## Symmetry of Molecules and Crystals

## What does symmetry mean?

Symmetry (Greek = harmony, regularity) means the repetition of a motif and thus the agreement of parts of an ensemble (Fig. 1).


Fig. 1 Examples of symmetric objects
Symmetry can also mean harmony of proportions, or stability, order, and beauty.

## Definition:

An object is symmetric if it is left invariant by a transformation, i.e., cannot be distinguished before and after transformation.

## Symmetry transformations, operations, elements are:

| Symbol* |  | Symmetry operation |
| :---: | :---: | :---: |
| Sch | HM | * Notation of symmetry elements after Schönflies (Sch for moleculs) and International Notation after Hermann/Mauguin (HM for crystals) |
| E | (1) | identity (E from "Einheit" = unity, an object is left unchanged) |
| $\mathrm{C}_{\mathrm{n}}$ | (n) | properrotation through an angle of $2 \pi / \mathrm{hrad}$. |
| $S_{n}$ |  | improperrotation through an angle of $2 \pi / \mathrm{n} \mathrm{rad}$. followed by a reflection in a plane perpendicular to the axis (rotation-reflection axis) |
|  | $\bar{n}$ | improperrotation through an angle of $2 \pi / \mathrm{hrad}$. followed by a reflection through a point on the axis (rotationinversion axis) |
| i | 1 | inversion (point reflection) $\left(\overline{1} \equiv \mathrm{~S}_{2}\right) \rightarrow$ ( $\mathrm{x}, \mathrm{y}, \mathrm{z} \rightarrow-\mathrm{x},-\mathrm{y},-\mathrm{z}$ in Cartesian coordinates) |
| $\sigma$ | m | mirror plane (from "Spiegel") |
| $\sigma_{\text {h }}$ |  | horizontal reflection in a plane passing through the origin and perpendicular to the axis with highest symmetry |
| $\sigma_{\mathrm{v}}$ |  | vertical reflection in a plane passing through the origin and the axis with highest symmetry |
| $\sigma_{\text {d }}$ |  | diagonal reflection in a plane as $\sigma_{v}$ and bisecting the angle between the two-fold axis perpendicular to the axis of highest symmetry |
|  | $\overrightarrow{\mathrm{t}}$ | translation $\vec{t}=\mathrm{n}_{1} \cdot \vec{a}+\mathrm{n}_{2} \cdot \vec{b}+\mathrm{n}_{3} \cdot \vec{c}$ |
|  |  | 1. column: notation after Schönflies (molecules) |
|  |  | 2. column: notation after Hermann/Mauguin (crystals) |

Symmetry classes and combinations $\Rightarrow$ point groups (see Table 1) (in a point group at least one point in space is left invariant by the operation)

