CALCAXES: A PROGRAM FOR COMPUTATION OF CALCITE CRYSTALLOGRAPHIC AXIS ORIENTATIONS

BY

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Abstract—Organisms with skeletons composed of single-crystal calcite often show considerable intraspecific constancy in the orientation of the calcite crystal lattice of each single-crystal component of their skeleton. The orientation of the calcite lattice may be described in terms of the angular relationship between specific crystallographic axes and anatomically defined reference axes. Patterns in crystallographic axis orientation may relate to several aspects of an organism's biology, including its phylogenetic history. A non-destructive method for determining crystallographic axis orientations involves growing crystals of calcite, under laboratory conditions, in crystallographic continuity with exposed skeletal surfaces. Orientations of these crystals are then measured with an optical goniometer. The program CALCAXES calculates calcite crystallographic axis orientations from goniometer measurements and offers a variety of options for data management and display. It thereby facilitates description and analysis of variation in calcite crystallographic axis orientation.

INTRODUCTION

Skeletonized organisms use a wide variety of inorganic and organic phases, combined in a no less impressive range of microfabrics, to form the structural components that make up their skeletons (Carter, 1990). Within this diversity, echinoderms stand out as one of the few groups to use a mineral phase that approximates the organization of a single crystal within each skeletal element. This is a well known feature (Smith, 1990), forming the basis for one of the most widely used field methods for recognizing echinoderm fossil material—the flash of sunlight reflected from crystal faces on broken or diagenetically overgrown skeletal elements. The original mineral phase of echinoderm skeletons is predominantly high-magnesium calcite. In many respects its structure is indistinguishable from that of a single crystal (Donnay and Pawson, 1969), but high-resolution studies suggest that it forms instead as a series of strongly, though not perfectly, aligned, submicron-scale, crystallographic domains (Blake and Peacor, 1981; O'Neill, 1981; Berman et al., 1993). In fossil material, neomorphic alteration during diagenesis commonly enlarges domains and transforms high-magnesium calcite to low-magnesium calcite within which occur scattered, minute dolomite crystals sequestering at least some of the original magnesium (Lohmann and Meyers, 1977). This transformation takes place without alteration of crystallographic orientation from that of the original high-magnesium calcite (Blake et al., 1982). Diagenesis may also involve deposition of low-magnesium calcite

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cement within the pores of the stereom microstructure characteristic of echinoderms, but this typically forms as a syntaxial overgrowth of the original or neomorphically altered calcite (Raup, 1962; Blake et al., 1982) and therefore only reinforces the single-crystal character of echinoderm skeletal material. The single-crystal nature of individual skeletal elements is thus a fundamental aspect of echinoderm biomineralization that is accessible for analysis in fossil and living material.

Single-crystal skeletal structure forms the basis for a class of phenotypic features that may be highly informative, namely the orientation of the crystal lattice of each structural unit of the skeleton, relative to recognized anatomical reference directions. Raup (1959, 1962), in a study of echinoids, showed that patterns of lattice orientation are relatively constant within species and some higher level taxa but vary among other higher level taxa. This suggests that such patterns are heritable and relatively conservative on short to intermediate evolutionary time scales, but subject to change on longer evolutionary time scales. This behavior makes them a promising source of evidence for inferring phylogenetic history. A different application was demonstrated by Emlet (1985, 1989), who showed that patterns of lattice orientation in certain skeletal elements of echinoids are indicative of mode of larval development. Such patterns may thus provide indirect evidence for aspects of life history, which in turn can be used to address both ecological and evolutionary questions.

The crystal lattice of calcite, whether in an inorganic or an organic context, has well known symmetry properties expressed in terms of crystallographic axes (Klein and Hurlbut, 1985). It has one c axis, an axis of 3-fold rotational symmetry, normal to the planes defined by oxygen atoms in CO_3 groups, and three a axes, each an axis of 2-fold rotational symmetry, separated by 120° within those same planes (Fig. 1). The orientation of the calcite crystal lattice can therefore be described by specifying the orientation of the c axis and one a axis. The most common method of measuring crystallographic axis orientations in previous studies of echinoderms has involved polarized light microscopy of oriented thin sections, using a universal stage (e.g., Raup, 1962; Emlet, 1989). In its standard form, this approach allows only the orientation of the c axis to be measured. X-ray techniques allow measurement of both c and a axis orientations and have been used for definitive investigation of various properties of echinoderm skeletal material (e.g., Donnay and Pawson, 1969; Blake et al., 1984; Berman et al., 1993), but not for surveying significant numbers of taxa. A third approach is based on the demonstration by Jones (1955) that micron-scale rhombohedral crystals of calcite can be artificially grown on specimen surfaces, in optical continuity with underlying calcite. This technique is known as "calcite decoration" and has been used in several studies of the orientation of calcite crystallographic axes in Recent echinoderm skeletal material (Okazaki and Inoué, 1976; Okazaki et al., 1981; Dillaman and Hart, 1981). The form and orientation of the calcite rhombohedra (i.e., the orientations of their edges and faces) reveal both c and a axis orientations. Most applications of calcite decoration have relied on scanning electron microscopy to measure the orientation of calcite rhombohedra grown on specimen surfaces (Dillaman and Hart, 1981), but a more precisely quantifiable method is to use an optical goniometer. Our first experience with this instrument was in determining crystallographic axis orientations from rhombohedral cleavage faces on naturally fractured fossil specimens of stylophoran echinoderms (Fisher, 1982), but this quickly demonstrated the ease with which decorated specimens, with or without fractures, could be accommodated. In this modification of the usual calcite decoration procedure, the optical goniometer measures the orientations of face poles of calcite rhombohedra, and the known angular relationship of these to crystallo-graphic axes (Fig. 1) is used to deduce the orientations of the latter. Although individual rhombohedra grown by the calcite decoration technique are too small to discriminate with the modest magnification typical of an optical goniometer, their common relationship to underlying skeletal calcite produces strong alignment of faces associated with single-crystal domains, and this is optically equivalent to a crystal with faces of macroscopic extent.   Subsequent studies
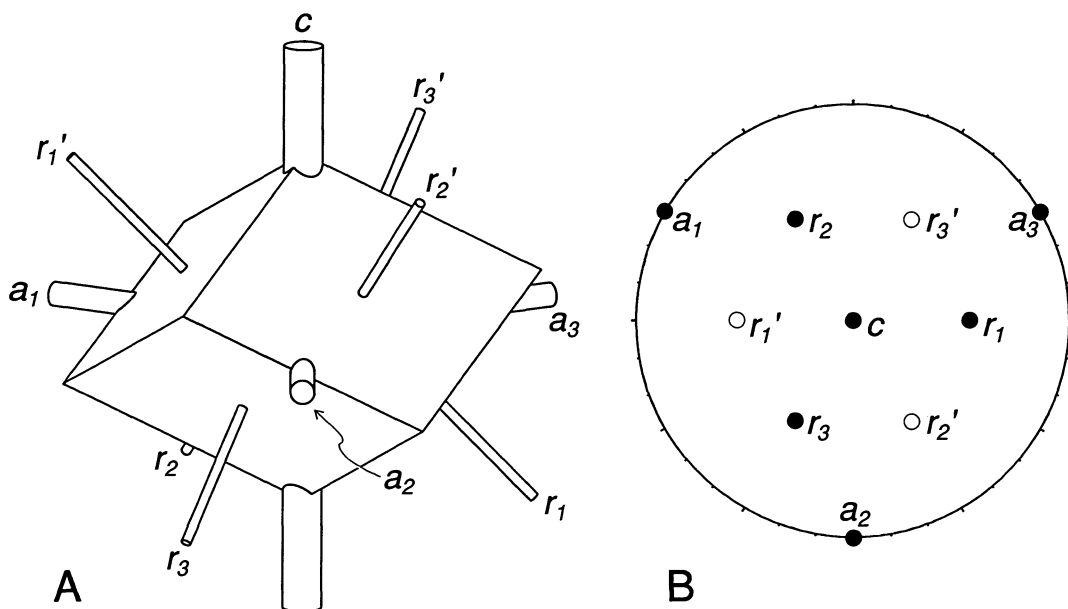
FIG. 1—Geometric relationships among key features of the calcite crystal lattice and the rhombohedral habit. A: isometric projection of a calcite rhombohedron, showing the orientations of rhombohedral faces, c axis (thick cylinder extending along axis of 3-fold rotational symmetry), a axes (intermediate cylinders extending along axes of 2-fold rotational symmetry), and rhombohedral face poles (thin cylinders normal to rhombohedral faces). View is from slightly above the plane of a axes. B: stereogram of rhombohedron shown in A (from above, with c axis vertical) showing orientations of c and a crystallographic axes and rhombohedral face poles (equal-area projection). Solid symbols represent axes or poles plotting on the lower hemisphere or equator, and open symbols represent poles plotting on the upper hemisphere. Angles between features shown here are from Palache et al. (1951, p. 142-143): $c \wedge a_1$, a_2, or $a_3 = 90°$; $a_1 \wedge a_2$, $a_2 \wedge a_3$, and $a_3 \wedge a_1 = 120°$; $c \wedge r_i = 44° 36.5'$; $r_1 \wedge r_2$, $r_2 \wedge r_3$, and $r_3 \wedge r_1 = 74° 55'$; $r_i \wedge r_i' = 180°$.

(Fisher and Cox, 1987; Bodenbender, 1990, 1992) have confirmed that this approach offers both ease of specimen preparation and considerable precision of measurement.

Although calcite decoration, coupled with optical goniometry, provides an effective source of information on c and a axis orientations, the weak link in this chain has been the processing of goniometer data. Goniometer data can be reduced to crystallographic axis orientations by manual plotting and manipulation of stereographic projections, but this tends to degrade precision and is inconvenient for handling large amounts of data. CALCAXES was written to solve this problem. It provides an analytical solution for c and a axis orientations, based on measurements of calcite rhombohedral face pole orientations. It also incorporates routines for evaluating the congruence of multiple measurements on a single specimen, for recognizing misleading measurements (e.g., face pole orientations observed on different skeletal elements or on fractured and displaced fragments of a single skeletal element), for handling incomplete data (e.g., when specimen topography interferes with observation of some face poles), for evaluating the degree of clustering of data from multiple specimens, for merging data collected in different specimen orientations, for editing data, and for displaying data on equal-area stereograms.

CALCAXES is written and compiled in Turbo Pascal version 5.5 (Borland International, Inc.) for use on MS-DOS microcomputers. The compiled program, in the file "calcaxes.exe" (ca.

200 Kb), and the source code (ca. 130 Kb, comprising ca. 3,700 lines of code) are available from the authors. CALCAXES uses many procedures derived from Calcite and Calcite3, programs written by Sanford Ballard under the direction of DCF.

We discuss program design and rationale below, covering issues such as the design of optical goniometers, establishment of an anatomical reference system, specimen mounting, the phi and rho coordinate system, display conventions, further details of calcite crystallography, and the algorithms for computing axis orientations. We then describe detailed procedures for using the software. Several geometric concepts pervade this discussion and are best noted at the beginning. The first of these is the distinction between location and orientation, within a space of given dimensionality. Location is a matter of distance from specified reference points and is adjusted by translation, while orientation is a matter of direction relative to reference points and is adjusted by rotation. In 3-dimensional space, there are three degrees of translational freedom for specification of location, and three degrees of rotational freedom for specification of orientation. Orientation is a potentially polar concept (e.g., positive and negative, toward and away from), but some geometric entities (e.g., lines) are by convention treated as nonpolar, or of ambiguous polarity. We will discuss both polar and nonpolar linear features. We use the term "position" in a sense that includes both location and orientation.

PROGRAM DESIGN AND RATIONALE

Design of Optical Goniometers

As introduced above, CALCAXES computes crystallographic axis orientations from the orientations of poles normal to the rhombohedral faces of calcite crystals. On the crystals typically produced by the calcite decoration technique, these faces are the only ones that develop; they have the same orientation as the principal cleavage faces of calcite. These faces are designated by the Miller index $\{10\bar{1}1\}$ (notation conventions for crystal forms are discussed in Klein and Hurlbut, 1985, p. 39-42), and the orientations of the poles normal to them are designated r. We will hereafter refer to these poles simply as face poles, although most of our comments address only the poles of rhombohedral faces, and not other known faces (such as a basal cleavage face) of calcite crystals.

To measure any face pole orientation with an optical goniometer, the user rotates a specimen until a crystal face, or a set of aligned crystal faces, is oriented so that light from an illumination source (Figs. 2 and 3) is reflected off the face(s) and down the axis of a viewing telescope. When this condition is met, the corresponding face pole orientation can be read as a coordinate pair of values on two orthogonal rotational scales, phi (ϕ) and rho (ρ). Phi and rho axes are at one level abstract elements of a spherical coordinate system, but a goniometer is designed to provide mechanical counterparts of phi and rho axes that allow controlled manipulation and viewing of a specimen. In most, but not all, instances, we refer to these abstract and mechanical axes without discrimination. Relationships among these and other features of goniometer design are illustrated in Figs. 2 and 3.

