PROCEEDINGS OF SOCIETIES

THE CRYSTALLOGRAPHIC SOCIETY OF AMERICA

William Parrish, *Secretary-Treasurer, c/o Philips Laboratories, Inc.,*
Irvington-on-Hudson, New York.

The fourth annual Spring meeting was held at University of Michigan, Ann Arbor, Michigan, April 7–9, 1949. 97 members and visitors registered for the meeting.

The officers for 1949 were:

President: Professor J. D. H. Donnay, The Johns Hopkins University.

Vice-President: Mr. Samuel G. Gordon, The Academy of Natural Sciences of Philadelphia.

Secretary-Treasurer: Dr. William Parrish, Philips Laboratories, Inc.

Councilors: Professor Raymond Pepinsky, Pennsylvania State College. Professor George Tunell, University of California at Los Angeles.

After more than a year's discussion the Society voted to join with American Society for *X*-ray and Electron Diffraction to form a single new Society, the *American Crystallographic Association,* which will carry on the functions of the two previous Societies. Information on the new Society may be obtained from the Secretary, Dr. Howard T. Evans, Jr., c/o Philips Laboratories, Inc., Irvington-on-Hudson, N.Y.

Abstracts of papers given at the technical sessions are given below in order of presentation.

CRYSTAL STRUCTURE

Chairmen: I. Fankuchen, Polytechnic Institute of Brooklyn,
A. Pabst, University of California, Berkeley, California.

CRYSTALLOGRAPHIC SYMMETRY IN RECIPROCAL SPACE AND IN VECTOR SPACE

M. J. Buerger, *Massachusetts Institute of Technology.*

The transformation of objects into reciprocal space and into vector space is important in crystal structure studies, so it is not only of theoretical interest, but of some practical importance to see how crystallographic symmetry is revealed in these spaces.

Application of the origin-shift theorem shows that a symmetry operation through the origin, and having translation component of c/q, appears as the same symmetry operation in reciprocal space, except that it causes a phase shift between fields of $e^{2\pi il/q}$. It follows that the fields related by the several operations of a symmetry element through the origin have phases related by $e^{2\pi ipl/q}$, where p is the power of the operation relating the fields. If the symmetry element occurs displaced from the origin by $xa+yb$, then the phase of the point is further shifted by $e^{2\pi i(xh+yk)}$. Hence the symmetry of reciprocal space is the same as the point-group symmetry of direct space, except that the phases of the fields are shifted in accordance with the discussion above. Obviously each space group has a unique reciprocal representation consisting of point-groups symmetry, reciprocal lattice point locations, and phase fields.

The transformation from crystal to vector space involves the transfer of each image-point of a symmetrical set to the origin of vector space. Furthermore, the periodicity of vector space is identical with that of crystal space. From this it follows that to each space group in crystal space the corresponding symmetry in vector space is the arithmetic space group. The translation components of the symmetry elements in crystal space appear in vector space as a collection of point images removed by that translation from the origin. Taking into account the centrosymmetrical aspect of vector space, it follows that all space groups in crystal space can be distinguished in vector space except those particular pairs which are differentiated by the operation $\bar{1}$ only, such as $R3$ and $R\bar{3}$. This result corresponds with the implication-theory result given at the Lake George meeting of the *A.S.X.R.E.D.* in June, 1946.

ON THE DERIVATION OF HARKER-KASPER INEQUALITIES*

CAROLINE H. MACGILLAVRY, *Alabama Polytechnic Institute* (temporarily).

The derivation given by Harker and Kasper of the inequalities relations between structure factors[1] involves quite laborious calculations for others than the simplest space groups and does not show clearly the fundamental meaning of the constant term, which is evidently $1/n$ where n is the symmetry number of the space group. It was shown that the fundamental Harker-Kasper inequalities can be easily found by straightforward group-theoretical methods[2] for any space group.

Moreover, it was pointed out that Harker-Kasper inequalities hold only if the electron density is a positive function; that is, if the scattering can be considered as Thomson-scattering from free electrons.

* This work was partly supported by the Office of Naval Research, Contract No. N7onr-377 with the Auburn Research Foundation.