Table 1 Point groups of molecules and polyhedra*

| Point gr. | Sym elements* | h*** | Point gr. | Sym elements* | h*** |
| :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathrm{C}_{1}$ | E | 1 | $\mathrm{C}_{\mathrm{i}}$ | i | 2 |
| $\mathrm{C}_{\text {s }}$ | $\sigma$ | 2 | $\mathrm{C}_{\mathrm{n}}$ | $\mathrm{C}_{\mathrm{n}}$ | n |
| $\mathrm{S}_{\mathrm{n}}$ | $\mathrm{S}_{\mathrm{n}}$ | n | $\mathrm{C}_{\mathrm{nv}}$ | $\mathrm{C}_{\mathrm{n}}, \mathrm{n} \sigma_{\mathrm{v}}$ | 2n |
| $\mathrm{C}_{\text {nh }}$ | $\mathrm{C}_{\mathrm{n}}, \mathrm{\sigma}_{\mathrm{h}}$ | 2n | $\mathrm{D}_{\mathrm{n}}$ | $\mathrm{C}_{\mathrm{n}}, \mathrm{nC}_{2} \perp \mathrm{C}_{\mathrm{n}}$ |  |
| $\mathrm{D}_{\text {nd }}$ | $\mathrm{C}_{\mathrm{n}}, \mathrm{nC}_{2} \perp \mathrm{C}_{\mathrm{n}}, \mathrm{n} \mathrm{\sigma}_{\mathrm{d}}$ | 4 n | $\mathrm{D}_{\text {nh }}$ | $\mathrm{C}_{\mathrm{n}}, \mathrm{nC}_{2} \perp \mathrm{C}_{\mathrm{n}}, \sigma_{\mathrm{h}}, \mathrm{n} \mathrm{\sigma}_{\mathrm{v}}$ | 4 n |
| $\mathrm{C}_{\text {ov }}$ | linear no i | $\infty$ | $\mathrm{D}_{\text {oh }}$ | linear with i | $\infty$ |
| T | tetrahedral | 12 | O | oktahedral | 24 |
| $\mathrm{T}_{\mathrm{d}}$ |  | 24 | $\mathrm{O}_{\mathrm{h}}$ | (cubic) | 48 |
| $\mathrm{T}_{\mathrm{h}}$ |  | 24 |  |  |  |
| $\begin{aligned} & \hline \mathrm{I} \\ & \mathrm{I}_{\mathrm{h}} \\ & \hline \end{aligned}$ | ikosahedral | $\begin{gathered} \hline 60 \\ 120 \end{gathered}$ | $\mathrm{K}_{\mathrm{h}}$ | spherical | $\infty$ |

* Schoenflies notation, ** Important symmetry elements, *** Order h (number of repetitions)

The point groups of some inorganic and organic compounds and the schematic representation of the symmetries of some important objects and polyhedra with their orders (repetitions) $n=2,3,4,5,6$ and $\infty$ are shown in Figs. 2a und 2b.










chiral!

$\mathrm{C}_{60} \mathrm{I}_{\mathrm{h}}$

Abb. 2a Point groups of some inorganic and organic molecules


Figure 12-8
Atkins Physical Chemistry, Eighth Edition
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Fig. 2b Schematic representation of some figures and polyhedra with their symmetry properties, orders $n$ and point groups

The point group notation after Hermann-Mauguin is given in the part Crystal symmetry.

As exercise (find, note and systematize), the symmetry elements and point groups of some molecules (without electron pairs) are listed in Fig. 3. A symmetry flow chart is given in Fig. 4.


Fig. 3 Point groups and symmetry elements of some molecules

## Systematic search for a point group of a given molecule



Figure 7-9
Shriver \& Atkins Inorganic Chemistry, Fourth Edition
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Fig. 4 Symmetry flow chart for the determination of point groups

## Representation/demonstration of symmetry properties

To demonstrate the symmetry properties of three-dimensional (spatial) objects (e.g. molecules, optional figures or frames, polyhedra, crystals) in a plane, projections like e.g. the stereographic projection are used (Fig. 5).


Fig. 5 Principle of a stereographic projection
The treated object, polyhedron, crystal etc. is positioned at the center of a sphere so that his main symmetry axis (axis of highest symmetry) is oriented perpendicularly to the equatorial plane. Its surface normals or center beams will meet the surface of the sphere at the so called point or plane pole P . The connecting line of the point or plane pole P with the opposite sphere pole (north or south pole) will meet the equatorial (projection) plane at the projection point $P$ ' of the point or plane pole $P$.
The angle between two point or plane poles corresponds to the angle between two center beams or the normal angles of two of the figure or crystal faces (normal angle $=180^{\circ}$ - plane angel), respectively, and gives the equatorial angle (azimuth $\beta$ ) and the vertical angle ( $90^{\circ}$ - pole altitude $\alpha$ ).
I.e., the stereographic projection is isogonal (s. Fig. 6 und 7).


Fig. 6 Stereographic projection of a tetragonal prism (a) and tetragonal pyramid (b). The angle coordinates $\varphi=\beta$ and $\delta=\alpha$ of the planes of the pyramid are also given.


Fig. 7 Plane poles and stereographic projection of a galenite crystal
The plane poles of a crystal mostly are positioned on few great circles. The corresponding planes belong to so called crystal zones. The zone axis is oriented perpendicularly to the plane of the respective great circle.
With the help of stereographic projections one can show/demonstrate, point or plane poles, plane angles, and thus the symmetry properties of molecules, polyhedra, or crystals.