We have used two goniometers, each representing a different portion of the range of goniometer design of which we are aware. We discuss both below, in order to elucidate some of the complications that may be encountered by users of different goniometers. The first instrument is of undocumented origin, probably manufactured early in this century, and is housed in the Mineralogical Laboratory of the Department of Geological Sciences, University of Michigan. It represents the general design of two-circle reflecting goniometer illustrated by Klein and Hurlbut (1985, p. 6, fig. 1.5d) and Groth (1905, p. 680) and referred to by Groth (1905, p. 678) as a "Fedorowsche Universalgoniometer." However, of the various goniometer designs developed around this time period (e.g., Goldschmidt, 1893; Fedorow, 1893; Stöber, 1898; Stöckl, 1904) ours is most closely approximated by the instrument illustrated by Gold-
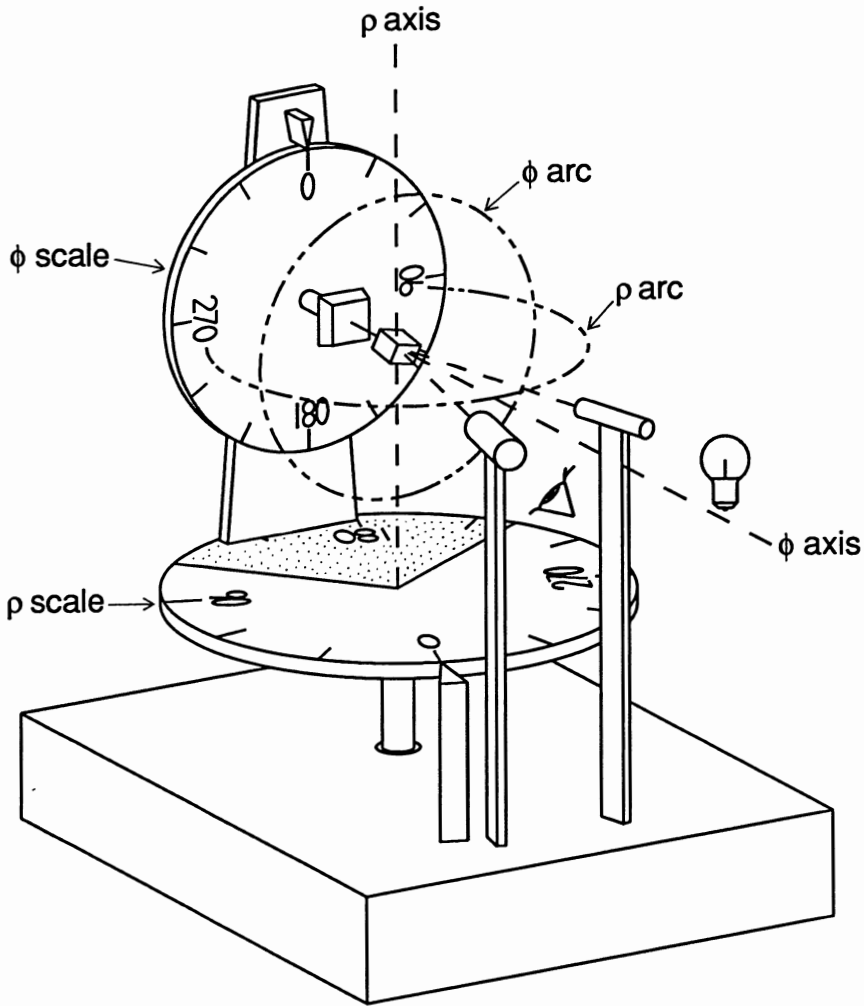
FIG. 2—Schematic design (isometric projection) of the Goldschmidt goniometer described in the text. Both this and the Nedinsco goniometer illustrated in Fig. 3 have a viewing telescope (cylinder aligned with eye icon), a light source and collimator (cylinder aligned with light bulb icon), a phi mechanism, a rho mechanism, and a goniometer head (truncated pyramid, or frustum) for mounting the specimen (rhombohedron) on the phi mechanism. Axes of rotation of the phi and rho mechanisms are perpendicular. The phi (ϕ) axis is the axis about which the specimen rotates to change the phi value without altering rho. A phi arc is an arc traced by a point in the anatomical reference frame as such rotation occurs, and the phi scale is a physical representation of a phi arc graduated for measuring phi values. Likewise, the rho (ρ) axis is the axis about which rotation changes rho values without altering phi. A rho arc is an arc traced by a point on the rho mechanism, during rho adjustment, and the rho scale is a physical representation of a rho arc graduated for measuring rho values. The sector of precluded rho measurements (about 120° to 220°) is shown in stippled pattern. The user sits in the right foreground, in a position to look down the viewing telescope.

schmidt (1898, Taf. VII). We therefore refer to it simply as the "Goldschmidt goniometer." It has a light source and viewing telescope that occupy stationary positions along a rho arc, within the plane of rho observation (Fig. 2). The rho scale is horizontal and spins (i.e., rotates

about its own axis) through an angle of about 260°, carrying with it the support for the mechanical phi axis. The phi axis, carrying the specimen, spins and also swings (i.e., rotates about an axis lying at an angle, in this case perpendicular, to itself) in the plane of rho observation. The second design, the "Nedinsco two-circle optical goniometer" manufactured by the N. V. Nederlandsche Instrumenten Compagnie of Venlo, Netherlands, has an inclined phi axis (shown in Fig. 3 as vertical), on which the specimen spins but does not swing, and an identically inclined rho arc. The eyepiece of the viewing telescope is stationary, but the access port for the reflected light beam (shown in Fig. 3), together with the light source, swings through the arc of rho adjustment (with light reflected to the stationary eyepiece by mirrors). As different as these designs are in some respects, they correspond to the same *relative* spatial relationships among the main mechanical components of the goniometer. These relationships represent such fundamental aspects of the phi and rho coordinate system that we expect them to be constant features of goniometer design.

A third goniometer design is represented by the "Huber two-circle reflection goniometer" (illustrated by Klein and Hurlbut, 1985, p. 49) manufactured by Huber Diffraktionstechnik, in Rimsting, Germany. It is essentially like the Goldschmidt goniometer except that the plane defined by incident and reflected light beams is vertical rather than horizontal (R. B. Emlet, pers. comm., 1993). Because this difference has consequences for the procedure for defining a standard specimen orientation, we also include occasional comments on the Huber goniometer.

In descriptions below, it will sometimes be useful to discuss features of goniometer design and specimen orientation in terms of a general reference frame 'attached to' the stable base of the goniometer and extending even to the observer and beyond. We shall call this the *external reference frame*. The external reference frame has already served implicitly above, for it is the natural context for a description of instrument configuration. For each goniometer, the observer has a standard position, seated 'in front of' and facing the instrument, in the right foreground of Figs. 2 and 3. These figures essentially offer a view over the left shoulder of the instrument operator. The relation between observer and instrument also provides a basis for describing directions of rotation within the external reference frame. For instance, on the Goldschmidt goniometer, an observer seated in standard position can look along the phi axis with an instrument setting close to that shown in Fig. 2, and when doing so, rotation about this axis can be described as clockwise or counterclockwise. Rotational position could also be described within the external reference frame as up, down, left, or right, but it is preferable to use a clock model (12 o'clock, 6 o'clock, 9 o'clock, or 3 o'clock, respectively), because this is more directly transferable to the Nedinsco goniometer. On the Nedinsco goniometer, the observer can only look along the phi axis by peering somewhat over the instrument, but then the same clock description applies, whereas a different description (far, near, left, or right, respectively) would be required if only the cardinal directions in the external reference frame were used. The rho axis on the Nedinsco goniometer lies along the observer's normal line of sight in the external reference frame, allowing straightforward application of the clock model. The same description extends to the Goldschmidt goniometer, although with it, the observer must peer over the instrument to look along the rho axis. Where necessary or convenient, descriptions couched in terms of the external reference frame will be supplemented or replaced by descriptions based on an anatomical reference frame and a telescope reference frame, both of which are discussed below.

Returning to goniometer design, the numbering of phi and rho scales is critical to the choice of values to represent a given orientation. Both scales, in principle, measure continuously from 0° through 360°, although this is in fact true only of the phi scale. The phi scale is numbered so that values engraved on the scale increase in a clockwise direction as one looks at the scale from a vantage point across the rho arc from the mechanical phi axis, the perspective described above as the standard relation of the observer to this axis. The rho scale is numbered so that it reads 0° or 360° for a face pole aligned with the phi axis, observed from across the rho arc
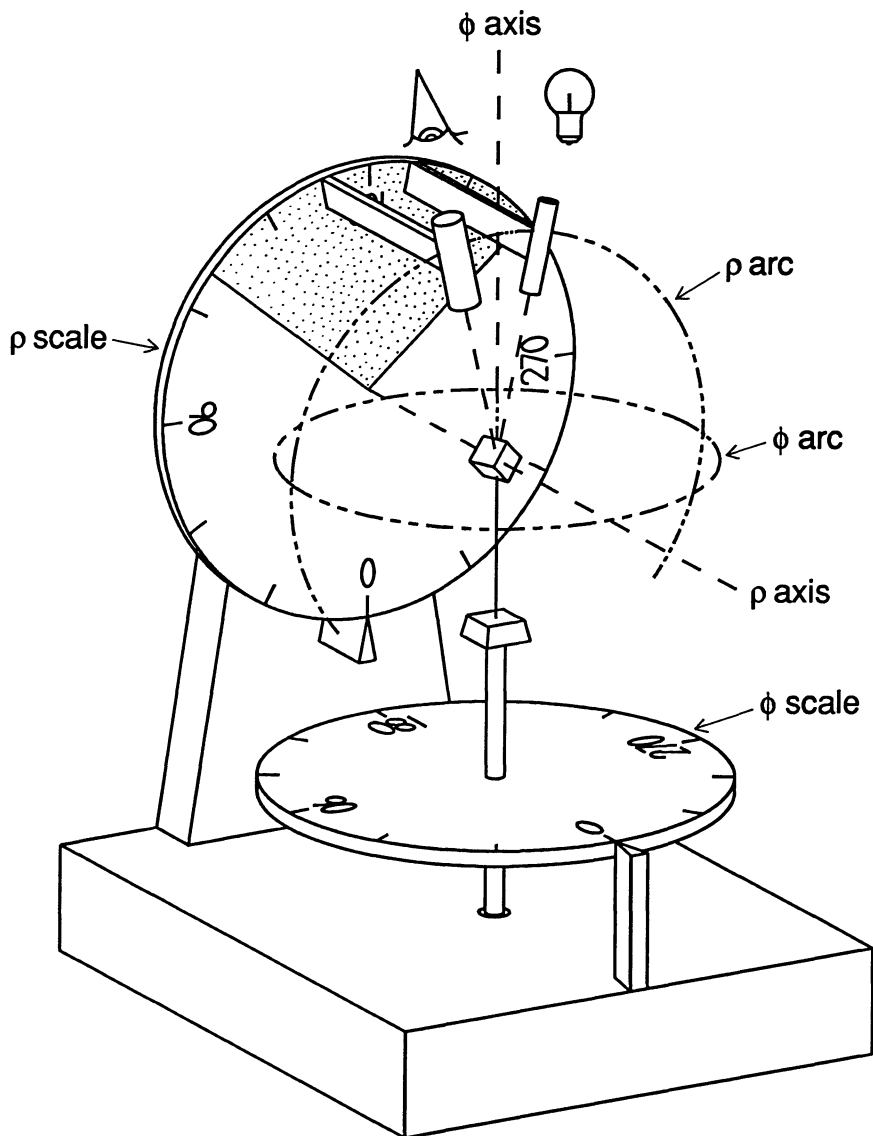
FIG. 3—Schematic design (isometric projection) of the Nedinsco two-circle optical goniometer. Principal features are identified in the caption of Fig. 2, except that the cylinder aligned with the eye icon now represents the access port for the reflected light beam, which is transmitted by a mirror system to the viewing telescope (not shown) in a position accessible to the user, sitting again in the right foreground. The sector of precluded rho measurements (about 130° to 230°) is shown in stippled pattern. In the actual design, the rho scale is situated between the specimen and the observer, but for clarity, it is here shown on the far side of the specimen.

from the mechanical phi axis. Rho values engraved on the scale increase in a clockwise direction as viewed from the standard observer position (looking down on the Goldschmidt goniometer, and from the front of the Nedinsco goniometer). Because the light source and telescope (or its access port) are both located on a rho arc, on these two goniometers, the

mechanical phi axis is excluded from the arc sector between them. This interference precludes rho readings in about the 120° to 220° range on the Goldschmidt goniometer and about the 130° to 230° range on the Nedinsco goniometer. The Huber goniometer's vertically oriented plane of incident and reflected light reduces somewhat the range of precluded rho readings, but the breadth of the phi axis mechanism is still great enough that rho readings in the 140° to 220° range are inaccessible (R. B. Emlet, pers. comm., 1993). The arrangement of scales on all of these goniometers is equivalent. This may be a feature of other goniometers as well, but like any convention involving handedness, it is based on arbitrary choices. Users of CALCAXES should verify that their goniometer is compatible with the design described here; if it is not, some modification of the program or its output may be necessary.

Specimen Orientation and Mounting

Orientations of face poles and crystallographic axes can be specified relative to one another, as done above, without reference to their relation to a specimen, but biological application of data on crystallographic axis orientation depends on some system for relating observations to an *anatomical reference frame*. This requires specification of several anatomical landmarks, in combinations that account for three degrees of orientational freedom. We commonly use one polar reference axis (e.g., anteroposterior, oral-aboral), which we call the *primary anatomical reference axis*, to lock in two degrees of orientational freedom. We then select a *secondary anatomical reference axis*, also polar (e.g., dorsoventral, left-right, a-ambulacral) and of known relationship to the first. Considered by itself, this carries as much orientational information as the primary anatomical reference axis, but since the two are not independent, this information is partly redundant to that carried by the primary axis. The remaining independent information nonetheless suffices to lock in the third degree of freedom. Comparisons between specimens depend on assuming that the landmarks used for recognition of anatomical reference axes are comparable, or homologous, for each specimen on which they are observed, but this is not a unique requirement imposed by crystallographic data.

Although one anatomical reference frame must be chosen for any single set of comparisons, we commonly consider alternative anatomical reference frames, depending on the problem and available data. For dealing with whole, articulated skeletons, we often use a whole-organism reference frame, considering all skeletal elements in the same context. However, if the form of the organism changes during ontogeny or evolution, the landmarks used to recognize anatomical reference axes may shift position relative to one another. This raises the possibility that some local (rather than whole-organism) reference frame, or some series of reference frames, may allow a more conservative representation of crystallographic patterns. In this event, or when dealing with isolated, disarticulated skeletal elements, it may be useful to define reference frames based on landmarks intrinsic to each skeletal element.