[1] Harker, D., and Kasper J. S., *Acta Cryst.*, **1,** 70 (1948).

[2] See for example Zachariasen, W. H., Theory of X-Ray Diffraction in Crystals, John Wiley, 1945

THE PHASES AND MAGNITUDES OF THE STRUCTURE FACTORS

J. KARLE AND H. HAUPTMAN, *U. S. Naval Research Laboratory, Washington, D. C.*

A fundamental set of inequalities exists among the Fourier coefficients which represent a positive function. It is found that if the first n coefficients are given, the $n+1$ coefficient must be restricted to within narrow bounds if a positive function is to be represented. This idea finds application in the determination of the structure of crystals since the electron density function is a positive function whose Fourier coefficients are the structure factors. The investigation considered here is the generalization of the pioneer work of Harker and Kasper.[1] The relationships of Harker and Kasper follow from our derivation. In addition, we obtain infinitely more inequalities.

It is not only possible to determine the signs of real coefficients but it is also possible to pin down the values of the real and imaginary parts of complex coefficients. By using the relationships which are necessary and sufficient, it is possible to derive coefficients beyond the range in which their magnitudes may be experimentally determined.

[1] Harker, D., and Kasper, J. S., *Acta Cryst.*, **1,** 70 (1948).

ONE-DIMENSIONAL REPRESENTATION OF TRIPERIODIC FUNCTIONS

J. D. H. DONNAY, *The Johns Hopkins University,*
AND
GABRIELLE E. HAMBURGER, *Massachusetts Institute of Technology.*

Any triperiodic function, say the electron density in a crystal, can be represented by a one-dimensional function. The latter is evaluated along the row $[n^2n1]$. Provided n is sufficiently large and the function is computed at enough points, evaluating the function along the period of the row approximates evaluating it throughout the cell. Let $n=1000$ and let the function be computed at any one of n^3 equidistant points within the period. Let X be the new x coordinate and H the new h index after transformation $n^2n1/0n1/001$. Since $\mathrm{H}=n^2h+nk+l$, there is a unique H for every hkl. We may therefore replace F_{hkl} by F_{H} and $\sum_h\sum_k\sum_l$ by $\sum_{\mathrm{H}}$. The point on the row that most closely corresponds to a given xyz is $\mathrm{X}_1=z'+y'/n+x/n^2$, where $y'=y$ if $x<0.5$ and $y'=y-0.001$ if $x\geqq 0.5$, and likewise $z'=z$ if $y<0.5$ and $z'=z-0.001$ if $y\geqq 0.5$. Conversely, to a given point $\mathrm{X}(0\leqq \mathrm{X}<1)$ there corresponds an equivalent point with trimetric coordinates $x=n^2\mathrm{X}$, $y=n\mathrm{X}$, $z=\mathrm{X}$ (owing to periodicity, only the decimal parts of x and y are used). Hence $hx+ky+lz=(n^2h+nk+l)X=HX$. We may therefore write for the electron density at X,

$$\rho(X)=(1/V)\sum_H F_H e^{-i1000HX},$$

where the angle is expressed in millicycles ($1mC=2\pi/1000$), as obtained directly from the calculations, in order to take advantage of the decimalization of the circumference (Villarceau)[1] and of recently calculated tables.[2]

[1] Villarceau, Yvon, *C. R. Ac. Sc. Paris*, **70,** 1233–1236; **71,** 362–368 (1870).

[2] Donnay, J. D. H., and Hamburger, G. E. (1948), Tables for Harmonic Synthesis giving the terms of Fourier series to one decimal at every millicycle tabulated for coefficients 1 to 100 and fiducial cosine values to eight decimals. Baltimore, Md. (1948).

OPERATION OF THE TWO-DIMENSIONAL FOURIER TRANSFORMER*

RAY PEPINSKY, *Alabama Polytechnic Institute.*

Computations of density functions and structure factors are illustrated, as carried out by our two-dimensional Fourier transformer.[1] The sources of error in the instrument are analyzed, and procedures for minimizing these described. A discussion is given of operational test procedures; of methods for addition, subtraction, multiplication and differentiation of functions; of simultaneous storage of density and scattering functions in the machine, when the density function is centrosymmetric; of the method for extension of range of coefficients; and of application of the machine in special analytical methods.

