Point Group Symmetries

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Basic Definitions

Symmetry Element:	a point, line or plane about which a symmetry operation is performed
Symmetry Operation:	a real or imagined movement of a body about a symmetry element, such that after movement, every point on the object is coincident with an equivalent point.
Proper Rotation:	No change of handedness occurs
Improper Rotation:	A change of handedness occurs

Elements of symmetry

- Point
- Line
- Plane
- Translation
- Combination of above

Symmetry elements and operations

Element	Operation	Symbol
none	identity	*E*
Proper rotation axis	Rotate by 360°/n	Cn
Mirror plane	Reflection	σ
Inversion center	Inversion	*i*
Improper rotation axis	Rotate by 360°/n, then reflect perpendicular to axis	Sn

Symmetry elements and operations

E: identity operation, all molecules have E

$E = C_1$

C_n: proper rotation

n principal (highest) axis

C_2 axis perpendicular to central C_n, called C_2' axis

σ: mirror plane

σ parallel to C_n is vertical: σ_v

σ parallel to C_n and bisecting 2 C_2' is dihedral: σ_d

σ perpendicular to C_n is horizontal: σ_h

i = inversion center

all atoms moved through the inversion center to an equal distance on the opposite side

i may or may not be atomic center

Sn = improper rotation axis

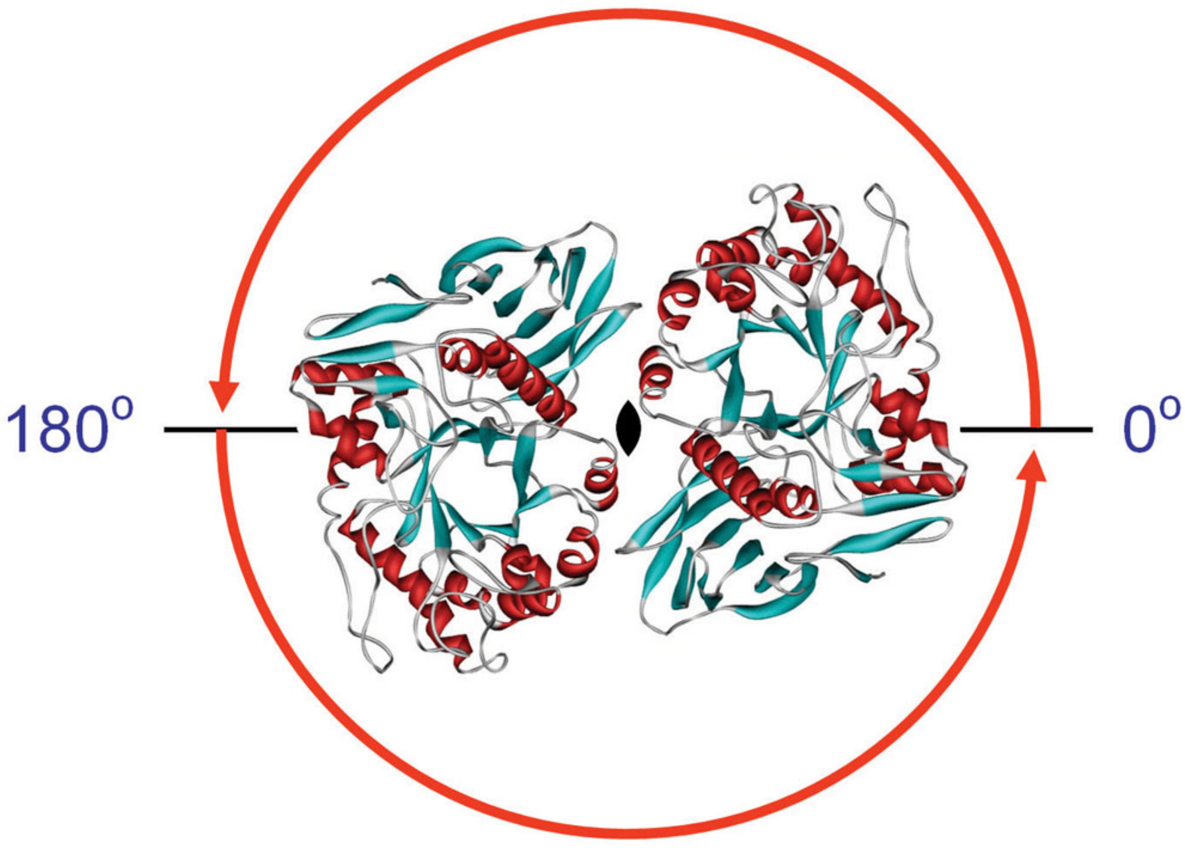
combination rotation/reflection

n_{odd} requires both C_n and σ_h

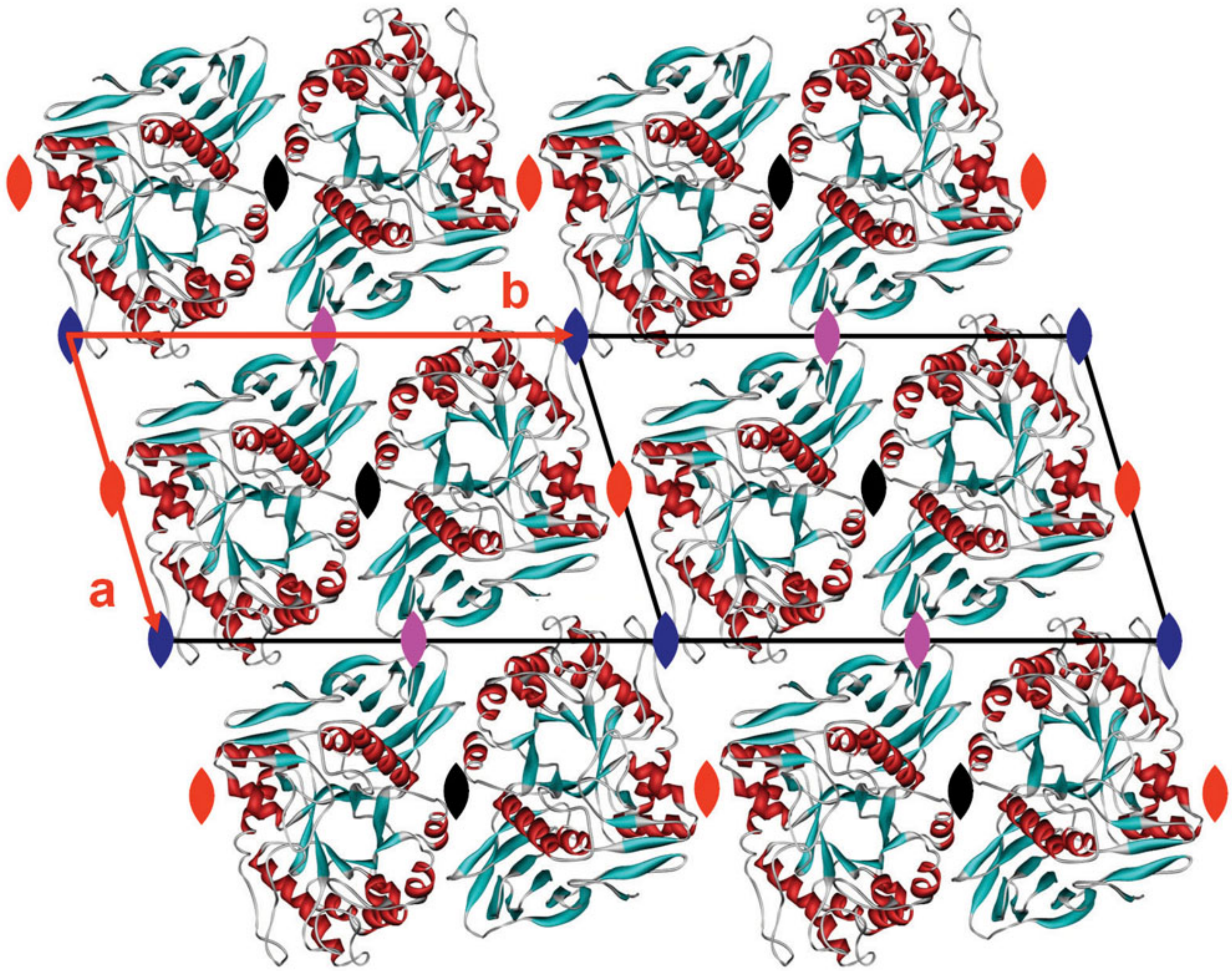
n_{even} may or may not have C_n and σ_h

