

1 **Revision 1**

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3 **EXCALIBR to EXCELIBR and the Optical Orientation of Minerals: Correcting the Optical Orientation of**
4 **Clinoamphiboles.**

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Abstract

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11 The crystallographic orientation of $C 2/m$ amphiboles has been depicted incorrectly since the
12 standardization of amphiboles in $C 2/m$. Texts citing the early optical work on amphiboles reference structures
13 drawn in the $I 2/m$ cell, for which the optical orientation is correct. When $C 2/m$ became the standard space group,
14 the optical orientation, (hkl), and crystallographic axes depicted in crystal form drawings were never revised. Using
15 the methods outlined by Gunter and Twamley (2001) combined X-ray and optical methods on single crystals of
16 amphiboles reveal the discrepancy between axes. In the correct orientation of a typical $C 2/m$ amphibole, the
17 physical optical orientation should have never changed from its position outlined in the Tschermak setting as shown
18 in Ford and Dana (1932), however, the crystallographic axes and (hkl) should have changed to accommodate the
19 difference between the $I 2/m$ cell and the $C 2/m$ cell. This error may perpetuate a misunderstanding between the
20 crystallographic setting and optical orientation of clinoamphiboles, which is an important relationship for
21 orientation-dependent analytical methods. Enclosed in this study is the correction of crystallographic axes for crystal
22 form drawings for $C 2/m$ amphiboles, along with an outline of methodology and updates to the spreadsheet
23 EXCELIBR. The methods applied in this study utilize relationships between crystallographic and optical vectors and
24 include an addendum to those presented by Gunter and Twamley (2001), which is applicable to arbitrary reference
25 positions on spindle stages.

26 **Keywords:** optical orientation, clinoamphiboles, crystallographic setting, EXCELIBR, EXCALIBR

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Introduction

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Inconsistencies in the crystallographic settings of minerals could be a source of confusion when depicting crystal form drawings, such as those found in Nesse (2013), Deer et al. (2013), and Tröger and Bambauer (1979). Many of the crystal depictions are based on data collected during, or even prior to the early years of X-ray crystallography. Discrepancies in the optical orientation of minerals may be due one of two circumstances. The first, is rearrangement of the orientations of the crystallographic axes **a**, **b**, and **c** since the original characterization of the optical and crystallographic axes. This scenario is unlikely to lead to errors in the literature since the old choice of axes were inherited to suit the space group of the X-ray structure solution. An example of this is with forsterite, where space group is *Pbnm*, though if forsterite was solved under the current standards, the space group would be *Pnma*, which would be the same cell as *Pbnm*, but with the definition of **b** and **c** switched. The second, is the use of an entirely different lattice from the original characterization of the mineral. This scenario is far more likely to result in discrepancies, particularly with monoclinic and triclinic minerals, since the original axes may have been selected prior to X-ray diffraction, and there can be multiple similar lattices centered in different orientations. In the case of mesolite, its structure was originally solved in *C2*, and since the two-fold axis of monoclinic minerals must be the **b**-axis, **b** corresponded with Y optical vector, which was also parallel to the long-axis of the form of the crystal (Deer et al. 1967). Later, mesolite was solved in larger cell but of higher metric symmetry, which was in the *Fdd2* space group where **a** = X, **b** = Z, **c** = Y (Gunter and Ribbe 1993).

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In the case of *C 2/m* clinoamphiboles, originally, two crystallographic settings were used to denote the symmetrical relationships between crystal faces. Though this is a correction of the optical orientation of clinoamphiboles, it is important to note that the error is in the depiction of their crystallographic setting.

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Methods

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Crystallographic orientation was collected with a single crystal X-ray Diffractometer (SC-XRD) using a Bruker SMART XRD system with an APEX1 detector (Bruker 2014). Diffraction data were processed and indexed

57 for lattice type and orientation with the Apex3 software suite. Principal optical vectors were located using the
58 spindle stage methods, along with the program EXCELIBR (Bloss 1981; Steven and Gunter 2017). The method
59 used to relate crystallographic axes collected on the SC-XRD to the coordinate system used on the polarized light
60 microscope (PLM) is outlined by Gunter and Twamley (2001). To summarize, the orientation matrix of a $C 2/m$ cell
61 in reciprocal space is converted to the direct orientation for the **a**, **b**, and **c** axes by taking the cross-product of the
62 orthonormal reciprocal axes to the direct crystallographic axes: $\mathbf{a} = \mathbf{b}^* \times \mathbf{c}^*$, $\mathbf{b} = \mathbf{c}^* \times \mathbf{a}^*$, $\mathbf{c} = \mathbf{a}^* \times \mathbf{b}^*$. An accurate
63 orientation matrix is listed in the Apex3 software suite after integrating X-ray frames and is also written into the p4p
64 file. The cartesian coordinates for **a**, **b**, and **c** on the SC-XRD are then transformed to match their coordinates in the
65 system used on the PLM. The correct transformation of coordinates is verified with orthorhombic minerals, where
66 the optical vectors coincide with the crystallographic axes.

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EXCELIBR

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70 EXCELIBR is a Microsoft Excel spreadsheet that determines the orientation of the optical indicatrix of
71 crystals on a spindle stage using numerical methods, like those used in the program EXCALIBR (Steven and Gunter
72 2017). The version of EXCELIBR used in this research is designed to locate crystallographic axes and optical
73 vectors on the same crystal, using spindle stage methods and SC-XRD. The current version of EXCELIBR includes
74 new calculations to relate principle optical vectors and crystallographic axes, particularly for those of monoclinic
75 minerals (Figure 1). Previous versions of EXCALIBR and EXCELIBR output spherical coordinates, cartesian
76 coordinates, and a stereogram of the location of axes to orient principle vibration directions either North-South, or
77 East-West with lower polarizer. However, the cartesian plot depends on the readout convention of both the PLM
78 stage, and the spindle stage or whether the numbers increase clockwise, or counterclockwise. Though the readout
79 convention of the PLM stage is accommodated for in EXCALIBR and previous versions of EXCELIBR, the spindle
80 stage readout is not. This does not affect the alignment of vectors East-West or North-South, but it does affect the
81 cartesian output of where vectors lie in space. The new standard output of EXCELIBR plots vectors in direct space,
82 and outputs cartesian coordinates in direct space, which depends on whether the PLM stage readout increases
83 clockwise or counterclockwise, and if the spindle stage increases clockwise or counterclockwise when viewing
84 towards the goniometer mount surface. This feature eliminates one potential step when converting the X-ray

85 coordinate system to the PLM coordinate system, since not all spindle stage readouts increase clockwise.
86 EXCELIBR also only plots upper hemisphere vectors, so it will project any lower hemisphere vectors to the upper
87 hemisphere, and will rename axes accordingly (i.e., a lower hemisphere **a**-axis will be projected as **-a** in the upper
88 hemisphere). EXCELIBR and its supplemental guide is available in the Mineralogical Society of America's
89 Monographs page.

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Converting Coordinate Systems

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93 As mentioned above, the cartesian coordinates of the SC-XRD are converted to match the coordinate
94 system used on the PLM. Specifically, the cartesian basis runs in the orientation shown in Figures 2a and 2b. The
95 goniometer mount for the PLM stage is depicted in the zero position for both the spindle axis and PLM stage. At the
96 zero position, a reference notch is denoted relative to the cartesian basis and resembles the line from the spindle axis
97 to the mount pin as the long line, and direction the goniometer points at zero as the short line. This is to
98 accommodate differences in the location of the notch on the spindle stage, since the notch position may be
99 adjustable or manufactured differently among spindle stages. The goniometer mount for the SC-XRD is in the
100 mount position, which reads zero for 2θ , ϕ , and ω , but with a fixed χ of 54.8° . The reference notch on the SC-XRD
101 is shown in the restored zero position on the SC-XRD relative to the cartesian basis. In this instance, after
102 superimposing the reference notches of the PLM and SC-XRD, the conversion to the basis of the PLM is $x = -z$, $y =$
103 $-y$, $z = -x$.