* This development has been supported by the Office of Naval Research, under Contract N7onr-377 with the Auburn Research Foundation.

[1] Pepinsky, R., *Jour. Appl. Phys.*, **18,** 601 (1947).

PATTERSON-HARKER MAPS OF PROTEIN CRYSTALS

DOROTHY WRINCH, *Smith College.*

In using 'experimental' Patterson-Harker maps of protein crystals to test any theory of protein structure, the question arises as to the relation between these maps of *crystals* comprising molecules in a water medium and maps of the *molecules* alone.

(1) Since the vector maps of the molecules+medium and of the molecules differ by the interactions of the medium with itself and with the molecules, we cannot derive one from the other without knowing the structure of the molecules.

(2) However, if 2 crystals in S_1 differ by a constant at every point, their S_2 vector maps, differing by the interactions of a *constant* distribution with itself and with another distribution, also have this property. Hence by suitably reducing every entry in a P-H map, we obtain the S_2 map of the 'reduced' crystal with a zero intermolecular density, thereby replacing the molecules by 'reduced' molecules in which the true electron density is replaced by its deviation from the intermolecular density.

(3) To test any 'experimental' P-H map against a proposed structure, we therefore require the vector map, not of the structure, but of the structure reduced to the appropriate level.

In testing the cyclol theory of protein structure against published P-H maps of proteins, we make, at this stage, the simplifying assumption of constant densities outside and inside the molecular cage skeletons. In a calculation involving over 150,000 terms, vector maps have been obtained for point atom distributions representing the C_1 cage and its interior reduced to a series of levels. The resulting maps show a highly characteristic morphology, their step by step derivation permitting us to diagnose the features in S_1 which are responsible.

The maps are compared with published 'experimental' P-H maps of protein crystals.

THE STRUCTURE OF AMMONIUM DIHYDROGEN PHOSPHATE, $NH_4H_2PO_4$

B. CHALMERS FRAZER, *Alabama Polytechnic Institute.*

The structure of ammonium dihydrogen phosphate[1] was determined by us in September, 1948. Some time later we learned[2] that R. Uedo[3] had published the structure in May, 1948. The results of the two investigations agree fairly well crystallographically, and are in conclusive agreement on the one point of real interest, namely, the existence of an N-H · · · O as well as an O-H · · · O system of hydrogen bonds in the structure. This should be of considerable importance in accounting for the electrical peculiarities of this crystal.

The results of the two structure determinations are discussed and compared with the well-known KH_2PO_4 structure.[4] Principal attention is centered on the hydrogen bond system and the possible hydrogen configurations as related to the normal and the polarized state. Speculations concerning the normal and polarized states are made from the viewpoint of a transition from $I\bar{4}2d$ to Fdd.

[1] Frazer, B. C., *Stroboscopic X-ray Diffraction Investigation of Piezoelectrically Oscillating Crystals,* Auburn Research Foundation, Tenth Quarterly Report to the U. S. Army Signal Corps, Contract No. W 36–039 sc-32031, 15 September, 1948.

[2] Private communication from A. L. Patterson.

[3] Uedo, R., *X*-Rays (Japan) **5,** 21 (1948).

[4] West, J., *Zeit. Krist.,* **74,** 306 (1930).

THE CRYSTAL STRUCTURE OF SiC, TYPE 10-H

L. S. RAMSDELL AND J. A. KOHN, *University of Michigan.*

A crystal of SiC, which did not correspond to any of the known types on the basis of crystal measurements, was shown by Weissenberg photographs to have a 10-layer hexagonal structure, and is accordingly designated type 10-H. Such a structure does not fit into any of the previously suggested series, and therefore no clues were available for indicating which of the various geometrical possibilities might be involved. Intensity calculations were carried out for eight different possible structures. The only one in harmony with the observed intensities is designated by the symbol 3223. This represents the zig-zag sequence of the Si (or C) atoms along the three symmetry axes in the $11\bar{2}0$ plane.

This arrangement has the symmetry $C3m$, which should appear on the films as $C\bar{3}m$. However, both the films and the calculated intensities show 6-fold symmetry. The explanation of this apparently higher symmetry is given.

