Lecture 2) (1

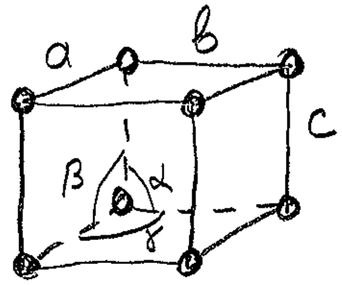
Classification of Bravais lattices and Crystal structures

7 Crystal systems

The symmetry of the Bravais lattices can be characterised by the symmetry of its building block - unit cell. 5 different 2d Bravais lattices from Lecture 1 were determined by the symmetry of parallelogram → rectangle → square → rhombus → rhombus with angle = 60°.

In the same way we can define symmetrie of the 3d Bravais lattice. We start with most symmetric cubic lattice and will deform it reducing symmetry step by step.

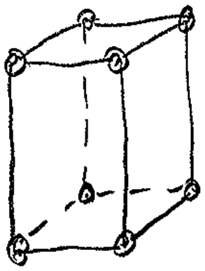
1. The most symmetric is the <u>cubic</u> system



$a = b = c$

$\alpha = \beta = \gamma = 90^\circ$

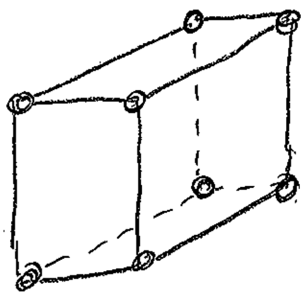
2. Stretching it along the c axis we obtain <u>tetragonal</u> system



$a = b \neq c$

$\alpha = \beta = \gamma = 90^\circ$

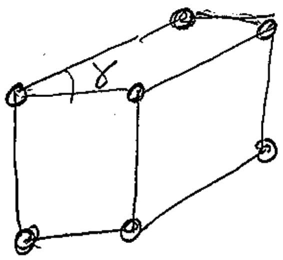
3. We can further reduce symmetry by stretching it along the a (or b) axis making rectangular base out of square one.
Such lattice system is called orthorhombic



$a \neq b \neq c$

$\alpha = \beta = \gamma = 90^\circ$

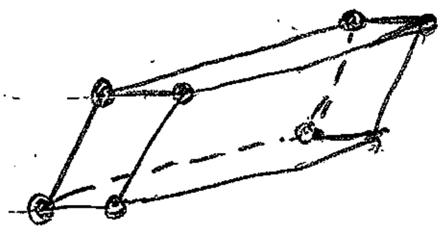
4) One can reduce ortho-rhombic symmetry by deforming top and bottom rectangular faces $\perp$ c into parallelogram $\Rightarrow$ Monoclinic



$a \neq b \neq c$

$\gamma \neq \alpha = \beta = 90^\circ$

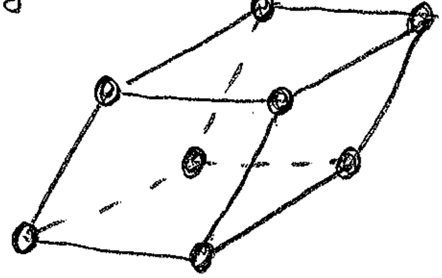
5) Shifting top face with respect to the bottom we obtain the crystal system with the least symmetry – triclinic



$a \neq b \neq c$

$\alpha \neq \beta \neq \gamma \neq 90^\circ$

6) If we stretch the cube along its body diagonal we obtain the trigonal or rhombohedral system

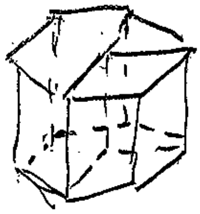


$a = b = c$

$\alpha = \beta = \gamma \neq 90^\circ$

7) l.m.

7) Last system is hexagonal it is obtained from monoclinic by making parallelogram to rhombus with $\gamma = 120°$. It has obvious analog with the 2d hexagonal Bravais lattice.



