3.60 SYMMETRY, STRUCTURE AND TENSOR PROPERTIES
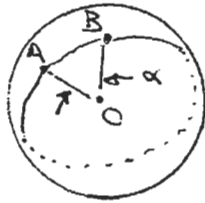
of MATERIALS

NOTES ON SPHERICAL TRIGONOMETRY

SPHERICAL TRIGONOMETRY DIFFERS FROM EUCLIDIAN PLANE GEOMETRY IN THAT ALL OF THE ACTION TAKES PLACE ON THE SURFACE OF A SPHERE WHICH, FOR CONVENIENCE, WE CAN TAKE AS HAVING UNIT RADIUS.

A GREAT CIRCLE IS DEFINED AS THE CIRCLE OF INTERSECTION (UNIT RADIUS) OF THE SPHERE AND ANY PLANE PASSED THROUGH THE CENTER OF THE SPHERE.

A SMALL CIRCLE (R<1) IS THE CIRCLE OF INTERSECTION WITH THE SPHERE OF ANY PLANE WHICH INTERSECTS THE SPHERE BUT DOES NOT PASS THROUGH ITS CENTER

DISTANCE BETWEEN TWO POINTS   CONSIDER TWO POINTS A & B ON THE

SURFACE OF THE SPHERE. THE "DISTANCE" BETWEEN A & B IS NOT THE LINE CONNECTING THEM (AS IN PLANE GEOMETRY) AS WE MUST REMAIN ON THE SURFACE OF THE SPHERE. POINTS A & B AND O, THE CENTER OF THE SPHERE, DEFINE A PLANE WHICH INTERSECTS THE SPHERE IN A GREAT CIRCLE. WE DEFINE THE DISTANCE BETWEEN A & B AS THE SHORTER OF THE TWO ARCS CONNECTING THE POINTS ALONG THE GREAT CIRCLE, AND MEASURE THE LENGTH $\overarc{AB}$ IN TERMS OF THE ANGLE $\angle AOB = \alpha$ SUBTENDED BY THE ARC AT THE CENTER OF THE SPHERE. (NOTE THAT THIS DEFINITION MAKES LENGTHS INDEPENDENT OF THE RADIUS OF THE REFERENCE SPHERE. MOREOVER, AS "LENGTHS" ARE MEASURED IN ANGLES, ONE CAN SPEAK OF TRIGONOMETRIC FUNCTIONS OF LENGTHS, MIND-BOGGLING AS THIS MIGHT BE IN PLANE GEOMETRY)

Pole OF AN ARC OR OF A GREAT CIRCLE
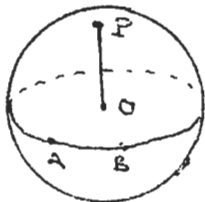
WE DEFINE AS THE Pole OF ARC $\overarc{AB}$ THE POINT OF INTERSECTION WITH THE SPHERE OF A PERPENDICULAR LINE CONSTRUCTED AT THE CENTER OF THE SPHERE AND NORMAL TO THE PLANE OF THE GREAT CIRCLE WHICH DEFINES $\overarc{AB}$. (eg, THE EARTH'S NORTH Pole IS THE Pole OF THE EQUATOR)
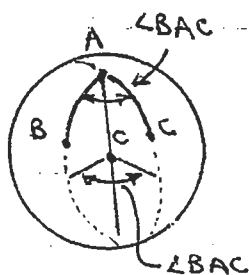
A PROPERTY OF A Pole IS THAT IT IS A "DISTANCE" OF 90° AWAY FROM ANY POINT ON ARC $\overarc{AB}$
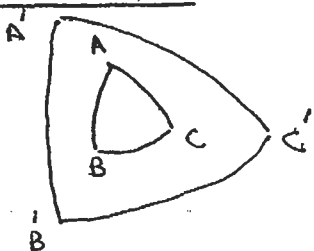
SPHERICAL TRIANGLES
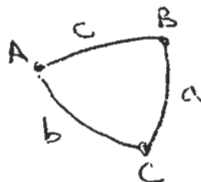
CONSIDER THREE POINTS A, B & C ON THE SURFACE OF THE SPHERE. A SPHERICAL TRIANGLE IS CONSTRUCTED FROM THEM BY PASSING GREAT CIRCLES THROUGH THESE POINTS TWO AT A TIME -- i.e, BY CONSTRUCTING THE ARCS $\overarc{BC} = a$, $\overarc{AC} = b$, $\overarc{AB} = c$.