$S_1 = \sigma$, $S_2 = i$

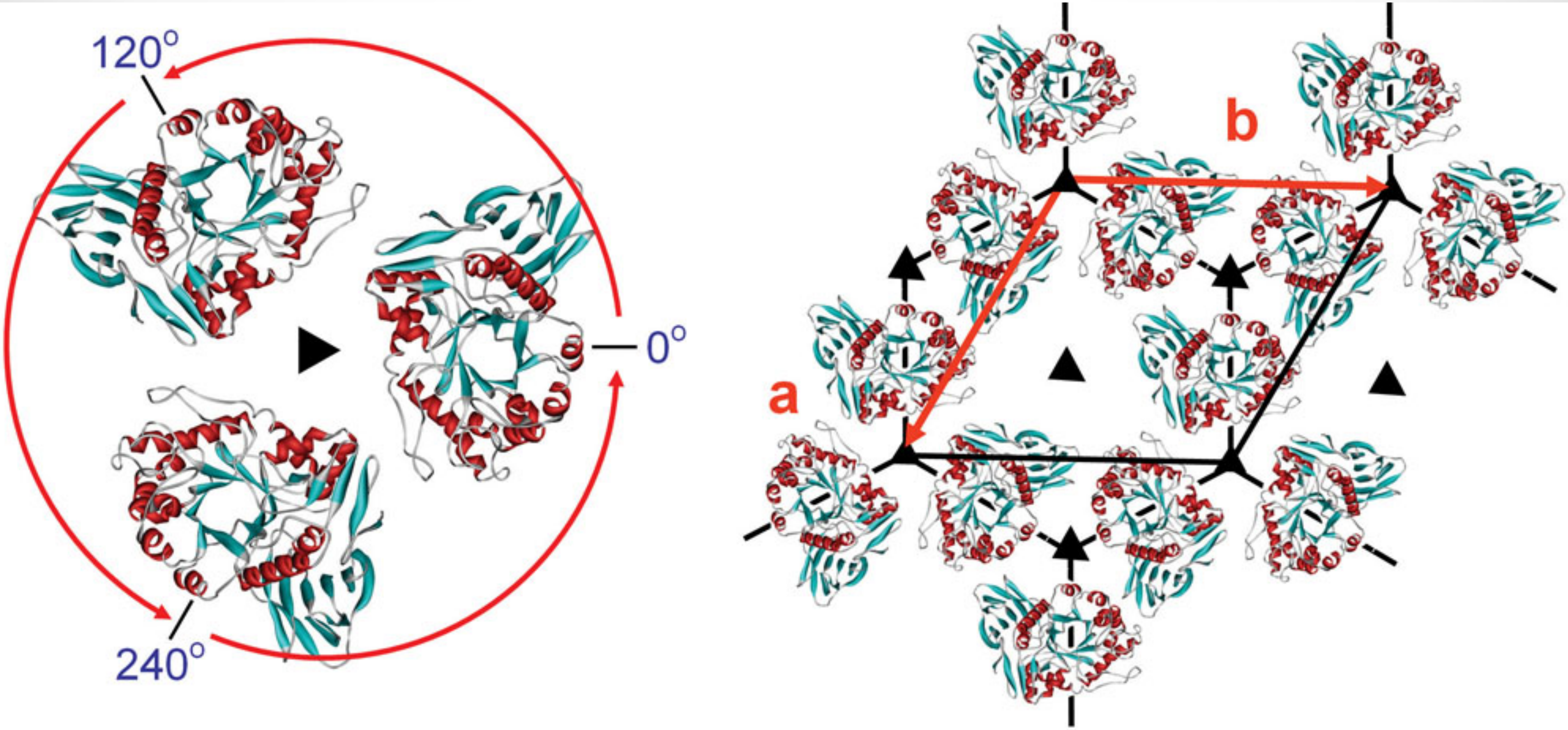
Rotation



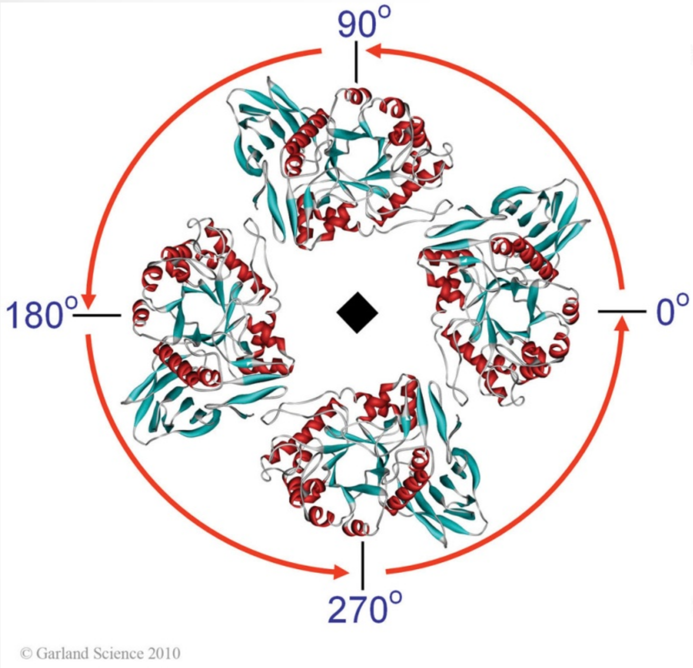
p2 plane group

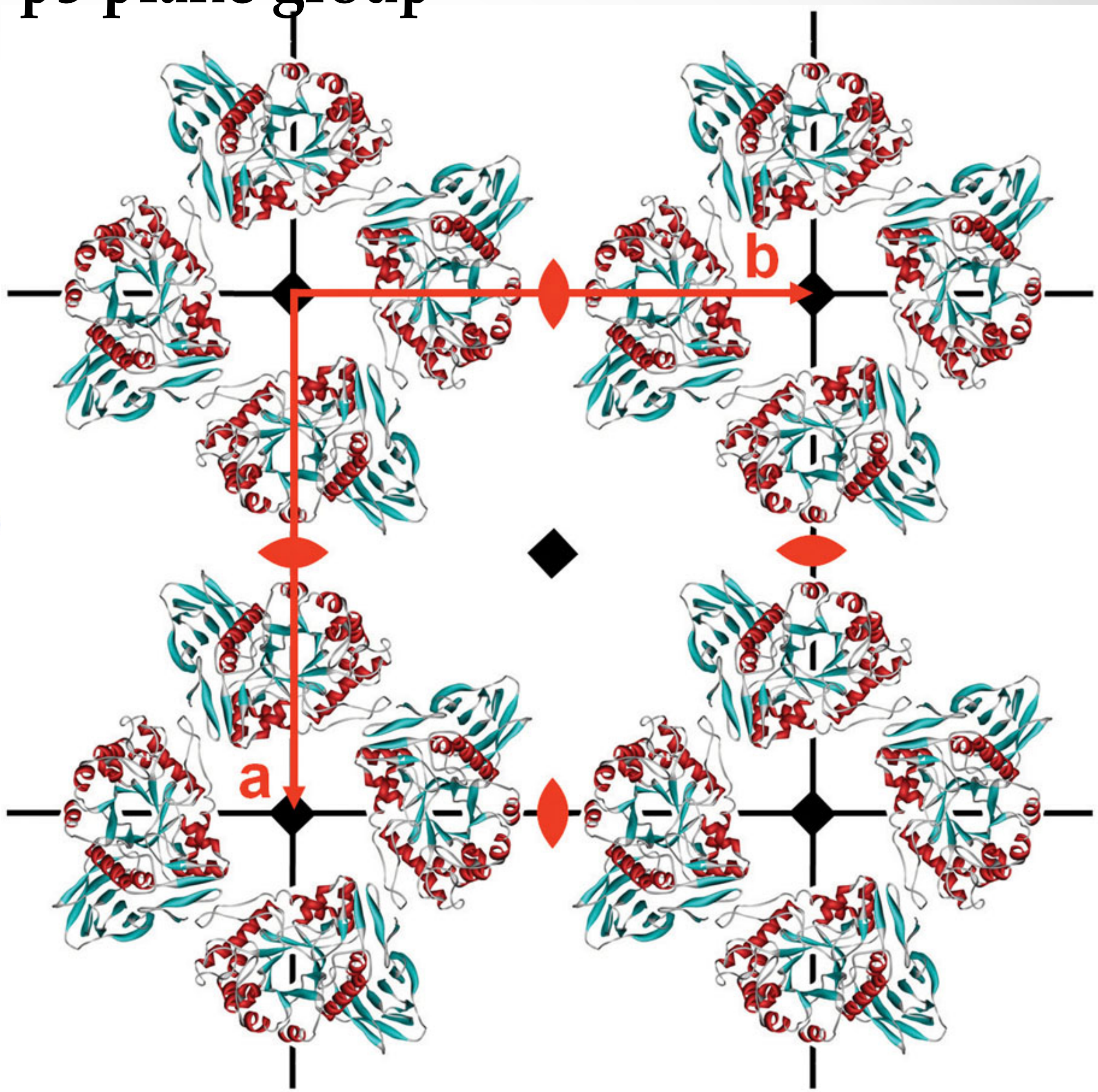


p3 plane group



p3 plane group

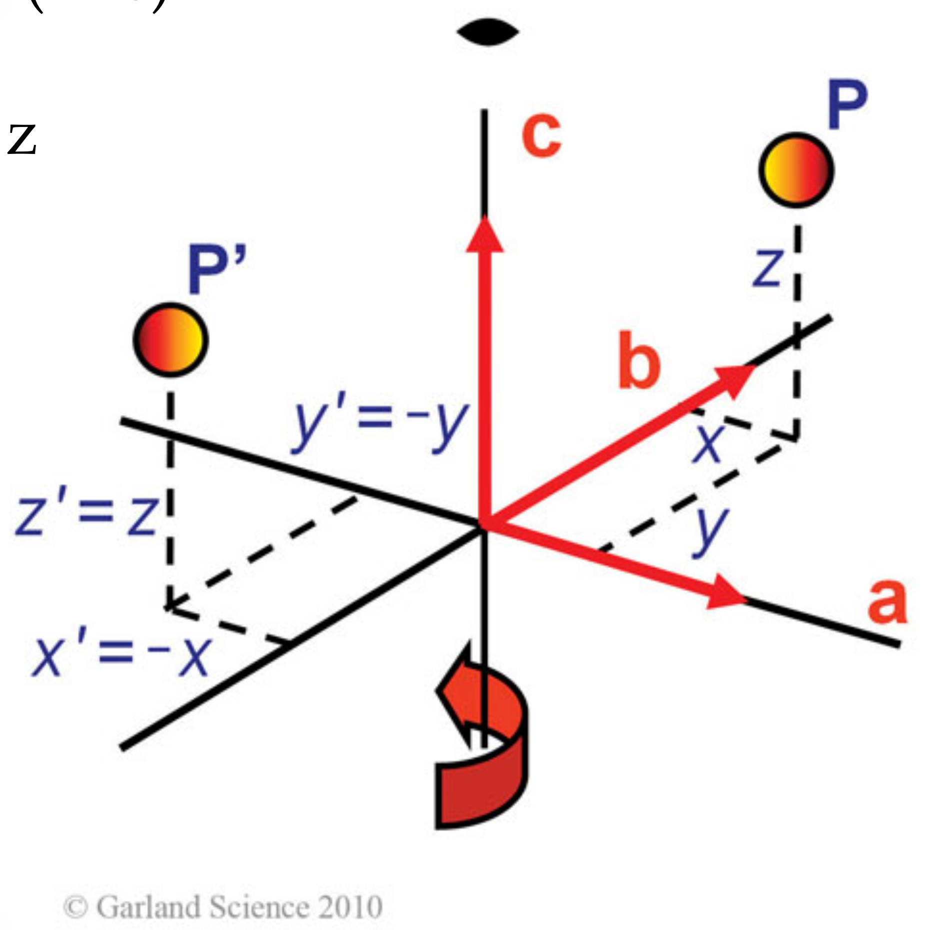


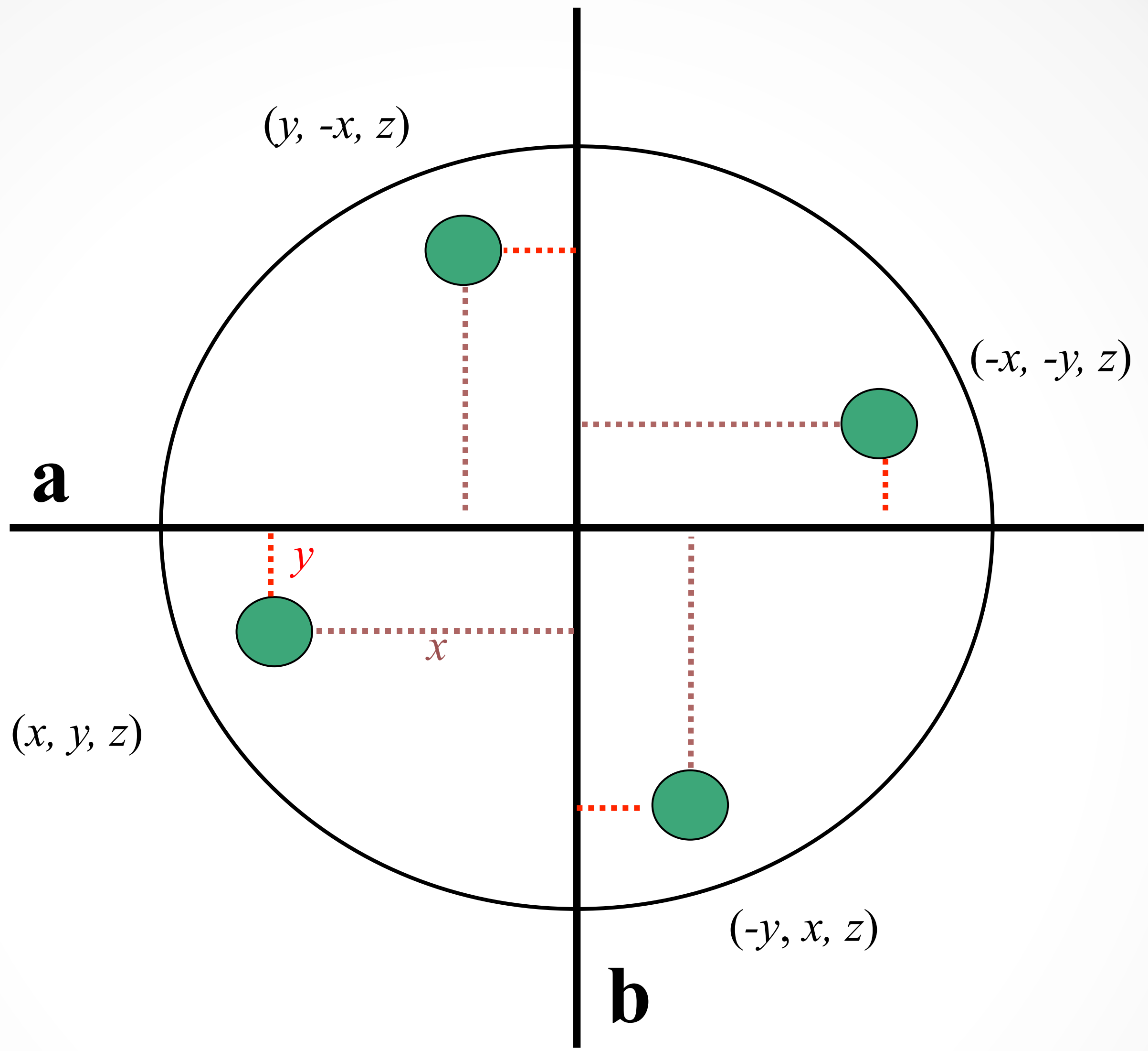


Rotation in 3D