## Symmetry and geometry of crystals

The basic feature of the crystalline state is (idealized) the high degree of order, i.e., the components of crystals (atoms, molecules, ions) are repeated in a regular way, i.e., are 3D periodic (Kepler, 1611; Hooke, 1665; Bergmann, 1773; Haüy, 1782)


CRYSTAL STRUCTURE
Fig. 8 Representation of a (2D) crystal structure
Crystals can be described as consisting of a structural motif (one or more atoms, molecules, ions) belonging to one lattice point and being repeated by a 3D lattice translation (Fig. 8).
Structural motiv (basis) + 3D translation (crystal lattice) $\rightarrow$ Crystal structure Unit cell: Parallelepiped representing crystal lattice+crystal structure (Fig. 9)


Fig. 9 Unit cells with unit cell vectors (lattice translations) $\vec{a}, \vec{b}, \vec{c}$.

Motif (basis), unit cell, crystal lattice and crystal structure have a definite, combined symmetry (Fig. 9).


Fig. 9 Translational repetitions of symmetric motifs.
The asymmetric unit is repeated by symmetry $m$ (a) and 4 (b), resulting in 2D lattice arrangements of symmetry $m$ (a) and 4 (b), respectively.

## Crystallographic symmetry elements/operations

Since crystals are 3D translational subjects, only space filling symmetry elements are allowed. Besides a mirror plane (m) and an inversion center ( $\overline{1}$ ), those space filling symmetry elements are the rotation axes $1,2,3,4$, and 6 only (Figs. 10, 11, 12).










| rotation axes: 1,2,3,4,6 | mirror plane: m | translations: $\vec{a}, \vec{b}, \vec{c}$ |
| :--- | :--- | :--- | as well as their combinations including $\overline{1}$ (Hermann/Mauguin)

Fig. 10 Space filling symmetry elements $(\mathrm{n}=5,7,8, \ldots$ not allowed)


Table 1-1 Conventional designation of improper axes

| Rotoinversion <br> axis | Rotoreflection <br> axis | Conventional designation |  |
| :--- | :--- | :--- | :--- |
| $\overline{1}$ | $\tilde{2}$ | Center of symmetry | $\overline{1}$ |
| $\overline{2}$ | $\tilde{1}$ | Mirror plane | $m$ |
| $\overline{3}$ | $\tilde{6}$ | 3 -fold rotoinversion | $\overline{3}$ |
| $\overline{4}$ | $\overline{4}$ | 4-fold rotoinversion | $\overline{4}$ |
| $\overline{6}$ | $\tilde{3}$ | 6-fold rotoinversion | $\overline{6}$ |


1

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2

3

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4


$\tilde{4}$



I

$\overline{2}$

$\overline{3}$

$\overline{4}$


Fig. 11 Demonstration, designation, and stereographic projections of proper and improper crystallographic (space filling) axes


Fig. 12 The 10 crystallographic (space filling) point group elements

## Crystal classes (crystallographic point groups)

Omitting translations, there are exactly 32 combinations possible for crystals, resulting inexactly 32 crystallographic point groups or crystal classes.
They are used for the description of the morphology of crystals and represented e.g. in form of stereographic projections (Fig 13).


Fig. 13 Stereographic representation of the 32 crystal classes

## Lattice symmetry (holoedric classes, crystal systems)

Also crystal lattices and the related parallelepipeds (unit cells) have a special symmetry (exactly 7 possibilities) $\rightarrow$ holoedric classes and crystal systems with different orientations/relations of the crystal axes (Figs. 14, 15).