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Methods of Locating Crystallographic Axes on a Spindle Stage

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107 In addition to locating crystallographic axes by transforming SC-XRD coordinates, crystallographic axes of
108 some monoclinic minerals may also be located using the spindle stage. For example, with monoclinic amphiboles, a
109 crystallite is commonly elongate on the line of the **c**-axis. However, for a randomly oriented crystal on a spindle
110 stage, it is challenging to discern when the long axis of the crystal is in the plane of the stage when viewing in the
111 PLM, and therefore, true orientation of the **c**-axis is challenging to find. One solution is to find any two intersecting
112 planes that do not intersect the **c**-axis, $(hk0)$, $(0k0)$, or $(h00)$. The cross-product of any two planes that do not

113 intersect the **c**-axis will intersect along a vector that is parallel to the **c**-axis, and in the case of tremolite-
114 ferroactinolite amphiboles, the optic normal is the orthogonal vector to the optic axial plane which is parallel to
115 (010), so indexing any (*hk0*) or (*0k0*) results in the solution of **c** in EXCELIBR (Figure 3). In the example from
116 Figure 3, the **c**-axis is parallel with the (*hk0*), even though it is tilted down out of the plane of the stage. After
117 indexing the (*hk0*) from Figures 3 and 4a, the cross product of the coordinates of the optic normal and the orientation
118 of the (*hk0*) results in the calculated orientation that will align the **c**-axis East-West and in the plane of the stage
119 (Figure 4b). Calculations for the method outlined above are contained within the program EXCELIBR (Steven and
120 Gunter 2017).

121 After locating the **c**-axis, EXCELIBR will solve for the **b**-axis by taking the cross-product of **c** and each of
122 the principle vibration directions. With monoclinic minerals, two of the cross-products will be the same orientation
123 and thus will be the **b**-axis. In the case of tremolite-ferroactinolite amphiboles, $Z \times c = X \times c$, and therefore,
124 $b = Y$.

125 The remaining axis to find is **a**, and, admittedly, the **a**-axis of clinoamphiboles cannot be directly located
126 with the spindle stage methods, since there is no plane of reference in a crystallite for the **a**-axis. However, since the
127 **a**-axis also lies in the orthogonal plane to **b**, the **c**-axis can be rotated by the common β angle of amphiboles of
128 104.7° along the optic axial plane. Then, the problem is that the rotation direction is unknown. At this point, the
129 method would then rely on crystal form drawings for where the **a**-axis should be relative the optical vectors and the
130 **b** and **c**-axes. In the published crystal form drawings of amphiboles in the tremolite-ferroactinolite series, the **a**-axis
131 is $\sim 104.7^\circ$ from **c** and normal to **b** rotated towards *Z*, as is depicted in Figure 5. When rotated in this way, the **a**-axis
132 of the *C 2/m* XRD orientation does not align with the spindle stage orientation solution. However, when rotated the
133 opposite direction, shown in Figure 6, the **a**-axis closely coincides with the SC-XRD orientation solution, which is
134 what is given for the spindle stage orientation solutions for actinolite samples given in Table 1. The probable
135 explanation for this inconsistency, is that the crystallographic setting depicted in crystal form drawings of
136 clinoamphiboles, have drawn the crystallographic axes and (*hkl*) in the *I 2/m* setting, despite listing *C 2/m* as the
137 space group. This would mean that Tschermak's setting is parallel to the *I 2/m* setting which is closely related to the
138 axes used for *C 2/c* pyroxenes (Figures 5 and 7).

139 The results of this method are compared to the X-ray orientation for **a**, **b**, and **c** with a residual angle to
140 demonstrate the efficacy of the method. For the clinopyroxene samples, the same method was applied to locate the **a**

141 and **c**-axes which matches the x-ray orientation. For the orthopyroxene sample, the **a**, **b**, and **c**-axes coincide with
142 the optical vectors, so the crystallographic axes on the spindle stage were directly located by the optical solution.

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144 **Crystal Form**

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146 Since the discrepancy in clin amphiboles is in the crystal axes, nothing changes in the crystal form of
147 amphiboles, however, the labeling of some of the (*hkl*) is different. In a typical clin amphibole, the crystal form is a
148 prism terminated by a clinodome, which is formed by the *r* faces Figure 8. Note that the setting of axes for
149 clinopyroxene and clin amphibole in Figure 8 are drawn parallel and are both labelled in their respective Tschermak
150 settings. In the Tschermak setting, the *r* faces are (011) and *p* face is (-101) (Ford and Dana 1932). In the alternate
151 setting, the *r* face is (-111) and the *p* face is (001) (Ford and Dana 1932). Experimentally, a growth crystal of a
152 tremolite was selected to verify the crystal faces with the SC-XRD, and the clinodome was found to be terminated
153 by (-111) and (-1-11) shown in Figure 9.

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155 **Discussion**

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157 The combined use of the spindle stage methods, and SC-XRD used in conjunction with EXCELIBR allow
158 for an unambiguous determination of the location of optical vectors, and crystallographic vectors for a particular
159 lattice setting. These methods may be used to check the crystallographic settings of minerals, and orient crystals for
160 orientation-dependent analytical methods. The spindle stage methods outlined in the research offer a convenient way
161 of locating optical vectors and reference axes based on crystal morphology, which also establishes handedness for
162 the reference axes of monoclinic crystals. The discrepancy in the crystallographic axes of monoclinic amphiboles,
163 likely stems from the adoption of the *I*2/*m* lattice setting.

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165 The choice of axes for monoclinic amphiboles dates back to the work of Tschermak in the late 1800s,
166 before X-ray crystallography (Tschermak 1897). Tschermak's setting is one of two crystallographic settings used in
167 the early years of crystallography for amphiboles and is perhaps the easiest setting to visualize with the common
168 crystal form of amphiboles, shown in Figure 8. However, Ford and Dana (1932) noted that some authors used an
alternate setting where the *p* crystal face is marked as (001) rather than (-101) in the Tschermak setting (Ford and

169 Dana 1932). In the Tschermak setting, clinopyroxenes and clinoamphiboles are indexed so that their crystal axes and
170 crystal faces coincide. Later, Warren (1929) published the first X-ray structure solution for a monoclinic amphibole,
171 which was for tremolite. The structure was solved in the $I2/m$ space group with an acute β angle, which was used so
172 that the crystallographic axes, relative to the structure, would coincide with the crystallographic axes of diopside,
173 also with an acute β angle, solved in $C2/c$ (Warren and Bragg 1928). The choice of axes for $C2/c$ pyroxenes is
174 depicted in Figure 8, which is the setting parallel to those used by Tschermak, and besides a 180° rotation of the **b**
175 and **a**-axes, the obtuse β setting, the axes as used by Warren and Bragg has not changed for $C2/c$ pyroxenes since
176 (Warren and Bragg 1928).

177 One discrepancy of the setting of clinoamphiboles, is in Strunz (1966), where the lattice of clinoamphibole
178 is stated to be $C2/m$, yet the Tschermak setting is adopted. As stated above, relative to their structures, the $C2/c$
179 lattice setting of clinopyroxenes is parallel to the $I2/m$ lattice of clinoamphiboles, which coincides with the
180 Tschermak setting. Whittaker and Zussman (1961) had discussed the relationship between the $I2/m$ of
181 clinoamphibole, and the $C2/c$ of clinopyroxene, as well as the confusion surrounding the choice of axes for
182 clinoamphibole since both lattices setting share similar cell parameters. Figure 10 depicts the relationship between
183 the I and C monoclinic lattice settings as described by Whittaker and Zussman. Despite this, several authors adopted
184 the Tschermak setting, presuming the axes were parallel to the axes of the $C2/m$ lattice setting. Since about 1961,
185 clinoamphiboles have all been solved in $C2/m$, which currently used as the standard centered monoclinic lattice.

