1. An experiment reveals that within experimental uncertainty, $a = b = c$ and $\alpha = \beta = \gamma = 90^\circ$. Write true or false against these options.
   (a) The crystal system is necessarily cubic. **False**
   (b) The symmetry of the physical properties will determine the point group and hence the crystal class. **True**
   (c) One must determine the arrangement of atoms within the crystal structure to assign the complete symmetry. **True**

2. There is only one two fold axis of rotation or a mirror plane in which of the following system(s)?
   (a) Triclinic
   (b) Monoclinic
   (c) Orthorhombic
   (d) Tetragonal.
   **Answer**
   Monoclinic.

3. A regular octahedron is shown. To which class does the point group symmetry of this object belong?
(a) Tetragonal
(b) Orthorhombic
(c) Cubic
(d) Hexagonal.

Answer
Cubic.

4. Label the eight faces, using Miller’s notation, of the octahedron shown. If the octahedron is stretched along $\pm \vec{c}$, index the faces. What are the families of plane in the stretched and unstretched case?

Answer

![Octahedron Diagram](image)

Miller Indices for the planes of the octahedron

(a) Shows the front facing and (b) the back facing faces. These indices can also be easily determined by looking at the $c$ projections as shown in (c) and (d). (c) is the projection for faces with $z < 0$ and (d) for $z > 0$. For a regular octahedron (in the
stretched and unstretched case) family \{111\} represents eight planes

\[(111); (\bar{1}11); (11\bar{1}); (\bar{1}1\bar{1}); (\bar{1}\bar{1}1); (\bar{1}1\bar{1}); (1\bar{1}1); (1\bar{1}1) \Rightarrow \{111\}.\]

5. A lattice has 4-fold axis of rotation. To what system does lattice belong to?
   (a) Orthorhombic
   (b) Only Tetragonal
   (c) Only Cubic
   (d) Either tetragonal or cubic.
   \textbf{Answer}
   Either tetragonal or cubic.

6. Show that in the cubic system, angle between the cube edge and the body diagonal is \(54.74^0\).
   \textbf{Answer}
   The vectors corresponding to the cube edge and body diagonal are \(\overrightarrow{OA} = \vec{a}\) and \(\overrightarrow{OB} = \vec{a} + \vec{b} + \vec{c}\). Their dot product is,
\[
\overrightarrow{OA} \cdot \overrightarrow{OB} = |\overrightarrow{OA}| |\overrightarrow{OB}| \cos \phi \\
\vec{a} \cdot (\vec{a} + \vec{b} + \vec{c}) = a\sqrt{a^2 + b^2 + c^2} \cos \phi \\
\vec{a} \cdot \vec{a} = a\sqrt{3}a^2 \cos \phi \\
a^2 = \sqrt{3}a^2 \cos \phi \\
1 = \sqrt{3} \cos \phi \\
\phi = \cos^{-1}\left(\frac{1}{\sqrt{3}}\right) \\
= 54.74^\circ.
\]

7. Rutile (TiO$_2$) crystallizes in the space group $P4_2/mnm$ with $a = 4.594$ Å, $c = 2.958$ Å. Ti is in 2$a$ and O in 4$f$ positions with $x = 0.305$. Find the coordinates of the O atoms. Draw a projection down $\vec{c}$ of the rutile structure. The space group information of atomic positions taken from the International Tables is appended.

**Answer**

Rutile (TiO$_2$) has tetragonal structure with $a = b = 4.594$ Å and $c = 2.958$ Å. Atomic coordinates:

- Ti in 2$a$ at $(0, 0, 0), \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)$
- O in 4$f$ at $(x, x, 0), (1-x, 1-x, 0), \left(\frac{1}{2} - x, \frac{1}{2} + x, \frac{1}{2}\right), \left(\frac{1}{2} + x, \frac{1}{2} - x, \frac{1}{2}\right)$

Taking the value of $x = 0.305$, the coordinates of O atoms are:

- $O_1 \equiv (0.305, 0.305, 0)$, $O_2 \equiv (0.695, 0.695, 0)$, $O_3 \equiv (0.805, 0.195, 0.5)$, $O_4 \equiv (0.195, 0.805, 0.5)$. 