Monoclinic



Orthorhombic


Trigonal


Hexagonal

Figure $3-2$
Shriver \& At
Shriver \& Atkins Inorganic Chemistry, Fourth Edition
Fig. 14 Crystal systems and lattice constants

| System | Number of lattices in system | Lattice symbols | Nature of unitcell axes and angles ${ }^{(1)}$ | Lengths and angles to be specified | Symmetry of lattice ${ }^{(2)}$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Triclinic | 1 | $P$ | $\begin{aligned} & a \neq b \neq c \\ & a \neq \beta \neq \gamma \end{aligned}$ | $\begin{aligned} & a, b, c \\ & a, \beta, \gamma \end{aligned}$ | I |
| Monocimic ${ }^{(3)}$ | 2 | 1st setting $\left\lvert\, \begin{aligned} & P \\ & B\end{aligned}\right.$ | $\begin{aligned} & a \neq b \neq c \\ & a=\beta=90^{\circ} \neq \gamma \end{aligned}$ | $a, b, c$ | 2/m |
|  |  | 2nd setting $\left\{\begin{array}{l}P \\ C\end{array}\right.$ | $\begin{aligned} & a \neq b \neq c \\ & a=\gamma=90^{\circ} \neq \beta \end{aligned}$ | $\underset{\beta}{a, b, c}$ |  |
| Orthorhombic | $4$ | $P$ $C^{(4)}$ $I$ $F$ | $\begin{aligned} & a \neq b \neq c \\ & a=\beta=\gamma=90^{\circ} \end{aligned}$ | $a, b, c$ | mmm |
| Tetragonal | 2 | $\begin{aligned} & P^{(s)} \\ & I \end{aligned}$ | $\begin{aligned} & a=b \neq c \\ & a=\beta=\gamma=90^{\circ} \end{aligned}$ | $a, c$ | $4 / \mathrm{mmm}$ |
| Cubic | 3 | $P$ $I$ $F$ | $\begin{aligned} & a=b=c \\ & a=\beta=\gamma=90^{\circ} \end{aligned}$ | $a$ | m3m |
| Trigonal | 1 | $R^{(\theta)}$ | $\begin{aligned} & a=b=c \\ & a=\beta=\gamma \\ & <120^{\circ}, \neq 90^{\circ} \end{aligned}$ | a | 3 m |
| Hexagonal | -1 | $P^{(7)}$ | $\begin{aligned} & a=b \neq c \\ & a=\beta=90^{\circ} \\ & \gamma=120^{\circ} \end{aligned}$ | a, c | $6 / \mathrm{mmm}$ |

Fig. 15 Crystal systems, unit cell axes and angles of the 7 holoedric classes

## Bravais lattices (centered cells/lattices)

Normally there is only 1 lattice point per unit cell (P), but for special axis relations $\left(\vec{t}_{1} \cdot\left(\vec{t}_{2}-\vec{t}_{1}\right)\right)$ a higher symmetry (with orthogonal axes) is possible under increase of the lattice point number per unit cell to 2 or $4 \rightarrow$ centered cells C (2), I (2), R (2), F (4) $\rightarrow 14$ Bravais lattices.


Fig. 16 The 14 Bravais lattices with their coordinate systems, lattice constants, and space group symbols

## Space groups (3D symmetry groups)

Inclusion of translation $\vec{t}$ results in further symmetry elements, the so-called translation symmetry elements, the screw axis and glide planes (Fig. 17)


Fig. 17 Effect of an inversion center, a screw axis, and a glide plane

## Translation symmetry elements are:

a) screw axis: $n_{m}$

Rotation by $2 \pi / \mathrm{n}$ and translation II to the screw axis by $\mathrm{m} / \mathrm{n} \cdot|\vec{t}|$ $\left(2_{1}, 3_{1}, 3_{2}, 4_{1}, 4_{3}, 4_{2}, 6_{1}, 6_{5}, 6_{2}, 6_{4}, 6_{3}\right.$ are possible, see Fig. 18).