THE PROBLEM OF THE GRAPHITE STRUCTURE

JOSEPH S. LUKESH, *Knolls Atomic Power Laboratory,* General Electric Company,*
AND
LINUS PAULING, *California Institute of Technology.*

Certain experimental observations cannot be explained readily if the structure of graphite is as generally accepted. A new structure is suggested having the following constants: $a_0 = 2.456$ Å, $b_0 = 4.254$, $c_0 = 6.696$. Space-group: $D_{2h}^{23} - Fmmm$. There are eight atoms in the cell at O, ±U, O, where U is nominally one-sixth.

Observations of angular relations of individuals indicate that the C-C bonds are not all equal. This is supported by structure factor computations and by theoretical considerations of bond numbers in resonance systems. Further work is necessary before the suggested structure can be unequivocally accepted.

* The work reported here was carried out for the Atomic Energy Commission under contract No. W-31-109 Eng-52.

A STRUCTURAL CLASSIFICATION OF THE ALUMINO-FLUORIDES

Address of the Retiring President of the Crystallographic Society of America

A. Pabst, *University of California.*

(To be printed in full in *The American Mineralogist*)

SYMPOSIUM ON TWINNING

Chairmen: J. D. H. Donnay, *The Johns Hopkins University.*
M. J. Buerger, *Massachusetts Institute of Technology.*

THE NEW APPROACH TO THE STUDY OF TWINNING

J. D. H. Donnay, *The Johns Hopkins University.*

THE DETERMINATION OF THE TWIN LAWS IN CRYSTAL PROJECTIONS

M. A. Peacock, *University of Toronto.*

THE GENESIS AND STRUCTURE OF TWINS

M. J. Buerger, *Massachusetts Institute of Technology.*

THE GENESIS OF GROWTH TWINS

C. Frondel, *Harvard University.*

THE ORIGIN OF ANNEALING TWINS

Robert Maddin, *Yale University.*

The slip process in face-centered metals is never as simple as the conventional Taylor and Elam analysis, for there is always a second cooperating plane which contains the same slip direction as the primary plane. There is also another cooperating plane which is commonly called the conjugate slip plane, previously observed to function only when the rotation due to the action of the first plane brought about a symmetrical condition producing equal shear stresses on the two systems.

Annealing twins in face-centered metals could arise from preformed nuclei which could be described as twin faults produced in a two-stage slip process. Such a process, which has been postulated by C. H. Mathewson for many years, is one in which the $\{111\}$ planes can move stepwise in two adjacent $\langle 112\rangle$ directions integrating into the $\langle 110\rangle$ slip direction. In the present investigation carefully tapered single crystals were strained and annealed at a high temperature, and twins were found with their composition planes parallel to the active slip planes and with no others observable. This can be interpreted as a very strong evidence in favor of the two-stage slip process.

X-ray study of the strained single crystals exhibited a sharp rise in the shear-strengthening curves at a value of shear of about 0.22. Recrystallization was found to begin at this value of shear. The orientations of ten of the new grains, determined by x-rays, were related to the parent lattice by a rotation about lines perpendicular to the three acting slip planes.

EFFECTIVE LATTICE ROTATIONS PERMITTED BY SHORT DISPLACEMENTS OF LATTICE POINTS

M. L. Kronberg and F. H. Wilson, *American Brass Company.*

If a lattice is rotated parallel to one of its nets about a lattice point in the net, there is a series of angular positions in each of which a definite proportion of the lattice points will coincide with points of the lattice before rotation. These points define a multiple of the primitive lattice. The relationship between a pair of orientations, consisting of the original and any one of the series, can also be considered as a 180° rotation about a line in the net through the point of rotation and the nearest coincidence site. The relationship is developed in detail for the specific example of a 38° rotation of a face-centered cubic lattice about a [111] axis. This development shows that because of the periodicity of coincidence sites, one orientation can convert to the other by relatively simple displacements of the remaining lattice sites. The existence of this coincidence mechanism was found during an attempt to understand the experimental observation that copper can give rise to a recrystallization orientation that is related to the parent orientation by a 38° rotation about a [111] axis. Other similar examples have been observed in metals.

