Geometry of Crystals

Crystal is a solid composed of atoms, ions or molecules that demonstrate long range periodic order in three dimensions.
## The Crystalline State

<table>
<thead>
<tr>
<th>State of Matter</th>
<th>Fixed Volume</th>
<th>Fixed Shape</th>
<th>Order</th>
<th>Properties</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gas</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>Isotropic</td>
</tr>
<tr>
<td>Liquid</td>
<td>Yes</td>
<td>No</td>
<td>Short-range</td>
<td>Isotropic</td>
</tr>
<tr>
<td>Solid (amorphous)</td>
<td>Yes</td>
<td>Yes</td>
<td>Short-range</td>
<td>Isotropic</td>
</tr>
<tr>
<td>Solid (crystalline)</td>
<td>Yes</td>
<td>Yes</td>
<td>Long-range</td>
<td>Anisotropic</td>
</tr>
</tbody>
</table>
Crystal Lattice

Not only atom, ion or molecule positions are repetitious – there are certain symmetry relationships in their arrangement.

\[
\text{Crystalline structure} = \text{Basis} + \text{Lattice}
\]
Crystal Lattice

One-dimensional lattice with lattice parameter $a$

$$r = ua$$

Two-dimensional lattice with lattice parameters $a, b$ and $\gamma$

$$r = ua + \nu b$$
Crystal Lattice

\[ \mathbf{r} = u \mathbf{a} + v \mathbf{b} + w \mathbf{c} \]
Crystal Lattice

- Lattice vectors, lattice parameters and interaxial angles

A lattice is an array of points in space in which the environment of each point is identical.
Crystal Lattice

Lattice

Not a lattice
Crystal Lattice

Unit cell content
- Coordinates of all atoms
- Types of atoms
- Site occupancy
- Individual displacement parameters
Crystal Lattice

- Usually unit cell has more than one molecule or group of atoms
- They can be represented by symmetry operators
Symmetry

- Symmetry is a property of a crystal which is used to describe repetitions of a pattern within that crystal.
- Description is done using symmetry operators

**Translation**

\[ R \rightarrow R \rightarrow R \]

**Rotation** (about axis O)

\[ \alpha = 360^\circ / n \]

where \( n \) is the *fold* of the axis

\( n = 1, 2, 3, 4 \) or 6)

**Mirror reflection**

\[ \overline{R} \mid \overline{R} \]

**Inversion**

\[ \overline{R} \rightarrow i \overline{R} \]
Two-dimensional Symmetry Elements

1. One-fold axis (no symmetry)
2. Vertical mirror line
3. Vertical and horizontal mirror lines
4. Two-fold rotation axis
5. Three-fold rotation axis
Two-dimensional Symmetry Elements

6. Tree-fold axis + vertical mirror line
7. Four-fold axis
8. Four-fold axis + mirror lines
9. Six-fold axis
10. Six-fold axis + mirror lines

10 two-dimensional crystallographic or plane point groups
The Five Plane Lattices

The oblique $p$-lattice

The rectangular $p$-lattice

The rectangular $c$-lattice

The square $p$-lattice

The hexagonal $p$-lattice
Two-dimensional Symmetry Elements

Reflection glide or glide line of symmetry
Two-dimensional Symmetry Elements

The Seventeen Plane Groups

Lattice type: $p$ for primitive, $c$ for centred.
Symmetry elements: $m$ for mirror lines, $g$ for glide lines, 4 for 4-fold axis etc.

Notes: Each group has a symbol and a number in ( ). The symbol denotes the lattice type (primitive or centered), and the major symmetry elements. The numbers are arbitrary, they are those of the International Tables Vol. 1, pp 58 - 72

Bravais Lattices and Crystal Systems

In three dimensions: point symmetry elements and translational symmetry elements.

For point symmetry elements:
- centers of symmetry
- mirror planes
- inversion axes

For translational symmetry elements:
- glide planes
- screw axes

We end up with 230 space groups (was 17 plane groups) distributed among 14 space lattices (was 5 plane lattices) and 32 point group symmetries (instead of 10 plane point symmetries)
The 14 Space (Bravais) Lattices

- The systematic work was done by Frankenheim in 1835. Proposed 15 space lattices.