$a = b \neq c$

$\alpha = \beta = 90°, \gamma = 120°$

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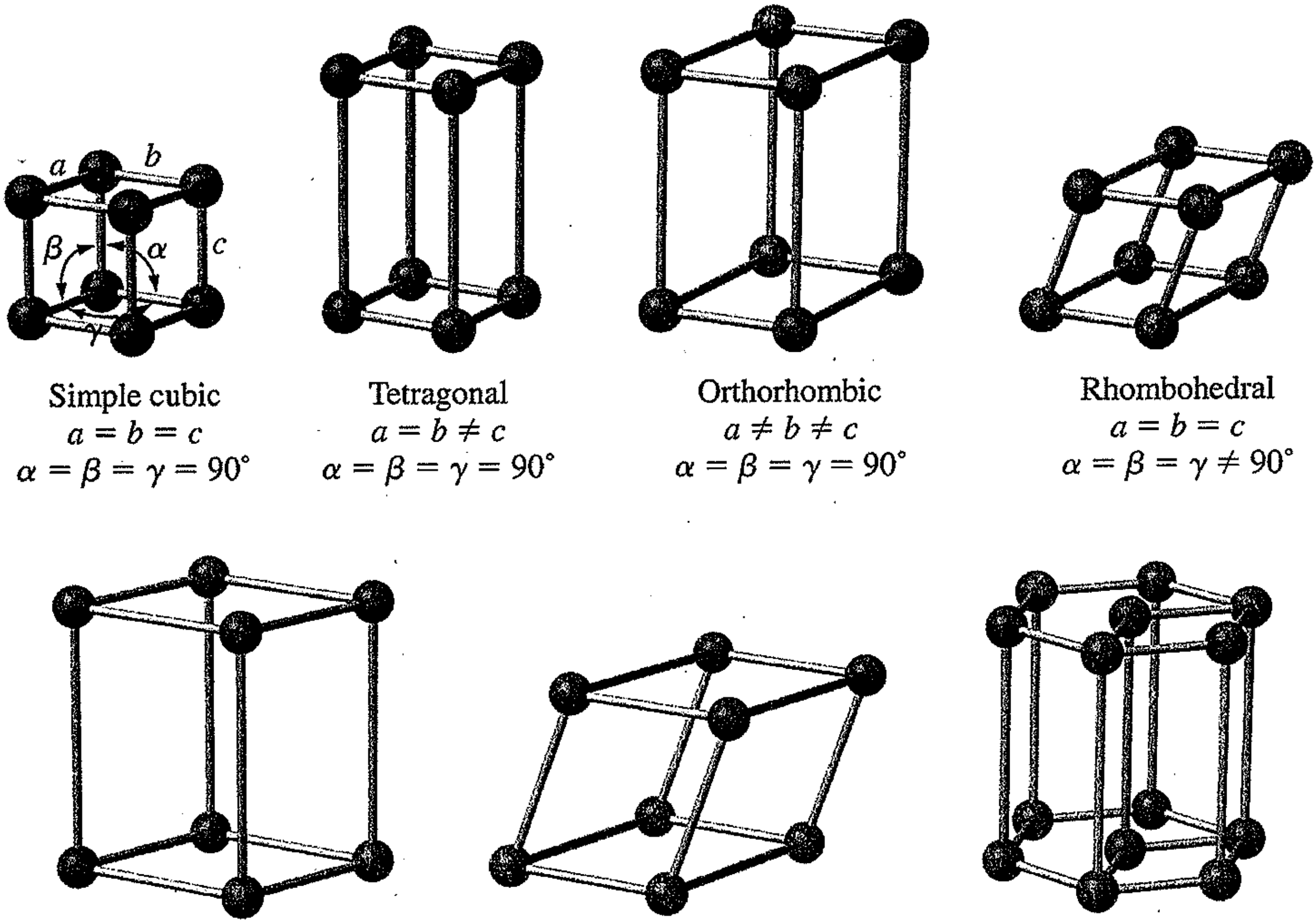


