accepting crystal faces as limiting lattice planes, the whole metrical aspect of crystal morphology can be developed from the crystal lattice and the auxiliary conception of the reciprocal lattice. The fourteen lattice types and the six metrical groups (provisional crystal systems) with their characteristic types of elements (axial ratios) may first be derived; the notation for crystal faces and edges is easily explained and, with the necessary geometry and trigonometry, their representation in stereographic and gnomonic projections is conveniently dealt with; and the derivation of cell elements from single-circle and two-circle measurements, and the converse calcula-

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[1] In the course in Mineralogy in the University of Toronto morphological crystallography, crystal measurement, and x-ray crystallography are prescribed in the second, third, and fourth undergraduate years, respectively.

tion of angles from established elements, can be treated in this sequence. Importance should be attached to the choice of the crystal lattice from angular measurements; this should, but for the rarest exceptions, correspond to the structural lattice as determined by x-rays. It is instructive to make this choice on morphological grounds without reference to the röntgenographic findings; and for this purpose the Bravais principle, especially as generalized by Donnay, and its gnomonic expression in the Harmonic-Arithmetic Rule, are effective and reliable aids.

The foregoing work can be developed with little reference to crystal symmetry, which can now be studied in a systematic manner, preferably with the use of the Hermann-Mauguin notation which requires rotation and rotation-inversion rather than rotation-reflection. Anticipating the needs of structural crystallography the thirty-two crystal classes should be rigorously deduced and grouped in the Laue Symmetries, and the possibilities of electrical polarity and optical activity in each class should be mentioned. At this point it would be well to redefine the crystal systems on the basis of symmetry, as seven rather than six groups of classes, in which any lattice element may fortuitously take special values which are incompatible with the provisional metrical definitions of crystal systems. The principles on which the space-groups are built can now be explained and the striking influence of glide-planes and screw-axes on crystal morphology, discovered by Donnay and Harker, can be illustrated. And finally the common occurrence of metrical pseudo-symmetry in crystals and its intimate relation to crystal twinning, so beautifully developed by Friedel, deserves more than passing mention.

This theoretical work always proceeds from the general to the special—the triclinic to the cubic—and consequently the practical work would logically follow the same course. Although contrary to current practice it might prove quite feasible to commence with a triclinic crystal and learn the full complexities at the outset. Exercises in the higher symmetries could then be carried through rapidly as relatively easy special cases.   •

THE TEACHING OF X-RAY CRYSTALLOGRAPHY

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Present day students of mineralogy need to learn the use of the x-ray powder diffraction method on account of its great utility and ease of application in the identification of crystalline substances. One lecture and one laboratory exercise in the beginning mineralogy course should suffice for this purpose. Students of elementary mineralogy also need at least an introduction to the structures of some of the commoner minerals in order to gain an insight into their chemical constitution and such physical properties as cleavage and refractive index.

Most students intending to specialize in mineralogy will wish to learn the methods of determining unit cell dimensions (edge lengths and inter-edge angles) by the diffraction of essentially monochromatic x-rays by single crystals. The equation existing between the unit cell volume, the density, and the chemical composition is an important aid to the mineralogist in checking these data, and its application is worthy of emphasis.

Those students of mineralogy especially interested in crystallography will go on to learn the detailed methods of determining the atomic arrangements in crystals by the analyses of the intensities of x-ray beams diffracted by single crystals and by powder specimens. These methods involve the use of Fourier series to calculate the distributions of electron densities in the unit cells as well as the use of the results of the theory of space groups. The study of atomic arrangements is beginning to provide a new quantitative picture of chemical bonds as well as of some of the important physical properties. An advanced course devoted to these topics will naturally include laboratory exercises with x-ray equipment, the optical goniometer, and the petrographic microscope.