TWINNING IN NESQUEHONITE, $MgCO_3 \cdot 3H_2O$

May Risch Kinsolving, Caroline MacGillavry and Ray Pepinsky,
Alabama Polytechnic Institute.

It was shown by one of us[1] that nesquehonite, described as orthorhombic in the literature, has actually a lower symmetry; the pseudo-orthorhombic symmetry is caused by repeated twinning, as shown by close doubling of many maxima on oscillation diagrams. From Weissenberg diagrams it has now become possible to determine the true unit cell and the twin law. The crystals are monoclinic, the ortho-axis being identical with that formerly called the *c*-axis. If we take the axes corresponding to the originally assigned orthorhombic cell, the space group is found to be $P2_1/n—C_{2h}^5$; $a=7.68$ Å, $b=5.39$ Å (formerly called *c*), $c=12.00$ Å (formerly called *b*), $\beta=90.45°$. The angle β was measured accurately on Weissenberg diagrams in which a 9 cm. shift of the film corresponded to a rotation of 12.7° of the crystal. The twinning occurs on the monoclinic (001) plane. A complete structure determination is now in progress.

[1] Pepinsky, R., *Phys. Rev.*, **59**, 925 (1941).

TWINNING IN MICROCLINE

Fritz Laves, *University of Chicago.*

Some observations on twinned microcline indicate that four different twin positions are related to each other so as to produce one set of planes in reciprocal space. *X*-ray photographs show that the four spots corresponding to planes with the same *hkl* values are joined by faint streaks. The probable explanation of this effect is discussed.

CRYSTAL GROWTH

Chairman: J. W. Gruner, *University of Minnesota.*

OBSERVATIONS ON THE FLAME FUSION GROWTH AND STRUCTURE OF RUTILE CRYSTALS

Charles H. Moore, L. Merker and L. E. Lynd,
Titanium Division, National Lead Co.

In the growth of single crystals of rutile by the present process, certain fundamental differences are noted from the synthesis of corundum or spinel by the Verneuil process. The tendency of TiO_2 to lose oxygen near its melting point necessitates that the crystal be grown in an oxygen-rich atmosphere. Even under these conditions, the resulting crystal is black in color, although apparently identical with the colorless material, judging from unit-cell measurements and *x*-ray powder patterns. Upon subsequent oxidation the crystal can be made substantially colorless.

Variations from stoichiometric proportions of constituents are permissible with rutile, indicating a structural flexibility not heretofore emphasized. A discussion of the mechanism of these variations is given, and differences in physical and electrical properties with degree of oxidation are described. The technique and theory of growth is discussed, as well as the possibility of extending the same principles to the growth of oxides of other members of the atomic transition series.

THE FLAME FUSION SYNTHESIS OF MULLITE

W. H. Bauer, I. Gordon and C. H. Moore, *Rutgers University.*

In conjunction with the O.N.R. project on tourmaline synthesis, a single crystal of an incongruently melting silicate, mullite ($3Al_2O_3 \cdot 2SiO_2$), has been grown by the flame fusion process. The equipment consists of a feeding device, burner, lowering apparatus and suitable gas controls. A modified Verneuil type burner employing hydrogen and oxygen was used. A feed of extreme purity and low density was developed by calcining a stoichiometric mixture of alum [$Al_2(SO_4)_3 \cdot (NH_4)_2SO_4 \cdot 24H_2O$] and pure silica gel.

X-ray and optical data show the resulting boule to be a single crystal of mullite. The *d/n* values obtained all correspond to those reported in the *A.S.T.M.* cards and no evidence of the existence of any crystalline alumina or silica was noted. The largest single crystal grown was 2 cm. in length and 1 cm. at its thickest point.

This synthesis presents a new approach to the field of silicate research. It indicates that the flame fusion technique is feasible for the study and possible single crystal growth of certain anhydrous silicates, provided that such problems as feed preparation, viscosity of the molten surface, and possible polymorphous inversions can be successfully solved or circumvented.