186 Inconsistencies in crystallographic settings in reference literature are a demonstrable source of confusion if
187 Bravais lattice is not listed with the set of axes depicted. With accurate reference material, the methods listed above
188 allows a user to obtain the full crystallographic orientation of a $C2/m$ amphibole just by knowing orientation of the
189 c-axis and optical vectors. These relationships are helpful when orienting a large number of crystals for analytical
190 methods that depend on orientation, which is particularly useful if SC-XRD is not available.

191 Beyond the clinoamphiboles, inconsistencies in settings may still exist in depictions of other minerals.
192 Mesolite would have benefitted from investigating the optical setting as a possible crystallographic setting, since
193 principle optical vectors work as a reliable set of reference vectors for a crystal, though their orientation may depend
194 on composition in monoclinic and triclinic crystals. In contrast, the optical setting for scolecite deviates from any
195 translational lattice with orthogonal axes, and therefore the optical setting informs that the crystal system must be
196 monoclinic or triclinic. In one crystallographic setting, scolecite is nearly face-centered orthorhombic, belonging to

197 the nonstandard monoclinic *F1d1* lattice. When processing SC-XRD data from scolecite, the crystal would appear to
198 be face-centered orthorhombic until scaling the data, where large discrepancies in supposed symmetrically
199 equivalent intensity maxima arise. Additionally, when relating the orientation of the principle optical vectors to the
200 axes to the pseudo-orthorhombic cell, it is clear that the **b**-axis corresponds with the Z optical vector (Figure 11c),
201 while the X and Y optical vectors don't correspond with the other axes of the lattice, suggesting a monoclinic lattice.
202 Further, for crystallographers solving scolecite in the *Cc* space group, the correct C monoclinic lattice must be
203 centered for the best refinement results, since multiple C-centered monoclinic lattices can be centered to a crystal
204 that is nearly face-centered orthorhombic (Figure 11).

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Implications

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208 The methods listed above were compiled for projects involving orientation-dependent spectroscopic
209 methods, though they are also useful for rectifying inconsistencies in crystallographic settings in compilation
210 reference material. The relationship between the principal optical vectors and crystallographic axes are extremely
211 important for orientation-dependent spectroscopic methods, since anisotropic absorption behavior of light may be, in
212 part, analogous to anisotropic behavior of other wavelengths of electromagnetic radiation, such as visible light (Dyar
213 et al. 2002). For example, an X-ray absorption spectrum will depend on several variables including, bond
214 characteristics and chemical speciation, but importantly, will depend on the orientation of the vibration path of the
215 photon source through an anisotropic crystal. Therefore, in empirical studies of XANES spectra of mineral series, an
216 effort must be made to compare like-orientations. Anisotropic diffusion of halogens in apatite during Electron Probe
217 Microanalysis (EPMA) is a known source of analytical error in halogen count rate per beam exposure time (Stormer
218 et al. 1993). This can be partially mitigated by preparing oriented mounts such that the polished surface runs parallel
219 to the (100) plane of apatite, rather than the (001) plane, where there is more variation in count rate per beam
220 exposure time. The optical and crystallographic orientation of minerals mounted on a spindle stage allows a user to
221 prepare oriented grains or grain mounts of crystals for spectroscopic analysis. The updated version of EXCELIBR
222 includes calculations for relating crystallographic and principle optical vectors of crystals from single crystal X-ray
223 data and extinction data, which can be used for characterizing new minerals, or for minerals where the relationship
224 between the optic indicatrix and crystallographic vectors is unknown.

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227 1754268.

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References

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232 Bloss, F. D. (1981) The spindle stage: principles and practice. Cambridge University Press.

233 Bruker (2014) SADABS, SAINT, SMART, and SHELXTL. Bruker AXS Inc., Madison, Wisconsin.

234 Cameron, M., and Gibbs, G. V. (1973) The crystal structure and bonding of fluor-tremolite: a comparison with

235 hydroxyl tremolite. American Mineralogist, 58(9-10), 879-888.

236 Deer, W. A., Howie, R. A., and Zussman, J. (2013) An introduction to the rock-forming minerals (3rd ed., pp. 147-

237 171). London: The Mineralogical Society.

238 Deer, W. A., Howie, R.A., and Zussman, J. (1967) Rock-forming minerals: framework silicates (Vol. 4, p. 358).

239 John Wiley and Son. New York, N.Y.

240 Dyar, M. D., Gunter, M. E., Delaney, J. S., Lanzirotti, A., and Sutton, S. R. (2002) Use of the spindle stage for

241 orientation of single crystals for microXAS: Isotropy and anisotropy in Fe-XANES spectra. American

242 Mineralogist, 87(10), 1500-1504.

243 Ford, W. E., and Dana, E. S. (1932) A textbook of mineralogy. John Wiley & Sons (3rd ed., pp 571-573).

244 Gunter, M. E., Bandli, B. R., Bloss, F. D., Evans, S. H., Su, S. C., and Weaver, R. (2004) Results from a McCrone

245 spindle stage short course, a new version of EXCALIBR, and how to build a spindle stage. The

246 Microscope. 52(1), 23-39.

247 Gunter, M. E., and Ribbe, P. H. (1993) Natrolite group zeolites: Correlations of optical properties and crystal

248 chemistry. Zeolites, 13(6), 435-440.

249 Gunter, M. E., and Twamley, B. (2001) A new method to determine the optical orientation of biaxial minerals: a

250 mathematical approach. The Canadian Mineralogist, 39(6), 1701-1711.

251 Mottana, A., Rossi, G., Kracher, A., & Kurat, G. (1979) Violan revisited: Mn-bearing omphacite and

252 diopside. Tschermaks mineralogische und petrographische Mitteilungen, 26(3), 187-201.

- 253 Nesse, W. D. (2013) Introduction to Optical Mineralogy (4th ed., pp. 212-224). Oxford university press.
- 254 Palmer, D. (2015) CrystalMaker Software. CrystalMaker Software Ltd, Oxfordshire, England.
- 255 Steven, C.J., and Gunter M.E. (2017) EXCELIBR: An Excel Spreadsheet for Solving the Optical Orientation of
256 Uniaxial and Biaxial Crystals. *The Microscope* 65 (4), 147-152.
- 257 Stormer, J. C., Pierson, M. L., & Tacker, R. C. (1993) Variation of F and Cl X-ray intensity due to anisotropic
258 diffusion in apatite during electron microprobe analysis. *American Mineralogist*, 78(5-6), 641-648.
- 259 Strunz, H. (1966) *Mineralogical Tables*, 162 (p. 369). Mineralogical tables.
- 260 Tröger, W. E., and Bambauer, H. U. (1979) Optical determination of rock-forming minerals, Part I. English edition
261 of the fourth German edition by HU Bambauer, F. Taborszky and HD Trochim. Schweizerbartsche
262 Verlagsbuchhandlung, Stuttgart.
- 263 Tschermak, G. (1897) *Lehrbuch der mineralogie*. A. Hölder.
- 264 Warren, B. (1929) The structure of tremolite $H_2 Ca_2 Mg_5 (SiO_3)_8$. *Zeitschrift fure Kristallographie*. 72: 42-57.
- 265 Warren, B., and Bragg, W. (1928) The structure of diopside, $Ca Mg (Si O_3)_2$. *Zeitschrift fure Kristallographie*.
266 69: 168-193.
- 267 Whittaker, E. J. W., and Zussman, J. (1961) The choice of axes in the amphiboles. *Acta Crystallographica*, 14(1),
268 54-55.
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Figure Captions

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275 **Figure 1:** EXCELIBR tab for locating optical vectors and crystallographic axes of monoclinic minerals. The output
276 is for actinolite1, and includes the inputs in blue, and the output location of crystallographic axes using spindle stage
277 methods, optical orientation, and transformed X-ray orientation. The cartesian coordinates and plot are given in real
278 space so that the coordinate system of a SC-XRD can be directly converted to the microscope coordinate system.