Fig. 18 Crystallographic screw axes $\mathrm{n}_{\mathrm{m}}$
b) glide planes: $a, b, c, n, d$

Reflection and translation parallel to the mirror plane by $\vec{a} / 2$ II $\vec{a}$ for $a ; \vec{b} / 2 \| \vec{b}$ for $b ; \vec{c} / 2$ II c for $c$ by $|\vec{a}+\vec{b}| / 2,|\vec{b}+\vec{c}| / 2,|\vec{a}+\vec{c}| / 2$ parallel $\vec{a}+\vec{b}, \vec{b}+\vec{c}, \vec{a}+\vec{c}$ for $n$ by $|\vec{a}+\vec{b}| / 4,|\vec{b}+\vec{c}| / 4,|\vec{a}+\vec{c}| / 4$ parallel $\vec{a}+\vec{b}, \vec{b}+\vec{c}, \vec{a}+\vec{c}$ for $d$ (for I and F cells only)

Combination of axes/planes and translations are restricted by the 3D periodicity of the crystal lattices.

Combination of the 14 Bravais lattices with the "space filling" point groups/ symmetry elements results in the 230 (3D) space groups (e.g. Fig. 19).

Point groups: describe the symmetry of crystal faces. Space groups: describe the symmetry of crystal bulks.

A summary of all symmetry elements of the 230 space groups are given in the International Tables for Crystallography, Vol. A (see e.g. Fig. 19).


Fig. 19 Example of space group information

## Atomic coordinates, equivalent positions

There are 3 possibilities for the description of crystal structures:

1. Every (translatorial) independent type of atom has its own crystal lattice and the total crystal structure is given as the sum of all the (shifted) "atomic translation lattices" all with the same basic translations $\vec{a}, \vec{b}, \vec{c}$.
2. The crystal structure is given as the sum of the motiv or basis and the translation or Bravais lattice.
3. Basis and lattice translations are represented/extracted by/from the parallel epiped (unit cell: P, C, I, F, R) built by the basic lattice translations $\vec{a}, \vec{b}, \vec{c}$.

The best and simplest description/representation of a crystal structure is the unit cell with its basic translations $(\vec{a}, \vec{b}, \vec{c})$ or the lattice constants ( $\mathrm{a}, \mathrm{b}, \mathrm{c}, \alpha$, $\beta, \gamma)$ and its content (atoms, ions, molecules etc.).

The atomic positions in the unit cell are given by the position vectors

$$
\vec{r}_{\mathrm{j}}=\mathrm{x} \cdot \vec{a},+\mathrm{y} \cdot \vec{b}+\mathrm{z} \cdot \vec{c}
$$

or (abbreviated) by their (contravariant) vector components $x, y, z$.
If the space group is known, the non-symmetric part of the unit cell, i.e. the asymmetric unit, is sufficient for describing the complete (ideal) crystal structure by using the equivalent positions listed in the International Tables.

## Lattice planes, sets (families) of lattice planes, Miller indices

Parallel planes through all the points of a crystal lattice form sets of planes with equidistant atoms and spacings (distances $d$ of the planes of such a set of planes), where the atomic distances and spacings depend on the orientation of those planes with respect to the lattice/unit cell vectors $\vec{a}, \vec{b}$, and $\vec{c}$ (Fig. 20).


Lattice or unit cell vectors $\vec{a}, \vec{b}, \vec{c} \quad$ Miller indices (hkl) $\quad$ Spacings $\mathrm{d}_{(\mathrm{hkl})}$

Fig. 20 Sets of lattice planes (hkl) with different orientation and spacings $d_{n}$ (or $\mathrm{d}_{(\mathrm{hkl})}$ ) for a monoclinic 3D point lattice projected parallel $-\vec{c}$

Each set of planes divide the lattice axes $\vec{a}, \vec{b}$, and $\vec{c}$ into an integral number of equal parts (see Fig. 20). These fractional intercepts h (for $\vec{a}$ ), k (for $\vec{b}$ ), and 1 (for $\vec{c}$ ) are the so-called Miller index triples or Miller indices (hkl).

A specific set of planes is characterized by the Miller indices (hkl) and also by its normal vector $\vec{n}$ (length 1) and the respective spacing $\mathrm{d}_{\mathrm{n}}$ or $\mathrm{d}_{(\mathrm{hkl})}$ (Fig. 21).


