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The compression pathway of quartz

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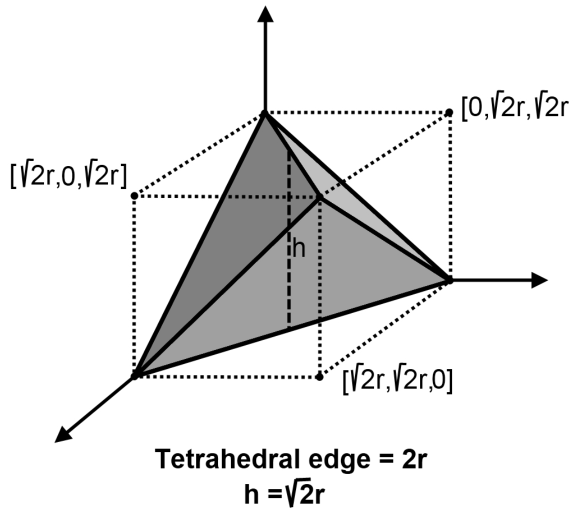
Appendix

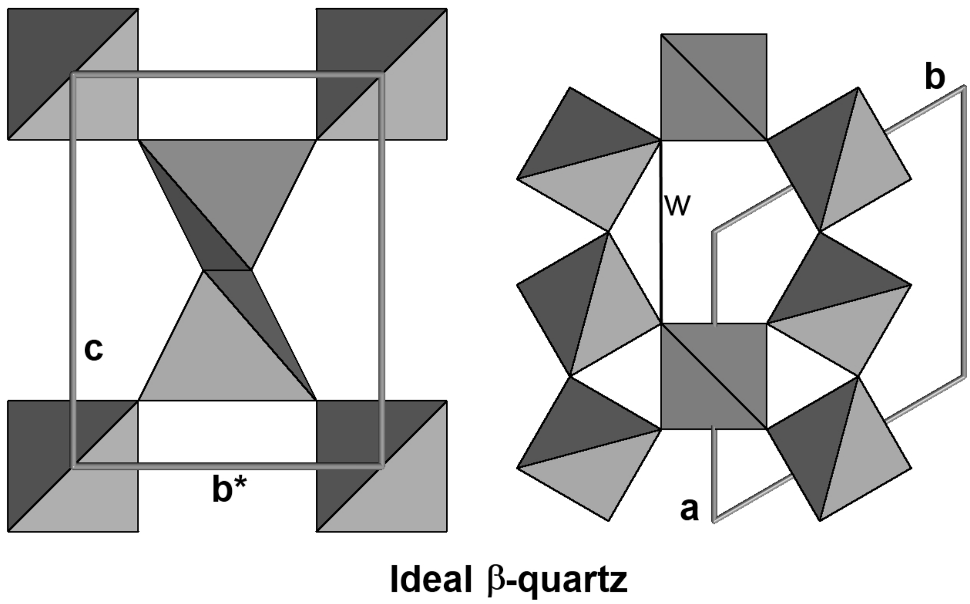
This appendix presents the derivation of the ideal quartz structures. All tetrahedra are perfectly regular with edge length 2r. Appendix Figure 1[1] illustrates an important quantity in the derivations. The dashed line segment, *h*, passing through the center of the tetrahedron is the portion of the tetrahedral twofold within the tetrahedron, and has length √2r. Alternatively, it can be described as the line segment connecting the midpoints of opposing tetrahedral edges.

Ideal β-quartz is relatively easy to derive. Appendix Figure 2 illustrates its unit cell. **c** = 3h = 3√2r and **a** = w + h = (√6 + √2)r. Appendix Figure 3 allows the derivation of the oxygen x-coordinate. Because O is on a special position, $x_{O3} = x_{O1}/2$, so $x_m = 3x_{O1}/4$, and $x_{Si} = 1/2$, so $(1/2 - 3x_{O1}/4)/(3x_{O1}/4) = (\sqrt{2}/2)/(\sqrt{6}/2)$, giving $x_{O1} = 1 - 1/\sqrt{3}$.