Specimens are initially mounted for measurement so that a single anatomical reference axis (generally the primary one) is aligned with the phi axis of the goniometer. This is accomplished through the intermediary of the goniometer head, a device that attaches to the mechanical phi axis and has two translational slides and two rotational arcs that allow the location and orientation of the specimen to be critically adjusted (Fig. 4). In general, the specimen is mounted on a rigid post, or other support, which is then attached securely to the goniometer head. The mounting of the specimen onto the rigid post need not involve precise control of orientation because subsequent adjustments of the rotational arcs on the goniometer head are ordinarily responsible for refining the alignment of the primary anatomical reference axis to the phi axis of the goniometer. This alignment may be evaluated by checking for wobble of the primary anatomical reference axis while viewing the specimen along a direction normal to the phi axis and spinning it about the phi axis. When complete, this alignment controls for two of the three degrees of orientational freedom needed to relate the anatomical
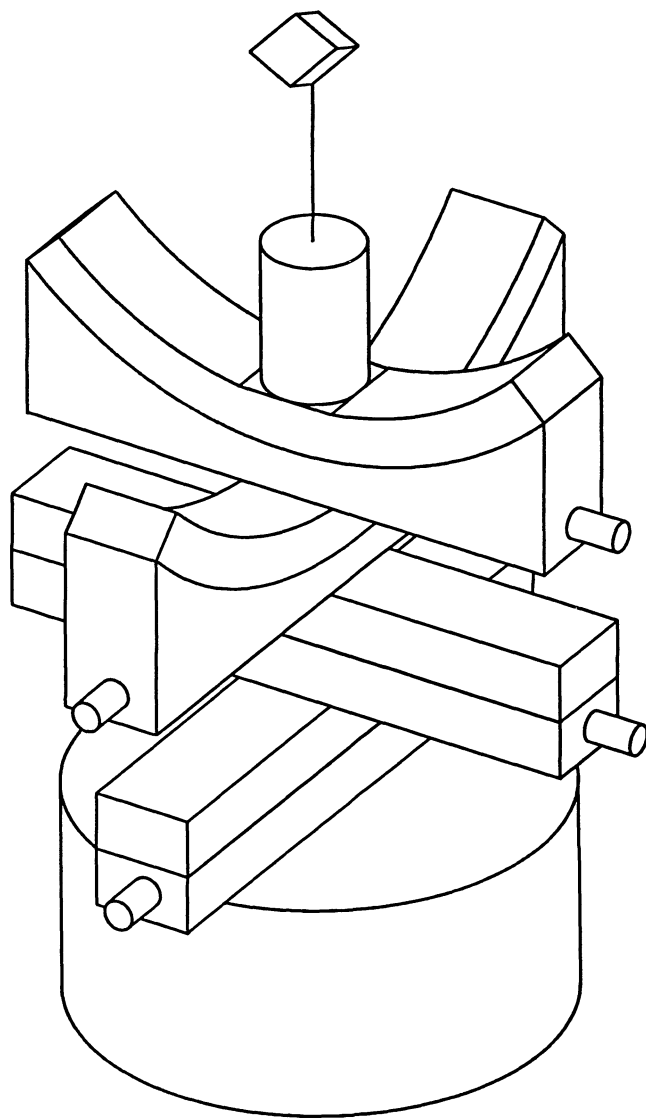
FIG. 4—Schematic diagram (isometric projection) of a goniometer head. The translational slides are used, together with a goniometer adjustment for translation along the phi axis, to bring a selected point on the specimen to the intersection of phi and rho axes. The arcs are used to align the primary anatomical reference axis of the specimen (rhombohedron) with the phi axis of the goniometer. The base is attached to the mechanical phi axis of the goniometer.

reference frame to the phi and rho coordinate system. The final degree of freedom, that specified by the secondary anatomical reference axis, is discussed below.

An alternative approach to specimen mounting is to use a custom-designed jig (illustrated elsewhere; Bodenbender, in prep.) to control the mounting of the specimen on the rigid post. We have, for instance, used such a jig to align the oral-aboral axis of blastoids with the long axis of a mounting post. The mounting post is then inserted into a prepared receptacle on the

goniometer head, the goniometer head arcs are set to 0°, and no further alignment of the primary anatomical reference axis is necessary.

Since the orientations of crystallographic axes are to be reported in a coordinate system based on anatomical reference axes, the ultimate precision of the data, and therefore the resolution that can be achieved in comparisons among specimens, depends on the repeatability, or uncertainty, in alignment of anatomical reference axes. This, in turn, depends on the nature of the landmarks used to define anatomical reference axes and the care taken in locating them. Under optimal circumstances, uncertainties on the order of 1-2° are achievable using morphological landmarks.

The Phi and Rho Coordinate System

The Globe-Specimen Model

To understand the relationship between the anatomical reference frame and the phi and rho coordinate system, it is useful to discuss a specimen as if it were located within an imaginary globe—i.e., a conventional model of planetary geography. The primary reference axis of a globe is its north-south axis of rotation, and in our globe-specimen model, the north-south axis of the globe is set parallel to or coincident with the primary anatomical reference axis of the specimen. A secondary reference axis for the globe could be represented by a vector passing from its center through any fixed point (such as Greenwich, England) on its surface (other than the north and south poles), or if we prefer a secondary reference axis perpendicular to the primary reference axis (as is common in anatomical systems), it could be the vector from the center of the globe through the intersection of its equator and the arc passing from north pole to south pole through any fixed point. In our globe-specimen model, the secondary reference axis of the globe is set parallel to or coincident with the secondary anatomical reference axis of the specimen. Thus, the specimen is rotationally fixed within the imaginary globe, but free to translate so that any chosen point on the specimen can be made to occupy the exact center of the globe. In other words, the globe represents the rotational (or orientational) aspect of the anatomical reference frame, and features of interest are brought to its center for assessment of their orientation.

As briefly introduced above, we attach the globe-specimen to the goniometer head by a pin mounted in the position of the south pole and, by adjustment of the goniometer head arcs or use of a jig, align the primary anatomical reference axis of the specimen, and hence the north-south rotational axis of the globe, with the phi axis of the goniometer (Fig. 5). Once this alignment is accomplished, the center of the globe is effectively located at the intersection of the goniometer's phi and rho axes, and rotations about these axes can be used to designate points on the globe surface. To measure the orientation of a feature such as a face pole on the specimen, we first use the goniometer head slides (and/or a third adjustment on the mechanical phi axis itself) to translate the area of interest on the specimen—i.e., the portion of a skeletal element on which a rhombohedral face is located—to the center of the globe and the intersection of phi and rho axes. The orientation of a pole normal to this face is recorded in terms of the position at which it would intersect the globe surface. The phi reading is essentially a measurement of the longitude of this intersection with the globe surface, and the rho reading is essentially a measurement of its latitude. One qualification required by this analogy concerns the numbering of the rho scale. Rho values, like latitudes, are read within a plane containing the north and south poles, perpendicular to the plane of the equator. However, unlike latitudes, rho = 0° only at the north pole (not anywhere along the equator), and rho values increase through a full 360° rather than quadrant by quadrant. They are first traced around the globe from north to south, such that rho = 90° at the equator, and 180° at the south pole. Values greater than 180° then go from south to north, so that rho = 270° again at the equator. Rho values between 0° and 90°, and between 270° and 360°, describe
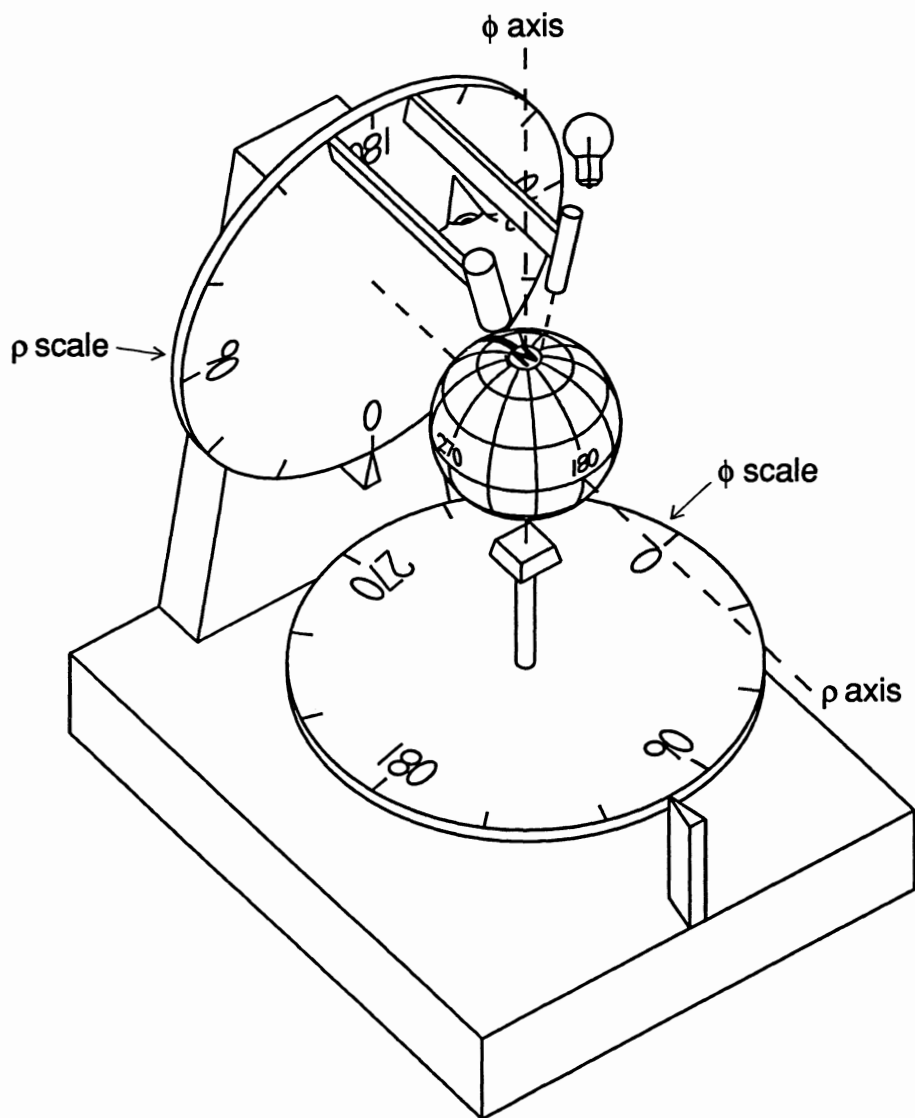
FIG. 5—Schematic diagram (isometric projection) of the Nedinsco goniometer (Fig. 3) in operation, with a specimen mounted on the goniometer head in standard orientation. The anatomical reference frame of the specimen is represented by a globe whose rotational axis coincides with the phi (ϕ) axis of the goniometer and whose center coincides with the intersection of the phi and rho (ρ) axes of the goniometer. The specimen is free to translate, but not rotate, within the globe. The north pole of the globe is indicated by the letter "N" and the line of 0° longitude is marked by a bold line, disappearing over the far side of the globe. Lines of 180° and 270° are also indicated. Note that these lines of 'longitude,' representing loci of equal phi value in the standard coordinate system, need not be (and in general, are not) aligned with corresponding values on the phi scale. The phi scale reading obtained with the globe-specimen in standard orientation is referred to as the phi offset value (phi$_0$) and is here illustrated as being 103°.

features in the northern hemisphere, while rho values between 90° and 270° describe features in the southern hemisphere.

Direction of Rho Increase

Readers may note that the above description of rho values is ambiguous as to their direction of increase. This is because the similarity of goniometer designs described above, with the numbers engraved on both rho scales increasing in a clockwise direction, viewed from the observer's standard position (looking down on the Goldschmidt goniometer and at the front of the Nedinsco goniometer), hides a deeper difference (which will resolve into another, still deeper similarity). On the Goldschmidt goniometer, the rho values assigned to poles on the globe-specimen, viewed along the rho axis, from the observer's standard position, increase in a clockwise direction, like the engraved rho numbers. This is because during rho movement (without moving phi), the rho scale of the Goldschmidt goniometer is stationary within the anatomical reference frame. In contrast, on the Nedinsco goniometer, the rho values assigned to poles on the globe-specimen, viewed along the rho axis, from the observer's standard position, increase in a *counter*clockwise direction. The inverted order of engraved numbers as compared to rho coordinates is due to the rho measurement strategy employed by the Nedinsco goniometer, wherein the rho scale moves within the anatomical reference frame during rho movement, even with phi locked in position. For a linear analogy, consider using a tape measure to determine the heights of a person's knees, waist, and shoulders above the floor. Placing the zero end of the tape on the floor and unrolling it as necessary corresponds to the Goldschmidt goniometer's rho strategy; the numbers on the tape increase in the same direction as height. The Nedinsco goniometer, however, performs the equivalent of placing the zero end of the tape by each anatomical feature and unrolling the tape to reach the floor; the numbers on the tape now increase in a direction opposite to that in which height increases, and for each measurement the tape must be moved within the reference frame in which height is measured. This difference does not, however, lead to different rho assignments to the same face pole measured on the two goniometers because the Nedinsco goniometer is, in relevant respects, equivalent to the Goldschmidt goniometer tipped up on its far edge. The standard view of the observer along the rho axis, in the external reference frame, is therefore opposite (i.e., equivalent to looking along the rho axis from the underside of the Goldschmidt goniometer); the similarity in direction of increase of engraved rho values is, by itself, misleading; and the Nedinsco's reverse relationship between engraved rho values and direction of increase in the rho coordinate yields coordinates identical to those measured on the Goldschmidt goniometer.

Completion of the Geographic Analogy

The analogy between phi values and longitude also needs qualification. Rather than running from 0° to 180° in two directions around the globe, phi values, viewed from the north pole, run clockwise around the globe through a full 360°. The phi scale is fixed relative to the globe surface, but rotation of the globe about its north-south axis moves the globe-specimen (and the phi scale) relative to the rho scale. Lines of equal phi, but varying rho, like lines of longitude, are great circles passing through the north and south poles. Lines of equal rho, but varying phi, like lines of latitude, are small circles lying within planes parallel to the plane of the equator.

This geographic analogy is applicable to any linear feature that can be represented by a vector passing from the center of the globe through a point on its surface. It is thus the means by which we describe the orientation of crystallographic axes as well as face poles.

Redundancy in the Phi-Rho System

This system leaves open the possibility of redundant observations, since a single point on the globe surface (i.e., a single orientation) can be specified by either of two sets of phi and rho coordinates. For example, setting rho to 1° with phi at, say, 10° will record a point 1° from the north pole. Keeping rho at 1° and rotating phi (and the specimen) a half turn to 190° will record a new point 1° from the north pole, and 2° from the first point, which has been

rotated to the opposite side of the pole. Now, rotating rho over the pole from 1° to 359° records the first point again, but this time its phi and rho coordinates are (190,359), whereas they were originally observed as (10,1). CALCAXES treats such redundant observations as equivalent in its calculations and interactive responses. At first, the potential for such redundancy may seem to imply that the direction of rho increase, discussed above, does not really matter; either way, the example in this paragraph would yield one rho value of 1° and another of 359°. However, this neglects the fact that it takes two coordinates to specify orientation in this system. If one direction of rho increase yields redundant coordinates (10,1) and (190,359), the other direction of rho increase would yield (10,359) and (190,1), implying a mirror-image orientation.

Coordinates vs. Scales and Index Marks

As noted above, both goniometers assign a rho value of 0° to a pole coincident with the north pole of the globe-specimen, but this does not necessarily mean that 0° on the rho scale must be aligned with the north pole. What determines the spatial relationship between a pole and its corresponding value on a scale is the location of the index mark against which the scale is read. The numbers on the rho scale and the rho index mark could be shifted to various degrees around a rho arc as long as the scale reads 0° when a pole in the position of the north pole is observed for measurement—i.e., placed so that its face reflects an incident beam into the viewing telescope. The same relativity pertains to the numbers on the phi scale and the location of the phi index.