Fig. 21 Three different sets of lattice planes of a monoclinic 3D point lattice (lattice vectors $\vec{a}, \vec{b}$, and $\vec{c}$, projected parallel $-\vec{c}$ ) with their normal vectors $\vec{n}_{\mathrm{i}}$, spacings $\mathrm{d}_{\mathrm{i}}$, and Miller indices (hkl)

Sets of planes, crystal faces, sets of symmetry equivalent planes or faces, and directions in a crystal or point lattice are described as follows:
(hkl) define sets of lattice planes and crystal faces
e.g. $(100) \equiv \mathrm{yz}$ or bc plane, $(010) \equiv \mathrm{xz}$ or ac plane, $(001) \equiv \mathrm{xy}$ or ab plane
\{hkl\} define symmetry equivalent sets of planes and crystal faces
e.g. $\{100\}_{\text {cubic }} \equiv(100),(010),(001),(-100),(0-10),(00-1)$
[uvw] define directions in a crystal lattice and a crystal corresponding to the components of the translation vector $\vec{t}=\mathrm{u} \cdot \vec{a}+\mathrm{v} \cdot \vec{b}+\mathrm{w} \cdot \vec{c} \quad$ e.g. $[100] \equiv \mathrm{x}$ or a axis, $[010] \equiv \mathrm{y}$ or b axis, $[001] \equiv \mathrm{z}$ or c axis

Some examples of sets of lattice planes with their spacings $d_{(\mathrm{hkl})}$ and of origin nearest lattice planes representing specific sets of lattice planes and the corresponding Miller indices are given in Fig. 22. For the definition of directions see Fig. 23.


$d_{110}=1 / 2 \sqrt{2} a$

$d_{111}=1 / 3 \sqrt{3} a$

$d_{222}=1 / 2^{1 / 1 / 3} \sqrt{3} a$

$d_{200}=a / 2$


Origin at lower left front


Fig. 22 Examples of lattice planes and plane sets with their Miller indices

To construct the origin nearest lattice plane of a lattice plane set (hkl) please:

1. select the origin 000,
2. mark intercepts $1 / \mathrm{h}, 1 / \mathrm{k}, 1 / \mathrm{l}$ of the plane (hkl) on $\vec{a}, \vec{b}$, and $\vec{c}$, 3. draw the plane.

For negative indices, first shift the origin accordingly.


Fig. 23 Directions [hkl] in crystal lattices and crystals

## Reciprocal lattice (labelling of lattice planes and lattice plane sets)

Lattice plane sets of a crystal or crystal lattice with basis vectors $\vec{a}, \vec{b}$, and $\vec{c}$,are characterized by their plane normals $\vec{n}_{(\mathrm{hkl})}$ and spacings $\mathrm{d}_{(\mathrm{hkl})}$.
The endpoints of vectors $\left(1 / \mathrm{d}_{\mathrm{n}}\right) \cdot \vec{n}_{\mathrm{n}}$ or $\left(1 / \mathrm{d}_{(\mathrm{hkl})}\right) \cdot \vec{n}_{(\mathrm{hkl})}$, respectively, form a point lattice named reciprocal lattice (Fig. 24)


Fig. 24 Relation between crystal lattice (left) and reciprocal lattice (right)

The relation between the basis vectors $\vec{a}^{*}, \vec{b}^{*}, \vec{c}^{*}$ of the reciprocal lattice and the basis vectors $\vec{a}, \vec{b}$, and $\vec{c}$, of the crystal lattice is demonstrated in Fig. 25.


Fig. 25 Relation between crystal lattice planes and the reciprocal lattice
The respective vector equations are

$$
\overrightarrow{a^{*}}=\frac{\vec{b} \times \vec{c}}{\vec{a} \cdot \vec{b} \times \vec{c}} ; \quad \overrightarrow{b^{*}}=\frac{\vec{c} \times \vec{a}}{\vec{a} \cdot \vec{b} \times \vec{c}} ; \quad \overrightarrow{c^{*}}=\frac{\vec{a} \times \vec{b}}{\vec{a} \cdot \vec{b} \times \vec{c}}
$$

with the reciprocal lattice vectors vectors

$$
\overrightarrow{\delta_{h k l}}=h \overrightarrow{a^{*}}+k \overrightarrow{b^{*}}+l \overrightarrow{c^{*}} \text { or } \overrightarrow{H_{h k l}}=h \overrightarrow{a^{*}}+k \overrightarrow{b^{*}}+l \overrightarrow{c^{*}}
$$