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280 **Figure 2:** (a) Cartesian coordinate basis used on a SC-XRD. This example is of a fixed χ goniometer, and reference
281 notch is drawn in the restored zero position for the diffractometer. The reference notch resembles the line from the ϕ
282 axis to the mount pin as the long line, and direction the goniometer points as the short line in the restored zero
283 position. (b) The goniometer mount for the microscope stage depicted at the zero position for the spindle axis and
284 microscope stage. The reference notch is positioned relative to the cartesian basis and resembles the line from the
285 spindle axis to the mount pin as the long line, and direction the goniometer points at zero as the short line.

286

287 **Figure 3:** Representation of the clinoamphibole actinolite1 mounted on a spindle stage. For actinolite, the
288 intersection of the optic axial plane, and an $(hk0)$ forms a vector parallel to the **c**-axis. Indexing any two intersecting
289 $(hk0)$, $(0k0)$, or $(h00)$ may be used to locate **c**, for example, the (110) cleavage planes.

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291 **Figure 4:** (a) Microscopic view of actinolite1 of the position in Figure 3. An $(hk0)$, $(0k0)$, or $(h00)$ is indexed by
292 aligning the **c**-axis with the N-S crosshair even if it is plunging into the plane of the microscope stage. (b) The
293 calculated position of the **c**-axis aligned E-W and in the plane of the microscope stage after taking the cross product
294 of an $(hk0)$ and the coordinates of the optic normal, which is equivalent to $(0k0)$ for actinolite.

295

296 **Figure 5:** A stereogram, crystal structure, and crystal form of the $I2/m$ setting of a clinoamphibole. The stereogram
297 and crystal form drawing depict (hkl) , crystallographic axes, and optical vectors. Optical vectors are drawn in an
298 orientation similar to that of a typical tremolite. The internal crystal structure (solution from Warren, 1929) is drawn
299 viewing down the **b**-axis using the CrystalMaker software and, relative to their structures, is oriented in line with the
300 clinopyroxene structure in Figure 7.

301 **Figure 6:** A stereogram, crystal structure, and crystal form of a $C 2/m$ amphibole in the tremolite-ferroactinolite
302 series. The stereogram and crystal form drawing depict (hkl), crystallographic axes, and optical vectors. Optical
303 vectors are drawn in an orientation similar to that of a typical tremolite. The internal crystal structure (solution from
304 Cameron and Gibbs 1973) is drawn viewing down the **b**-axis using the CrystalMaker software, and, relative to their
305 structures, is oriented in line with the clinopyroxene structure in Figure 7.

306

307 **Figure 7:** A stereogram, crystal structure, and crystal form of $C 2/c$ pyroxenes. Optical vectors are drawn in an
308 orientation similar to that of a typical diopside. The stereogram and crystal form drawing depict (hkl),
309 crystallographic axes, and optical vectors. The internal structure (solution from Mottana et al. 1979) was drawn in
310 CrystalMaker, and, relative to their structures, is oriented in line with the clinoamphiboles from Figures 5 and 6.

311

312 **Figure 8:** The common crystal form of clinopyroxene with faces labeled in lettering form, axes and Miller indices
313 denoted using the C monoclinic lattice (left) and clinoamphibole with faces labeled in lettering form, axes and
314 Miller indices denoting faces in the Tschermak I monoclinic lattice setting (right).

315

316 **Figure 9:** Image of a portion of a growth crystal of tremolite. Crystal faces are indexed in the Apex3 software after
317 collecting the unit cell. The full growth crystal was cleaved in half on (110) for experimental purposes. The crystal is
318 a tremolite sample from Gouverneur talc mine, New York, and corresponds to the sample name actinolite2 in Table
319 1. Outside of the (110) cleavage face in the back, the crystal is bounded by growth faces and clinodome is
320 terminated by (1-1-1) and (11-1).

321

322 **Figure 10:** Depiction of the relationship between the centering of the C monoclinic lattice in bold, and the I
323 monoclinic lattice shaded in grey with axes denoted by subscripts for the C and I lattice settings, modified after
324 Whittaker and Zussman (1961).

325

326 **Figure 11:** Stereograms depicting the orientation solution for a scolecite crystal in a) the $F1d1$ lattice b) an incorrect
327 monoclinic C lattice centering where no optical vector corresponds with a crystallographic axis and c) the correct Cc
328 lattice where $b = Z$

329 Tables and Figures

330

331 **Table 1:** Tables of the converted XRD coordinates and the spindle stage coordinates of an orthopyroxene,
 332 clinopyroxene, and five clinoamphiboles. The spindle stage coordinates for the **a**-axis and **c**-axis of the monoclinic
 333 minerals are located using the method outlined in the text, and the difference in the coordinates are given as an angle
 334 on the right. The consistency in the orientations demonstrate the efficacy of relating crystallographic vectors
 335 between the spindle stage methods and X-ray orientation solution. Discrepancies for clinopyroxenes tend to be
 336 larger due to its high dispersion, which influences extinction measurements and ultimately the orientation
 337 determined from the optical solution.

338

orthopyroxene1

	X-ray Orientation				Spindle Stage Orientation			discrepancy (degrees)		
	-a	-b	-c		-a	-b	-c	-a	-b	-c
x	-0.2099	0.4383	0.8740	x	-0.2091	0.4437	0.8714	1.0	1.1	0.8
y	0.0580	0.8979	-0.4364	y	0.0402	0.8943	-0.4457			
z	0.9760	0.0408	0.2139	z	0.9771	0.0581	0.2048			

clinopyroxene1

	X-ray Orientation				Spindle Stage Orientation			discrepancy (degrees)		
	-a	b	-c		-a	b	-c	-a	b	-c
x	0.6061	0.0780	-0.9311	x	0.5911	0.0027	-0.9413	2.4	4.4	4.4
y	-0.4386	0.8630	-0.1159	y	-0.4126	0.8603	-0.1700			
z	0.6635	0.4992	0.3459	z	0.6931	0.5098	0.2918			

clinopyroxene2

	X-ray Orientation				Spindle Stage Orientation			discrepancy (degrees)		
	a	-b	-c		a	-b	-c	a	-b	-c
x	-0.1807	-0.1462	-0.9841	x	-0.1776	-0.1833	-0.9777	3.4	3.7	2.5
y	-0.2228	0.9693	-0.1629	y	-0.2801	0.9513	-0.2028			
z	0.9580	0.1978	0.0707	z	0.9434	0.2480	0.0550			

actinolite1

	X-ray Orientation				Spindle Stage Orientation			discrepancy (degrees)		
	-a	b	-c		-a	b	-c	-a	b	-c
x	-0.2999	-0.52	0.85	x	-0.3138	-0.5290	0.8427	2.4	2.8	1.1
y	0.95358	-0.19	-0	y	0.9471	-0.2324	-0.0268			
z	0.02756	0.83	0.53	z	0.0670	0.8162	0.5378			

actinolite2

	X-ray Orientation				Spindle Stage Orientation			discrepancy (degrees)		
	-a	-b	c		-a	-b	c	-a	-b	c
x	0.6448	-0.3191	0.8367	x	0.6906	-0.3266	0.7994	3.9	0.8	4.1
y	0.7260	-0.0287	-0.4778	y	0.6781	-0.0178	-0.5386			
z	0.2392	0.9473	0.2674	z	0.2514	0.9450	0.2661			