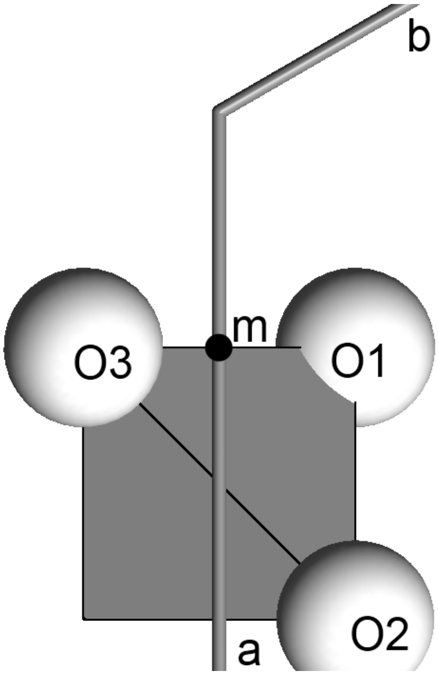
Ideal α-quartz is more complicated. Coordinates for O2 (Appendix Fig. 3) are derived below in terms of a series intermediate parameters illustrated in Appendix Figure 4 and 6 and ultimately in terms of the tetrahedral rotation angle, ϕ, and the model oxygen radius, *r*. From this, the coordinates can be recast in terms of the Si-O-Si angle, θ, and used to calculate the position of O1 and Si



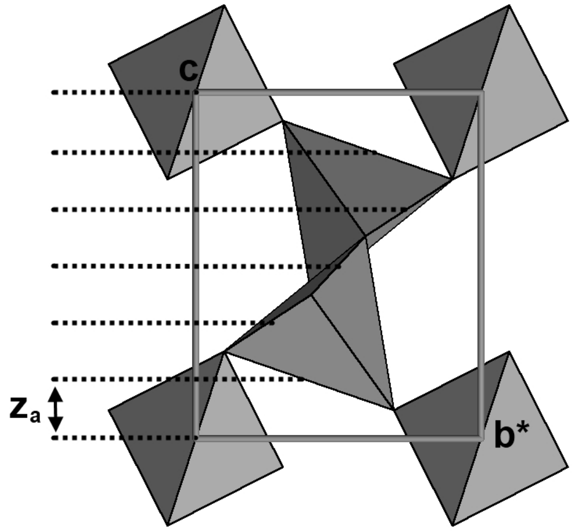
Appendix Figure 1. Tetrahedral geometry. The line segment, h, connecting the midpoints of opposing edges in a regular tetrahedron with edge length 2r has length √2r.



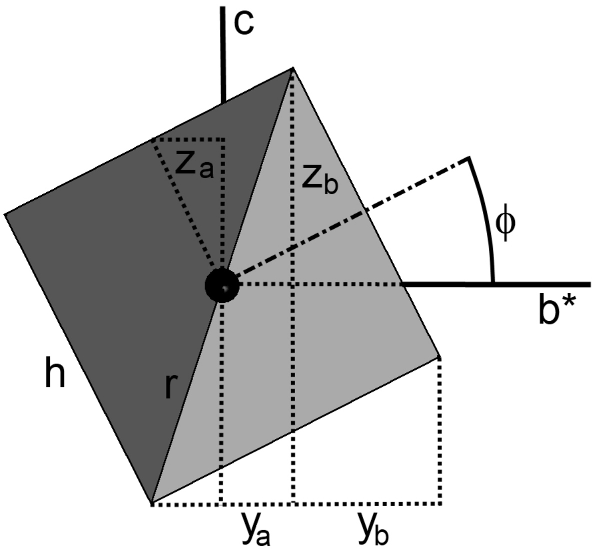
Appendix Figure 2. Cell parameters of ideal β-quartz. c = 3√2r, a = √6r.



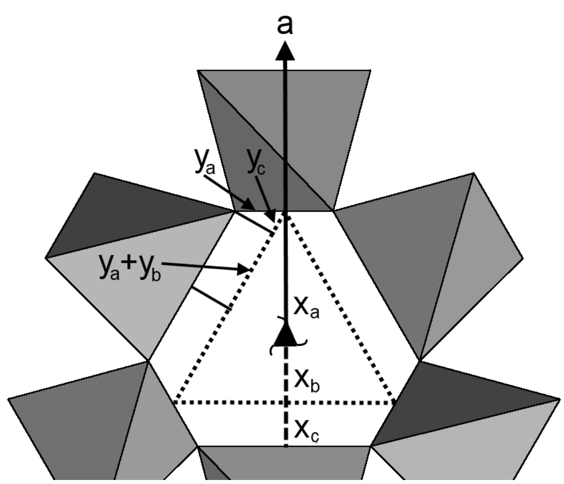
Appendix Figure 3. Deriving the oxygen x-coordinate of ideal β-quartz.