Date: 13 February, 2013
Generators selected  
(1) \( t(1,0,0); t(0,1,0); t(0,0,1) \); (2); (3); (5); (9)

**Positions**

<table>
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<tr>
<th>Positions</th>
<th>Coordinates</th>
<th>Reflection conditions</th>
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<tbody>
<tr>
<td>16 ( k ) 1</td>
<td>( (1) x,y,z ) ( (2) \bar{x},\bar{y},\bar{z} ) ( (3) \bar{y}+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2} ) ( (4) y+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2} )</td>
<td>General: ( { 0kl : k+l = 2n } ) ( { 00l : l = 2n } ) ( { h00 : h = 2n } )</td>
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<td>( (5) \bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2} ) ( (6) x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2} ) ( (7) y,x,\bar{z} ) ( (8) \bar{y},\bar{x},\bar{z} )</td>
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<td>( (9) \bar{x},\bar{y},\bar{z} ) ( (10) x,y,\bar{z} ) ( (11) y+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2} ) ( (12) \bar{y}+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2} )</td>
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<tr>
<td>( (13) x+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2} ) ( (14) \bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2} ) ( (15) \bar{y},\bar{x},z ) ( (16) y,x,\bar{z} )</td>
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</table>

8 \( j \) m | \( x,x,z \) \( \bar{x},\bar{x},z \) \( \bar{x}+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2} \) \( x+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2} \) | no extra conditions |

8 \( i \) m | \( x,y,0 \) \( \bar{x},\bar{y},0 \) \( \bar{y}+\frac{1}{2},x+\frac{1}{2},\frac{1}{2} \) \( y+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2} \) | no extra conditions |

8 \( h \) 2 | \( 0,\bar{z},z \) \( 0,\bar{z},z+\frac{1}{2} \) \( 0,\bar{z},z+\frac{1}{2} \) \( 0,\bar{z},z+\frac{1}{2} \) | \( hkl : h+k,l = 2n \) |

4 \( g \) m | \( x,\bar{x},0 \) \( x,\bar{x},0 \) \( x+\frac{1}{2},x+\frac{1}{2},\frac{1}{2} \) \( \bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2} \) | no extra conditions |

4 \( f \) m | \( x,x,0 \) \( \bar{x},\bar{x},0 \) \( \bar{x}+\frac{1}{2},x+\frac{1}{2},\frac{1}{2} \) \( x+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2} \) | no extra conditions |

4 \( e \) \( 2,mm \) | \( 0,0,z \) \( \frac{1}{2},\frac{1}{2},\frac{1}{2} \) \( \frac{1}{2},\frac{1}{2},\frac{1}{2} \) \( 0,0,\bar{z} \) | \( hkl : h+k+l = 2n \) |

4 \( d \) \( 2 \) | \( 0,\frac{1}{2},\frac{1}{2} \) \( 0,\frac{1}{2},\frac{1}{2} \) \( \frac{1}{2},0,\frac{1}{2} \) \( \frac{1}{2},0,\frac{1}{2} \) | \( hkl : h+k,l = 2n \) |

4 \( c \) \( 2,mm \) | \( 0,\frac{1}{2},0 \) \( 0,\frac{1}{2},0 \) \( \frac{1}{2},0,\frac{1}{2} \) \( \frac{1}{2},0,\frac{1}{2} \) | \( hkl : h+k,l = 2n \) |

2 \( b \) \( m,mm \) | \( 0,\frac{1}{2},0 \) \( \frac{1}{2},0,\frac{1}{2} \) \( \frac{1}{2},0,\frac{1}{2} \) | \( hkl : h+k+l = 2n \) |

2 \( a \) \( m,mm \) | \( 0,0,0 \) \( \frac{1}{2},\frac{1}{2},\frac{1}{2} \) \( \frac{1}{2},\frac{1}{2},\frac{1}{2} \) | \( hkl : h+k+l = 2n \) |

**Symmetry of special projections**

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<th>Along</th>
<th>( [001] )</th>
<th>( p4gm ) ( a' = a ) ( b' = b ) ( \text{Origin at 0,} \frac{1}{2},z )</th>
<th>( [100] )</th>
<th>( c2mm ) ( a' = b ) ( b' = c ) ( \text{Origin at x,} 0,0 )</th>
<th>( [110] )</th>
<th>( p2mm ) ( \text{Origin at 0,} 0,0 )</th>
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**Maximal non-isomorphic subgroups**

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<th>[2] ( P4n2 ) (118)</th>
<th>1; 2; 7; 8; 11; 12; 13; 14</th>
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<td>[2] ( P42,2 ) (94)</td>
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<td>[2] ( P4,1m11 ) (P4,1m, 84)</td>
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<td>[2] ( P2/m12 ) (Cmm2, 65)</td>
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<td>[2] ( P2/m,2/n1 ) (P4mm, 58)</td>
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**Maximal isomorphic subgroups of lowest index**

| IIc | [3] \( P4,1mnm \) (\( c' = 3c \)) (136); [9] \( P4,1mnm \) (\( a' = 3a, b' = 3b \)) (136) | | | | |

**Minimal non-isomorphic supergroups**

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