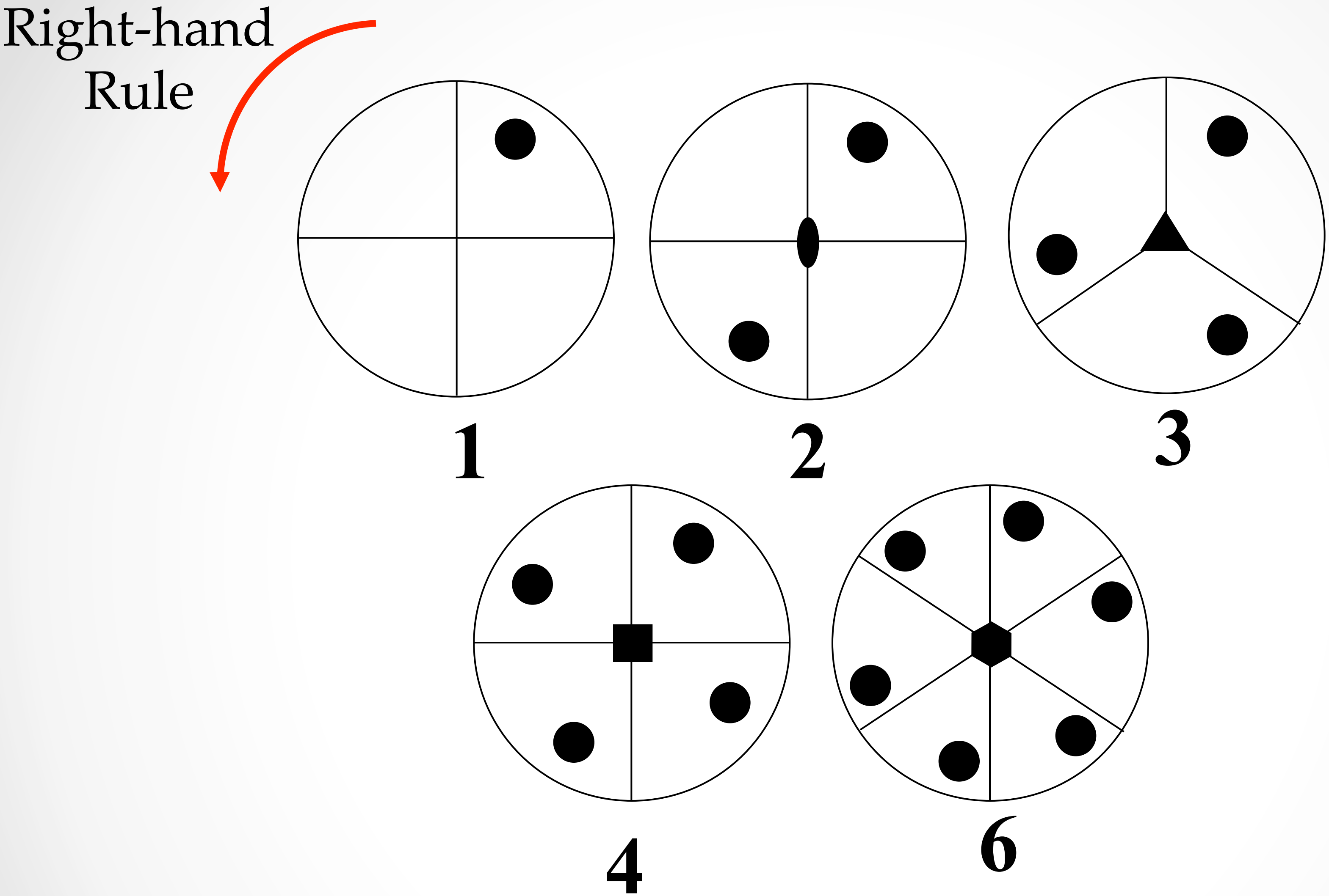
About an axis (line)

x, y, z = -x, -y, z





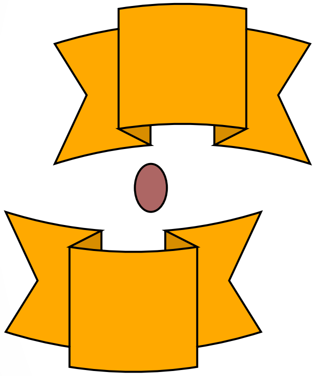
Equivalent positions for a 4-fold proper rotation



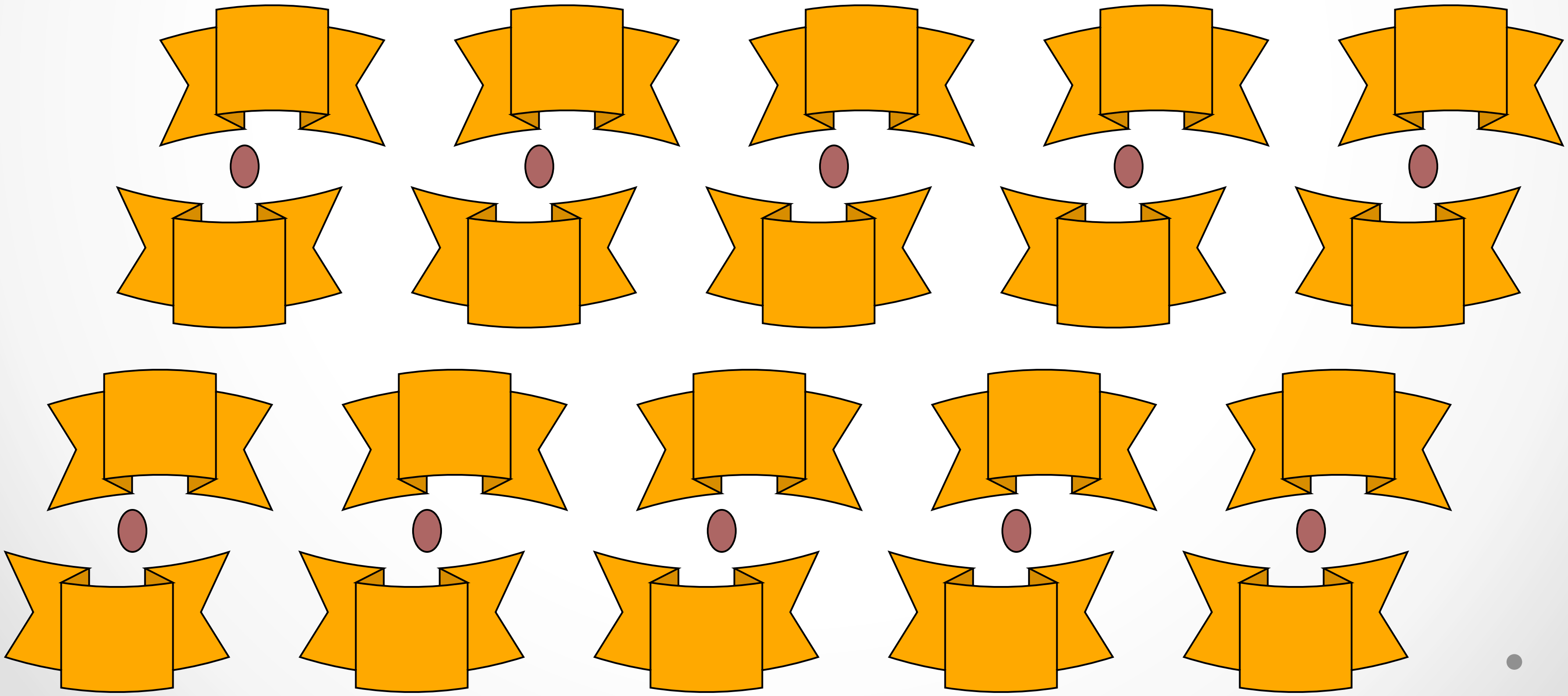
Stereograms of the proper rotation axes

Only rotations allowed: 2, 3, 4, 6 (Crystallographic Restriction theorem)