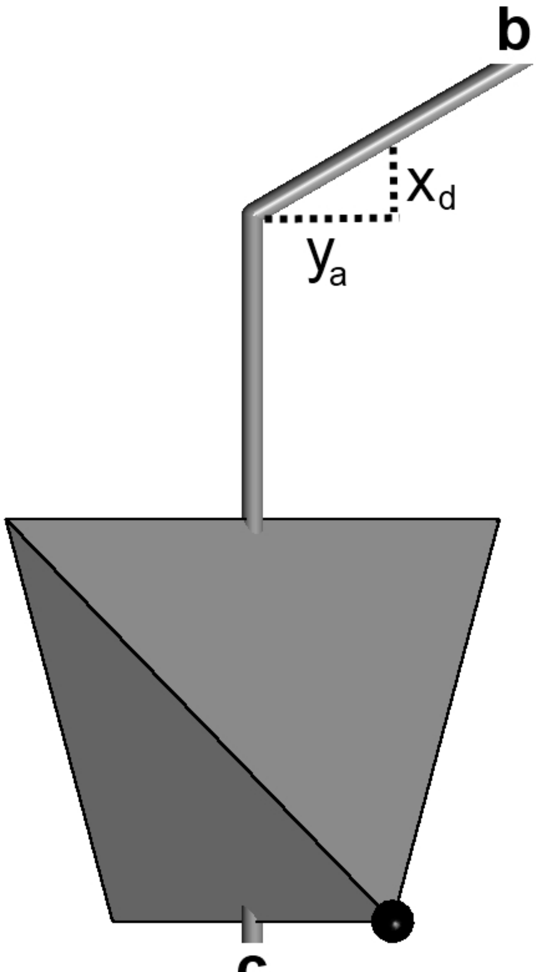
Appendix Figure 5. Deriving the c cell edge of ideal α-quartz. Each dotted line passes through the midpoints of the edges of tetrahedra. Thus, the same vertical percentage of each tetrahedron is between dotted lines and c = 6za.



Appendix Figure 4. Deriving the oxygen positional coordinates of ideal α-quartz. za represents the length of the vertical line segment forming the right-hand side of the dotted triangle. zb represents the length of the dotted vertical line segment originating at and perpendicular to the ab-plane and ending at the uppermost corner of the tetrahedron. The ideal quartz structure in this example has an Si-O-Si angle of 130° and a tetrahedral rotation angle, φ, of 26.9°.



Appendix Figure 6. Important quantities in deriving a, xO2, and yO2. This ideal quartz structure in this example has an Si-O-Si angle of 145° and a tetrahedral rotation angle, φ, of 15.4°.



Appendix Figure 7. Deriving xO2 and yO2.

(see text). From Appendix Figure 4:

$h = \sqrt{2}r$
$z_a = r \cdot \cos\phi/\sqrt{2}$
$z_b = r \cdot \sin(\phi + 45°)$

by inspection of Appendix Figure 5, $c = 6z_a$

$z_{O2} = z_b/c$
$y_a = r \cdot \cos(\phi + 45°)$
$y_b = h \cdot \cos\phi - 2y_a = \sqrt{2}r \cdot \cos\phi - 2r \cdot \cos(\phi + 45°) = \sqrt{2}r \cdot \sin\phi.$

From Appendix Figure 6:

$y_c = y_a/2$
$x_a = (2/\sqrt{3}) \cdot (y_a + y_b + y_c)$
$x_b = x_a/2$
$x_c = (\sqrt{3}/2) \cdot y_a$
$a = x_a + x_b + x_c + h.$

From Appendix Figure 7:

$y_{O2} = (2y_a/\sqrt{3})/a$
$x_{O2} = (x_b + x_c + x_d + h)/a.$

Finally:

$x_{Si} = (x_{O2} + y_{O2} + 1)/4$
$x_{O1} = -x_{O2} + y_{O2} + 1$
$y_{O1} = -x_{O2} + 1$
$z_{O1} = z_{O2} - 1/3.$

To derive the relation between ϕ and the Si-O-Si angle, θ, examine the oxygen atom O2 at [x, y, z]. Form the vectors $\mathbf{v}$ = *O2Si1* and $\mathbf{w}$ = *O2Si2*, where Si1 = [$(x + y + 1)/4$, 0, 0] and Si2 = [1, $(x + y + 1)/4$, 1/3]. Solve the equation $\cos\theta = \mathbf{v} \cdot \mathbf{w}/(||v||\ ||w||)$, substitute the expressions for x, y, and z as functions of ϕ, and complete the square.