- In 1848 Bravais pointed that two of his lattices were identical (unfortunate for Frankenheim).

- Today we have 14 Bravais lattices.

\[ a, b, c – \text{unit cell lengths}; \alpha, \beta, \gamma - \text{angles between them} \]
## Crystal Symmetry

<table>
<thead>
<tr>
<th>Centering of the lattice</th>
<th>Lattice points per unit cell</th>
<th>International symbol</th>
<th>Lattice translation(s) due to centering</th>
</tr>
</thead>
<tbody>
<tr>
<td>Primitive</td>
<td>1</td>
<td>P</td>
<td>None</td>
</tr>
<tr>
<td>Base-centered</td>
<td>2</td>
<td>A</td>
<td>1/2(b+c)</td>
</tr>
<tr>
<td>Base-centered</td>
<td>2</td>
<td>B</td>
<td>1/2(a+c)</td>
</tr>
<tr>
<td>Base-centered</td>
<td>2</td>
<td>C</td>
<td>1/2(a+b)</td>
</tr>
<tr>
<td>Body-centered</td>
<td>2</td>
<td>I</td>
<td>1/2(a+b+c)</td>
</tr>
<tr>
<td>Face-centered</td>
<td>4</td>
<td>F</td>
<td>1/2(b+c); 1/2(a+c); 1/2(a+b)</td>
</tr>
<tr>
<td>Rhombohedral</td>
<td>3</td>
<td>R</td>
<td>1/3a+2/3b+2/3c; 2/3a+1/3b+1/3c</td>
</tr>
</tbody>
</table>
# The 14 Space (Bravais) Lattices

<table>
<thead>
<tr>
<th>System</th>
<th>Axial lengths and angles</th>
<th>Bravais lattice</th>
<th>Lattice symbol</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cubic</td>
<td>Three equal axes at right angles</td>
<td>Simple</td>
<td>P</td>
</tr>
<tr>
<td></td>
<td>$a = b = c, \quad \alpha = \beta = \gamma = 90^\circ$</td>
<td>Body-centered</td>
<td>I</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Face-centered</td>
<td>F</td>
</tr>
<tr>
<td>Tetragonal</td>
<td>Three axes at right angles, two equal</td>
<td>Simple</td>
<td>P</td>
</tr>
<tr>
<td></td>
<td>$a = b \neq c, \quad \alpha = \beta = \gamma = 90^\circ$</td>
<td>Body-centered</td>
<td>I</td>
</tr>
<tr>
<td>Orthorhombic</td>
<td>Three unequal axes at right angles</td>
<td>Simple</td>
<td>P</td>
</tr>
<tr>
<td></td>
<td>$a \neq b \neq c, \quad \alpha = \beta = \gamma = 90^\circ$</td>
<td>Body-centered</td>
<td>I</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Base-centered</td>
<td>C</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Face-centered</td>
<td>F</td>
</tr>
<tr>
<td>Rhombohedral*</td>
<td>Three equal axes, equally inclined</td>
<td>Simple</td>
<td>R</td>
</tr>
<tr>
<td></td>
<td>$a = b = c, \quad \alpha = \beta = \gamma \neq 90^\circ$</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Two equal coplanar axes at 120°,</td>
<td>Simple</td>
<td>P</td>
</tr>
<tr>
<td></td>
<td>third axis at right angles</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>$a = b \neq c, \quad \alpha = \beta = 90^\circ \quad (\gamma = 120^\circ)$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Hexagonal</td>
<td>Three unequal axes, one pair not at right angles</td>
<td>Simple</td>
<td>P</td>
</tr>
<tr>
<td></td>
<td>$a \neq b \neq c, \quad \alpha = \gamma = 90^\circ \neq \beta$</td>
<td>Base-centered</td>
<td>C</td>
</tr>
<tr>
<td>Monoclinic</td>
<td>Three unequal axes, unequally inclined</td>
<td>Simple</td>
<td>P</td>
</tr>
<tr>
<td></td>
<td>and none at right angles</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>$a \neq b \neq c, \quad (\alpha \neq \beta \neq \gamma \neq 90^\circ)$</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

*Also called trigonal.