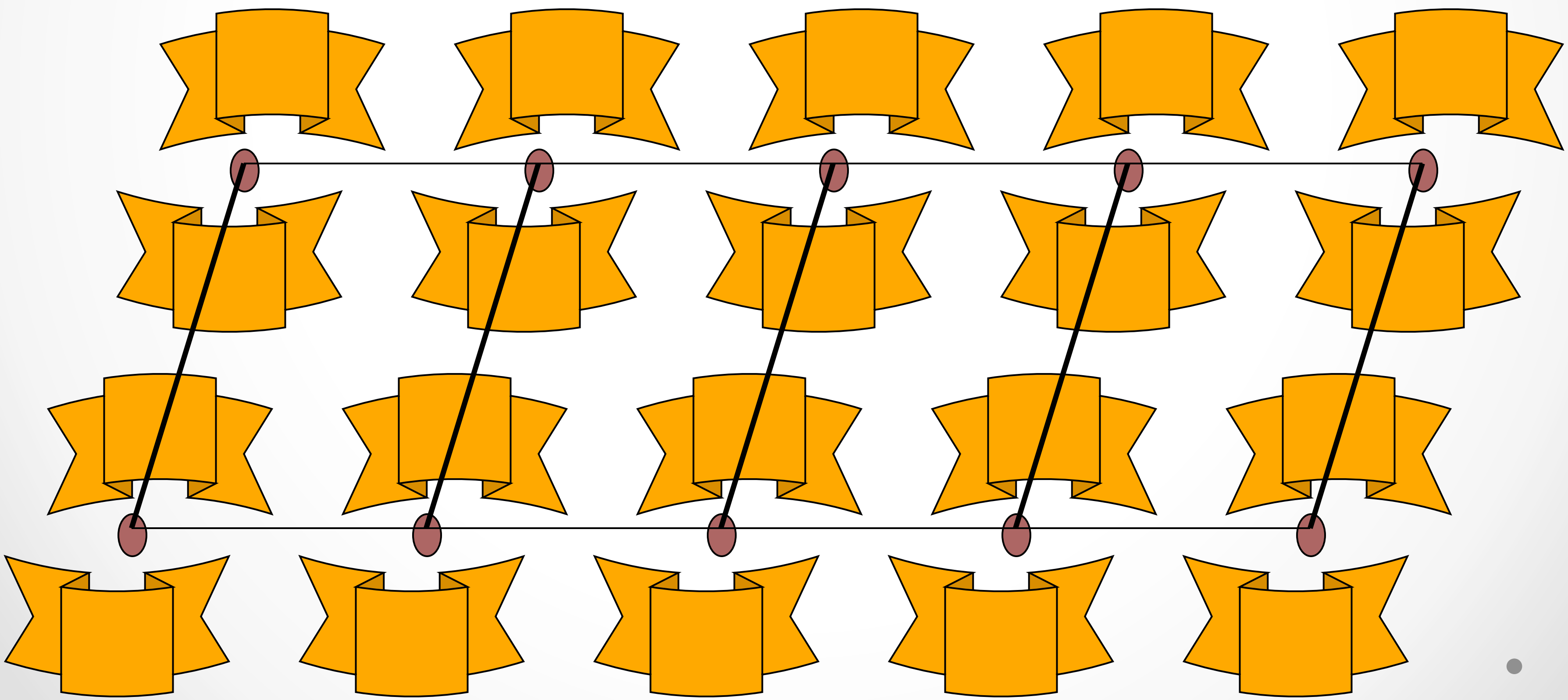
Rotation and translation



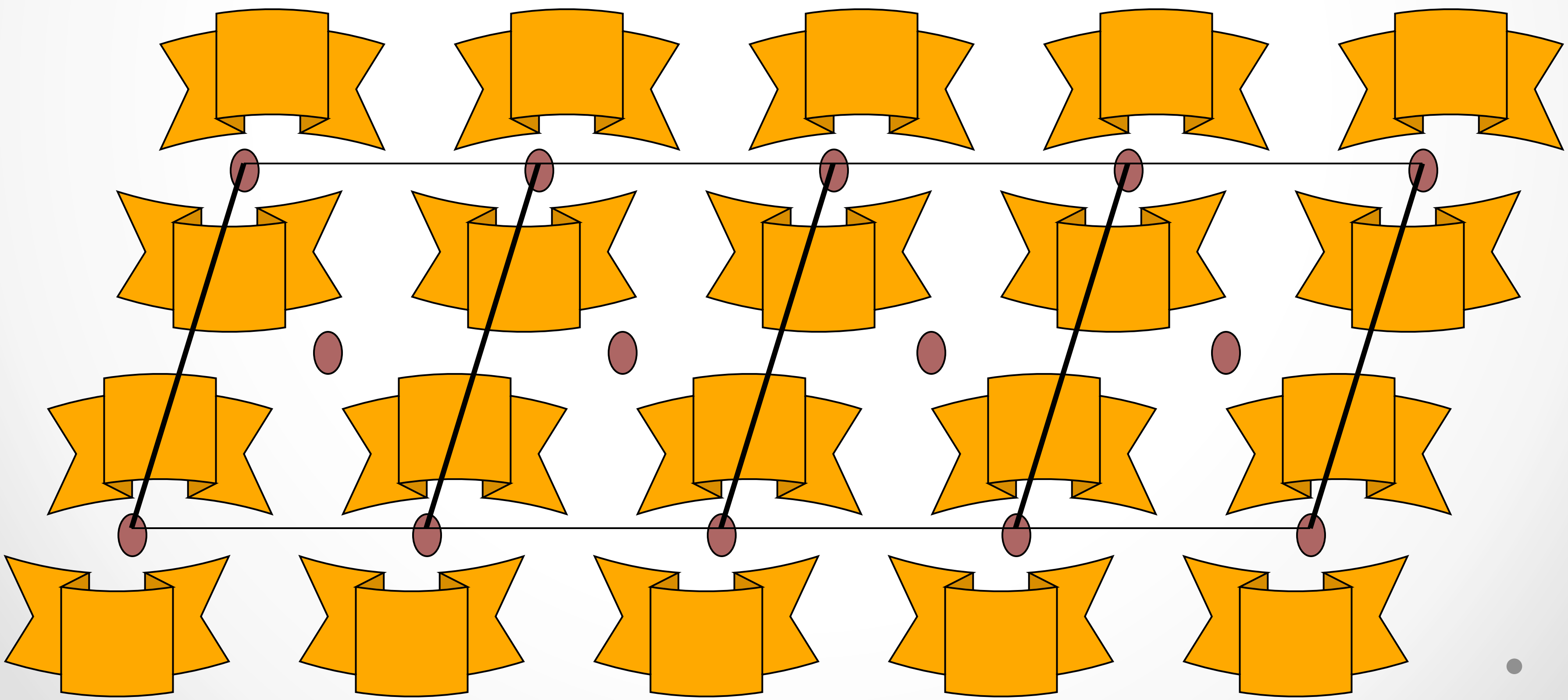
Rotation and translation



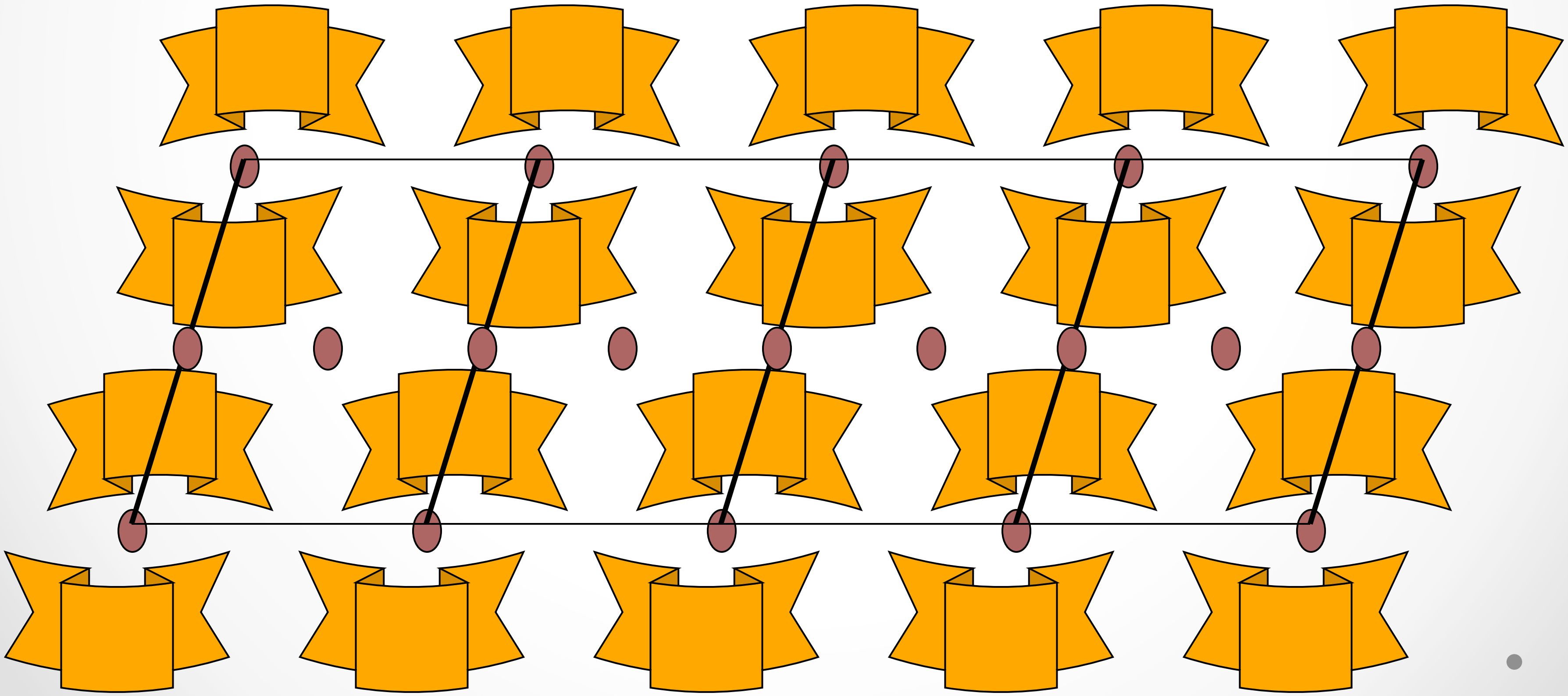
Rotation and translation



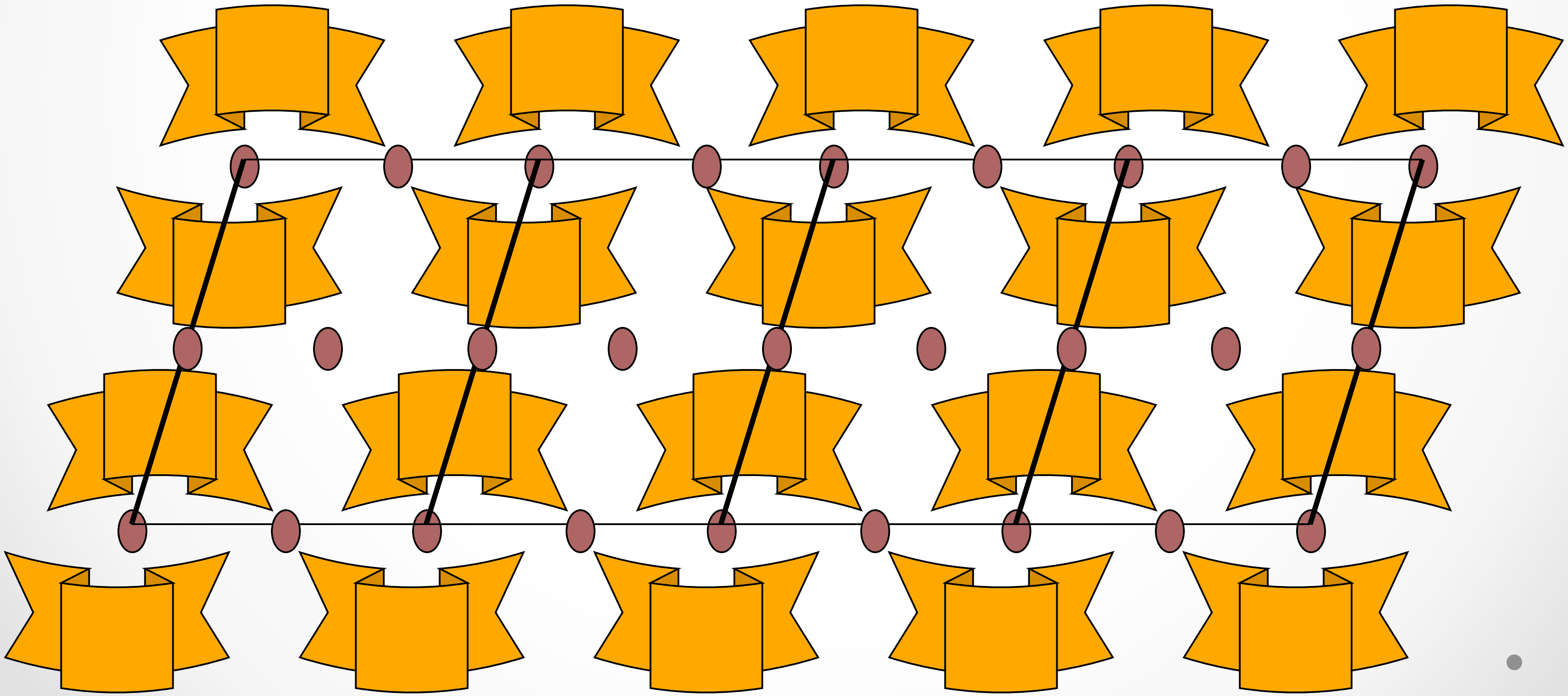
Rotation and translation



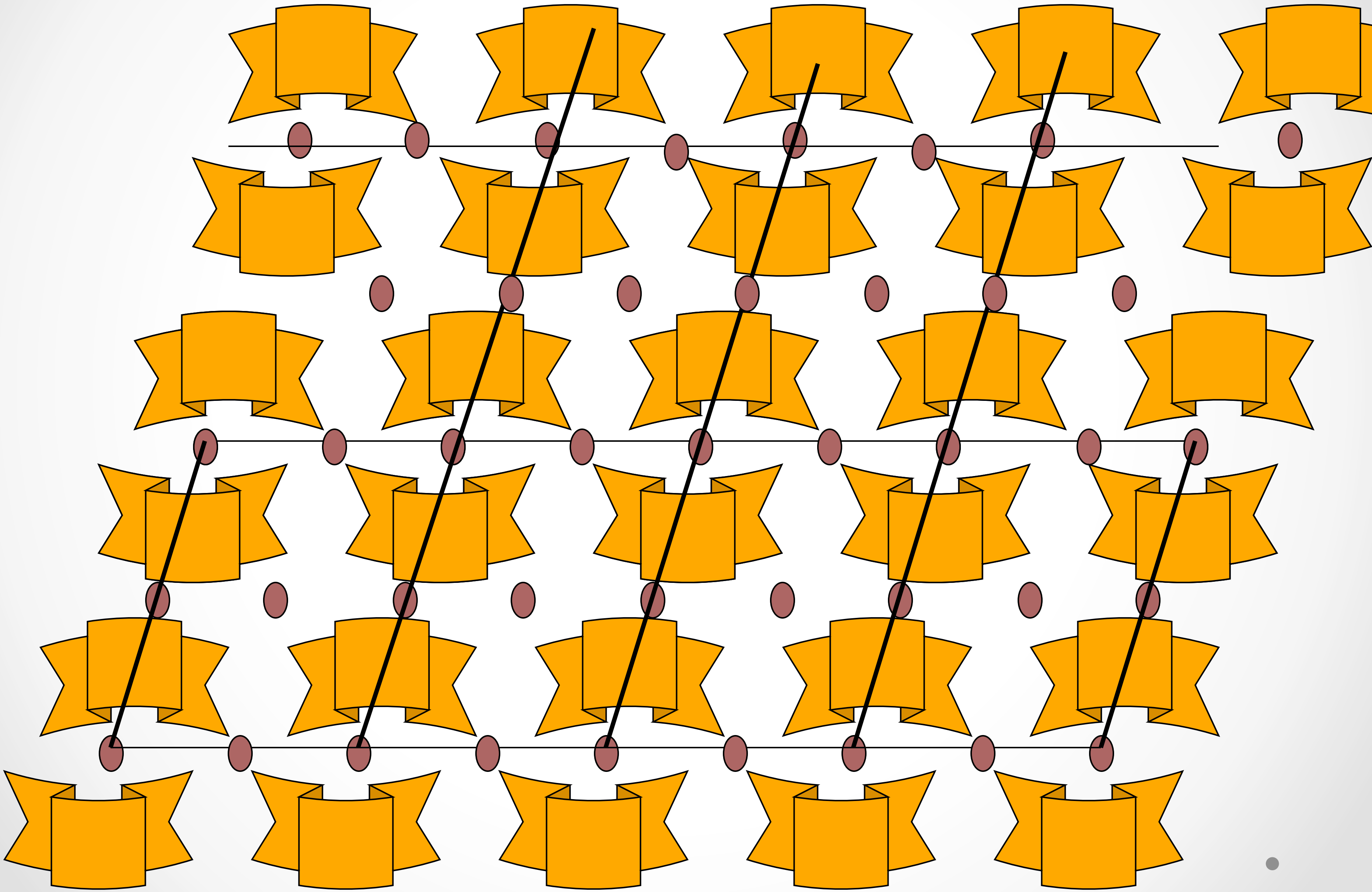
Rotation and translation