actinolite3

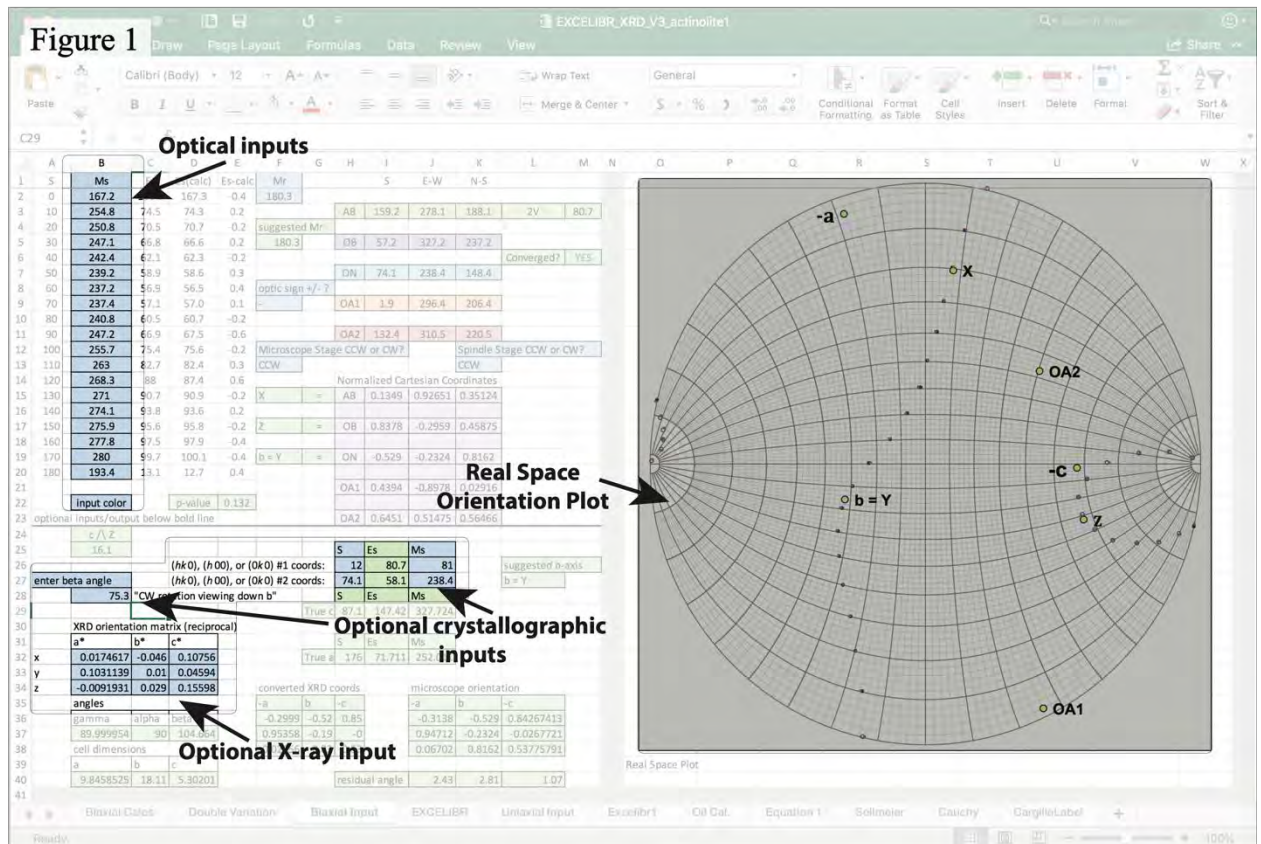
	X-ray Orientation				Spindle Stage Orientation			discrepancy (degrees)		
	-a	b	-c		-a	b	-c	-a	b	-c
x	0.2868	-0.2866	0.8108	x	0.3024	-0.3085	0.7947	0.9	1.5	1.8
y	0.9572	0.0469	-0.5201	y	0.9524	0.0607	-0.5320			
z	0.0390	0.9569	0.2684	z	0.0374	0.9493	0.2923			