THE MUTUAL MODIFICATION OF THE CRYSTAL HABIT OF AMINO ACIDS AND SODIUM CHLORIDE

Charles P. Fenimore, *The Johns Hopkins University*
AND
Arthur Thrailkill, *Aberdeen Proving Ground.*

Glycine, pyridine betaine, and β alanine in aqueous sodium chloride solutions modify the crystal habit of growing sodium chloride: the first causes the formation of dodecahedra, the other two give octahedra. Glycine and β alanine are themselves modified by sodium chloride. The largest or most unexpected (on the basis of the modified law of Bravais) new form developed on the amino acid by sodium chloride is compared with the form developed on sodium chloride by the amino acid. A fairly good correspondence of mesh dimensions is found in both cases and a structural correspondence is found in the case of glycine.

DISORDER IN BORNITE, Cu_5FeS_4

Alfred J. Frueh, Jr., *Massachusetts Institute of Technology.*

Diffraction data from single crystals of bornite, from Bristol, Connecticut, indicate that bornite in its ordered form is tetragonal with cell dimensions: $a = 21.91$ Å, $c = 10.95$ Å. When quenched from above 225° C. the crystals become isometric, $a = 10.95$ Å. This can be explained by disordering between the copper and iron,

$$Cu_5FeS_4 \overset{225°}{\rightleftarrows} \underset{\text{dynamic disordered}}{\left\{\begin{matrix} Cu_5 \\ \\ Fe \end{matrix}\right\} S_4} \xrightarrow{\text{quench}} \underset{\text{static disordered}}{\left\{\begin{matrix} Cu_5 \\ \\ Fe \end{matrix}\right\} S_4}.$$

The absorption of heat that accompanies the disordering has been observed by means of a thermal analyzer.

The appearance of super structure lines and their consequent disappearance upon heating has been observed in powder patterns of bornite from various localities, both statically and dynamically, with the aid of a high temperature camera. It has been found possible to reorder the disordered material by slow cooling from 225° C.

CRYSTAL OPTICS

Chairman: A. N. Winchell, *University of Virginia.*

THE FREQUENCY-DISTRIBUTION OF THE OPTICAL PROPERTIES OF CRYSTALS

A. F. Kirkpatrick, *American Cyanamid Company.*

A study has been made of the frequency-distribution of approximately 1000 crystalline phases, both inorganic and organic, among the following classes: isotropic, uniaxial positive, uniaxial negative, biaxial positive, and biaxial negative. The distribution of the refractive indices, N, N_O, N_E, N_X, N_Y, N_Z, of specific gravity, and of oblique and parallel extinction has also been examined within the above classes.

The relationships of the results to the examination of crystalline substances in an industrial analytical laboratory are discussed. For example, a narrower interval in refractive index between individual standard immersion liquids is needed near the index with the greatest frequency of occurrence than at index ranges of low frequency. Emphasis is placed on the relations of the distributions to the certainty of the identification of an unknown phase by the determination of its optical properties.

CRYSTAL OPTICS ON MICROSCOPIC VIEWS—A MONOCLINIC CASE

W. A. O'Brien, *Celanese Corporation of America,*
AND
J. D. H. Donnay, *The Johns Hopkins University.*

In the microscopical study of crystals, measurements of refractive indices and determinations of fast and slow extinction directions may be made on various faces. While the morphology of the crystal can be determined by microscope goniometry[1] it is also desirable to derive the principal refractive indices and the optical orientation from the measured optical properties. The procedure will vary with the nature of the data. Graphical methods are presented for the transformation, when the available data are the fast and slow extinction directions in two faces, the refractive indices in one of the two faces, and the orientation of the two faces with respect to each other and to a plane of optical symmetry. (The faces must not be perpendicular to a plane of optical symmetry.) This case arises in monoclinic crystals. The transformation of the measured refractive indices into principal refractive indices is based on Mertie's monogram[2] used for the solution of the ellipse from angular data determined from the stereographic projection. The determination of the optical orientation is based on finding the locus of possible optic axis positions for each face and noting the intersection of the loci for the two faces. This is done by stereographic projection methods.

[1] Donnay, J. D. H., and O'Brien, W. A., *Ind. and Eng. Chem., Analyt. Ed.*, **17**, 593–597 (1945).

[2] Mertie, John B., *Am. Mineral.*, **27**, 538–551 (1942).