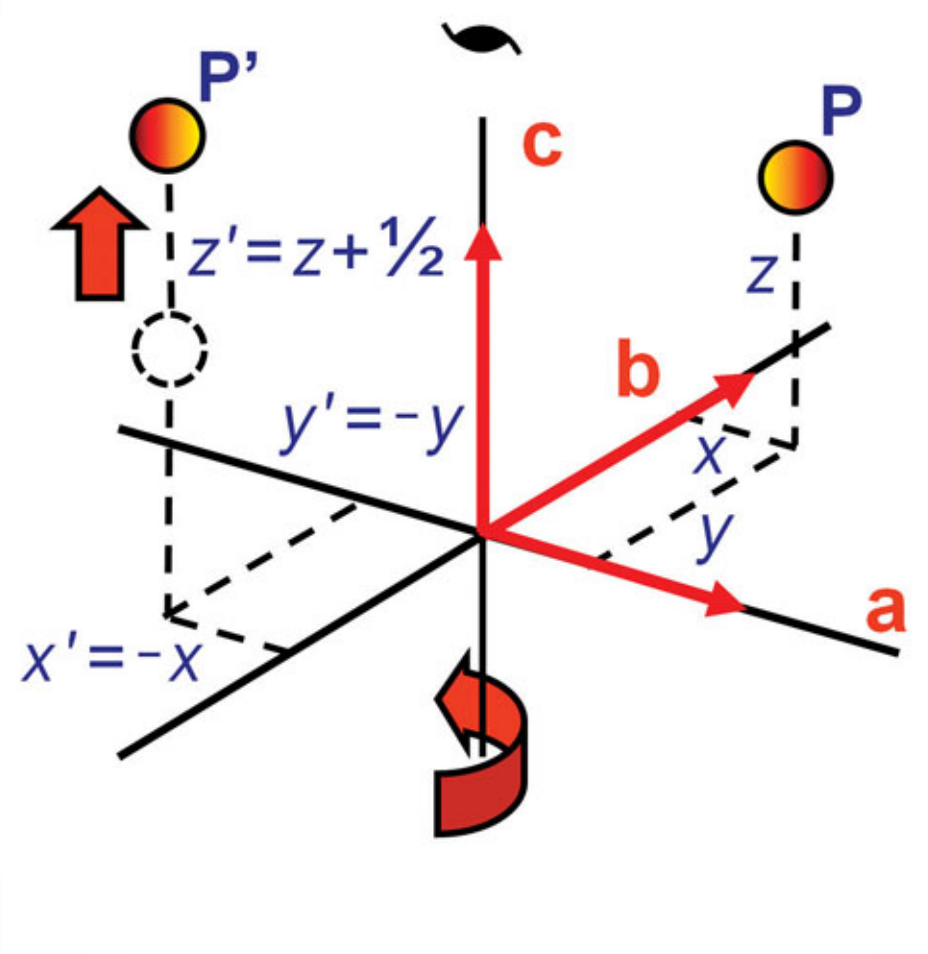
Rotation and translation



Rotation and translation

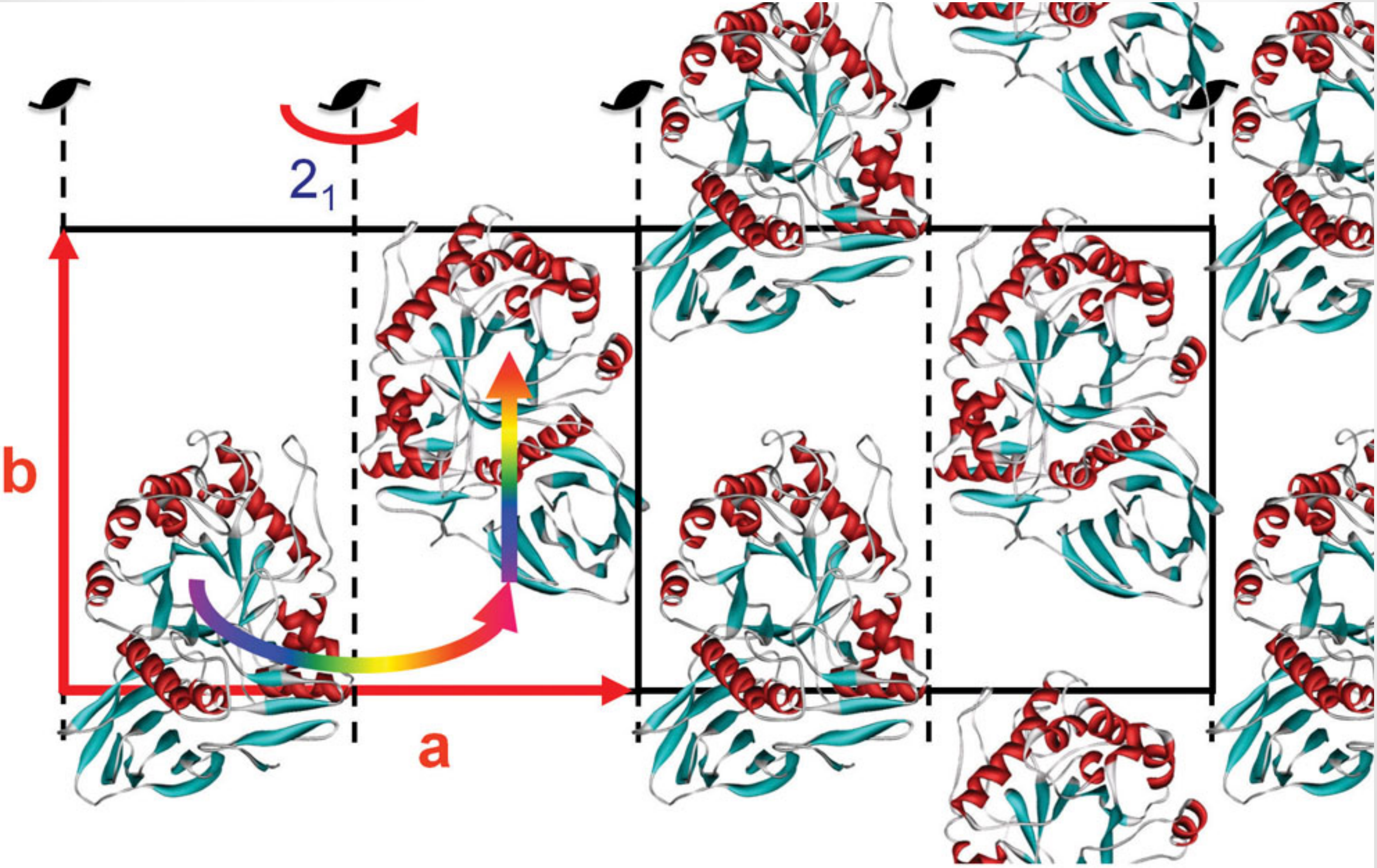


Rotation and translation – screw axis

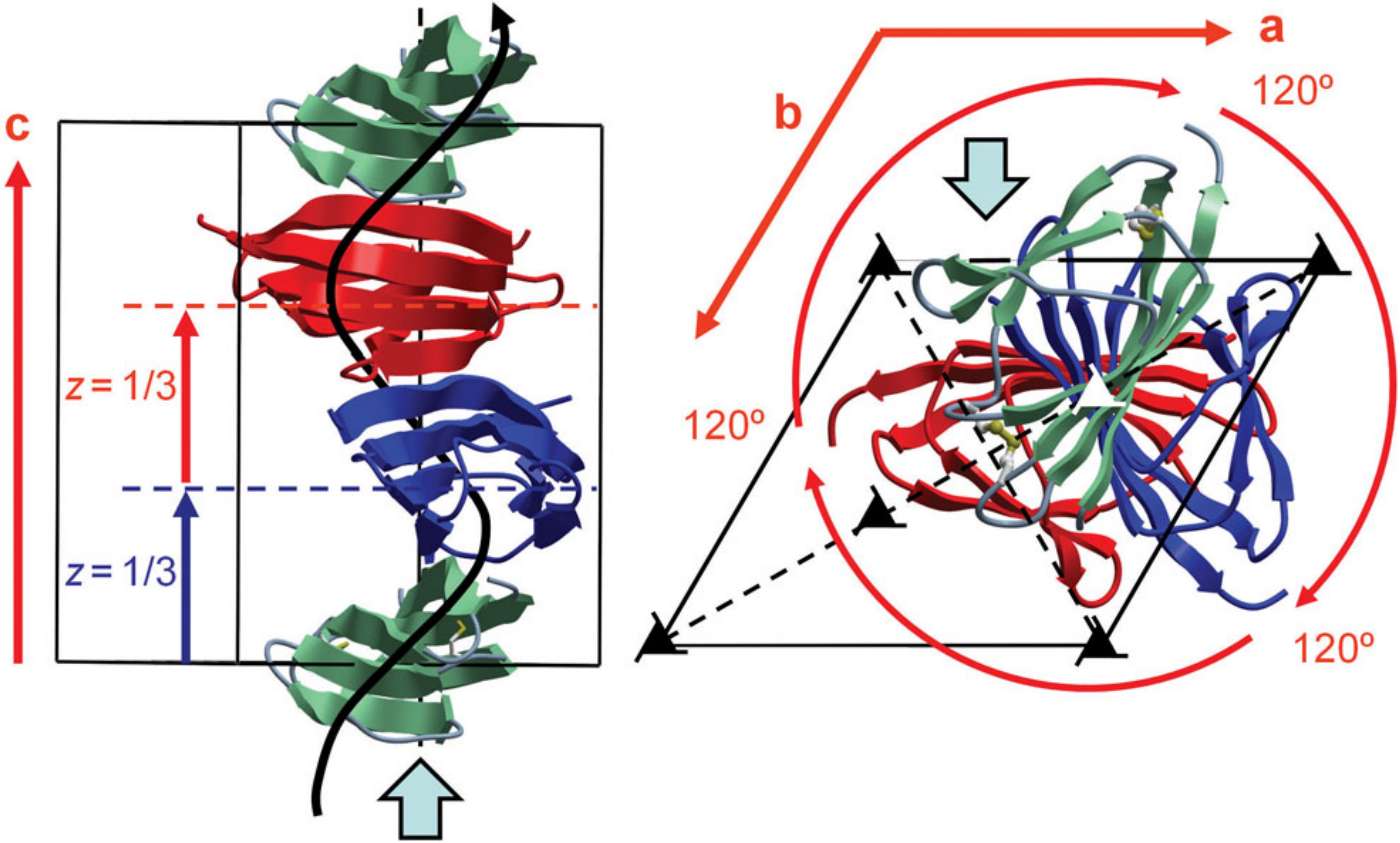


x, y, z = -x, -y, z+1/2

Rotation and translation – screw axis



Rotation and translation – screw axis



Mirror (σ)