SPHERICAL ANGLES

∠BAC

WE DEFINE, AS THE MEASURE OF THE SPHERICAL ANGLE ∠BAC IN A SPHERICAL TRIANGLE, THE DIHEDRAL ANGLE BETWEEN THE PLANES WHICH DEFINE THE GREAT CIRCLES OF ARCS $\widehat{BA}$ AND $\widehat{AC}$.

∠BAC

POLAR TRIANGLES

CONSIDER A SPHERICAL TRIANGLE ABC.

FIND A', THE POLE OF ARC $\widehat{BC}$
B', THE POLE OF ARC $\widehat{AC}$
C', THE POLE OF ARC $\widehat{AB}$

NOW, CONNECT A', B', C' WITH ARCS OF GREAT CIRCLES.

TRIANGLE A'B'C' IS SAID TO BE THE **POLAR TRIANGLE** OF TRIANGLE ABC

AN AMUSING FEATURE OF THESE TRIANGLES IS THAT THEY ARE MUTUALLY POLAR — THAT IS, IF A'B'C' IS THE POLAR TRIANGLE OF ABC, THEN ABC IS ALSO THE POLAR TRIANGLE OF A'B'C'.

Proof: B' IS POLE OF $\widehat{AC}$, ∴ B' IS 90° AWAY FROM ANY POINT ON $\widehat{AC}$, IN PARTICULAR POINT A.

C' IS POLE OF $\widehat{AB}$, ∴ C' IS 90° AWAY FROM ANY POINT ON $\widehat{AB}$, IN PARTICULAR POINT A.

POINT A IS NOW ESTABLISHED AS 90° FROM B', 90° FROM C', THUS A MUST BE THE POLE OF $\widehat{B'C'}$. SIMILAR ARGUMENTS SHOW THAT B IS THE POLE OF $\widehat{A'C'}$, C IS THE POLE OF $\widehat{A'B'}$ QED.

IN TWO POLAR TRIANGLES THE ANGLE IN ONE IS THE SUPPLEMENT OF THE OPPOSITE SIDE IN THE OTHER
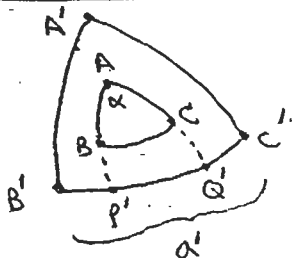
CONSIDER A PAIR OF POLAR TRIANGLES ABC AND A'B'C'

LET ANGLE ∠BAC = α
SIDE $\widehat{B'C'}$ = a'

THIS THEOREM THEN STATES $a' + \alpha = 180°$.

Proof: EXTEND THE GREAT CIRCLES WHICH DEFINE $\widehat{AB}$ AND $\widehat{AC}$ UNTIL THEY INTERSECT $\widehat{B'C'}$ AT POINTS P' AND Q', RESPECTIVELY.

B' IS POLE OF $\widehat{AC}$, ∴ $\widehat{B'Q'} = 90°$
C' IS POLE OF $\widehat{AB}$, ∴ $\widehat{C'P'} = 90°$

THUS $\widehat{B'Q'} + \widehat{C'P'} = 180° = (\widehat{B'P'} + \widehat{P'Q'}) + (\widehat{P'Q'} + \widehat{Q'C'})$
$= (\widehat{B'P'} + \widehat{P'Q'} + \widehat{Q'C'}) + \widehat{P'Q'} = a' + \widehat{P'Q'}$