Simple cubic
$a = b = c$
$\alpha = \beta = \gamma = 90°$

Tetragonal
$a = b \neq c$
$\alpha = \beta = \gamma = 90°$

Orthorhombic
$a \neq b \neq c$
$\alpha = \beta = \gamma = 90°$

Rhombohedral
$a = b = c$
$\alpha = \beta = \gamma \neq 90°$

Monoclinic
$a \neq b \neq c$
$\gamma \neq \alpha = \beta = 90°$

Triclinic
$a \neq b \neq c$
$\alpha \neq \beta \neq \gamma \neq 90°$

Hexagonal
$a = b \neq c$
$\alpha = \beta = 90°, \gamma = 120°$

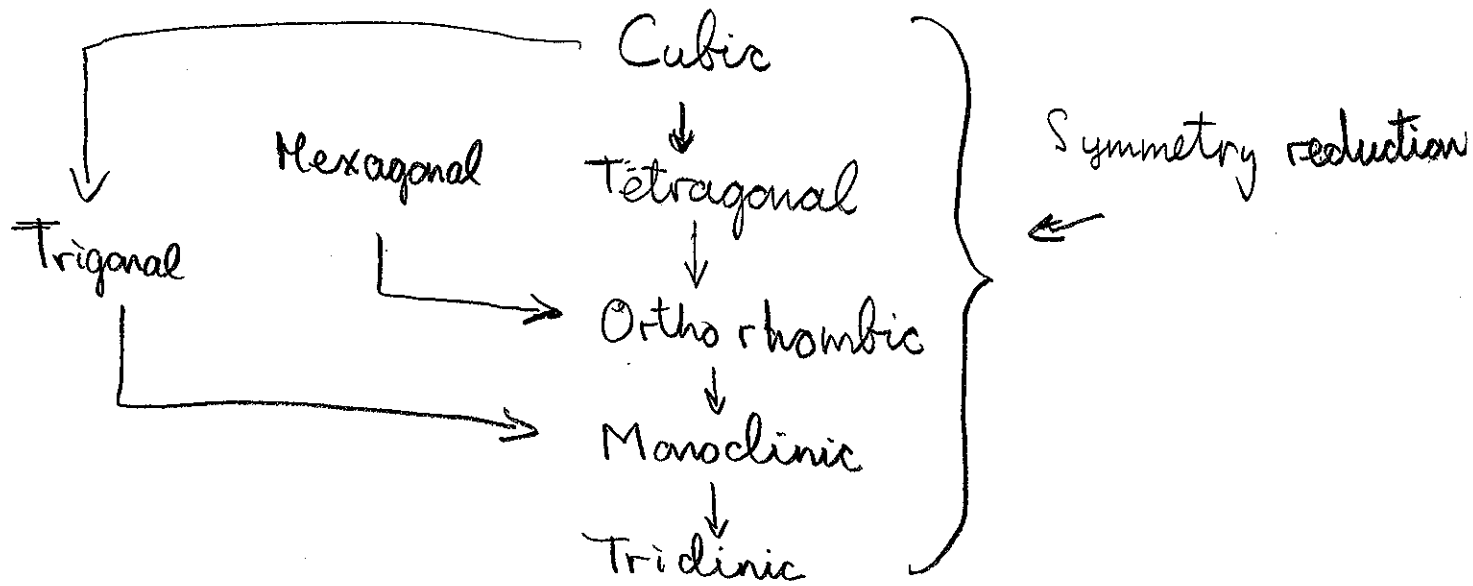
14 Bravais Lattices

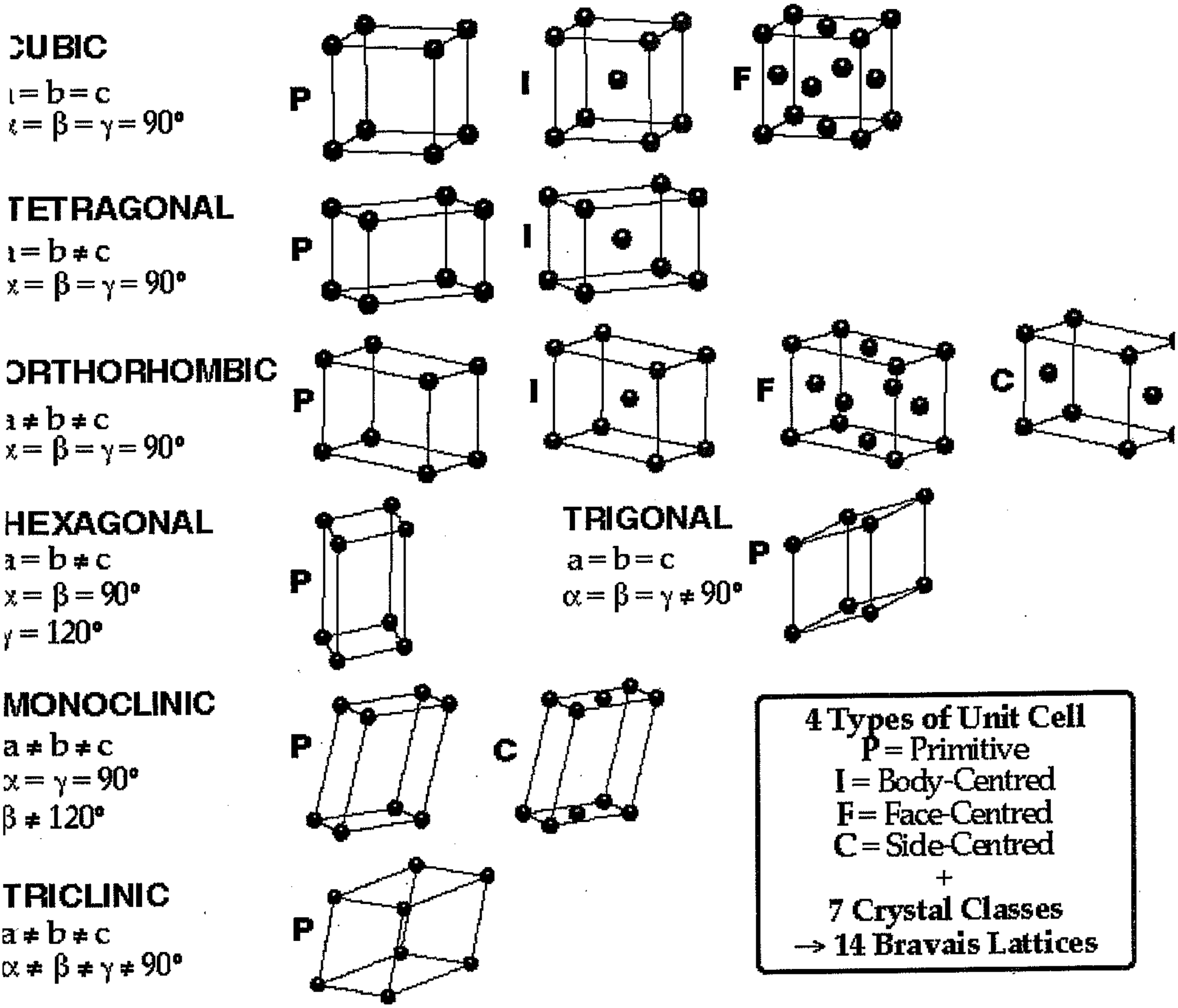
Next step is center some of the Bravais lattices. For the cubic system in addition to the simple cubic we will get body-centered cubic (bcc) and the face-centered (fcc)
It is relatively easy to see that stretching cube to tetragonal prism both bcc and fcc will produce the same body-centered tetragonal lattice (bct). To convince yourself consider stretched fcc and choose the unit cell by changing top and bottom square faces to squares made out of diagonals with the side $\sqrt{2}\,a$. Thus there are two Bravais lattices with tetragonal symmetry.
For the orthorombic we may have 4 Bravais lattices: simple one, body-centered, base centered (analog of the centered rectangular in 2d) and the face-centered

For the monoclinic lattice we have either simple or centered monoclynic where two opposite retangular sides are centered

For the triclinic, trigonal and hexagonal systems we have only simple Bravais lattices centering them doesn't bring anything new.