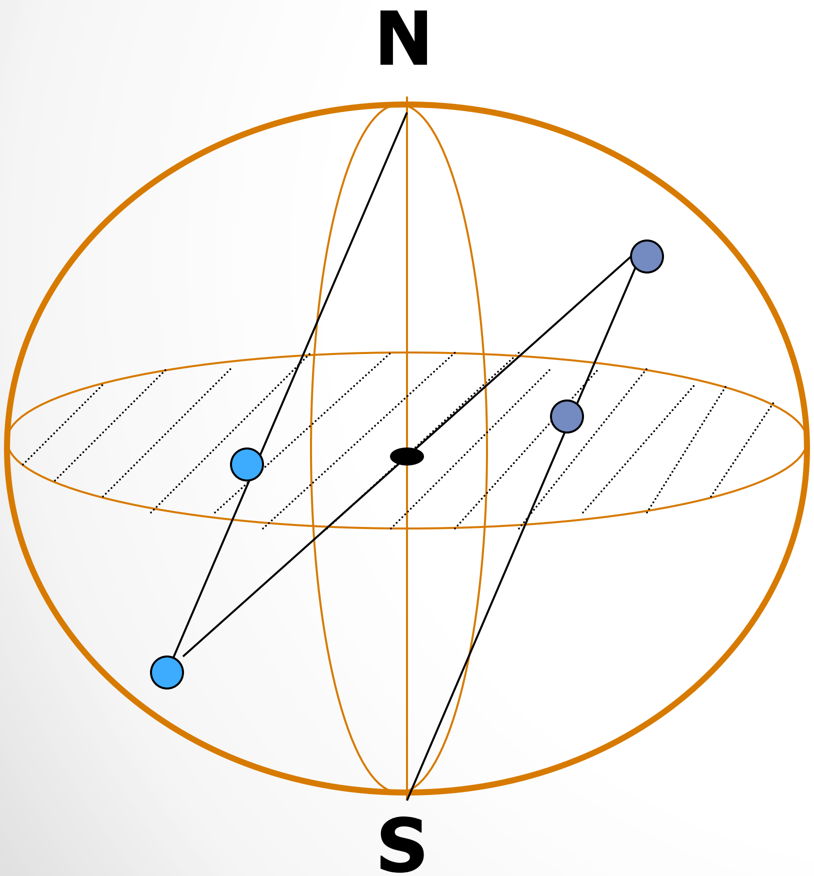
Reflection along a plane

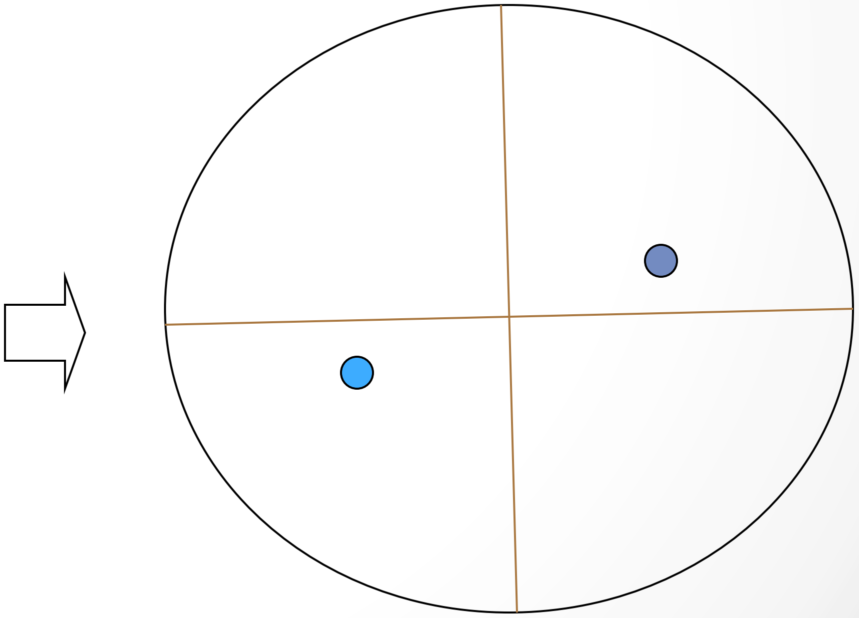
$$x,y,z \rightarrow x, -y, z \quad (\sigma \perp y)$$
$$x,y,z \rightarrow -x, y, z \quad (\sigma \perp x)$$
$$x,y,z \rightarrow x, y, -z \quad (\sigma \perp z)$$

Inversion (i)