The following relations are valid

$$
\begin{gathered}
\overrightarrow{a^{*}} \cdot \overrightarrow{b^{*}} \times \overrightarrow{c^{*}}=\mathrm{V}^{*}, \quad \vec{a} \cdot \vec{b} \times \vec{c}=\mathrm{V}=1 / \mathrm{V}^{*}, \vec{a} \cdot \overrightarrow{a^{*}}=\vec{b} \cdot \overrightarrow{b^{*}}=\vec{c} \cdot \overrightarrow{c^{*}}=1, \\
\vec{a} \cdot \overrightarrow{b^{*}}=\vec{a} \cdot \overrightarrow{c^{*}}=\vec{b} \cdot \overrightarrow{c^{*}}=\overrightarrow{a^{*}} \cdot \vec{b}=\overrightarrow{a^{*}} \cdot \vec{c}=\vec{c}=0 .
\end{gathered}
$$

In orthogonal lattice systems (all angles are $90^{\circ}$ ) one has

$$
a=1 / a^{*}, b=1 / b^{*}, c=1 / c^{*} .
$$

Relations between the spacings $\mathrm{d}(\mathrm{hkl})$, reciprocal spacings $1 / \mathrm{d}(\mathrm{hkl})$ and the lattice constants $\mathrm{a}, \mathrm{b}$, and c of the 7 crystal systems are given in Table 2.

Table 2 Reciprocal spacings $1 / \mathrm{d}((\mathrm{hkl}))$ and lattice vectors $\mathrm{a}, \mathrm{b}$, and c

| System | $1 / d_{h k l}^{2}$ |
| :--- | :--- |
| Cubic | $\left(h^{2}+k^{2}+l^{2}\right) / a^{2}$ |
| Tetragonal | $\frac{h^{2}+k^{2}}{a^{2}}+\frac{l^{2}}{c^{2}}$ |
| Orthorhombic | $\frac{h^{2}}{a^{2}}+\frac{k^{2}}{b^{2}}+\frac{l^{2}}{c^{2}}$ |
| Hexagonal and <br> trigonal (P) | $\frac{4}{3 a^{2}}\left(h^{2}+k^{2}+h k\right)+\frac{l^{2}}{c^{2}}$ |
| Trigonal (R) | $\frac{1}{a^{2}}\left(\frac{\left(h^{2}+k^{2}+l^{2}\right) \sin ^{2} \alpha+2(h k+h l+k l)\left(\cos ^{2} \alpha-\cos \alpha\right)}{1+2 \cos ^{3} \alpha-3 \cos ^{2} \alpha}\right)$ |
| Monoclinic | $\frac{h^{2}}{a^{2} \sin ^{2} \beta}+\frac{k^{2}}{b^{2}}+\frac{l^{2}}{c^{2} \sin ^{2} \beta}-\frac{2 h l \cos \beta}{a c \sin ^{2} \beta}$ |
| Triclinic | $\left(1-\cos ^{2} \alpha-\cos ^{2} \beta-\cos ^{2} \gamma+2 \cos \alpha \cos \beta \cos \gamma\right)^{-1}\left(\frac{h^{2}}{a^{2}} \sin ^{2} \alpha\right.$ |
|  | $+\frac{k^{2}}{b^{2}} \sin ^{2} \beta+\frac{l^{2}}{c^{2}} \sin ^{2} \gamma+\frac{2 k l}{b c}(\cos \beta \cos \gamma-\cos \alpha)$ |
|  | $\left.+\frac{2 l h}{c a}(\cos \gamma \cos \alpha-\cos \beta)+\frac{2 h k}{a b}(\cos \alpha \cos \beta-\cos \gamma)\right)$ |