7 crystal systems
Crystal Symmetry

- 7 axial systems + 32 point groups $\rightarrow$ 230 unique space groups
- A 3-D crystal must have one of these 230 arrangements, but the atomic coordinates (i.e. occupied equipoints) may be very different between different crystals

<table>
<thead>
<tr>
<th>Crystal Class</th>
<th>Non-centrosymmetric Point Group</th>
<th>Centrosymmetric Point Group</th>
<th>Minimum Rotational Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>Triclinic</td>
<td>1</td>
<td>$\bar{1}$</td>
<td>One 1-fold</td>
</tr>
<tr>
<td>Monoclinic</td>
<td>2, $m$</td>
<td>$2/m$</td>
<td>One 2-fold</td>
</tr>
<tr>
<td>Orthorombic</td>
<td>222, mm2</td>
<td>mmm</td>
<td>Three 2-folds</td>
</tr>
<tr>
<td>Tetragonal</td>
<td>4, 422, 4, 4mm, 42m</td>
<td>4/m, 4/mmm</td>
<td>One 4-fold</td>
</tr>
<tr>
<td>Trigonal</td>
<td>3, 32, 3m</td>
<td>$\bar{3}$, $\bar{3}m$</td>
<td>One 3-fold</td>
</tr>
<tr>
<td>Hexagonal</td>
<td>6, 622, 6, 6mm, 6m2</td>
<td>6/m, 6/mmm</td>
<td>One 6-fold</td>
</tr>
<tr>
<td>Cubic</td>
<td>23, 432, 43m</td>
<td>$m\bar{3}$, $m\bar{3}m$</td>
<td>Four 3-folds</td>
</tr>
</tbody>
</table>
The Symmetry of Bravais Lattices

Point group symmetry of the cube
- Nine mirror planes
- Three four-fold axes
- Four three-fold axes
- Six two-fold axes

Point group symmetry of the orthorhombic cell
- Three mirror planes
- Three two-fold axes
Crystal Axes and the Reciprocal Lattice
Crystal Lattice & Directions

One-dimensional lattice with parameter $a$

$$r = ua$$

Two-dimensional lattice with parameters $a$ and $b$

$$r = ua + vb$$

Two-dimensional lattice with parameters $a$ and $b$
Lattice Directions

For the lattice points $u, v, w$:

$$\mathbf{r} = u\mathbf{a} + v\mathbf{b} + w\mathbf{c}$$

For the points in space $u', v', w'$ that are not lattice points:

$$\mathbf{r} = u'\mathbf{a} + v'\mathbf{b} + w'\mathbf{c}$$

$$= (n + u_1)\mathbf{a} + (p + v_1)\mathbf{b} + (q + w_1)\mathbf{c}$$

$$= (n\mathbf{a} + p\mathbf{b} + q\mathbf{c}) + (u_1\mathbf{a} + v_1\mathbf{b} + w_1\mathbf{c})$$

$n, p, q$ – integers

$u_1, v_1, w_1$ – fractions
Indexing Lattice Directions

- Direction must pass through the origin
- Coordinates of point P (in fractions of $a$, $b$ and $c$) are $1$, $\frac{1}{2}$, $1$ \Rightarrow [212]
- For point Q coordinates are $\frac{1}{2}$, $\frac{1}{4}$, $\frac{1}{2}$ \Rightarrow [212]

[212] – defines direction for OL

For OS – the direction is [110]

\[
\mathbf{r}_{102} = 2\mathbf{a} + \mathbf{b} + 2\mathbf{c}
\]
\[
\mathbf{r}_{110} = \mathbf{a} + \mathbf{b} + 0\mathbf{c}
\]
Indexing Lattice Directions

Specific direction ⇒ [uvw]

Family of directions ⇒ <uvw>

Example:

<310>  

[3-10]
Indexing Lattice Directions

- Directions related by symmetry are called *directions of a form*.