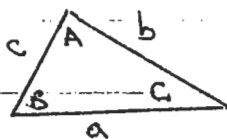BUT THE LENGTH OF $\widehat{P'Q'}$ IS NUMERICALLY EQUAL TO THE ANGLE USED TO MEASURE α (SEE DEFINITION OF SPHERICAL ANGLES, ABOVE)

∴ $a' + \alpha = 180°$ QED
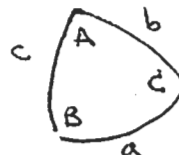
LAW of COSINES

     IN PLANE GEOMETRY, THE law of COSINES RELATES THE length of ONE SIDE of A TRIANGLE TO THE OTHER TWO SIDES AND THE ANGLE BETWEEN THEM. AN ANALAGOUS RELATION (GIVEN WITHOUT PROOF) EXISTS FOR SPHERICAL TRIANGLES.
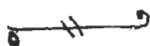
PLANE GEOMETRY

$$a^2 = b^2 + c^2 - 2bc \cos A$$

SPHERICAL GEOMETRY

$$\cos a = \cos b \cos c + \sin b \sin c \cos A$$

COMBINATION of TWO ROTATION OPERATIONS

     LET US CONSIDER THE OPERATION WHICH ARISES WHEN TWO ROTATION OPERATIONS A_α AND B_β ARE COMBINED. FOR THE TIME BEING WE WILL CONSIDER ONLY COMBINATIONS of SYMMETRY ELEMENTS WHICH PERTAIN TO A finite, closed CLUSTER of SYMMETRICALLY RELATED MOTIFS ABOUT SOME POINT IN SPACE. TO MEET THIS REQUIREMENT THE ROTATION AXES <u>MUST INTERSECT</u> AT A COMMON POINT. (OTHER ARRANGEMENTS of MORE THAN ONE ROTATION OPERATION ARE POSSIBLE — FOR EXAMPLE, PLACING A 4-fold ROTATION AT EVERY LATTICE POINT of A SQUARE NET — BUT THESE PERTAIN TO AN EXTENDED, INFINITE PATTERN)
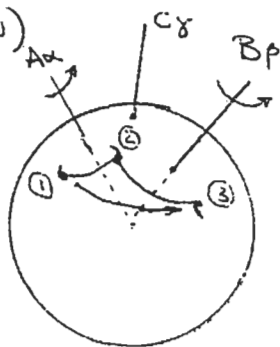
WE NOW ASK THE QUESTION $B_\beta \cdot A_\alpha = ?$

   LET A_α AND B_β BE COMBINED AT SOME ANGLE c. THE ANSWER TO OUR QUESTION MAY BE OBTAINED BY EXAMINATION of THE MOTION of A MOTIF ON THE SURFACE of A SPHERE. LET A SPHERE BE DRAWN ABOUT THE POINT of INTERSECTION of THE AXES. ROTATION A_α MOVES MOTIF ① TO ②. ROTATION B_β ACTING ON MOTIF ② MOVES IN TO ③. ALL THREE MOTIFS ARE of THE SAME "HANDEDNESS" AS ROTATION DOES NOT PRODUCE AN ENANTIOMORPH.

WHAT OPERATION ARISES WHICH RELATES ① DIRECTLY TO ③ ? WE MAY ANSWER THE QUESTION BY THE PROCESS OF ELIMINATION. ONLY 4 OPERATIONS ARE POSSIBLE IN A 3-DIMENSIONAL SPACE: TRANSLATION, REFLECTION, ROTATION, AND INVERSION. REFLECTION AND INVERSION CHANGE "HANDEDNESS" AND WON'T DO THE JOB. TRANSLATION PRODUCES AN OBJECT OF THE SAME "HANDEDNESS", BUT MOTIFS ① AND ③ ARE NOT PARALLEL. MOREOVER, THE DISTANCE BETWEEN ① AND ③ DEPENDS ON EXACTLY WHERE THE INITIAL MOTIF IS PLACED RELATIVE TO A_α. TRANSLATION WON'T WORK EITHER. THEREFORE, BY ELIMINATION, THE THIRD OPERATION MUST BE A ROTATION:

$$\boxed{B_\beta \cdot A_\alpha = C_\gamma}$$

WE CAN FIND THE LOCATION OF AXIS $\dot{C}$ BY FINDING THE SMALL CIRCLE WHICH CONNECTS ① AND ③ AND PASSING A PERPENDICULAR THROUGH THE CENTER OF THE SPHERE. NOTE THAT IF THE SENSE OF ROTATION OF A_α AND B_β IS THE SAME, AXIS C_γ ALSO ACTS IN THE SAME DIRECTION.