SOME PHOTOELASTIC CONSTANTS OF CRYSTALS $NH_4H_2PO_4$(ADP) AND KH_2PO_4(KDP)

C. D. West and A. S. Makas, *Polaroid Corporation.*

The results of our static measurements for these crystals, which belong to the class V_d—$\bar{4}2m$, are piezoelectric, and were supplied by the Brush Development Company, are found in the accompanying table. We also confirmed experimentally the correctness of Pockels' theory (1906) for tetragonal crystals, no examples of which were previously studied.

Line	Quantity	ADP	KDP
1	ω_D, ϵ_D	1.5246, 1.4792	1.5095, 1.4684
2	C_1, C_3	$-1.84\pm.17$, $32.2\pm.7$	$(>0, <0.5)$, $19.4\pm.4$
3	$2(s_{11}-s_{12})$, s_{66}^E	20, 164	43, 164
4	$(q_{11}-q_{12})$, q_{66}^E	1.04, -18.15	$(>-0.3, <0)$, -11.25
5	$\frac{1}{2}(c_{11}-c_{12})$, c_{66}^E	50, 6.1	24.2, 6.1
6	$\frac{1}{2}(p_{11}-p_{12})$, p_{66}^E	0.052, -0.1107	$(>-0.007, <0)$, -0.0685

Line 1 shows refraction indices after Topsoe and Christiansen (1873), lines 3 and 5 elastic shear compliance resp. stiffness after Mason (1946), lines 2, 4 and 6 are various expressions of photoelastic shear constants in the notation of Szivessy (1928). The wavelength 0.560 mμ applies to line 2. For lines 2, 3 and 4 the units are 10^{-13} cm.^{2}/dyne, for line 5 they are 10^{10} dyne/cm.^{2}

INFRARED MICROSCOPY

E. L. Perrine and W. C. McCrone, *Armour Research Foundation of Illinois Institute of Technology.*

Plans and details of construction for a very simple infrared microscope are shown and discussed. The unit involves essentially a high voltage transformer and a secondary photoemission tube (1-P-25) similar to those used during the war in the sniperscope. The instrument has been constructed to fit into any microscope in place of the ocular.

The applications of this instrument to crystallography and microscopy are briefly discussed. These include the examination of materials opaque to visible light (some of the minerals, organic dyes, etc.) and the study of crystal optics. The present limitations and possible improvements for the infrared microscope are considered.

AN INEXPENSIVE PETROGRAPHIC MICROSCOPE

Horace Winchell, *Yale University.*

A number of manufacturers have recently announced development of students' microscopes selling for about $100.00, which can be adapted for elementary petrographic work by the addition of inexpensive polaroid elements, and a simple rotating stage. The design of a stage and installation of polaroids are described.

MISCELLANEOUS PAPERS

Chairman: E. H. KRAUS, *University of Michigan.*

ELECTRICAL EVIDENCE ON THE CLASS OF SOME TRICLINIC CRYSTALS

W. L. BOND, *Bell Telephone Laboratories.*

An example of a crystal class should have two qualifications: there should be no doubt that it belongs to the class it "represents," and it should be readily available for study. It should not be unstable, as are the "examples" of class 1 quoted in crystallography texts. The "classical example" used in most mineralogy texts and in Bunn is calcium thiosulfate hexahydrate—it dehydrates in a day or so and probably belongs in class $\bar{1}$ since it is not piezoelectric and most crystals are of pinacoidal habit. Rubidium ferrocyanide dihydrate (Phillip's example) is stable, but is neither pyroelectric nor piezoelectric, and hence is probably of class $\bar{1}$. Strontium ditartrate tetrahydrate (Cady's example) is both pyroelectric and piezoelectric but extremely unstable, dehydrating violently in minutes. Phillips also says that axinite probably belongs to class 1, but since we find it to be neither pyroelectric nor piezoelectric, we think it belongs to class $\bar{1}$.

The liquid air tests for pyroelectricity are open to criticism as not testing at room temperature—conceivably a crystal could transform to a pyroelectric class before reaching liquid air temperature, then give a positive test. Piezoelectric tests are not open to this criticism.