Necessity of Phi Conventions

Although goniometer design effectively determines that the north pole of the globe-specimen will have a rho value of 0°, it does not completely determine how phi values relate to the standard orientation. It is up to the user to choose a convention for this. Our procedure is to mount the specimen so that its primary anatomical reference axis is aligned with the phi axis, and then rotate the specimen about the phi axis to a reproducible orientation that can be recognized for all comparable specimens. This is the step that calls for a secondary anatomical reference axis, and it is the placement of the secondary anatomical reference axis in a standard orientation that locks in the third degree of rotational freedom discussed above. To judge this orientation consistently, it is essential to pick an identical vantage point for observation of all specimens. This is particularly important on the Nedinsco goniometer, where the optical system for reflecting light from the access port to the viewing telescope induces a complex rotation of the image even when only rho is being changed. Using the Goldschmidt and Nedinsco goniometers, we have chosen to standardize specimen orientation relative to phi by first setting rho so that the goniometer telescope looks directly down the phi axis.

Explanation of our procedure now requires a brief digression on rho settings. Measuring a face pole orientation on the goniometer records the position of the bisector of the angle formed by the incident beam from the light source and the beam reflected off the crystal face, into the viewing telescope (Fig. 6). When looking at the specimen during measurement, one looks down the path of the reflected beam. In order to look directly down the phi axis, at 0° rho, the user must rotate the globe-specimen to look down a path of reflection associated with some bisector (or face pole) that has a non-0° rho value on the goniometer. On both goniometers we have used, the angle between incident and reflected beams is 25°, and a line of sight directly down the phi axis is obtained by setting rho to 347.5°. In general, the rho setting to use for standardizing phi depends on a goniometer's 0° rho position, the angle between incident and reflected beams, and the direction of displacement between them.

Once a standard line of sight, down the phi axis, has been obtained, it remains to bring the secondary anatomical reference axis into a standard orientation, without moving rho. To restate the task in terms of the globe model, we are now looking directly down on the north pole, but we have to make sure that Greenwich faces the same direction as we measure each
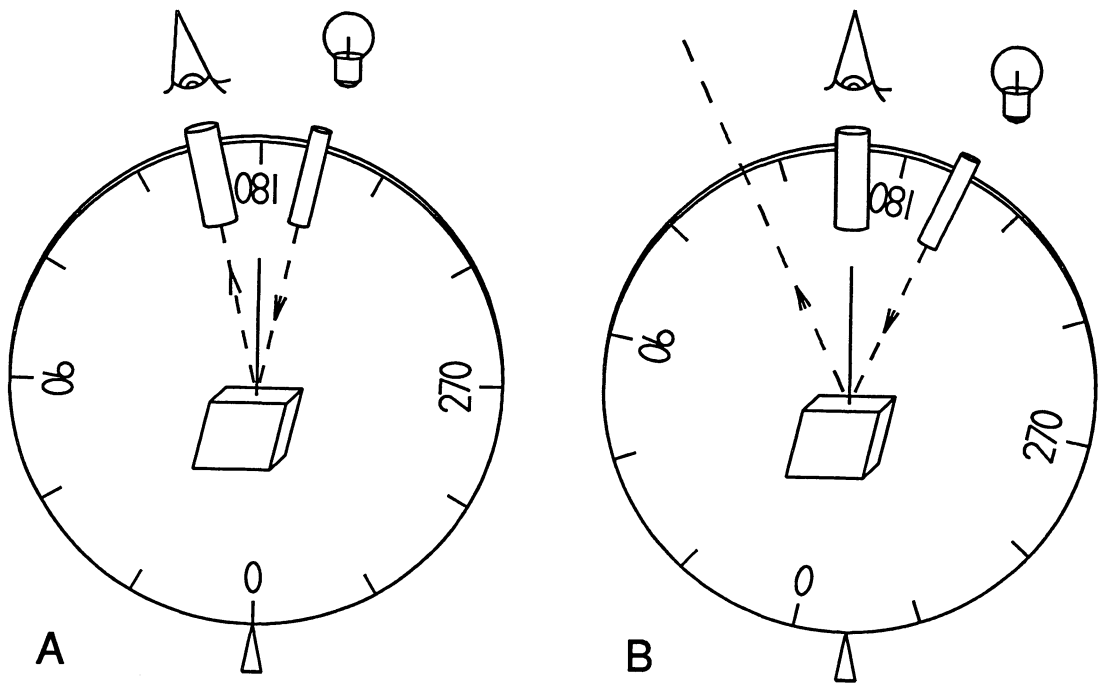
FIG. 6—Contrasting instrument settings for data collection and control of the line of sight. The specimen is an idealized rhombohedron on which one face has been oriented so that its pole is aligned with the phi axis. The goniometer is modeled after the Nedinsco goniometer, but the Goldschmidt goniometer is comparable. Incident and reflected beams are shown in dashed lines, with arrows indicating direction of travel. Only the rho scale is illustrated, and its index (against which rho values are read) is the small triangle at the bottom of each diagram. A: instrument set to measure the rho value of the face pole shown. The reading of 0° on the rho scale represents the face pole itself, not the line of sight of the telescope. B: instrument set so that the line of sight of the telescope is along the phi axis. The rho value associated with this view is 347.5°, and the reflected beam no longer enters the telescope.

globe (i.e., specimen) in our sample. This is done by rotating the specimen about the phi axis until the secondary anatomical reference axis reaches a predetermined position. Any repeatably recognizable position would serve to standardize samples, but the choice we make has complicated consequences. In addition to the issue of how to orient the secondary anatomical reference axis, there is a question of what coordinates to assign reference axes. To be sure, placing the secondary anatomical reference axis in a standard position, in the standard view, will yield *some* phi value (i.e., some reading on the phi scale) to make a coordinate pair along with the rho value of 0°. However, there are two problems with simply accepting this as the end of the matter. The first is that it is not really enough just to associate a given phi value with a particular orientation of the globe as a whole. In order to 'navigate' efficiently from one rhombohedral face to another, making sense of the spatial 'meaning' of various phi and rho coordinates, we also need to know what lines of longitude on the globe-specimen are being assigned the phi values of 0°, 90°, and so on. The second problem is that although the secondary anatomical reference axis can often be oriented with as much precision as the primary anatomical reference axis, goniometer design gives the user little control over what raw phi value will be associated with a given orientation of the secondary anatomical reference axis. In particular, once the specimen has been mounted and its primary anatomical reference

axis aligned with the phi axis, there is no provision for rotating the phi scale about the phi axis, independent of specimen movement, in order to apply a standard raw phi value to a standard specimen orientation. To some extent, it is possible to mount and align the same specimen, on different occasions, so that the standard orientation has nearly the same raw phi value. However, mounting the specimen on the goniometer head, and the goniometer head on the goniometer, followed by alignment of the primary anatomical reference axis with the phi axis, all introduce rotations whose net directions and magnitudes are difficult to anticipate or reproduce. The Nedinsco goniometer simplifies this somewhat by means of a machined slot that accepts a pin in the base of the goniometer head, but the Goldschmidt goniometer provides no such constraint. This means that anatomical reference axes (not to mention any other selected feature) generally have different raw phi coordinates after every mounting operation. The most practical solution to these problems is a rotational subtraction procedure, yielding transformed phi coordinates that have a standard relation to anatomical reference axes. Raw phi coordinates should not be used directly to compare among specimens or even among data measured on different mountings of the same specimen.

Virtues of the 9 o'clock Position
    We address these problems first by considering what would be ideal coordinates for reference axes. The primary and secondary anatomical reference axes differ in their rho values by 90°, and given a rho value of 0° for the primary anatomical reference axis, it is reasonable to assign the secondary anatomical reference axis a rho value of 90° (270° is the alternative). Because both reference axes are located along a single line of longitude, it seems sensible to give them the same phi value, and their reference status suggests this should be 0°. Admittedly, any phi value for the primary anatomical reference axis is arbitrary, like a longitude for the north pole, but this can still serve as a way to designate the particular view used for standardization. The catch is that these coordinate assignments will only work if the standard view (looking down the north pole-phi axis on the Goldschmidt or Nedinsco goniometers) places the secondary anatomical reference axis in the 9 o'clock position, or toward the observer's left in the external reference frame (telescope views are discussed below). This can be understood by remembering the stability of the rho axis in both goniometer designs—i.e., the specimen and/or parts of the goniometer swing about the rho axis, but the rho axis itself does not swing. In the external reference frame, the plane of rho observation is stationary; rho values must thus be measured for any point on the globe-specimen by bringing the desired point into the plane of rho observation, by adjusting phi, rather than bringing the plane of rho observation to the point. Therefore, the only way the goniometer can rotate from rho = 0° to rho = 90°, without changing phi, is to move directly from observation of the north pole position to observation of a pole located at the 9 o'clock position (again, looking down the phi axis, in the external reference frame). This is simply the direction in which a pole with rho = 90° is located relative to a pole with rho = 0°. If the standard view orients the secondary anatomical reference axis in any other than the 9 o'clock position, the standard view of the north pole and a view down the secondary anatomical reference axis will not have the same phi coordinates.

Virtues of the 12 o'clock Position
    Despite the factors favoring a standard orientation with the secondary anatomical reference axis in the 9 o'clock position, other complications are induced by this choice. As mentioned above, the optics of the Nedinsco goniometer reflect the image of the globe-specimen. The orientation of the effective mirror plane is such that the 9 o'clock position in the external reference frame is equivalent to a 3 o'clock position viewed through the telescope. Description of standardization procedures must then be qualified by noting whether landmarks are being discussed in the external or the *telescope reference frame* (i.e., spatial relationships as perceived by looking through the telescope). On the Goldschmidt goniometer, telescope optics rotate the

image of the globe-specimen 180°. This is in some ways easier to deal with visually because landmarks maintain their relative positions (within the telescope reference frame) without reflection, but the description of standardization in the external reference frame still differs from its description in the telescope reference frame. Using the Nedinsco goniometer, there is an option that permits the description of standardization in both these reference frames to be identical. This is to choose a standard view with the secondary reference axis located along either the 12 o'clock or the 6 o'clock position, where (because of the orientation of the mirror plane) image reflection does not change the position of a landmark. Choosing the 12 o'clock position (up, in the external reference frame of the Goldschmidt goniometer; away from the observer, in the external reference frame of the Nedinsco goniometer) also has the benefit of allowing the line of longitude used as our phi reference to occupy the same position on the goniometer (with the globe-specimen in standard orientation) as it does on the stereograms used for data display (which in turn have been standardized to reflect conventions familiar to most potential users of CALCAXES; see below). Finally, in working with many echinoderms, the oral-aboral axis is the easiest to align with the phi axis and therefore the natural choice for a primary anatomical reference axis, and the a-ambulacrum is then the linear feature that most nearly lies along a line of longitude that could be used as a phi reference. Anatomical illustration conventions typically place this ambulacrum at a 12 o'clock position, and it would be useful to maintain consistency with these.

An entirely independent argument for using a 12 o'clock standard position for the secondary anatomical reference axis emerges from considering the design of the Huber goniometer. With its telescope and light source occupying a vertical plane, perpendicular to the plane of rho movement, only the bisector of the angle between the telescope and light source can be aligned with the phi axis. The telescope itself cannot look directly down the phi axis. This does not interfere with alignment of the primary anatomical reference axis, for this would usually be judged by spinning the specimen about phi at a rho position of 90° or 270° (on the Huber goniometer). However, it rules out aligning the secondary anatomical reference axis by looking down the phi axis. Instead, the secondary anatomical reference axis must be 'centered' (i.e., placed along a vertical line of symmetry) in the oblique view that the Huber telescope provides of the 0° rho position. Any other standard placement of the secondary anatomical reference axis would suffer from inadequate visual symmetry cues for use in alignment from this perspective.

Phi Transformations

For these reasons, our convention for standardization is to rotate the secondary anatomical reference axis until it is directed toward the 12 o'clock position in the external reference frame described above and in the field of view of the Nedinsco telescope (Fig. 7B). Given this choice, even if we have primary anatomical reference axis coordinates of (0,0), the secondary anatomical reference axis will end up with coordinates of (90,90), as explained above, unless we adopt a transformation of phi coordinates. In order to accommodate our shift of phi reference location away from the 9 o'clock position, CALCAXES subtracts 90° from all raw phi values. Subtraction of a positive phi is appropriate because the 12 o'clock position of the line of longitude we have chosen for our phi reference is 90° (the *phi reference angle*) in a clockwise direction (the direction of phi increase, looking down on the north pole) from the 9 o'clock reference position favored when we consider only goniometer design. This yields transformed phi coordinates of (0,90) for the secondary anatomical reference axis, as desired, but unfortunately gives (270,0) as the coordinates of the north pole *in standard view* (Fig. 7A and B), apparently thwarting our goal of identical phi values for the primary and secondary anatomical reference axes. Can we not have our cake and eat it too? The real answer is of course, "No," but we may turn this into a qualified "Yes," by noting that we can after all get transformed coordinates of (0,0) for the primary anatomical reference axis, but only in a *rotated* standard view that places the secondary anatomical reference axis at 9 o'clock, in the
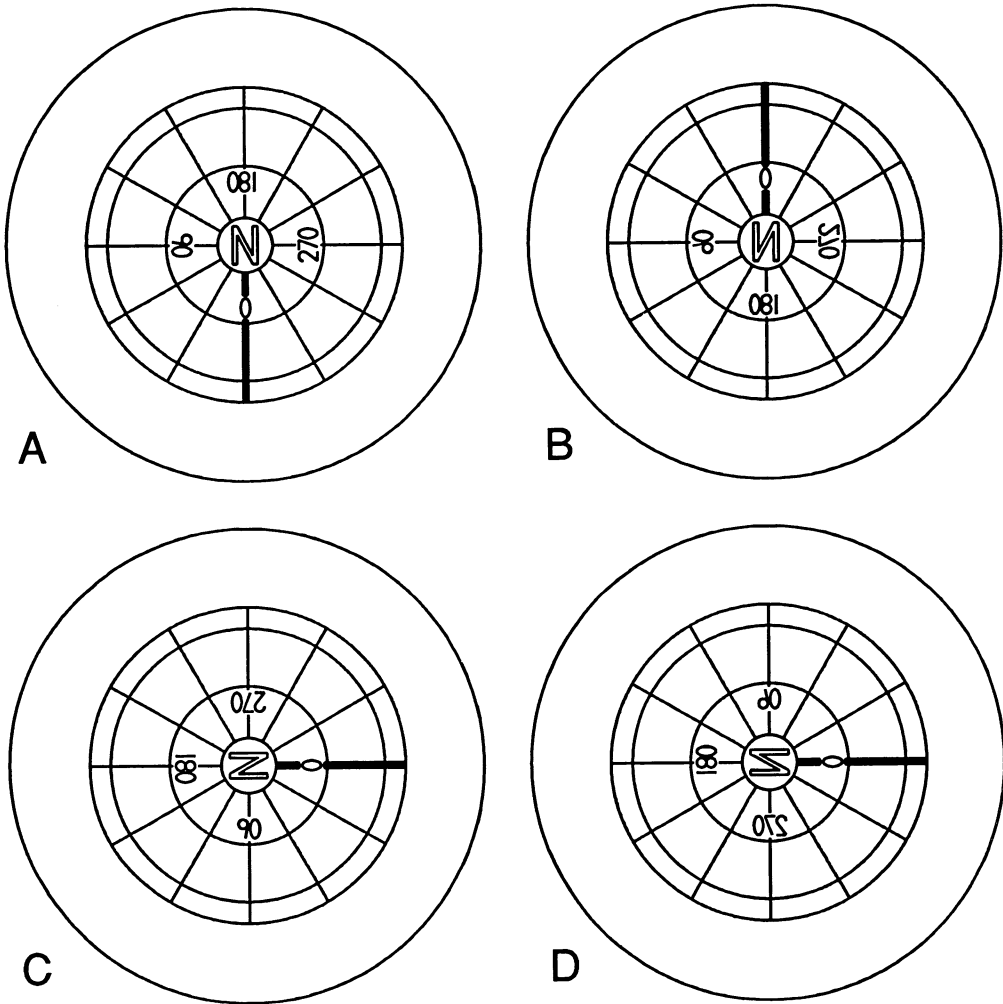
FIG. 7—Views of the north pole of the globe-specimen, looking through the goniometer telescopes with a line of sight directly down the phi axis. As explained in the text and Fig. 6, the rho value for all these views is 347.5°. In A and B, the globe-specimen is in standard orientation, with the arc of 0° phi in the 12 o'clock position in the external reference frame. The phi value for this setting, after subtraction of phi_0 and the 90° phi reference angle, is 270°. In C and D, the globe-specimen has been rotated about the phi axis to one of only two phi positions (arc of 0° phi in the 9 o'clock position in the external reference frame) at which the goniometer telescope can look directly down both the primary and secondary anatomical reference axes (by appropriate adjustment of rho). The phi value for this setting, after subtraction of phi_0 and the 90° phi reference angle, is 0°. A: view down the telescope of the Goldschmidt goniometer, showing the standard specimen orientation. The secondary reference axis *appears* to be at the 6 o'clock position because of image inversion. B: view down the telescope of the Nedinsco goniometer, showing standard orientation. The secondary reference axis appears at the 12 o'clock position, as it does in the external reference frame, because of the vertical orientation of the effective mirror plane for image reflection (from the reflected beam access port to the stationary viewing telescope). C: view down the telescope of the Goldschmidt goniometer, with the secondary reference axis rotated to the 9 o'clock position in the external reference frame (image inverted). D: view down the telescope of the Nedinsco goniometer, with the secondary reference axis rotated to the 9 o'clock position in the external reference frame (image reflected).