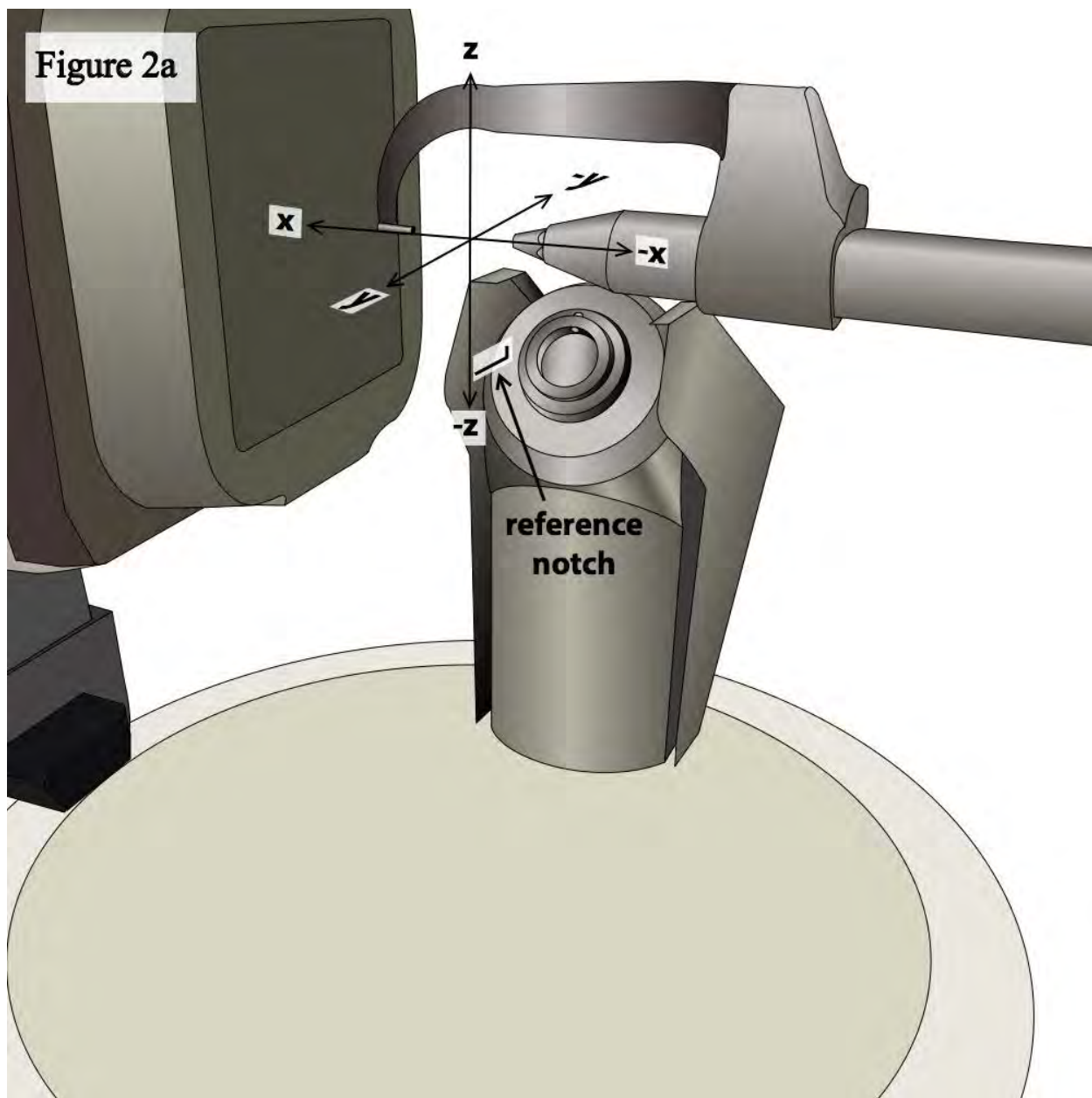
actinolite4

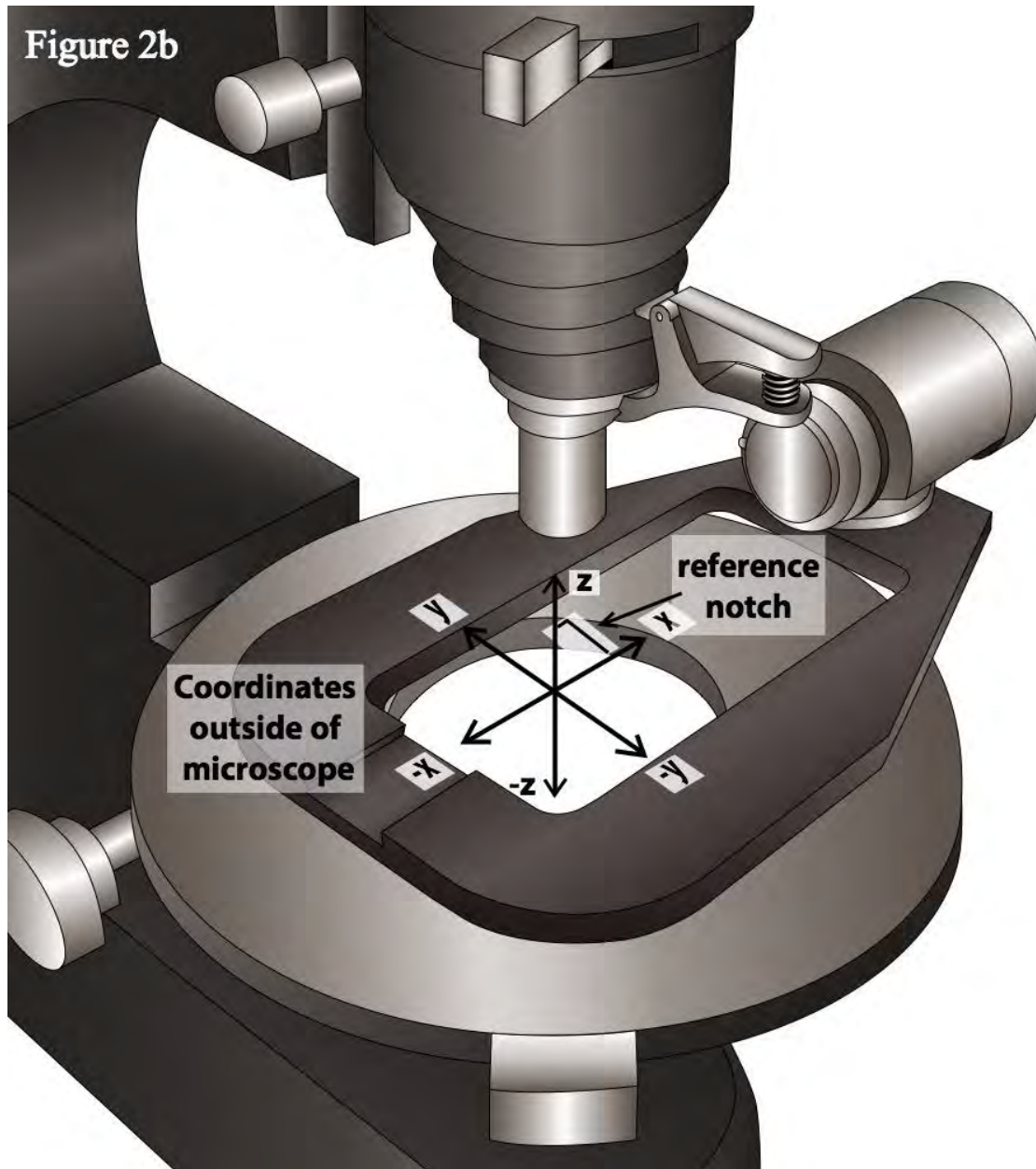
	X-ray Orientation				Spindle Stage Orientation			discrepancy (degrees)		
	-a	-b	-c		-a	-b	-c	-a	-b	-c
x	-0.1205	-0.3085	-0.9433	x	-0.1356	-0.2947	0.9494	2.6	2.3	1.6
y	-0.6550	0.7389	-0.3189	y	-0.6848	0.7180	0.2952			
z	0.7459	0.5990	0.0925	z	0.7160	0.6306	0.1076			

actinolite5

	X-ray Orientation				Spindle Stage Orientation			discrepancy (degrees)		
	-a	b	-c		-a	b	-c	-a	b	-c
x	-0.4598	-0.4326	0.8667	x	-0.4735	-0.4444	0.8557	0.9	1.5	1.2
y	0.2620	-0.9005	-0.4021	y	0.2552	-0.8956	-0.4173			
z	0.8485	0.0436	0.2953	z	0.8430	0.0215	0.3060			