Specific direction $\Rightarrow [uvw]$  
Family of directions $\Rightarrow <uvw>$

We have: [111], [-111], [-1-1-1], [11-1], ...
The Crystallographic Planes

\[
\begin{align*}
1 & 1 \\
2 & 1 \\
1 & 4 \\
1 & \infty \\
\end{align*}
\]

\[
\begin{align*}
1 & 1 \\
1/2 & 1 \\
1 & 1/4 \\
1 & 1/\infty \\
\end{align*}
\]

\[
\begin{align*}
1 & 1 \\
1 & 2 \\
4 & 1 \\
1 & 0 \\
\end{align*}
\]

\[
(11) \\
(12) \\
(41) \\
(10) \\
\]
Definition of the Miller Indices

Let's draw a plane at $2 \times a$, $5 \times b$, $2 \times c$.

<table>
<thead>
<tr>
<th></th>
<th>a</th>
<th>b</th>
<th>c</th>
</tr>
</thead>
<tbody>
<tr>
<td>The intercepts</td>
<td>2</td>
<td>5</td>
<td>2</td>
</tr>
<tr>
<td>The reciprocals</td>
<td>1/2</td>
<td>1/5</td>
<td>1/2</td>
</tr>
<tr>
<td>Multiply by 10</td>
<td>5</td>
<td>2</td>
<td>5</td>
</tr>
<tr>
<td>The Miller indices</td>
<td>(525)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Specific plane $\Rightarrow (hkl)$

Family of planes $\Rightarrow \{hkl\}$
Definition of the Miller Indices

- For plane A \(a/2, b/2, \text{ and } 1c \Rightarrow 2, 2, 1 \Rightarrow \text{ plane is } (221)\)
- For plane B \(1a, 1b, \text{ and } 2c \Rightarrow 1, 1, 1/2 \Rightarrow 2, 2, 1 \Rightarrow \text{ plane is } (221)\)
- For plane C \(3a/2, 3b/2, \text{ and } 3c \Rightarrow 2/3, 2/3, 1/3 \Rightarrow 2, 2, 1 \Rightarrow \text{ plane is } (221)\)
- For plane D \(2a, 2b, \text{ and } 4c \Rightarrow 1/2, 1/2, 1/4 \Rightarrow 2, 2, 1 \Rightarrow \text{ plane is } (221)\)

By the set of crystallographic planes \(hkl\), we mean a set of parallel equidistant planes, one of which passes through the origin, and the next nearest makes intercepts \(a/h, b/k, \text{ and } c/l\) on the three crystallographic axes.

The integers \(hkl\) are usually called the Miller indices.
Miller Indices
Miller Indices and Zone Axis Symbols

Closures for crystallographic indices

\([uvw]\) = square brackets designate a direction in the lattice from the origin to a point. Used to collectively include all the faces of a crystals whose intersects (i.e., edges) parallel each other. These are referred to as crystallographic zones and they represent a direction in the crystal lattice.

\(<uvw>\) – designate family of directions.

\((hkl)\) = parenthesis designate a crystal face or a family of planes throughout a crystal lattice.

\(\{hkl\}\) = "squiggly" brackets or braces designate a set of faces that are equivalent by the symmetry of the crystal. The set of face planes results in the crystal form. \(\{100\}\) in the isometric class includes \((100), (010), (001), (-100), (0-10)\) and \((00-1)\), while for the triclinic \(\{100\}\) only the \((100)\) is included.