position it would indeed have if we came to the primary anatomical reference axis directly from measuring the secondary anatomical reference axis at transformed coordinates (0,90), without changing phi. This rotated standard view is shown in Fig. 7C and D. In summary, the awkwardness of a standard view with coordinates of (270,0) and a primary anatomical reference axis with coordinates of (0,0) only in a rotated standard view, is simply the price we must pay for our choice to use a standard orientation with the secondary anatomical reference axis 90° above (in the external reference frame of the Goldschmidt goniometer) the plane of rho observation. If the user makes a different choice, the program will have to be modified or CALCAXES' output will have to be rotated to give proper phi values.

Although we now have a standard orientation and a coordinate system in which the primary and secondary anatomical reference axes have identical phi values, the mounting and alignment procedure still leaves us with no guarantee that this phi value will be 0°. CALCAXES solves this problem by another transformation. Once a specimen is positioned in its standard orientation relative to both phi and rho axes, the value read on the phi scale is recorded as the *phi offset value* (phi_0) for that specimen. CALCAXES subtracts each specimen's phi offset value from all phi values recorded for that specimen (as well as subtracting the 90° discussed above), yielding (further) transformed phi values. This cancels the effects of the essentially arbitrary component of phi yielded by mounting and alignment procedures. The result can be seen by comparing original phi values entered into the program with trends reported for those values in the *standard coordinate system* (i.e., the coordinates resulting from standardized specimen orientation and transformation of phi values). The trends differ from the original phi values by 90° plus the phi offset value. Phi values are entered into the program exactly as read from the goniometer for each specimen, yet results are reported (for standardized display) in the standard coordinate system.

The Relationship Between Specimen and Stereogram

Just as conventions must be defined for placing the specimen in a standard orientation on the goniometer, conventions must also be defined for displaying data from the goniometer on a stereogram. Our stereograms follow a pattern common in geological usage, with 0° phi (or, equivalently, 0° trend) at the top of the stereogram (12 o'clock), and with values increasing clockwise. 0° rho is plotted at the center of the stereogram (Fig. 8). The (transformed) phi and rho values we have chosen to represent our standard view of the specimen correspond to these stereogram conventions.

At times it is convenient to treat the stereogram as a full-sphere stereographic projection, distinguishing axes in the upper hemisphere from those in the lower hemisphere. When full-sphere projections are used, we plot axes from the upper hemisphere of the specimen (external reference frame, Nedinsco goniometer; i.e., the northern hemisphere of the globe-specimen) as falling in the upper hemisphere of the projection. Likewise, axes from the lower hemisphere of the specimen plot on the lower hemisphere of the projection. When it is not necessary to distinguish between hemispheres, we adopt the convention of projecting axes to the lower hemisphere. These conventions allow direct correspondence between axis orientations displayed on the stereogram and in the specimen's standard orientation (external reference frame) on the goniometer.

To facilitate use by those with more background in structural geology than in crystallography (a diagnosis we suspect applies to most potential users of the program) CALCAXES' output reports plunges rather than rho values. These differ in that rho values record angular divergence from the vertical radius in the upper hemisphere while plunges record angular divergence below a horizontal plane. Whereas rho would be plotted on a stereogram by starting at the center and counting toward the edge, plunges are plotted by starting at the edge
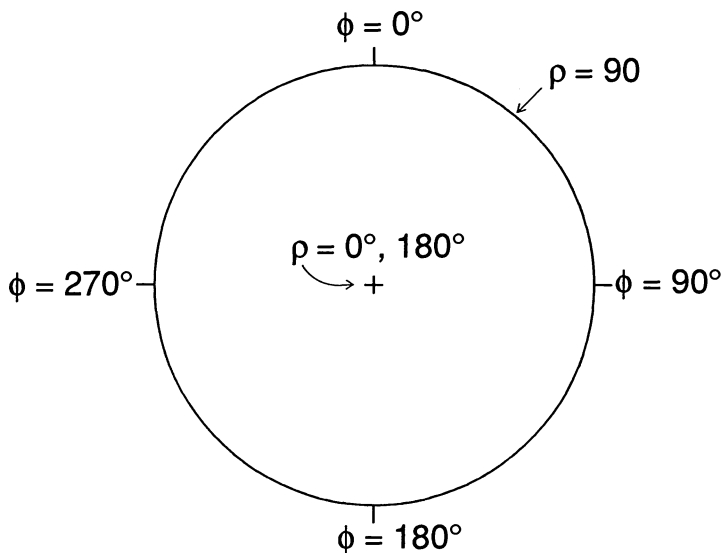
FIG. 8—Conventions used in displaying data on stereograms.

(the horizontal plane) and counting toward the center. Axes lying in the lower hemisphere have positive plunges. Axes lying in the upper hemisphere have negative plunges.

If a goniometer differs from the configuration described in the preceding sections, CALCAXES should still give good *relative* axis orientations for a group of specimens. What could differ is the position of the reference loci for phi and rho measurement, relative to the standard orientation of the specimen on the goniometer. If the absolute orientation of crystallographic axes relative to the specimen is important to the question at hand (as it probably will be), the program may have to be modified or different stereogram conventions adopted.

Crystallographic Background Information

The calcite crystal lattice (or a calcite rhomb) has six rhombohedral face poles, but these may be grouped as three pairs of antipodal mates (r_i and r_i' in Fig. 1). Each member of a given pair is parallel to its antipodal mate; they thus have the same nonpolar orientation (i.e., their orientation differs only in polarity). Antipodal face poles therefore give observationally independent information, but their coordinates still only constitute different estimates of the same nonpolar orientation (assuming an undeformed crystal lattice). Observation of one face pole with or without its antipodal mate constrains the c axis to lie somewhere along a small circle representing the locus of points 44.61° (44° 36.5'; Palache et al., 1951, p. 143) away from the observed face pole (or face pole pair). Observation of two nonantipodal face poles (with or without observing their antipodal mates) further constrains the c axis to two possible orientations along this small circle. Geometrically, the second nonantipodal face pole prescribes a second small circle that intersects the first at two points. Full constraint of c axis (and a axis) orientation is obtained only by observation of three mutually nonantipodal face poles. Antipodal face poles, if observed, are not redundant in the sense of the redundant phi and rho coordinate pairs discussed earlier, but they still specify only one of a required three axes needed to calculate c and a axis orientations.

In a calcite crystal, the two ends of the *c* axis are identical, as recognized by the 2-fold rotational symmetry about any of the *a* axes. The orientation of the *c* axis is thus nonpolar and can be designated by the phi and rho coordinates, or the trend and plunge, of either end of the *c* axis. The *a* axes, in contrast, are inherently polar, with positive and negative ends. The 3-fold rotational symmetry about the *c* axis (either end) means that successive *a* axes (either positive or negative), separated by 120°, have identical relations to the lattice, but the opposite ends of a given *a* axis, separated by 180°, do not. Since the two ends of a given *c* axis are equivalent, in its calculation procedure CALCAXES adopts the convention of projecting all *c* axes to the lower hemisphere, and reporting as best-fit face poles (see below) those poles which are at an acute angle to the projected *c* axis (whether all such face poles lie in the lower hemisphere or not). On the other hand, *a* axes are never projected, since the positive and negative ends are not equivalent in orientation relative to the orientations of face poles. CALCAXES always calculates the orientations of positive *a* axes. As with *a* axes, trends and plunges of observed face poles are not projected to the lower hemisphere but are simply reported (in the standard coordinate system) as observed on the specimen. Therefore, *c* axes always have positive plunges in the output from CALCAXES' calculation routine, but some face poles, best-fit face poles, and *a* axes can be expected to have negative plunges.

How Axis Orientations Are Calculated

The following is a brief overview of the rationale behind the algorithms used to calculate axis and face pole orientations and deviations. Additional information can be found in comments in the program source code.

As an initial step for all calculations, observed face poles that are approximately parallel or antiparallel (i.e., antipodal mates) are grouped together. The first face pole entered into the program defines one group; the next face pole that is neither subparallel nor subantiparallel (within 20°) to the first group defines a second group; and the next pole not sub(anti)parallel to either of these groups defines a third group. Only three groups of face poles should be found for any rhombohedral calcite crystal. Any observed poles that are not sub(anti)parallel to the first three groups are flagged with a warning and ignored in subsequent calculations of axis and face pole orientations. As new members are added to each group, they are projected, if necessary, so that all lie at acute angles to one another. Treating each pole as a unit vector, poles within groups are added, and when data collection is terminated, each group's resultant vector is normalized to unit length, yielding a mean pole for that group. These mean poles are then projected to lie at acute angles to one another.

If three different groups of face poles are represented by the observed data, the simplest route to an estimate of *c* axis orientation would be to calculate the mean of these three mean poles. If error in observing each face pole were uniformly distributed and several observations were made for each group, the mean pole orientation for each group would represent the best estimate of that group's true face pole orientation, and consequently would yield the best estimate of *c*.

It is possible, however, that error is distributed very nonuniformly, for instance, because of an isolated mistake in reading the phi or rho scale, or because a pole is observed from a crystal domain displaced from the rest of the lattice. Such errors could pass through the coarse filter of the angular divergence criterion described above and significantly degrade the accuracy of our estimate of crystallographic axis orientation. Misreading a scale is a potential problem in any quantitative study, and we usually have little defense against it beyond care and repetition of measurements. Reading face poles from multiple domains is a kind of error unique to crystallography, but crystallography also gives us an internal standard of consistency against which such errors might be recognized. As a way of evaluating the accuracy of measurement and the integrity of the crystal lattice, CALCAXES determines the angles between the mean face

poles for each of the three groups and compares these angles to the ideal angles expected between rhombohedral face poles on crystallographic grounds. Next, a set of three originally observed face poles, one from each group, or a combination of originally observed face poles and group means, one from each group, is selected. Interpolar angles are calculated for this set of three poles and compared to the ideal interpolar angles. This is repeated for all possible combinations of original observations and group means among the three groups, and the program retains the set of three originally observed face poles and/or mean poles that has the minimum sum of squared deviations from the ideal angles. This set of three poles is judged to be the set of best estimators of the crystal's true face poles. The user is informed of their identity by an onscreen message, and the c axis is computed as their mean. This procedure helps avoid the influence that single observations with large error have on a group mean, and is justifiable because the ideal interpolar angles are independently documented and a priori applicable. It is possible that correlated errors for different face poles could lead this procedure astray, but there is no mechanical or crystallographic reason to expect correlated errors.

If only two groups of face poles are represented by observations, the program takes the mean pole for each of the two groups present (projected to lie at an acute angle) and finds the bisector of the angle between them. This bisector is an estimate of e, the pole to the $\{01\bar{1}2\}$ twin plane in calcite. Next, the program finds the plane that contains this bisector and lies perpendicular to the plane of the two mean poles. This new plane contains the two possible c axes, each at 26.26° (26° 15.5′; Palache et al., 1951, p. 143) from the mean pole bisector (e). The new plane also contains the two possible orientations of the third group of face poles, like the c axes, one on each side of the mean pole plane. Trends and plunges of the two possible c axes are presented to the user, along with predicted phi and rho values of the corresponding rhombohedral face poles. As detailed below, if the user has some basis for choosing one of the two possible c axis orientations, the coordinates calculated by this method can be retained as the best available estimate of c and a axis orientations. Alternatively, the user may edit the input data to add additional face pole observations and return to the axis calculation routine described for three groups of face poles.

As the foregoing indicates, CALCAXES calculates c axes in two different ways depending on the input. Each method will produce the same results for face pole observations that have no error, but when error is present, some variation can be expected between the results of the two methods. This can be seen by entering two face poles that differ by, say, 95° rather than the ideal 74.92°(74° 55′; Palache et al., 1951, p. 142). With only two poles, the program asks the user to choose from two c axes calculated as explained above. The user should note the c axis values, then, as a test, edit the data and enter one of the suggested face poles. The resulting c axis differs from either of the c axis values originally offered as choices because c is now calculated as the mean of all three poles and therefore no longer lies at an ideal angle to the plane of the first two face poles. In practice, however, departures of interpolar angles from ideal values are much less pronounced than in this example, and differences between calculation methods are usually small.