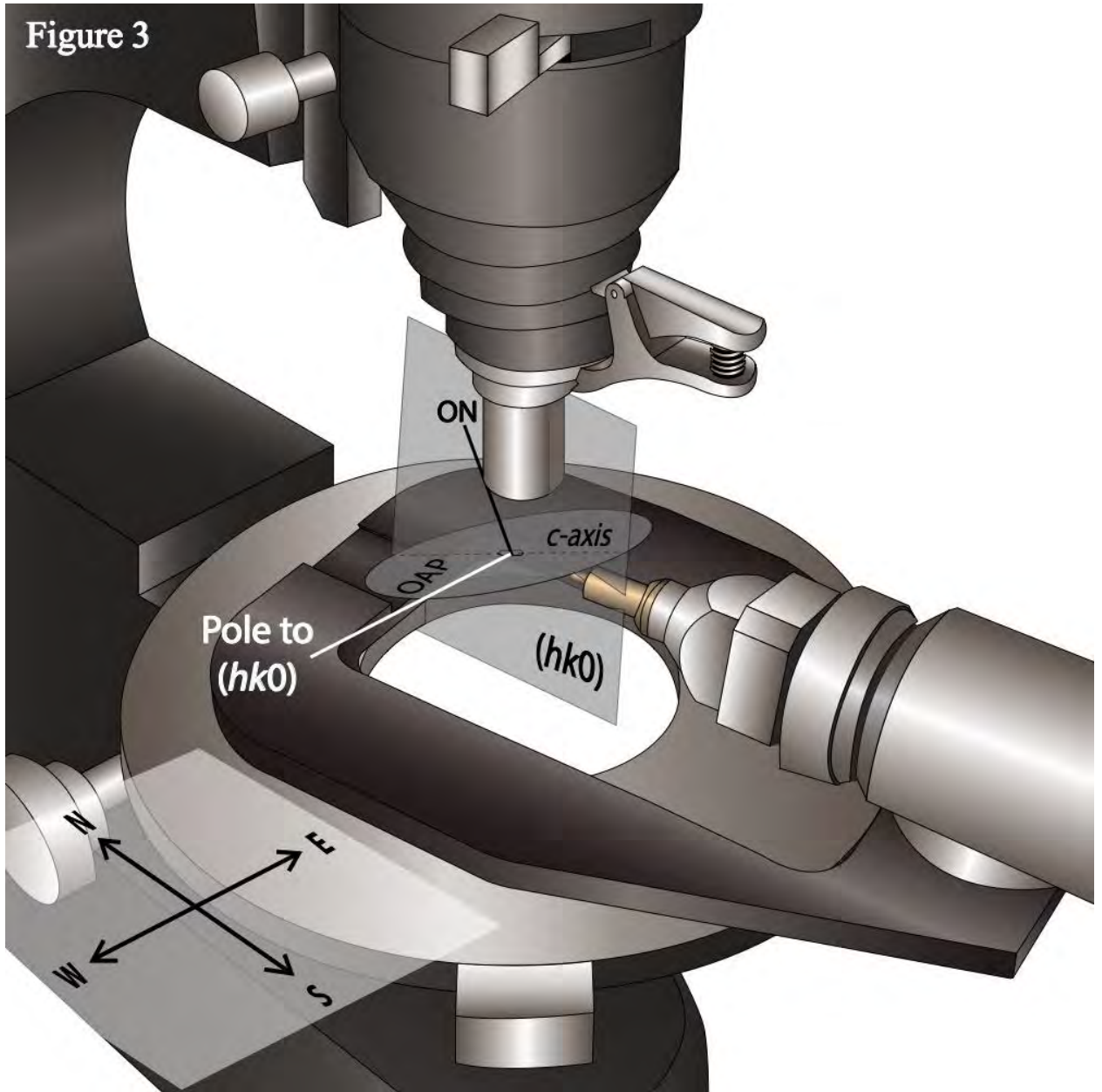


Figure 4a

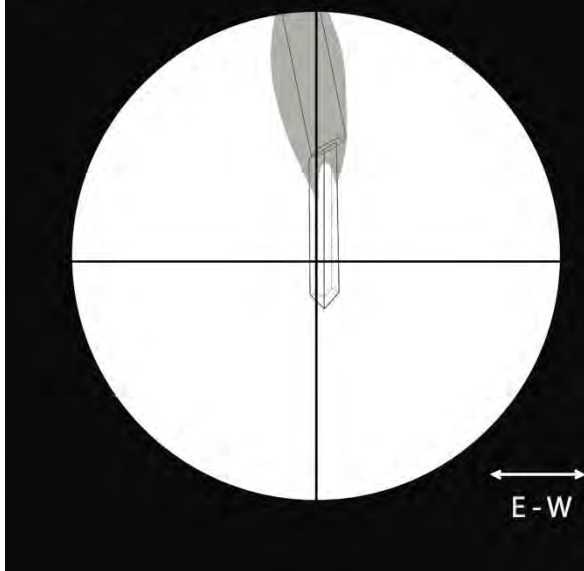
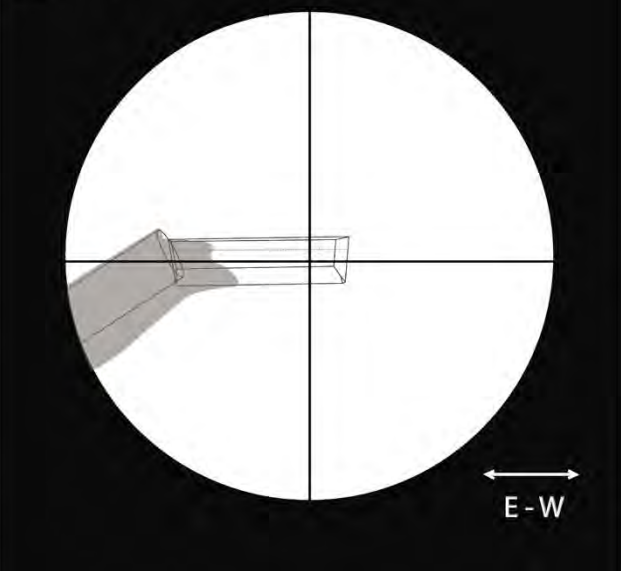
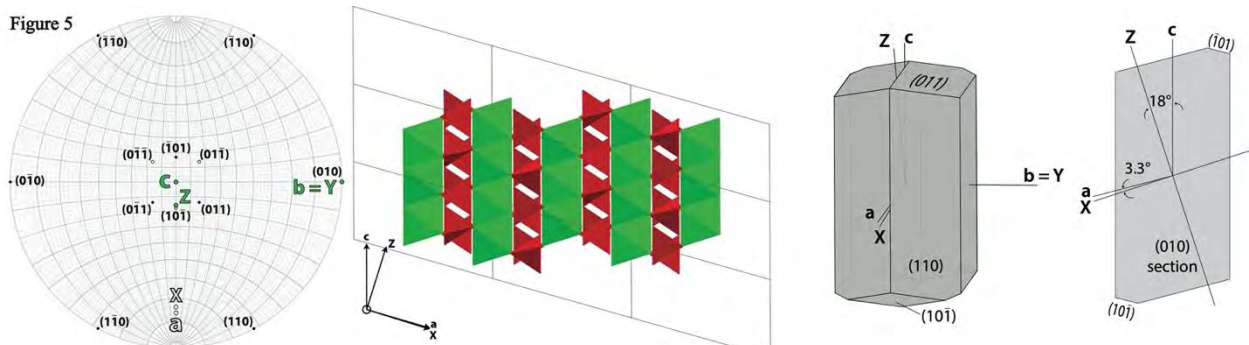


Figure 4b



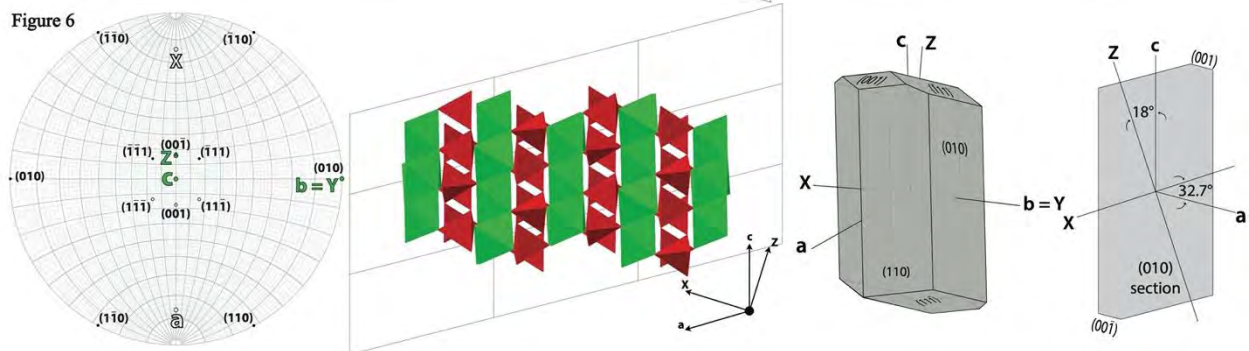
343

Figure 5

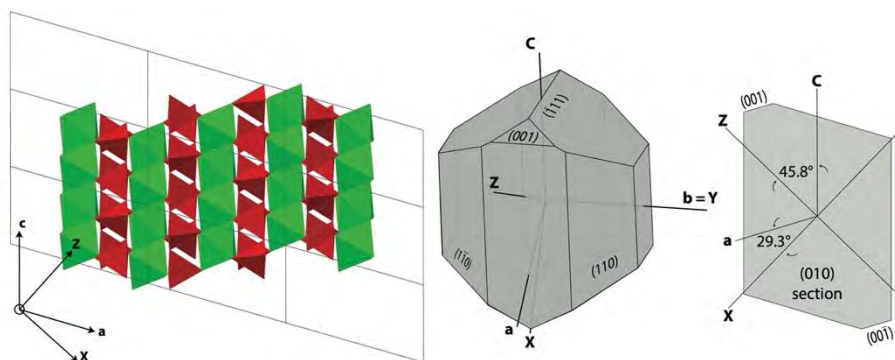
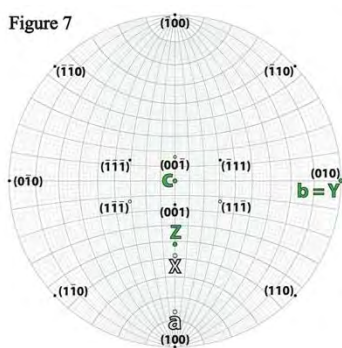