**d-spacing** is defined as the distance between adjacent planes. When X-rays diffract due to interference amongst a family of similar atomic planes, then each diffraction plane may be reference by it's indices \(d_{hkl}\).
Miller Indices and Zone Axis Symbols

For cubic crystal:

- Direction symbols
  - <100> ⇒ [100], [-100], [010], [0 -10], [001], [00 -1]
  - <111> ⇒ [11 -1], [-1 -11], [1 -11], [-11 -1], [-111], [1 -1 -1], [111], [-1 -1 -1]
  - <110> ⇒ 12 combinations

- Miller indices
  - {100} ⇒ (100), (-100), (010), (0 -10), (001), (00 -1)

---

Orthorhombic crystal
Lattice Plane Spacings

- For crystal with orthogonal axes:
  \[ OA \cos \alpha = ON \rightarrow (a / h) \cos \alpha = d_{hkl} \rightarrow \cos \alpha = \left( \frac{h}{a} \right) d_{hkl} \]

- For angles \( \beta \) and \( \gamma \):
  \[ \cos \beta = \left( \frac{k}{b} \right) d_{hkl} \]
  \[ \cos \gamma = \left( \frac{l}{c} \right) d_{hkl} \]

- Since for orthogonal axes:
  \[ \cos^2 \alpha + \cos^2 \beta + \cos^2 \gamma = 1 \]

- We write:
  \[ \left( \frac{h}{a} \right)^2 d_{hkl}^2 + \left( \frac{k}{b} \right)^2 d_{hkl}^2 + \left( \frac{l}{c} \right)^2 d_{hkl}^2 = 1 \]

- For a cubic crystal \( a = b = c \), hence
  \[ \frac{1}{d_{hkl}^2} = \frac{h^2 + k^2 + l^2}{a^2} \]
Lattice Plane Spacings

Cubic:
\[ \frac{1}{d^2} = \frac{h^2 + k^2 + l^2}{a^2} \]

Tetragonal:
\[ \frac{1}{d^2} = \frac{h^2 + k^2 + l^2}{a^2 + c^2} \]

Hexagonal:
\[ \frac{1}{d^2} = \frac{4(h^2 + h k + k^2)}{3a^2} + \frac{l^2}{c^2} \]

Rhombohedral:
\[ \frac{1}{d^2} = \frac{(h^2 + k^2 + l^2)\sin^2 \alpha + 2(h k + k l + h l)\cos^2 \alpha - \cos \alpha}{a^2(1 - 3\cos^2 \alpha + 2\cos^3 \alpha)} \]

Orthorhombic:
\[ \frac{1}{d^2} = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2} \]

Monoclinic:
\[ \frac{1}{d^2} = \frac{1}{\sin^2 \beta} \left( \frac{h^2}{a^2} + \frac{k^2 \sin^2 \beta}{b^2} + \frac{l^2}{c^2} - \frac{2h l \cos \beta}{a c} \right) \]

Triclinic:
\[ \frac{1}{d^2} = \frac{1}{V^2} \left( S_{11} h^2 + S_{22} k^2 + S_{33} l^2 + 2S_{12} h k + 2S_{23} k l + 2S_{13} h l \right) \]

\[ V = \text{volume of unit cell} \]
\[ S_{11} = b^2 c^2 \sin^2 \alpha, \]
\[ S_{22} = a^2 c^2 \sin^2 \beta, \]
\[ S_{33} = a^2 b^2 \sin^2 \gamma, \]
\[ S_{12} = abc^2 (\cos \alpha \cos \beta - \cos \gamma), \]
\[ S_{23} = a^2 b c (\cos \beta \cos \gamma - \cos \alpha), \]
\[ S_{13} = a b^2 c (\cos \gamma \cos \alpha - \cos \beta). \]
Special Case: Trigonal & Hexagonal Lattices

- (1 -10), (100), and (010) are indices different in type but describe crystallographically equivalent lattice planes.
- Introducing the fourth axis – U. We have Miller-Bravais indices \((hkil)\).
- All indices of the planes are of the same form – \(\{10\ -10\}\).

\[h + k + i = 0 \Rightarrow i = -(h + k) \Rightarrow \{hk.l\}\]
The Reciprocal Lattice

Reciprocal lattice vectors

\[ \mathbf{d}_1^* = K / d_1, \]
\[ \mathbf{d}_2^* = K / d_2, \]
\[ \mathbf{d}_3^* = K / d_3 \]

\( K \) – is a constant
The Reciprocal Lattice
The Reciprocal Lattice

Monoclinic unit cell planes \( \{h0l\} \)