Inversion through a point

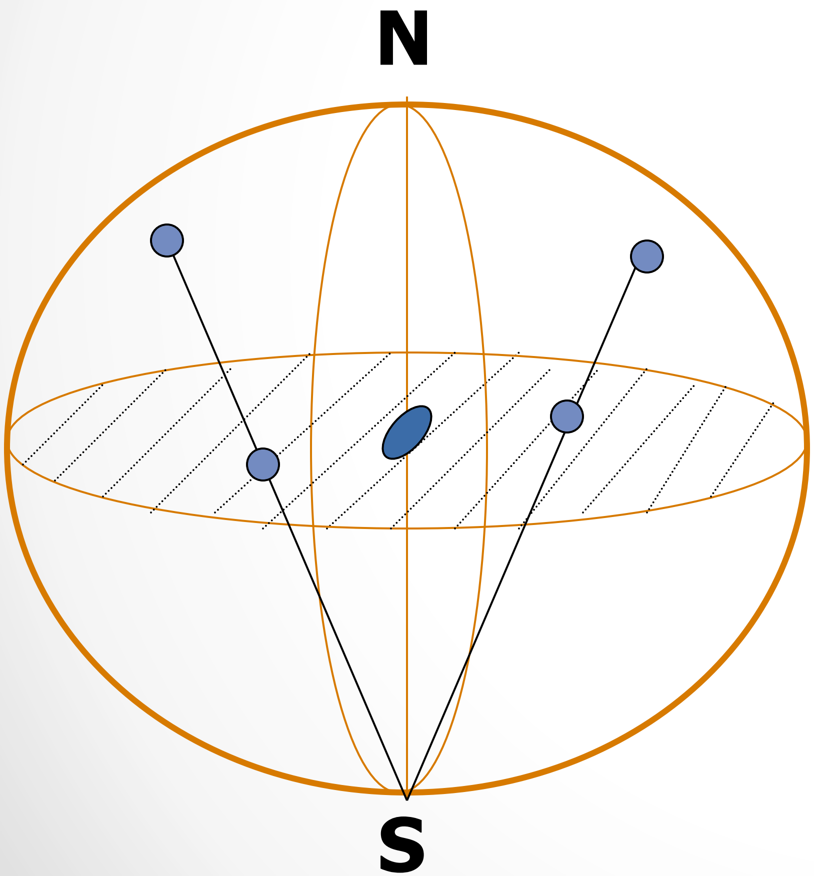
x, y, z $\rightarrow$ -x, -y, -z

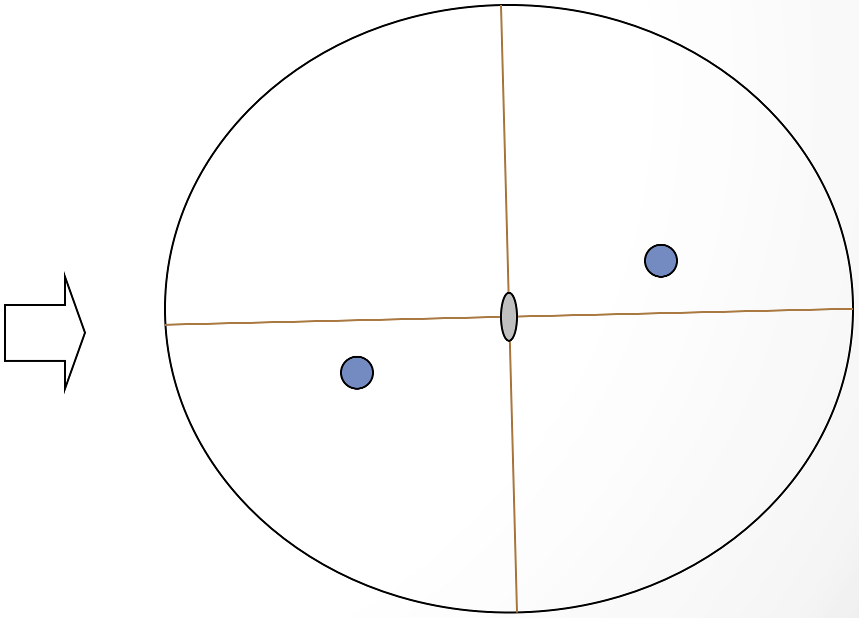




A 2-fold

x, y, z → -x, y, -z



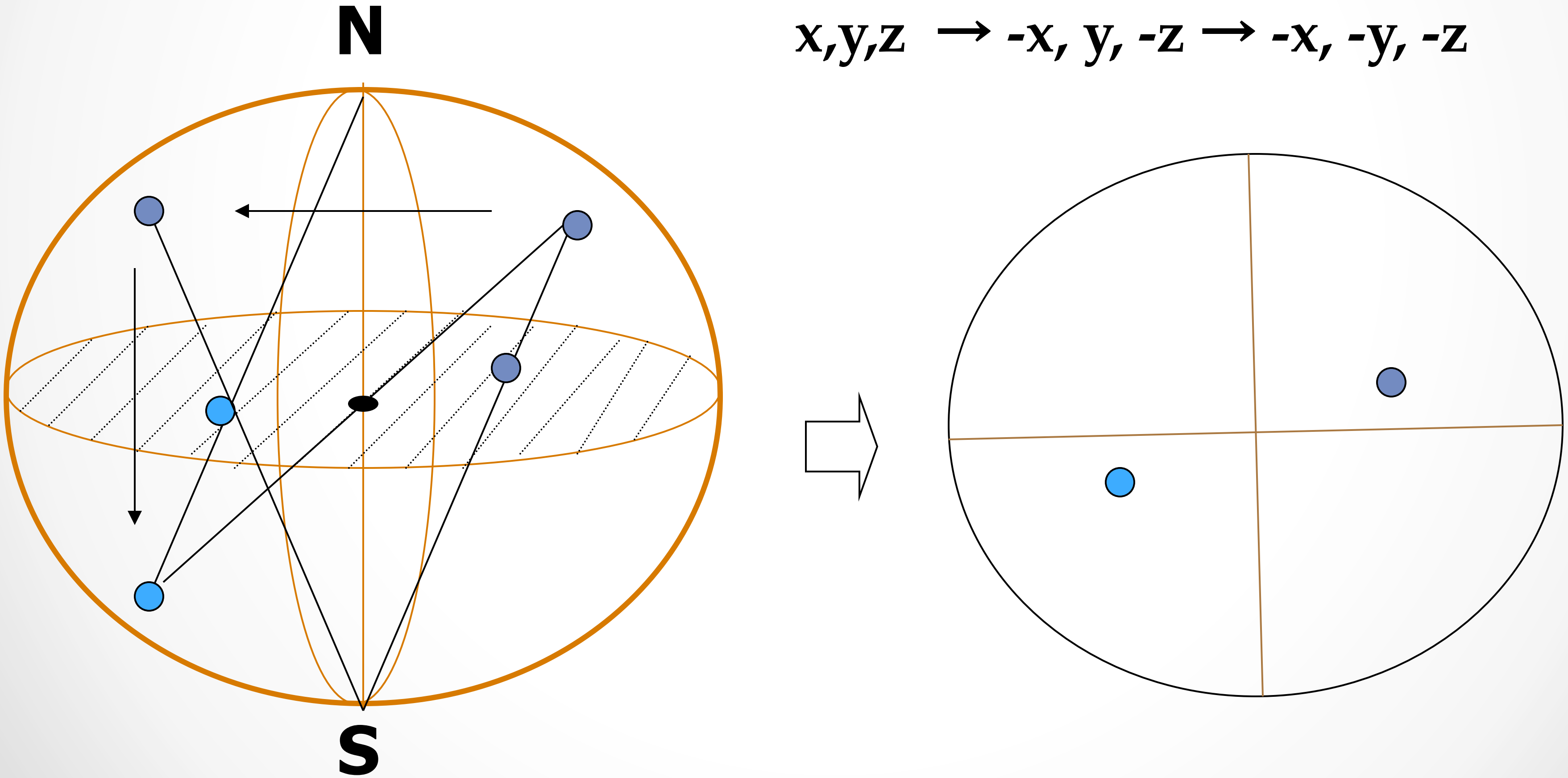


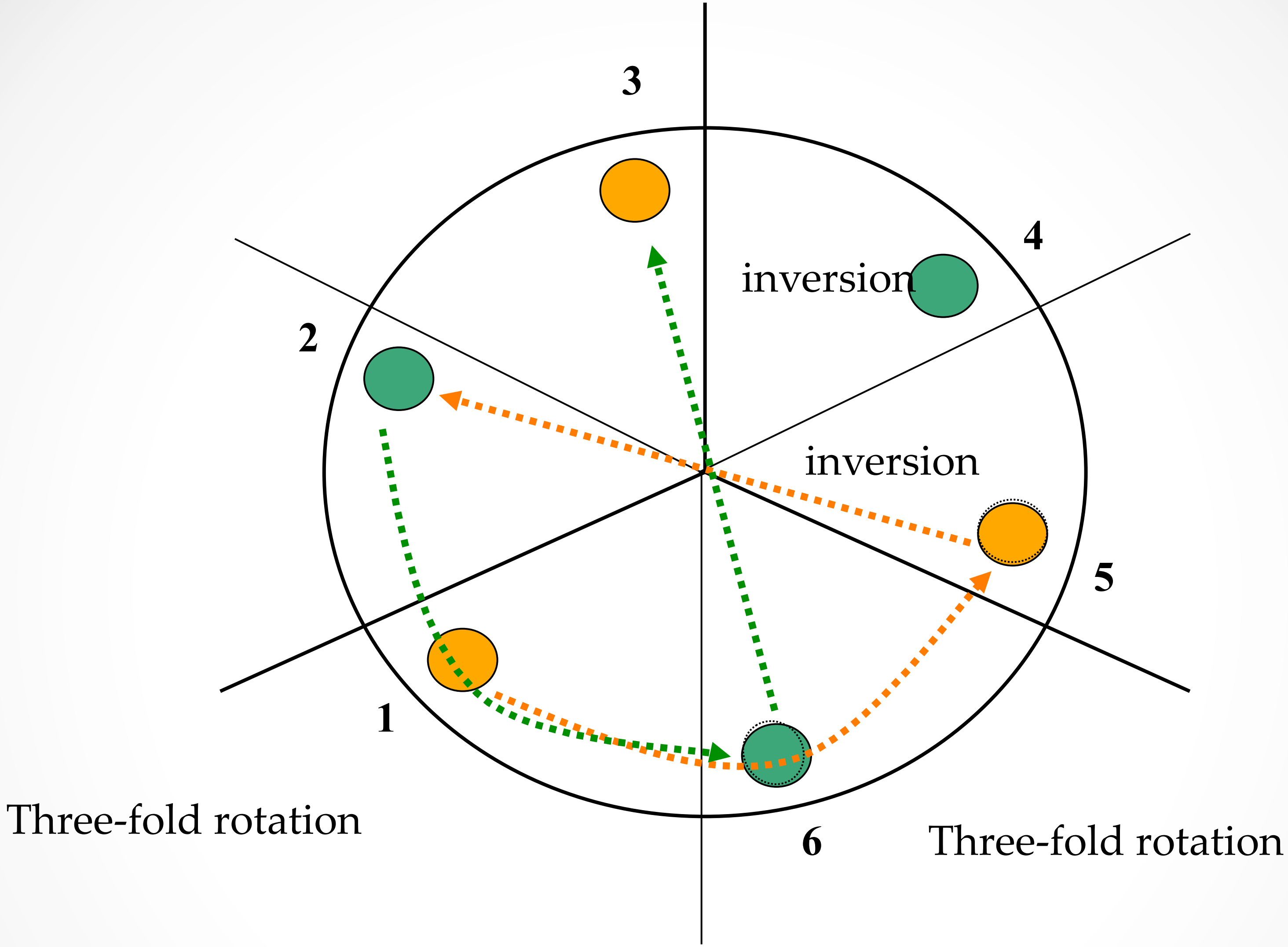
A 2 fold with ⊥σ

2/σ operation is same as inversion