Thus we have 3 cubic, 2 tetragonal, 4 orthorhombic, 2 monoclinic and 1 triclinic, 1 trigonal and 1 hexagal lattice, all together 14 different Bravais lattices that belong to 7 crystal systems.





CUBIC
a = b = c
α = β = γ = 90°
P
I
F
TETRAGONAL
a = b ≠ c
α = β = γ = 90°
P
I
ORTHORHOMBIC
a ≠ b ≠ c
α = β = γ = 90°
P
I
F
C
HEXAGONAL
a = b ≠ c
α = β = 90°
γ = 120°
P
TRIGONAL
a = b = c
α = β = γ ≠ 90°
P
MONOCLINIC
a ≠ b ≠ c
α = γ = 90°
β ≠ 120°
P
C
TRICLINIC
a ≠ b ≠ c
α ≠ β ≠ γ ≠ 90°
P
4 Types of Unit Cell
P = Primitive
I = Body-Centred
F = Face-Centred
C = Side-Centred
+
7 Crystal Classes
→ 14 Bravais Lattices

Point groups

Anisotropy of crystals means that different directions have different properties. Some directions are equivalent for high symmetry lattices. Thus anisotropy of physical properties of the crystal is determined by the symmetry of directions. Since translations do not change directions we should consider other symmetry elements like rotations or mirror reflections.

The full symmetry group of a Bravais lattice consists of translations through lattice vectors and operations (rotations, reflections) that leave a particular lattice point fixed.

When we discuss anisotropic properties of the crystal we are interested in these last operation.

The subset of the full symmetry group of the cristal that leaves a particular point fixed is called the <u>point group</u>

As we learned from Lecture 1 in a lattice we may have n-fold rotational symmetry with $n = 2, 3, 4, 6$. We may also have mirror reflection planes

Schonflies notations

C_n - group that contains only n-fold rotation axis

C_{nh} - group that has n-fol axis and a single mirror plane that is orthogonal to the rotation axis. Monoclinic system has C_{2h} symmetry group

C_{nv} - n-fold axis and a mirror plane that contains the rotational axis plus as many additional mirror planes that follow from the C_n symmetry

D_n - n-fold axis, a 2 fold axis $\perp$ to n-fold axis plus other 2 fold axes that follow from the C_n symmetry

D_{nh} - all elemens of D_n and horisontal mirror plane as for C_{nh}.

Orthorombic lattice has D_{2h} symmet

Tetragonal system has D_{4h} symmetry group
Hexagonal — D_{6h} — " —

D_{nd} – all elements of D_n plus mirror planes containing the n-fold axis which bisect the angles between the 2 fold axis

Trigonal system has D_{3d} symmetry group.

O_h - group symmetry of the cube (O- octahedron)

<u>32 Crystallographic point groups</u>

For the 7 crystal systems (or 14 Bravais lattices) we have 7 different point groups enumerated above. Since real crystals may have unit cell with a basis their symmetry is reduced. To classify it we should consider different subgroups of the above mentioned symmetry group. The crystal system of a crystallographic point group is that of the least symmetric of the seven Brave lattice point groups containing every symmetry operator of the crystallographic group

The cubic group we can reduce to 5 different subgroup before going to lower symmetry system (11

Table 7.2
OBJECTS WITH THE SYMMETRY OF THE FIVE CUBIC CRYSTALLOGRAPHIC POINT GROUPS[a]