344

Figure 6

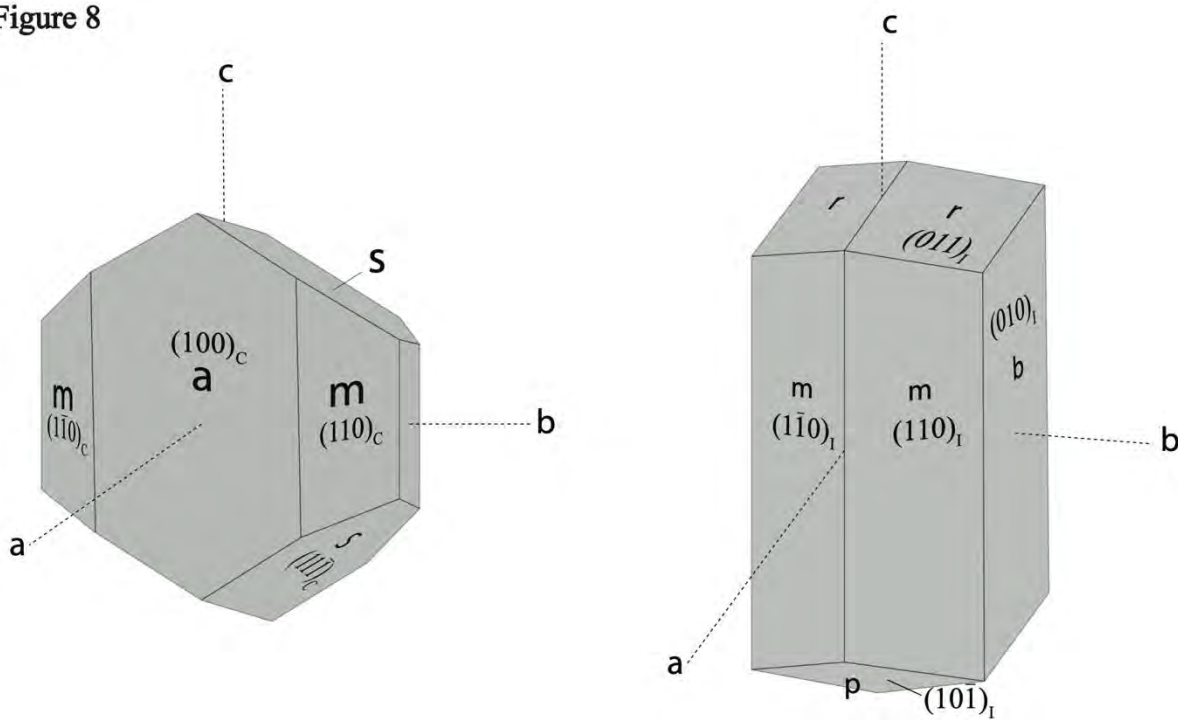


345

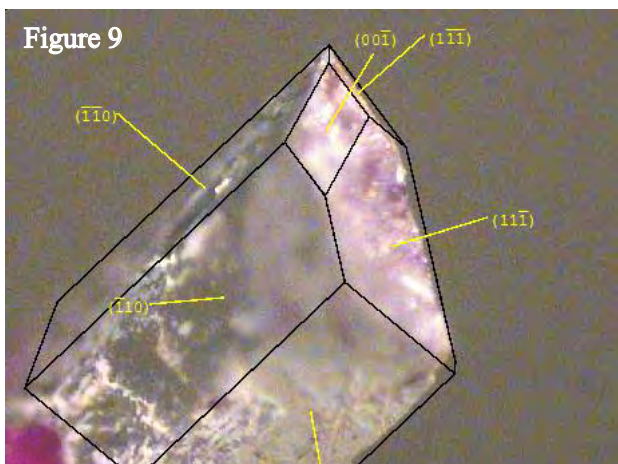


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Figure 8

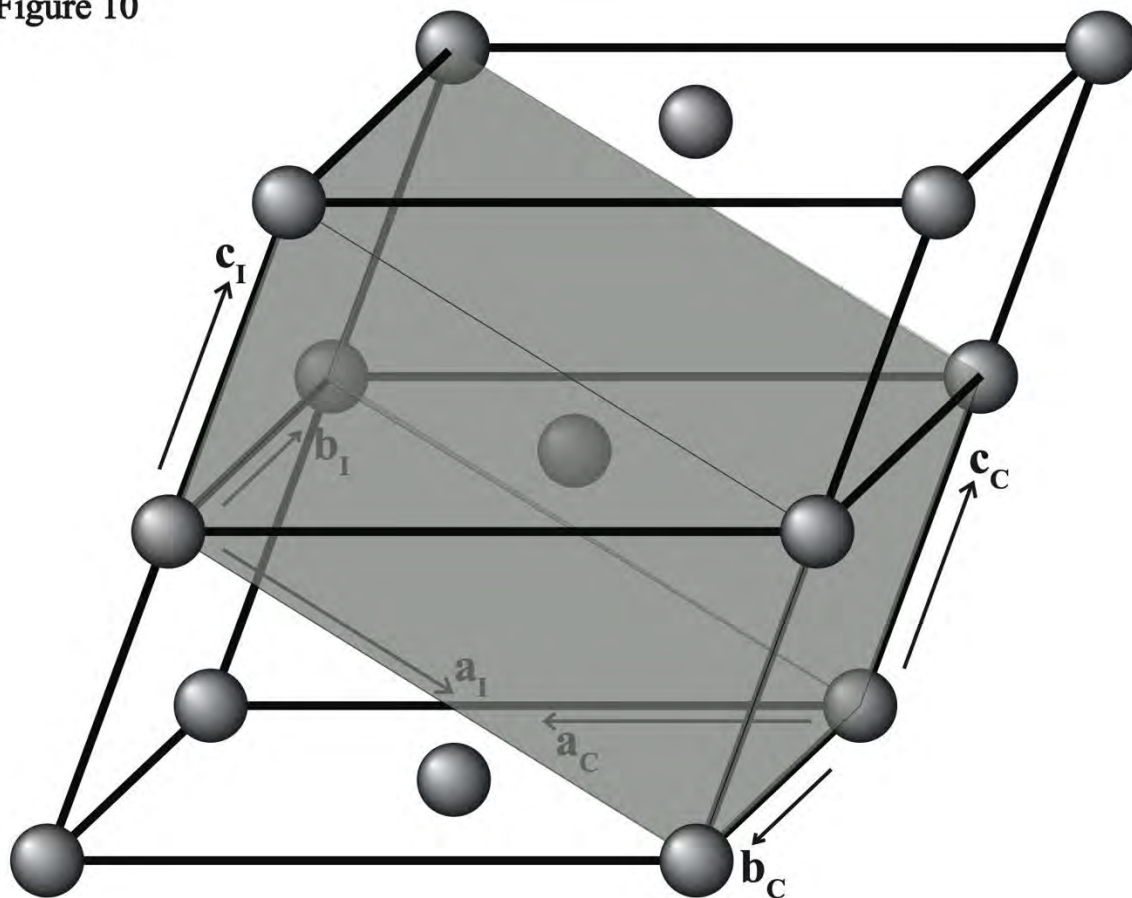


347

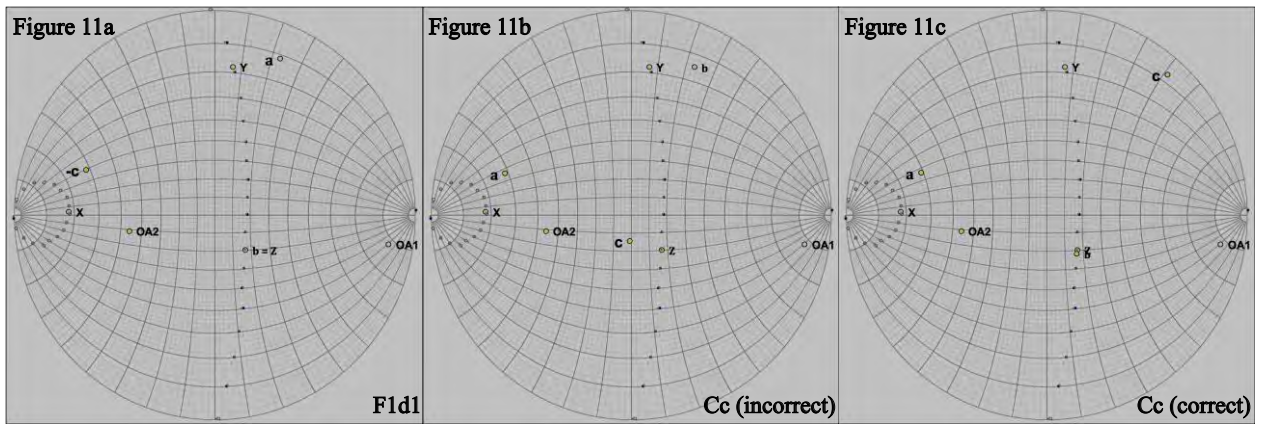


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Figure 10



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