Best-fit face poles are found by first rotating each group's best estimator of the true face pole orientation (whether derived from an individual face pole observation or from the mean of all observations in the group) to be subparallel with the best estimators from the other face pole groups. The estimators from each group are then summed and normalized, and this mean is adjusted (i.e., rotated toward or away from c) to lie at the ideal crystallographic angle from c (44.61°). This mean pole represents one of the three best-fit face poles; the other two are found by rotating the first about c by 120° and 240°.

The program finds a axes in a series of calculations that make use of the orientations of the c axis and a best-fit face pole. These calculations find the intersection of the plane perpendicular to c and a plane that includes both c and a best-fit face pole. The best-fit face pole chosen will lie at an acute angle to one end of the c axis. Looking toward the center of the globe-specimen, from this end of the c axis, a positive a axis is found by starting at the

intersection just discovered and then rotating 30° clockwise, within the plane perpendicular to *c*. The same series of operations based on either end of the *c* axis (as long as a best-fit face pole that lies at an acute angle to that end is selected) will yield the orientations of that crystal's positive *a* axes.

The program also calculates deviations for each face pole observation. These represent the angle (in degrees) between each observation (or its projection) and the nearest best-fit face pole.

RUNNING THE PROGRAM

The program is started by typing "calcaxes" (without quotes) at the DOS prompt and pressing ⟨**Enter**⟩ (keyboard entries are shown in the preceding typeface). If a printer is connected to the computer, it should be turned on. Once the program is running, menus and screen messages should be largely self-explanatory. Items in square brackets indicate default options. These can be selected simply by pressing ⟨**Enter**⟩. Selections from menus are activated by typing the single-letter abbreviation (case insensitive) listed with each menu item.

As the Main Menu indicates, CALCAXES is divided into two modules. The Calculation Module is described in this section and can be started by typing **C**. This module calculates crystallographic axis and best-fit face pole orientations from goniometer readings entered at the keyboard. It can be run while data are being gathered with the goniometer, to identify redundant face pole observations and suggest possible goniometer settings where additional face poles may be found. It creates a data file to record goniometer readings and axis calculations. The Graphics Module, described below, reads files produced by the Calculation Module and provides a number of options for data analysis and display. An additional item, the "Adjust settings" command, permits modification of some program defaults for the treatment of data. We will first describe program operation under CALCAXES's default settings, noting instances where user modification of settings affects program function. The "Adjust settings" command can be accessed from the Main Menu and from the Graphics Module; it is discussed fully in the documentation for the Graphics Module (below). The program can be exited by typing **Q** at the Main Menu.

Data Collection and Calculation

The Calculation Module has two different modes of operation. Mode 1 is designed for cases in which data are gathered from individual skeletal elements, mounted one at a time on the goniometer and standardized with respect to individual element morphology. Each mounting operation is likely to yield a different phi offset value, so the user will typically need to enter a new phi offset value for every new set of poles observed and axes calculated. Mode 1 therefore asks for a new phi offset with each sample (i.e., specimen or skeletal element).

Mode 2 is designed for cases where the user wishes to find axis orientations for many different skeletal elements on a single specimen and where these elements retain original spatial relationships so that a single reference frame is applicable to all. Axis orientations of individual skeletal elements in this case are reported with respect to the standard orientation of the whole specimen (that is, in a whole-organism reference frame). In Mode 2, the program asks for the phi offset value only once, to standardize the orientation of the whole specimen, and assumes that the same phi offset applies to all subsequent samples (i.e., skeletal elements) occurring on the same mounted specimen.

An intermediate case between isolated skeletal elements and tightly articulated multi-element specimens is the case of multi-element specimens with disarticulation and displacement of some or all elements. This may make landmarks intrinsic to each element the most precise guides for comparisons with other specimens and favor treatment in Mode 1. With this approach, the

specimen would be reoriented for observation of each element. Alternatively, data could be gathered in Mode 2, with respect to any chosen reference frame, and axis orientations could later be transformed by rotations calculated by the user to accomplish the equivalent of rearticulation.

After selecting the mode of operation, the user is prompted to enter the name of the file to which data will be sent (normal DOS filename restrictions apply). This file can be either new or old. If an old file is chosen, CALCAXES will either add data at the end of the file or replace the old data, at the user's discretion.

If in Mode 1, the program asks the name of the current sample. The user may type up to 30 characters of relevant data such as specimen numbers or anatomical identity of elements.

The program then asks for the phi offset value of the current sample. If the programs's default settings are used, the phi offset is entered in the format: degrees.minutes (e.g., 211° 20' is entered as **211.20**, and 10° 07' is entered as **10.7** or **10.07**). Note that the number of minutes is read literally; single-digit minute values represent the units place, not the tens place. The "Input notation" option in the "Adjust settings" command (see below) can be used to change from the default sexagesimal notation (degrees and minutes of arc) to decimal notation (degrees and decimal fractions of degrees).

If in Mode 2, CALCAXES asks for the phi offset value first. The user is then given the opportunity to enter approximate phi and rho readings for an anatomical reference axis. This may be either the primary or secondary anatomical reference axes discussed above or some third polar, linear feature recognizable on the specimen. This record of orientation of an anatomical reference axis is used in instances when a specimen that has been measured in standard orientation is remounted in a different orientation in order to make additional measurements. This may be necessary because interference between the mechanical phi axis and the arc sector occupied by the viewing telescope and light source prevents observation of features oriented too close to the mechanical phi axis. Knowing the orientations of an anatomical reference axis in standard orientation and in the new, nonstandard orientation simplifies calculation of the transformation necessary to express the new measurements in coordinates compatible with the standard orientation. This anatomical reference axis can be any relocatable, linear feature on the specimen, such as an axis of symmetry or the normal to a particular skeletal plate, as long as it is unidirectional. That is, the end that is recorded should be readily distinguishable from its projection through the specimen. The purpose of this axis is discussed in more detail in the "Merge" section of the CALCAXES Graphics Module (see below). If all measurements on a specimen will be made in standard orientation, no reference axis need be specified. If, on the other hand, the specimen will be remounted for additional measurements, approximate phi and rho readings for the axis should be entered both when the specimen is mounted in standard orientation and when it is remounted.

After entering preferences concerning an anatomical reference axis, the user is asked to name the current sample. This is done exactly as in Mode 1.

Next, for either mode, the user enters the coordinates of rhombohedral face poles as read from the goniometer. For each face pole, type the value for phi in degrees and minutes, separated by a decimal point (e.g., 15° 42' is typed as **15.42**), press ⟨Enter⟩, type the rho value in the same format, and ⟨Enter⟩ again (see the "Input notation" option in the "Adjust settings" command, below, for data entry in decimal notation rather than in degrees and minutes). Repeat the procedure for each face pole from the crystal currently under study. Up to 15 face pole observations may be entered.

As values are entered, the screen will display the original values, the phi and rho values transformed to the standard coordinate system, and the trends and plunges of the transformed values. At times, the user may notice that two different phi, rho coordinate pairs yield identical trend and plunge values, showing that redundant observations of a single face pole have been made, as described above.

When all phi and rho values are entered, press ⟨**Enter**⟩ an extra time. This terminates data acquisition for the current skeletal element.

If the user has made observations on three groups of face poles (as explained above), CALCAXES displays the original face pole phi and rho values in degrees and minutes, the standardized trends and plunges in degrees and decimal portions of degrees, and the deviation of each pole (or its projection on the other hemisphere) from the closest of the three best-fit face poles. Deviations are given to hundredths of degrees. Deviations of less than 3° from the best-fit face poles are often possible even with deformed specimens, and material with fair to good preservation typically yields deviations of less than 1°. High deviations serve as warning flags. They may result from error in operating or reading the goniometer, observation of poles from two different skeletal elements on a single specimen, error in recording or entering data, or (potentially) the presence of non-rhombohedral faces, or crystals other than calcite, on the specimen.

Along with the above information, CALCAXES displays the specimen name, the trend and plunge of an anatomical reference axis (if entered, for use with the "Merge" command), and the phi offset value. Finally, the trends and plunges (to hundredths of degrees) of the best-fit face poles and of the c and a axes are displayed.

A simple way to ensure that all three groups of face poles are recorded is to run CALCAXES while using the goniometer. Redundant observations of the same pole are frequent, and are indicated by their conversion to identical trends and plunges when the user enters phi and rho values. Observations of antipodal face poles show up as trends that are 180° apart and plunges that are opposite in sign. For the experienced user, a glance down the list of recorded poles may suggest possible ranges of coordinates where new face poles might lie, but CALCAXES can also take on some of this burden. If the user terminates data collection when, knowingly or unknowingly, poles from fewer than three groups have been observed, CALCAXES points this out and indicates how many face pole groups have been measured. If only one face pole group has been observed, the observer must go back to the specimen and find at least one more face pole group. If two face pole groups have been recorded, CALCAXES displays the two possible orientations in which the third group is constrained to lie, and gives the four goniometer settings for each orientation (i.e., two redundant sets of coordinates for each of two antipodal face poles). The user may then either select one of the calculated c axis orientations or edit the input data to add information.

The most common circumstance that brings the user to this point is that some range of orientations has simply been neglected in the search for face poles, but with CALCAXES' prompting, the prematurely terminated search can be efficiently resumed. The third pole is often found by systematically checking the predicted goniometer settings, and when one of these reveals the expected reflection, the *measured* coordinates should be added to the input data, whereupon CALCAXES recalculates axis orientations and best-fit face poles according to the routine reserved for three face pole groups.

A different situation is when all face pole settings for one possible c axis orientation turn out to be obscured by the goniometer head, by nearby portions of the specimen, or by intrinsic limits in the rotation of the goniometer. Despite the inaccessibility of these settings, they may be inferred to represent the true face pole orientation if any of the settings for the *other* possible c axis orientation are clearly visible and *fail* to show the reflection indicative of a face pole. At this point, the most straightforward approach is simply to accept CALCAXES' estimate of axis orientations based on the two face pole groups that were actually observed. For face poles that show little within-group scatter and a between-group divergence close to the crystallographic ideal, this can scarcely be improved upon. However, less confidence may be placed in this estimate if there is evidence of nonuniform distribution of error, as when one of the groups shows much more scatter than the other, or even a single outlying observation. In principle, it would be possible to do pairwise comparisons of face pole orientations in two groups comparable to what CALCAXES does for three groups, but because it is easier for two poles to

appear, by chance, at the right angular divergence than for three poles, by chance, to have the ideal *mutual* angular divergences, we have refrained from implementing such an approach. Instead, the user has the option of entering the appropriate estimated face pole coordinates *as if* they had been observed directly. Although a face pole entered in this fashion is entirely a function of other observations, it allows access to the routine devised for three face pole groups, including consideration of the possibility that certain face pole observations may be better estimates of face pole orientation than are the group means. Whether the user selects a *c* axis based on two face pole groups (and additional observation of candidate orientations) or inputs a candidate face pole orientation as data (again presuming an objective basis for the choice between candidates), the deviations reported by CALCAXES will be artificially low, because one of the orientations used for calculating best-fit face poles is already a calculated ideal orientation rather than an observed orientation.

Editing Data

After face poles have been entered and CALCAXES has calculated axis orientations, the user has the option of making changes. If no changes are to be made, just press ⟨Enter⟩ or type N; otherwise, type Y as indicated at the prompt. An Edit Menu appears at the bottom of the screen. The user can delete or add a pole, or change the specimen name, phi offset value, program mode, or anatomical reference axis orientation, by typing the appropriate letter or number preceding each option. One can change the coordinates of a pole by typing the number of the line on which the pole is displayed (the cue for this selection is "#" in the Edit Menu), but the coordinates listed are not updated until after quitting the edit mode. Likewise, deleting a pole causes all succeeding poles to be renumbered in memory, but the screen will not be immediately updated. If a user wishes to delete pole 1 and change pole 2's rho value, deleting pole 1 first will cause pole 2 to be renumbered as pole 1, although it still appears on the screen as pole 2. To avoid unwanted changes, edit higher-numbered face poles first. When finished making changes, type Q or ⟨Enter⟩.

Sending Output

Output can be sent to the output file, a printer, both the file and a printer, or nowhere. Pressing ⟨Enter⟩ sends data to the file only. Sending output to a printer that is not on-line will produce an error message and cause the program to abort.

Output to the printer is similar to the data on deviations and axis orientations displayed on the screen. Data sent to a data file have a slightly different format. In the data file, the first line for each specimen is devoted to the specimen name. The second line has two numbers: the phi offset value and the number of face pole observations recorded for the specimen. If an anatomical reference axis was specified while gathering data, its trend and plunge, in decimal notation, follow on the same line as these numbers. The next lines consist of original face pole phi and rho values in sexagesimal notation, standardized trends and plunges in decimal notation, and face pole deviations in decimal notation (one face pole per line). The last seven lines of data for a specimen list trends and plunges (to hundredths of degrees) of the *c* axis, best-fit face poles, and *a* axes.

The Calculation Module now repeats, asking for the name of the next sample to be entered. The user may exit the module at this point by simply pressing ⟨Enter⟩. To continue, type the next sample name and press ⟨Enter⟩.

On exiting the Calculation Module, the Main Menu allows the user to "Resume" calculations using the same mode, data file, and anatomical reference axis as before, by typing R. This is convenient for switching between the Calculation Module and the Graphics Module. To reenter

the Calculation Module with a clean slate, use the "Calculation Module" command rather than the "Resume" command.

Displaying Output

Output from CALCAXES can be displayed by the Graphics Module. This shows data in full-sphere, equal-area, stereographic projection. That is, the program distinguishes whether an axis is in the upper or lower hemisphere on the stereogram and uses projection conventions appropriate for looking at the dispersion of points on the sphere.

The Graphics Module of CALCAXES supports Hercules, CGA, EGA, VGA, AT&T 400 line, IBM 3270 PC, and IBM-8514 graphics. The code for the Graphics Module of CALCAXES makes calls to standard graphics files that are included with the Turbo Pascal compiler. If a complete Turbo Pascal 5.5 compiler package is not available, do not erase the compiled version.

Start the Graphics Module by typing **G** at the Main Menu. The following Graphics Menu will appear:

> F — File read
> L — Label group
> D — Display
> S — Statistics
> R — Rotate
> M — Merge
> P — Print/Plot
> W — Write to file
> A — Adjust settings
> Q — Quit

The screen also indicates what data file, if any, is active. If a data file was active in the Calculation Module, that file will remain active upon entry into the Graphics Module. If no data file is active, only the commands "File read", "Adjust settings", and "Quit" will respond until a data file is read using the "File read" command.