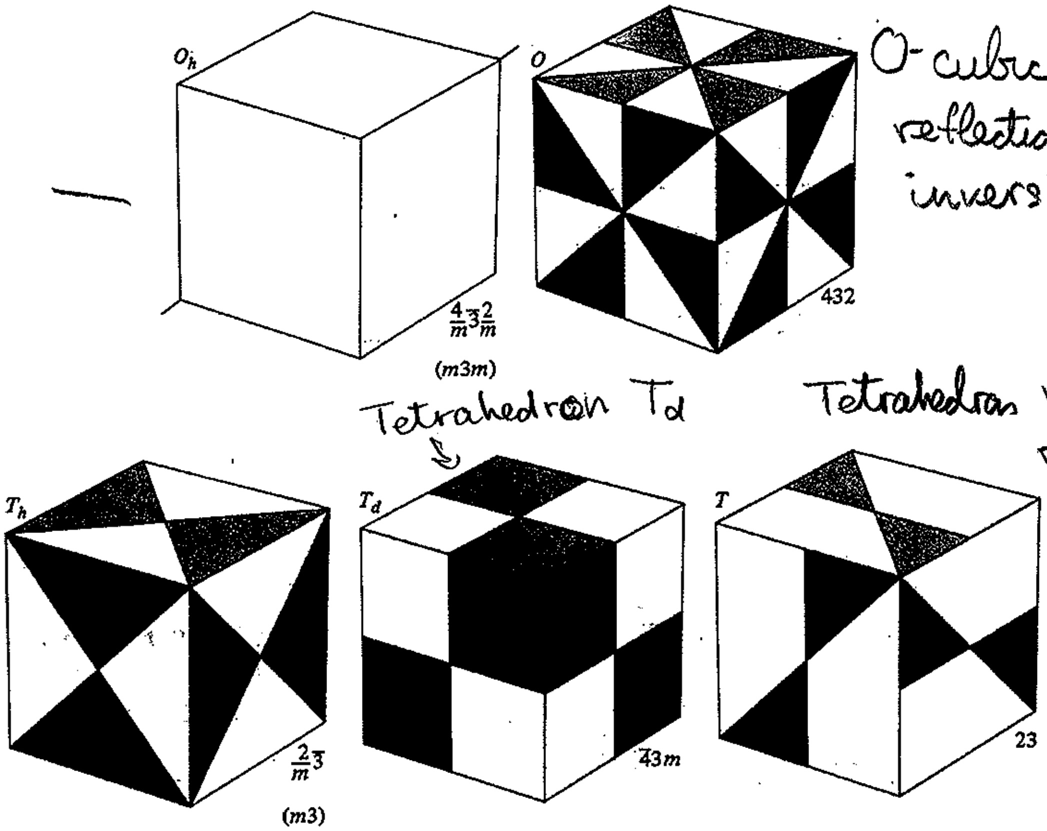
O_h cubic —

O - cubic without reflections and inversions

Tetrahedron T_d

Tetrahedron without reflection and inversi

Tetrahedron without reflections



[a] To the left of each object is the Schoenflies name of its symmetry group and to the right is the international name. The unpictured faces may be deduced from the fact that rotation about a body diagonal through 120° is a symmetry operation for all five objects. (Such an axis is shown on the undecorated cube.)

Breaking the symmetry of the other Bravais lattice point groups we get the following classificatias.

Triclinic	C_1 , S_2
Monoclinic	C_2, C_{2h}, C_{1h}
Orthorambic	C_{2v}, D_2, D_{2h}
Tetragonal	$S_4, D_{2d}, C_4, C_{4h}, C_{4v}, D_4, D_{4h}$
Trigonal	$C_3, S_6, C_{3v}, D_3, D_{3d}$
Hexagonal	$C_{3h}, D_{2h}, C_6, C_{6h}, C_{6v}, D_6, D_{6h}$
Cubic	T, T_h, T_d, O, O_h

All together 32 crystallographic point groups

230 Space groups

We should take into account that for some crystal systems there are several (centered) Bravais lattices). This will multiply the number of possible structures. Then

Number of point cubic group (5) × Number of cubic Bravais lattices (3) + Number of hexagonal p.g. × Number of hexagonal Bravais lattices + ... = 61

Then we can place trigonal basis to hexagonal lattice we get another 5 groups. Another 7 appears from the possibility to orient basis

All these 73 groups are called <u>symmorphic</u>

Another 157 nonsymmorphic groups contain additional operations such as screw axis (rotations × translation along it) and glide plane. (reflection × translation along the plane)