Reciprocal lattice vectors

Reciprocal lattice unit cell

\[
\mathbf{a}^* = d_{100}^* \quad \text{and} \quad |\mathbf{a}^*| = 1/d_{100};
\]

\[
\mathbf{c}^* = d_{001}^* \quad \text{and} \quad |\mathbf{c}^*| = 1/d_{001}.
\]
The Reciprocal Lattice

$h0l$ section

$h1l$ section
The Reciprocal Lattice

- Consider a real space unit cell with real lattice basis vectors \( \mathbf{a}, \mathbf{b} \) and \( \mathbf{c} \).
- We define a set of reciprocal lattice basis vectors by:

\[
\mathbf{a}^* = \frac{1}{V} (\mathbf{b} \times \mathbf{c}) = \frac{\mathbf{b} \times \mathbf{c}}{\mathbf{a} \cdot (\mathbf{b} \times \mathbf{c})}
\]

\[
\mathbf{b}^* = \frac{1}{V} (\mathbf{c} \times \mathbf{a})
\]

\[
\mathbf{c}^* = \frac{1}{V} (\mathbf{a} \times \mathbf{b})
\]

- \( \mathbf{c}^* \) \perp a-b plane
- Volume of real space unit cell

volume of real space unit cell

volume of real space unit cell
The Reciprocal Lattice

Just like we can define a real space lattice in terms of our real space lattice vectors, we can define a reciprocal space lattice in terms of our reciprocal space lattice vectors:

\[ \mathbf{r}^* = \mathbf{d}_{hkl}^* = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^* \]

The real and reciprocal space lattice vectors form an orthonormal set:

\[ \begin{align*}
\mathbf{a}^* \cdot \mathbf{b} &= \mathbf{a}^* \cdot \mathbf{c} = 0 \\
\mathbf{a}^* \cdot \mathbf{a} &= 1 \\
\text{similar for } \mathbf{b}^* \text{ and } \mathbf{c}^*
\end{align*} \]

We can define a reciprocal unit cell with volume \( V^* \):

\[ V^* = \mathbf{a}^* \cdot (\mathbf{b}^* \times \mathbf{c}^*) \]

\[ V^* \cdot V = 1 \]

Now we can write:

\[ \mathbf{r}_{uvw} = u\mathbf{a} + v\mathbf{b} + w\mathbf{c} \]

\[ \mathbf{d}_{hkl}^* = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^* \]
The Reciprocal Lattice

Plan of a cubic $I$ crystal \perp $z$-axis

Reciprocal lattice points
The Reciprocal Lattice

Cubic $F$ reciprocal lattice unit cell of a cubic $I$ direct lattice

Cubic $I$ reciprocal lattice unit cell of a cubic $F$ direct lattice
The Reciprocal Lattice

- **d-spacing of lattice planes**

  \[ d_{hkl}^* = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^* \]

  \[ d_{hkl}^* \cdot d_{hkl}^* = \frac{1}{d_{hkl}^2} = (h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*) \cdot (h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*) \]

  for orthorombic, tetragonal, cubic:  \[ \mathbf{a}^* \cdot \mathbf{b}^* = 0 \]

  therefore:

  \[ \frac{1}{d_{hkl}^2} = h\mathbf{a}^* \cdot h\mathbf{a}^* + k\mathbf{b}^* \cdot k\mathbf{b}^* + l\mathbf{c}^* \cdot l\mathbf{c}^* = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2} \]

  \[ \left( \mathbf{a}^* \cdot \mathbf{a}^* = \frac{1}{a^2} \right) \]

- **Angle \( \rho \)** between plane normals \((h_1 k_1 l_1)\) and \((h_2 k_2 l_2)\)

  the angle between two vectors is  \[ \cos \rho = \frac{\mathbf{a} \cdot \mathbf{b}}{ab} \]

  therefore:

  \[ \cos \rho = \frac{d_{h_1 k_1 l_1}^* \cdot d_{h_2 k_2 l_2}^*}{\left| d_{h_1 k_1 l_1}^* \right| \left| d_{h_2 k_2 l_2}^* \right|} \]