F — File read

This command reads data files into program memory. Data from several files may be held in memory simultaneously, but all files must have either the format of CALCAXES output or a simple format of one trend and plunge per line. The latter can be read if "general format" has been specified using the "Adjust settings" command (see below). The screen displays the settings currently in effect for the "File read" command.

Once a file has been read, the screen returns to the Graphics Menu, and the active data file is listed. Subsequent issue of the "File read" command offers the option to either "Clear" existing data from memory before reading a new file (type **C**; the new filename will replace the old as the active data file) or "Append" data from a new file to the data already in memory (type **A**; the active data file message is updated only by addition of a " +"). Typing **L** produces a "List" of files that are currently in memory. Data can come from any number of files, but the "List" command will only list the first 20 data files. For files in CALCAXES format, data (*c* axes, *a* axes, face poles, and best-fit face poles) from up to 500 crystals can be read into memory at one time. A total of 500 trends and plunges can be read from files having general format. In all following procedures the Graphics Module treats general format trends and plunges as *c* axes.

Pressing **Q**, from the "File read" menu, will cause the program to return to the Graphics Menu without reading new data or altering in any way the data currently in memory. Pressing ⟨**Enter**⟩ immediately after the "Clear" or "Append" command, at the prompt asking for the name of a new data file, will have the same effect.

L — Label group

This command is optional. It lets the user influence the labelling of best-fit face poles as "b1", "b2", and "b3", which in turn determines the labelling of the *a* axes associated with each specimen's best-fit face poles. For ease of keyboard entry, the numbers used here are not subscripted, and they do not correspond strictly to the subscript values used in crystallographic notation. They are instead simply labels of convenience used to designate groups of poles. When viewing data from multiple specimens whose axes cluster nicely, the initial numbering scheme may break up a cluster of best-fit face poles, designating some as "b1" and some as "b2" (or as "b2" and "b3", or as "b3" and "b1"). To prevent this, the "Label group" command displays all best-fit face poles, rotated such that the mean *c* axis orientation for the whole group of specimens is vertical (i.e., appearing in the center of the stereogram). The user can then move the cursor into a gap between clusters of best-fit face poles. The cursor position defines a vertical plane passing through the center of the stereogram. For each specimen (i.e., crystal) being considered, the first pole counterclockwise (as the user looks at the stereogram) from this plane will be numbered "1", the next "2", and the last "3". Move the cursor on the screen using the arrow keys or the number keys on the keypad: **4** = left, **8** = up, **6** = right, **2** = down. Odd numbers are diagonal. Exit this command by pressing ⟨**Enter**⟩.

D — Display

This command displays data on the computer screen and allows exploratory or permanent projection of *c* axes and observed face poles to the opposite hemisphere. The screen stereogram has 0° trend at the top, and trends increase clockwise. On color monitors, the program's default settings display all orientations on the lower hemisphere in white except for best-fit face pole orientations, which are displayed in green. Orientations on the upper hemisphere are shown in red. If the program's default settings are used, all originally observed face poles are projected to the lower hemisphere. If the user opts to deactivate face pole projection (see below and the "Face pole display" option under the "Adjust settings" command), upper hemisphere face poles will be displayed in yellow.

Two display modes are available. In Quick-plot Mode a single command causes all axes or poles of a given type in the data file to be plotted. In Stepwise Mode, orientations of the chosen type are plotted one at a time, in the order in which they occur in the data file. The newly plotted orientation is highlighted and the sample name associated with the orientation is displayed at the lower right corner of the screen. The next orientation is not plotted until a key is pressed. Typing **Q** during a stepwise display sequence changes from Stepwise to Quick-plot Mode and displays all orientations of the chosen type remaining in the data file. Typing **M** toggles between the two modes.

The Graphics Module of CALCAXES can display *c* axes (type **C**), face poles (type **R**, for rhombohedral face pole), individually labelled *a* axes (type **A1**, **A2**, and **A3**), and individually labelled best-fit face poles (type **B1**, **B2**, and **B3**). An **A** or **B** must be followed by a **1**, **2**, or **3** for the screen to respond (press ⟨**Enter**⟩ after **A** or **B** to cancel the command). A message at the lower right of the screen identifies the type or types of data currently displayed. To erase the current plot, type **0** (zero). Exit the "Display" command by pressing **Q** or ⟨**Enter**⟩.

The "Display" command permits the projection of *c* axes via the "Trial projection" (type **T**) or "Permanent projection" (type **P**) commands. These commands also permit projection of original face pole observations if the "Face pole display" option in the "Adjust settings" command (see below) has first been set to "display poles as written in file". When this setting

is in effect, the user is asked to select projection of c axes (type **C**) or face poles (type **R**). Choosing any of these commands causes a menu of projection options to appear. "All" upper hemisphere orientations of the chosen type can be projected to the lower hemisphere (type **A**), or the user can select individual points to be projected, choosing from all points in "Either" hemisphere (type **E**) or just from those in the "Upper" hemisphere (type **U**). When selecting individual orientations, points on the screen are highlighted in turn by a red and blue box and can be projected, or not projected, by pressing **Y** or **N**. Pressing **Q** halts the selection of points to project, while **A** projects all remaining points.

The "Trial projection" and the "Permanent projection" commands perform identical functions with the exception that the former command carries out the operation only on screen whereas the latter command permanently alters the data in memory. That is, projecting axes with the "Trial projection" command, clearing the screen, and redisplaying the axes will yield the initial rather than the projected orientations. The same operations with the "Permanent projection" command, however, will yield the projected orientations since they have replaced the initial orientations in computer memory. The "Trial projection" command is therefore useful as an exploratory tool, while the "Permanent projection" command is necessary if projected data are subsequently going to be rotated, plotted, printed, stored, or subjected to statistical analysis. It is important to note that neither command alters data stored in a data file. Rereading the data file with the "File read" command from the Graphics Menu will produce plots of the initial, nonprojected data. To save projected orientations to a file, use the "Write to file" command from the Graphics Menu (see below).

Readers may have noticed that a axes and best-fit face poles cannot be projected with the "Display" command. CALCAXES does not permit projection of a axes because doing so would mix positive and negative ends of a axes. Projecting best-fit face poles would tend to obscure the spatial relationships between trios of best-fit face poles and their associated c axes. These relationships are most apparent when all best-fit face poles are at acute angles to each other, but become less apparent when one of a trio is projected to the opposite hemisphere. Users who find a need for projection of a axes or best-fit face poles may edit their data files before running CALCAXES, adding 180° to trends and changing the signs of plunges in order to project data.

S — Statistics

This command calculates statistics for clusters of poles or axes. Indicate the type of pole or axis to be analyzed using the same labels as for output to the screen, such as **A1** or **B1**. To analyze face poles, the user must also specify the trend and plunge of a reference axis, and an angle about that axis. Only those face poles lying within the specified angle about the reference axis will be included in the statistical analysis.

For whichever type of pole or axis one chooses, the routine displays: the mean orientation; a precision parameter, K, which indicates the degree of nonrandom clustering of orientations; a 95% confidence interval, α_{95}, which is one half the apical angle of a cone within which the true mean orientation of the data is expected (with 95% confidence) to lie; θ_{95} and the circular standard deviation, θ_{63}, both of which are measures of the scatter of the data about the mean, representing radii of circles, drawn on the unit sphere, that would be expected to include 95% and 63% of the observations, respectively; and the number of samples, N. Large K values and small α_{95}, θ_{95}, and θ_{63} values indicate well-clustered data. For more information on K, α_{95}, θ_{95}, and θ_{63}, see Tarling (1971, p. 77-78) and Koch and Link (1971, p. 136-142).

An eigen analysis is also performed on the unit vector representations (i.e., the Cartesian coordinates of endpoints) of the chosen poles or axes. For orientational data consisting of unit vectors (or points on a unit sphere), the results of this analysis are described somewhat differently from results of the more familiar eigen analysis of a cloud of points in multivariate space. All eigenvectors pass through the center of the unit sphere. The first eigenvector represents the axis about which the data points (each treated as having unit mass) show the

minimum moment of rotational inertia (Watson, 1966). The second eigenvector lies within the plane perpendicular to the first and, of all orientations *within that plane*, represents the one that has the lowest associated moment of rotational inertia. The third eigenvector lies perpendicular to the first two; in a 3-dimensional system, its orientation is thus entirely constrained by theirs. It is associated with a moment of rotational inertia that is not necessarily maximal but is greater than that associated with either of the first two eigenvectors. All eigenvectors are reported in both Cartesian and spherical coordinates. The eigenvectors' Cartesian coordinate system is oriented with positive Y at $0°$ on the screen stereogram and positive X at $90°$. The positive Z axis is in the upper hemisphere, but the eigenvectors are always reported with positive plunges so their Z values will always be negative.

Describing eigenvectors as minimizing moment of inertia can be related to their more familiar characterization as maximizing variance if we consider orientational data to include not only single vectors, or points on the unit sphere, but also their projections onto the opposite hemisphere. Given all such points, the first eigenvector again can be thought of as maximizing variance. However, if one focuses on a single cluster of data without projection, the first eigenvector has an orientation similar to the *mean* orientation of the cluster (as determined by vector addition). The second eigenvector then indicates the direction of greatest spread *within* the cluster, while the third eigenvector is a direction of lesser variance. The eigenvalues corresponding to each eigenvector are negatively correlated with the moments of inertia of their respective eigenvectors, and are scaled to sum to 1. Watson (1966) and Koch and Link (1971, p. 142-146) give guidelines for interpreting different patterns in the relative magnitudes of eigenvalues that emerge from variously structured data sets.

Depending on the number or particular orientation of poles or axes in the data set, not all of the above statistics may be calculable. If some have not been calculated, it does not necessarily imply that there is something wrong with the input data; the data may simply have a structure that is not compatible with the particular descriptors calculated here. Exit the "Statistics" command by pressing **Q** or ⟨**Enter**⟩.

R — Rotate

This command rotates all c axes, a axes, face poles, and best-fit face poles in memory by a specified number of degrees about a specified axis of rotation. Enter the trend and plunge of an axis of rotation and the number of degrees of rotation, in decimal notation. The sign of the rotation angle follows the right-hand rule; positive angles rotate the data clockwise when looking from the center of the sphere outward along the axis of rotation, while negative angles rotate the data counterclockwise. Once data are rotated, the program automatically returns to the Graphics Menu. The annotation "rot'd" is added to the listing of the current data file, and the "Display" command is then available to display the rotated data. To cancel this command without completing a rotation, press ⟨**Enter**⟩ without inputting a numerical value.

Rotation of data is useful for transforming data from one coordinate system to another. For instance, in work on stylophoran homalozoans (Fisher, 1982; Fisher and Cox, 1987), an anteroposterior axis often makes the best choice for a primary anatomical reference axis, because it is easiest to align with the phi axis, but this results in stereograms that represent highly nonstandard anatomical orientation. We therefore rotate CALCAXES output to represent applicable anatomical conventions. In a similar fashion, data collected in a standard orientation based on intrinsic plate landmarks may need to be transformed to a whole-organism reference frame. This can be done by determining the required rotation and then applying this rotation through the "Rotate" command from CALCAXES' Graphics Menu. In the general case of two independently defined reference frames, two separate rotations are required to bring the reference frames into coincidence (MacConaill and Basmajian, 1969).

After the rotation command has been employed, an additional line, "U — Undo rotation 1", is added to the Graphics Menu. With each "Rotate" command that is executed, the rotation number is increased by one. Choosing the "Undo rotation" command (type **U**) re-rotates all

data about the most recently specified pole of rotation, through the same angle as the most recent rotation, but in the opposite direction. This new rotation affects all data currently in memory, even if some of the data were read subsequent to the last "Rotate" command. If several rotations were applied to the data, repeating the "Undo rotation" command will undo them in reverse sequence, undoing recent rotations before earlier ones. While any number of rotations can be applied to a data set, only the ten most recent rotations are retained by the "Undo rotation" command. After a rotation is undone, the prefix "Unrot'd" is added to the listing of the current data file. If the current data set is cleared from memory by using the "Clear" option within the "File read" command, all rotations available to the "Undo rotation" command are also cleared, and the "Undo rotation" command will not appear in the Graphics Menu until a new "Rotate" command has been issued.

M — Merge

This command implements rotation in a special context designed to combine two different groups of observations, each made on the same specimen, but with the specimen mounted in different orientations. When a specimen is mounted on the goniometer in its standard orientation, some skeletal elements may not be exposed well enough to allow observation of the three mutually nonantipodal face poles needed to calculate axis orientations. Our solution to this problem is to measure as many elements as possible in the standard orientation, then remount the specimen on the goniometer in an orientation in which the formerly obscured elements are better exposed. We then reobserve some of the elements that were measured in the standard orientation, in addition to observing the new elements to be measured. This results in two sets of coordinate values. The first set is recorded in the standard coordinate system, but the second set is recorded in a coordinate system that may initially have only an imprecisely determined, or even an undetermined, relation to the first. This is in part because the orientation for collecting the second set is intended to maximize visual access to new portions of the specimen rather than optimize the alignment of any anatomically defined reference axis. More to the point, however, goniometer design allows greater precision in measuring orientations of crystallographic features than in aligning morphologically recognized features. Duplicate measures of crystallographic features are therefore more effective reference axes for calculating the relation between the two coordinate systems involved in this problem than would be measured orientations of anatomical features. The goal of the merge procedure is to determine a transformation that will express the observations made in the unstandardized coordinate system in terms of the standard coordinate system. In principle, the duplicate records used to determine this transformation could be either face pole observations or crystallographic axis orientations calculated from them. However, even a small region of a specimen generally displays face poles in three or more orientations, and keeping track of these in two different specimen orientations (each of which may provide access to a different complement of faces) can be difficult. We therefore use only c axes (each readily attributable to an anatomical region) as duplicate features, although the transformation computed is eventually applied to all unstandardized coordinate values.

The "Merge" command performs a least-squares fit that as nearly as possible superimposes the unstandardized duplicate c axes (as a group) on their standardized counterparts, by minimizing the sum of the squared values of the angles between corresponding c axes. It then determines a pair of rotations that will accomplish this same reorientation more directly, and performs these rotations on all unstandardized coordinate values. The merge procedure can succeed using as few as two duplicate axes, but in general it is recommended that four or more different c axes be calculated in both orientations. Up to ten duplicate axes can be used at one time to merge data. The "Merge" command assumes that all coordinate values recorded in the standardized coordinate system precede all unstandardized coordinate values in the data file.