TO ANSWER OUR QUESTION QUANTITATIVELY WE NEED TO KNOW THE MAGNITUDE OF γ AND ALSO THE ORIENTATION OF C RELATIVE TO THE FIRST TWO AXES. IN OTHER WORDS,
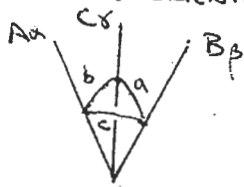
FOR A_α AND B_β COMBINED AT A PARTICULAR ANGLE c WE WISH TO KNOW THE VALUES OF γ AND THE TWO REMAINING INTER-AXIAL ANGLES a AND b.

CLEARLY, THE VALUES OF a, b AND γ DEPEND ON THE VALUES SELECTED FOR α, β AND c

CRYSTALLOGRAPHIC CONSTRAINTS

WE HAVE SHOWN THAT THE PATTERNS OF ATOMS IN CRYSTALS MUST, BY DEFINITION, BE TRANSLATIONALLY PERIODIC AND THAT ONLY 1-FOLD, 2-FOLD, 3-FOLD, 4-FOLD AND 6-FOLD ROTATION AXES MAY COEXIST WITH A TRANSLATION. ACCORDINGLY, IF WE RESTRICT OUR ATTENTION TO CRYSTALLOGRAPHIC ROTATION AXES, α & β CANNOT BE ANY OLD VALUES, BUT WILL BE RESTRICTED TO THE ANGULAR THROWS OF 1, 2, 3, 4 OR 6. THERE IS NOW A RATHER SEVERE CONSTRAINT, ON THE ANGLE c AT WHICH A AND B ARE COMBINED: γ ALSO CANNOT BE ANY OLD VALUE. IT MUST BE A SUBMULTIPLE OF 2π AND, IF THE SYMMETRY IS TO BE COMPATIBLE WITH TRANSLATION, MUST ALSO TURN OUT TO BE THE ANGULAR THROW OF EITHER 1, 2, 3, 4 OR 6.

EULER'S CONSTRUCTION

IT IS NOT EXACTLY OBVIOUS HOW ONE OBTAINS a b & γ IN TERMS OF α, β AND c. THE RELATIONSHIP MAY BE OBTAINED FROM A CONSTRUCTION DUE TO THE MATHEMATICIAN LEONHARD EULER (1707 - 1783).

① LOCATION OF THE AXIS C

CONSIDER THE POINTS A AND B WHERE AXES A_α AND B_β EMERGE FROM THE REFERENCE SPHERE. CONNECT A & B. BY A GREAT CIRCLE. THE LENGTH OF THE ARC $\overarc{AB}$ IS THUS EQUAL TO c, THE ANGLE AT WHICH A_α AND B_β ARE COMBINED.
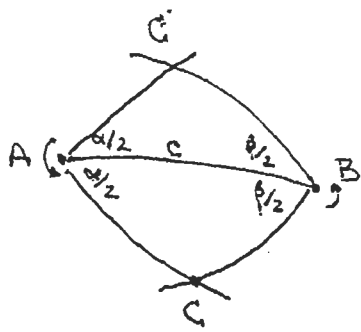
CONSTRUCT A GREAT CIRCLE THROUGH POINT A WHICH MAKES A SPHERICAL ANGLE $\alpha/2$ WITH $\widehat{AB}$ (ie, THE GREAT CIRCLE CONTAINING $\widehat{AC}$ IN THE DIAGRAM TO THE LEFT) THE ACTION of AXIS A_α ROTATES THIS GREAT CIRCLE THROUGH α TO A NEW LOCATION $\widehat{AC'}$

SIMILARLY, CONSTRUCT A GREAT CIRCLE THROUGH POINT B WHICH MAKES A SPHERICAL ANGLE $\beta/2$ WITH $\widehat{AB}$ (ie, THE GREAT CIRCLE CONTAINING $\widehat{BC'}$) B_β ROTATES THIS GREAT CIRCLE THROUGH β TO A NEW LOCATION $\widehat{BC}$.