Triclinic crystals containing an optically active organic acid are certainly of class 1 since the optically active component cannot have a center of symmetry. One developed at the Bell Telephone Laboratories is aminoethyl ethanolamine hydrogen tartrate. It is pyroelectric, piezoelectric and stable.

MAXIMUM HARDNESS VECTORS IN THE DIAMOND

C. B. SLAWSON AND J. A. KOHN, *University of Michigan.*

Since, in the lapping of diamonds, it is desirable to work on the so-called "on-grain" or softer lapping directions, little information is available concerning other hardness vectors. Qualitative determinations, by the use of standard diamond-lapping equipment, have been made on those "off-grain" lapping directions which parallel zonal lines connecting cube, octahedron, and dodecahedron faces.

When lapping parallel to a given direction, it is found that as one departs farther and farther from the "on-grain" position, a point is eventually reached where an abrupt variation in susceptibility to lapping occurs. These "limits" of "off-grain" lapping directions have been approximately evaluated and the results plotted on stereographic projections. All lapping directions investigated gave maximum hardness areas displaying three fold symmetry about the octahedron face and, likewise, two-fold symmetry about the dodecahedral position. Such areas beyond the "limits" offer the hardest and, therefore, most suitable directions for the working surfaces of diamond tools.

Several difficulties were encountered in the standardization of lapping conditions: (*a*) it is impossible to maintain a surface of uniform lapping efficiency over any extended period of time, (*b*) twinning lamellae were consistently present to a variable degree, (*c*) criteria for defining "limiting" conditions cannot be precisely established.

CRYSTALLOGRAPHIC DATA ON WAVELLITE FROM LLALLAGUA, BOLIVIA AND ON CACOXENITE FROM HELLERTOWN, PENNSYLVANIA

SAMUEL G. GORDON, *The Academy of Natural Sciences of Philadelphia.*

Wavellite, $[Al_3(PO_4)_2(OH, F)_3 \cdot 5H_2O]_4$, *Pcmn*. The unit-cell dimensions are: $a_0 = 9.60$ Å, $b_0 = 17.31$, $c_0 = 6.98$; $a_0/b_0 = 0.555$, $c_0/b_0 = 0.403$, $c_0/a_0 = 0.727$. By goniometry, $a = 0.554$, $c = 0.403$, $p_0 = 0.726$. $M = 1652$ (from formula), 1649 (calculated from cell). Sp. gr. $= 2.36$ (on weighing), 2.365 (calc.).

Cacoxenite, $[Fe_4(PO_4)_3(OH)_3 \cdot 12H_2O]_{12}$, *C*6/*mmm*(?). The unit-cell dimensions are: $a_0 = 27.6$ Å, $c_0 = 10.4$; $c_0/a_0 = 0.377$. $M = 9312$ (from formula), 9340 (calculated from cell). Sp. gr. $= 2.26$ (on weighing), 2.25 (calc.). A new chemical analysis on 50 mg. gave: Fe_2O_3, 40.5; P_2O_5, 26.8; H_2O, 32.4(=99.7). (The lattice constants on cacoxenite were determined by Dr. Joseph Singer.)

WHAT IS A MINERAL?

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The old definition of a mineral as a natural inorganic substance of definite chemical composition is criticized. A new definition is proposed and its effects are illustrated.

A COMPACT DEMOUNTABLE *X*-RAY DIFFRACTION TUBE AND POWER SOURCE[1]

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A compact diffraction unit has been constructed on the basis of earlier experience.[2] It contains a demountable *x*-ray tube with an electron gun to provide fine focus and grid control, a vacuum system, and stabilized high potential and current supplies. The tube body and electron gun are at ground level, the target being cooled by an oil circulating system to reduce leakage current to a few microamperes. The low average power demands of the unit permit the use of a stabilized radio-frequency high potential generator of the type used in electron microscopes. The table top is 33″ high and of dimensions 34″×42″, and the unit is mounted on casters.

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[1] Development supported by Signal Corps Engineering Laboratories, Contract W 36-039 sc-32031.

[2] Pepinsky, R., *Phys. Rev.*, **67**, 308 (1945); *Phys. Rev.*, **69**, 546 (1946); Long, H. M., and Pepinsky R., *Phys. Rev.*, **74**, 126 (1948).