As mentioned earlier, collection of data in Mode 2 (the mode in which data subjected to merging are likely to have been collected) offers the opportunity to record standardized and

unstandardized orientations of an anatomical reference axis (the primary, the secondary, or some other). This anatomical reference axis guides the program during the least-squares fit by helping to locate homologous ends of c axes. All c axes in the standardized and unstandardized data sets are projected to lie at an acute angle to their set's anatomical reference axis. If c axes and the anatomical reference axis were located without error, this would ensure that the alignment procedure was attempting to match the same ends of c axes in both data sets. In practice, however, many conceivable anatomical reference axes are not precisely measurable on the goniometer, and all axes are located with some measurement error, so the program permits up to about 30° error in estimating anatomical reference axis orientations.

On issuing the "Merge" command, the screen displays a numbered list of sample names in the file. The user should note the numbers labelling all duplicate samples (each of which has its own calculated c axis), and should also note the label of the first unstandardized sample in the data set. These labels are entered at the appropriate prompt: duplicate samples with standardized data first, then corresponding unstandardized samples (in the same order as used for the standardized samples), and then the label for the first unstandardized sample. Labels can be entered individually, with each number followed by an ⟨**Enter**⟩, or series of consecutive samples can be indicated by entering the first and last numbers in the series, separated by a hyphen (e.g., **3-7**) and followed by an ⟨**Enter**⟩. After the label for the last standardized sample has been entered, the ⟨**Enter**⟩ key must be pressed again to cue the prompt for unstandardized data. To cancel the "Merge" command, press ⟨**Enter**⟩ without inputting a numerical value, when first prompted for a given type of data.

The "Merge" command will probably be used most often on data from a single file, but it can handle data read into memory from multiple files. Any single issue of the command, however, can only handle data collected in one standard and one nonstandard orientation. The program searches the current files to find one that contains two different anatomical reference axis orientations and then uses the first such pair encountered to assist in the merge operation. If no anatomical reference axis orientations are found, the user is prompted for the approximate trend and plunge of an anatomical reference axis in standard and then in nonstandard orientation. If more than one file contains anatomical reference axis orientations, or if a file contains more than two different reference axis orientations, these additional orientations (i.e., beyond the first two in the same file) are ignored. It is important to note in this context that the "Rotate" command does not affect anatomical reference axes. Caution should therefore be used when merging data that have been rotated or that have been read from several different files. To avoid confusion in specifying anatomical reference axes, the user can set the "Anatomical axes" option (type **A**) under the "Adjust settings" command (see below) to allow manual entry of appropriate anatomical reference axis trends and plunges. The program then displays the trends and plunges of the standardized and unstandardized anatomical reference axis orientations used in the merge procedure, allowing the user an additional check on the program's operation.

When selecting c axes for duplicate expression in the standardized and unstandardized coordinate systems, the user should be aware that c axes that are nearly perpendicular to the anatomical reference axis used for guiding the fit are not ideal, because it is difficult to determine which ends of these axes are homologous between the two data sets. Duplicate records from several different skeletal elements reduce the chance that all duplicate c axes will fall into this category. When faced with an inauspiciously located duplicate axis, the program selects a provisionally homologous end, based on its relation to c axes whose ends have less ambiguous homologies. The program also issues warnings or cautionary statements if the data suggest potential difficulties during the procedure. After homologous ends of axes have been identified, the program rotates the set of unstandardized duplicate axes to coincide with the set of duplicates in standard orientation. The program reports the minimum deviation found between the two sets of axes, and an estimate of the average deviation between duplicate axes. Typically, superimposition of duplicate c axes will have been approximated through a long

series of rotations, but the program then calculates two rotations that are together equivalent to the foregoing series and can be applied to all the unstandardized data to bring them into standard orientation. If the calculations are successful, these rotations are displayed on the screen and automatically applied to the (unstandardized) data set. The results can be viewed by returning to the Graphics Menu and using the "Display" command.

The estimated error between duplicate axes calculated during the least-squares fit should be comparable to the measurement error for individual axes in the data set. If the estimated deviation is larger than expected, it may indicate an error in specifying comparable axes between the standardized and unstandardized data sets. Alternatively, it might indicate an error in specifying an anatomical reference axis. For example, selecting opposite ends of the anatomical reference axis in each data set will cause the program to attempt to align standardized duplicate axes with the projections of their corresponding unstandardized axes. Typically, a set of three or more axes cannot be made to align perfectly with its projection using rotations alone, so larger than normal deviations will result, and a stereogram of the merged data will show that the duplicate axes mirror each other instead of corresponding in orientation. Repeating the merge procedure on the original data set but entering the projection of one of the anatomical reference axes (i.e., adding 180° to the trend and changing the sign of the plunge) should yield properly merged rather than mirrored data, and a correspondingly lower estimated deviation.

P — Print/Plot

This command produces paper copies of stereograms. It writes files in HP-GL/2 graphics language, which can be printed or plotted on compatible printers and plotters. This command can be canceled by typing **Q** or ⟨**Enter**⟩.

Printer output. Typing **L** from the "Plot to:" menu turns on laser printing mode. In this mode, CALCAXES formats output for a Hewlett Packard LaserJet III printer. The user can send output directly to an attached printer by pressing ⟨**Enter**⟩ or entering **PRN** as the filename to receive data. Alternatively, the user can create a file on disk to copy to a printer later. The LaserJet output uses small, solid dots to indicate orientations on the lower hemisphere; open circles indicate orientations on the upper hemisphere. If the program's default settings are used, originally observed face poles are projected to the lower hemisphere for printing (see the "Face pole display" option in the "Adjust settings" command, below, for the effects of changing this setting).

Plotter output. Typing **P** from the "Plot to:" menu turns on plotting mode, in which CALCAXES creates a file containing commands for an HP 7550 plotter. The plot description file should be readable by any plotter compatible with HP 7550 plotter format. As with printing, the program's default is to project originally observed face poles to the lower hemisphere for plotting. The upper and lower hemispheres are differentiated by open and closed circles. Designating different pen colors will also make data in the two hemispheres more readily distinguishable.

W — Write to file

This command writes the trends and plunges (in decimal notation) of face poles, *c* axes, best-fit face poles, and *a* axes (i.e., all data currently in memory) to a file of the user's choosing. It is particularly useful for saving data after they have been projected, rotated, or merged. Data for each sample (i.e., crystal) are preceded in the data file by a line containing the specimen name and a line containing two numbers: 999.00 (a false phi offset value) and the number of face poles. Unlike normal CALCAXES files, files created by the Graphics Module do not include each face pole's original goniometer readings or deviations. Files written by the Graphics Module also differ from other CALCAXES files in that they never contain trends and plunges of anatomical reference axes. The Graphics Module can read either type of file,

or files containing combinations of output of both types, without difficulty. To cancel this command, press ⟨**Enter**⟩ without inputting a filename.

Changing the default program setting of the "Data format" option in the "Adjust settings" command (see below) from CALCAXES format to general data format alters the action of the "Write to file" command. When CALCAXES is set for general data format, the "Write to file" command outputs only c axes (in decimal notation), one trend and plunge per line. No face poles, a axes, or phi offset values are sent to file.

A — Adjust settings

This command can be called from the Main Menu or the Graphics Menu. The effects are identical when called from either point in program operation. The "Adjust settings" command lets users alter several default settings for the display of data on the screen and the treatment of data in the program. With it the user can reset the proportions of the screen display on the monitor, select different colors for text, the screen background, the stereogram, and data points, and modify the treatment of data as they are read into and written from the program. These modifications can be saved in a configuration file (see below), which will automatically apply them in future sessions. To cancel this command, press **Q** or ⟨**Enter**⟩.

Adjust stereonet. The "Calculate appropriate factor" and "Enter a new factor" commands adjust the screen display so that the stereogram shown on the computer screen is circular rather than oval. These commands compensate for differences in screen dimensions and pixel shape on different monitors by letting the user enter a factor by which width is multiplied relative to constant height. The "Calculate appropriate factor" command (type **C**) calculates the appropriate factor after asking the user to measure and enter the height and width of a figure on the computer screen (in any units, as long as they are the same for both dimensions). Once the proper factor is known, the "Enter a new factor" command (type **E**) can be used to enter it directly, rather than recalculating it each time. Better still, if a configuration file is saved (see below), the new factor will be recalled automatically each time the program is run.

Change program settings. The current settings for each of the five program options are highlighted beside each option. The "Literal input" (type **L**) option controls the treatment of c axes as they are first read from a data file. By default, the Graphics Module reads into memory and displays the orientations for all axes just as they are expressed in the data file. The two ends of a c axis are equivalent, however, and users are frequently interested in evaluating the clustering of axes. CALCAXES will therefore optionally examine all c axes as they are read from a data file and project axes when necessary so that all c axes lie at acute angles to the first c axis in memory. When projected, some c axes may show up in the upper hemisphere even though all c axes in the original data file were reported in the lower hemisphere. Pressing **L** toggles between activating and deactivating this projection convention. Deactivating projection allows the program to again read and display c axes literally.

The "Face pole display" (type **F**) option influences the projection of originally observed face poles during onscreen display and printing or plotting. Face poles are read and held in memory exactly as they appear in the data file, but to aid in assessing clustering, CALCAXES by default displays, prints, and plots the lower hemisphere projections of all face pole observations rather than the actual observations. Using the "Face pole display" option toggles between this default projection and an alternative, the display, printing, and plotting of the actual face pole orientations held in memory. Setting the "Face pole display" option to display face pole orientations as written in the file also makes the temporary and permanent projection options of the "Display" command available for use on face poles.

CALCAXES is ordinarily set to read and write data having the format of normal CALCAXES files written by the Calculation and Graphics Modules. To increase the program's applicability to a wider range of tasks, the "Data format" option (type **D**) toggles between the default CALCAXES format and a more general format consisting of one trend and plunge (in decimal

notation) per line. When the program is set for general data format, the "File read" command reads one trend and plunge (separated by a space) from each line of the data file. All data are treated as *c* axes for screen display, printing, plotting, statistical analysis, and merging. The *a* axes and best-fit face poles that would normally be associated with each *c* axis are assigned arbitrary values of 0° trend and 90° plunge, initially placing them at the center of the stereogram (the "Rotate" and "Merge" commands will move them from their initial orientation). Because of this arbitrary assignment, all data types other than *c* axes should be ignored in subsequent commands. Furthermore, data read in general data format should not be written to file in CALCAXES format, because the data on *a* axis and face pole orientations saved in CALCAXES files would merely reflect the arbitrary assignment. Writing data in general format (whether or not the data were initially read in general format) will output all *c* axes to a file, one trend and plunge per line. No *a* axes, face poles, or best-fit face poles will be sent to file.

The "Anatomical axes" option allows the user to enter orientations for anatomical reference axes manually even if reference axes have already been read from a data file. This is useful if rotations have been performed on the data before using the "Merge" command, or if files containing several anatomical reference axes have been read, and the user is uncertain which orientations will be applied to the data. Pressing **A** toggles between entering reference axes manually in the "Merge" command and using the first two anatomical reference axes read from a single data file.

The "Input notation" option (type **I**) lets the user choose the notation in which data are entered in the Calculation Module. The appropriate setting for this option depends on the goniometer used to gather data, since some goniometers report readings in sexagesimal notation (degrees and minutes of arc) whereas others display degrees of arc and decimal fractions of degrees. For sexagesimal notation, data are entered in the format: degrees.minutes (e.g., 211° 20′ is entered as **211.20**, and 10° 07′ is entered as **10.7** or **10.07**). For decimal notation, data are entered as a decimal number (e.g., 128.05° is entered as **128.05**, and 47.90° is entered as **47.9** or **47.90**) with units of degrees of arc assumed. The "Input notation" option affects data entry in the Calculation Module only; the Graphics Module accepts only decimal input. To avoid confusion, CALCAXES indicates which notation is expected when prompting the user for data entry.

Original goniometer readings are displayed on the screen and printed in their original notation, but in order to maintain standardization of data files, the Calculation Module writes all original goniometer readings to file using sexagesimal notation. All calculated values (trends and plunges of face poles in standard orientation, *c* axes, *a* axes, and best-fit face poles) are printed, displayed, and saved to file in decimal notation. Similarly, the "File read" command expects original goniometer readings to be in sexagesimal notation but all other data to be in decimal notation. In accordance with this convention, the trends and plunges in data files in general format must use decimal notation.

Reset colors. The "Reset colors" command (type **R**) permits the selection of different colors for text (both emphasized and normal), background, and a variety of different data points (upper hemisphere *c* axes and emphasized text are the same color). This is useful if a monitor's color settings tend to make some colors difficult to distinguish from others. The text for each type of entity is displayed in the current color. Each color has an associated number, which is also displayed. After selecting an entity type whose color is to be changed, the user is prompted to enter a new number. Numbers 0 through 15 produce different colors on EGA and VGA displays, but colors shown by entities when executed in graphics mode (the screen mode in which stereograms are drawn) may vary from the colors shown in text mode (the screen mode in which the menu options for the "Reset colors" command are displayed), and some colors that are distinct in one mode may be identical in the other. Since monitors and graphics cards vary, users may have to experiment to find acceptable color combinations. After viewing the effects of assigning different numbers to the various types of entities, the user

is asked to confirm resetting to the new color scheme. Type **Y** to put the changes into effect, or **N** to retain the previous color settings.

Save configuration. This command saves the current screen colors, screen width to height adjustment factor, and program options to a configuration file, "calcaxes.cfg". Each time CALCAXES is run, the program looks for the configuration file in the subdirectory in which CALCAXES is located. If the configuration file is found, CALCAXES automatically applies the settings saved there. Otherwise, CALCAXES notifies the user that the program's default settings are being used. To restore a modified configuration file to the default settings, delete the file, start CALCAXES again, and save a new configuration file.

The configuration file is an ASCII file containing a single line of 17 numbers. The first eleven integers are color codes for the stereonet outline and tickmarks, lower hemisphere *c* axes, upper hemisphere *c* axes, lower hemisphere *a* axes, upper hemisphere *a* axes, lower hemisphere best-fit face poles, upper hemisphere best-fit face poles, text color, and screen background color. The next number in the file is the factor for adjusting stereogram display, and the final five integers are codes indicating which of the "Literal input", "Face pole display", "Data format", "Anatomical axes", and "Input notation" program options are put into effect.

Q — Quit
This command quits the Graphics Module, returning the user to the Main Menu.

Final note
If the computer on which CALCAXES is run does not support Hercules, CGA, EGA, VGA, AT&T 400 line, IBM 3270 PC, or IBM-8514 graphics, the three commands that display stereograms on the monitor will not be available. These are: the "Label group" command; the "Display" command; and the "Calculate appropriate factor" command under "Adjust stereonet" in the "Adjust settings" menu. Calling any of these commands without acceptable graphics capabilities will cause the program to abort. All other functions, including the reading, rotating, merging, and printing of data and the writing of printer, plotter, and data files, can be performed regardless of graphics capabilities.

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