TO FIND THE LOCATION of AXIS C WE NOW INVOKE OUR DEFINITION of A SYMMETRY ELEMENT: IT IS THE LOCUS of POINTS LEFT UNMOVED BY AN OPERATION. IF $C_\gamma = B_\beta \cdot A_\alpha$, THE PLACE WHERE AXIS C EMERGES FROM THE SPHERE MUST BE THE

POINT WHICH IS LEFT UNMOVED BY THE SUCCESSIVE ROTATIONS A_α & B_β. LET US EXAMINE THE POINTS ALONG GREAT CIRCLE $\widehat{AC}$ WHICH SATISFY THIS CONDITION. IT OBVIOUSLY IS NOT fulfilled BY MOST POINTS ALONG THIS LOCUS. (IN THE DIAGRAM ABOVE, for EXAMPLE, POINT P ON $\widehat{AC}$ IS ROTATED TO LOCATION P' BY A_α. THE OPERATION B_β DOES NOT RESTORE P TO ITS ORIGINAL LOCATION, BUT INSTEAD MOVES IT TO A NEW LOCATION P'')
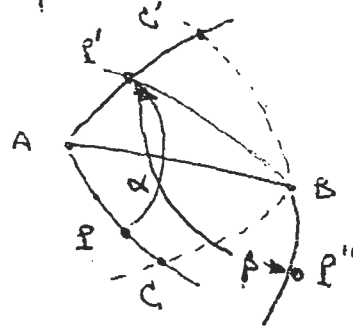
THE ONLY POINT IN OUR CONSTRUCTION WHICH IS RESTORED TO ITS ORIGINAL LOCATION BY THE SUCCESSIVE OPERATION of A_α AND B_β IS POINT C. THIS IS WHERE C_γ EMERGES FROM THE SPHERE. THE LENGTHS of ARCS $\widehat{AC}$ AND $\widehat{BC}$ REPRESENT THE ANGLES WHICH THE NEW AXIS MAKES WITH RESPECT TO A_α AND B_β.

② THE VALUE of γ

NEXT EXAMINE how A DIFFERENT POINT ON THE SPHERE IS MOVED. LET US CONSIDER POINT A.
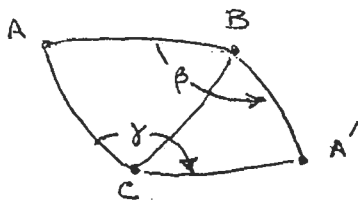
A_α LEAVES POINT A UNMOVED, AS IT SITS SMACK ON THE AXIS A_α

B_β MOVES POINT A TO A NEW LOCATION A'

CONNECT B & A' WITH GREAT CIRCLE $\widehat{BA'}$. CONNECT C & A' WITH GREAT CIRCLE $\widehat{CA'}$

NOW, $B_\beta \cdot A_\alpha = C_\gamma$ SO A MUST BE RELATED TO A' BY THE OPERATION C_γ. IT THEREFORE follows THAT SPHERICAL ANGLE

$\angle ACA' = \gamma$

NEXT EXAMINE SPHERICAL TRIANGLES BAC AND BA'C.

$\angle ABC = \angle A'BC = \beta/2$
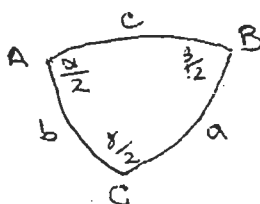$\widehat{AB} = \widehat{A'B}$ AS THEY ARE RELATED BY ROTATION
$\widehat{BC}$ IS COMMON TO THE TWO TRIANGLES

$\left. \right\}$ ∴ $\triangle ABC = \triangle A'BC$ AS THEY HAVE TWO SIDES AND AN INCLUDED ANGLE EQUAL

∴ $\angle ACB = \angle A'CB = \gamma/2$

WE NOW HAVE ALL QUANTITIES of INTEREST $\alpha/2$, $\beta/2$, $\gamma/2$ AND THE INTERAXIAL ANGLES a, b & c IN ONE SPHERICAL TRIANGLE.
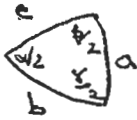
CAUTIONARY NOTE : The spherical angles in our final triangle are __HALF__ of the angular throw of the rotation axes and NOT the rotation angles themselves.

QUANTITATIVE RELATION BETWEEN ANGLES

The law of cosines when applied to a spherical triangle with sides u, v, w and angles U, V, W provides

$$\cos w = \cos u \cos v + \sin u \sin v \cos W$$

Applying this to the spherical triangle of Euler's construction yields

$$\cos c = \cos a \cos b + \sin a \sin b \cos \frac{\gamma}{2}$$

with similar equations for a & b. Each is a lovely equation. Unfortunately, they involve the parameters which we do __NOT__ know — namely, the unknown interaxial angles a & b — and not the variables which we may select (the crystallographic rotation angles α, β & γ.)

We can get around this problem by constructing the polar triangle of $\triangle ABC$, and making use of the fact that an angle in one triangle and the opposite side in the other are supplements
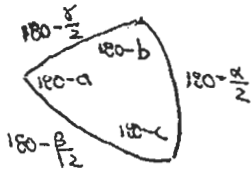
Applying the law of cosines to the polar triangle provides

$$\cos\left(180 - \frac{\gamma}{2}\right) = \cos\left(180 - \frac{\alpha}{2}\right)\cos\left(180 - \frac{\beta}{2}\right) + \sin\left(180 - \frac{\alpha}{2}\right)\sin\left(180 - \frac{\beta}{2}\right)\cos(180 - c)$$

Noting that $\cos(180 - \phi) = -\cos\phi$ and $\sin(180 - \phi) = \sin\phi$

$$-\cos\frac{\gamma}{2} = \cos\frac{\alpha}{2}\cos\frac{\beta}{2} - \sin\frac{\alpha}{2}\sin\frac{\beta}{2}\cos c$$

Solving for the cosine of the interaxial angle c

$$\boxed{\cos c = \frac{\cos\frac{\alpha}{2}\cos\frac{\beta}{2} + \cos\frac{\gamma}{2}}{\sin\frac{\alpha}{2}\sin\frac{\beta}{2}}}$$

If we pick an axis A with angular throw α, and an axis B with angular throw β, this relation tells us the angle c at which they must be combined in order to have the resulting third axis C produce a desired angle of rotation γ.

Note that we have __NOT__ specified the combination of axes until we find the location of the axis C — that is, we still need values for the interaxial angles a & b. These are, upon further application of the law of cosines :

$$\cos b = \frac{\cos\frac{\alpha}{2}\cos\frac{\gamma}{2} + \cos\frac{\beta}{2}}{\sin\frac{\alpha}{2}\sin\frac{\gamma}{2}}$$

$$\cos a = \frac{\cos\frac{\beta}{2}\cos\frac{\gamma}{2} + \cos\frac{\alpha}{2}}{\sin\frac{\beta}{2}\sin\frac{\gamma}{2}}$$

COMBINATIONS TO BE TESTED The number of combinations of crystallographic rotation axes $1, 2, 3, 4$ & 6, without concern for permutations, is provided in the following table

A\B	1	2	3	4	6
1	111 112 113 114 116				
2	212 213 214 216	222 223 224 226			
3	313 314 316	323 324 326	333 334 336		
4	414 416	424 426	434 436	444 446	
6	616	626	636	646	666

35 combinations are distinct but, of these, 4 of the type 11n are impossible as no rotation followed by no rotation cannot be equivalent to a net rotation.

Only a limited number of the remainder work. These are :

222   322   422   622

233   432