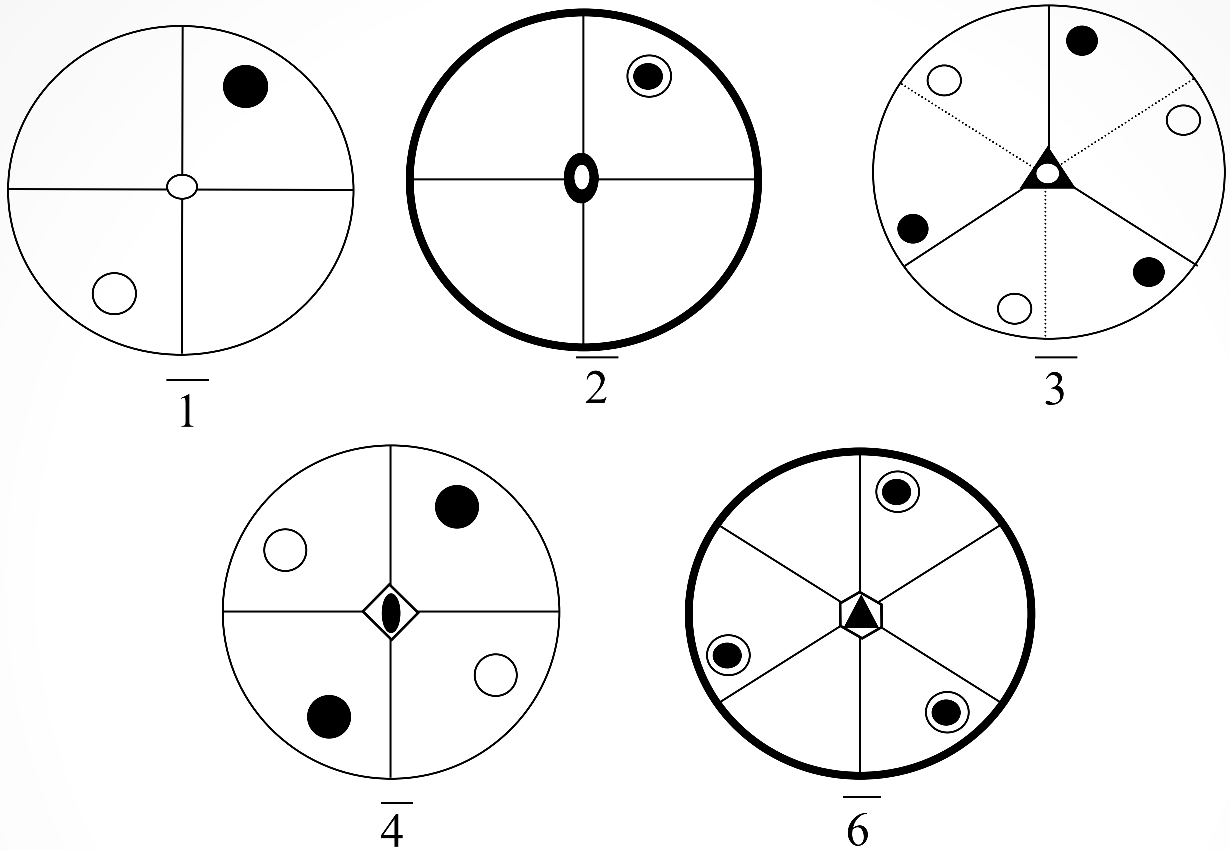
2| |y σ⊥y

x,y,z → -x, y, -z → -x, -y, -z





3-fold improper axis



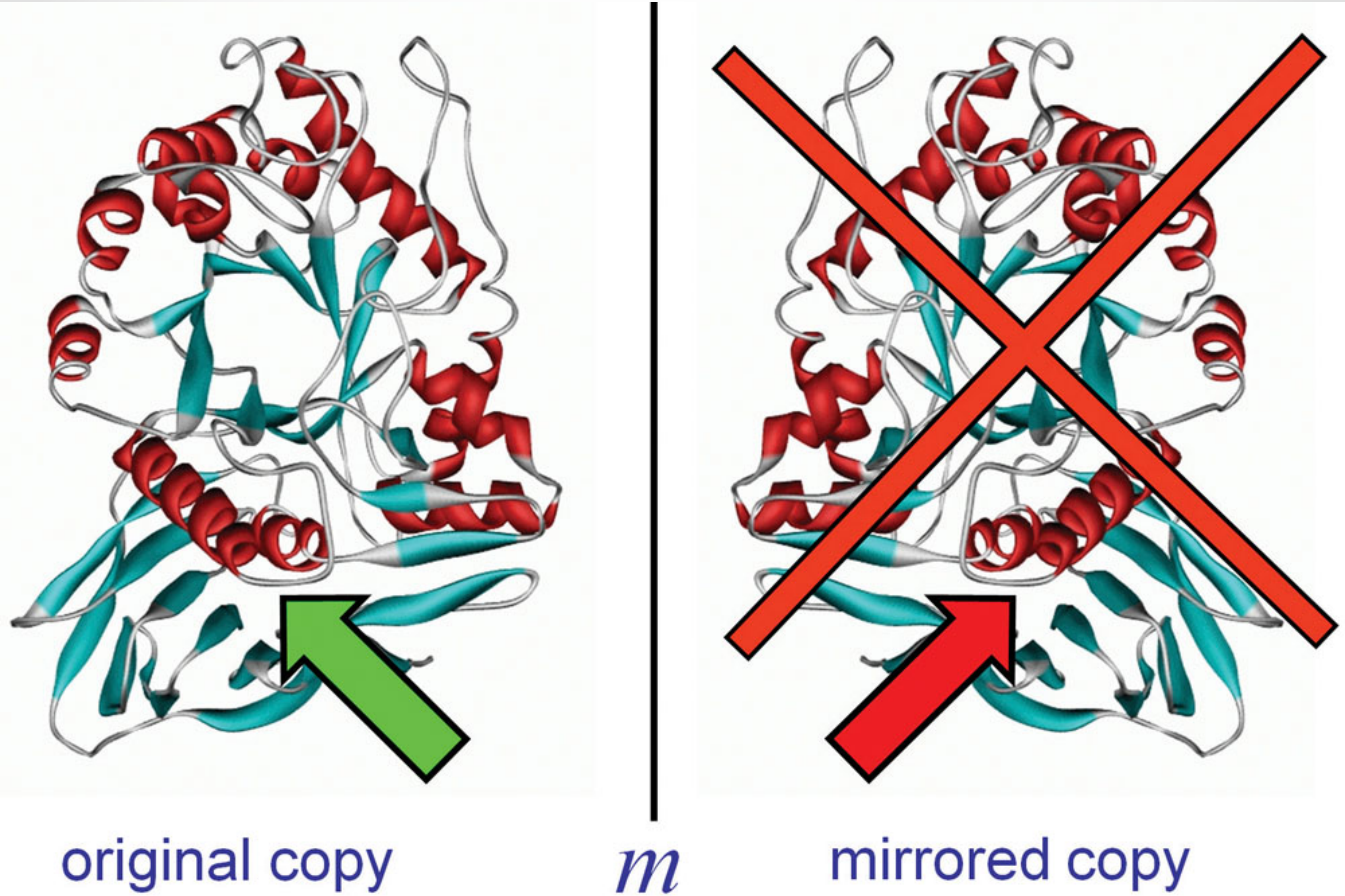
Stereograms of the five improper rotation axes

Point Group

Collection of symmetry elements
Symmetry elements (in a molecule) intersect at a point
Do not alter the molecule itself

Summarizes all symmetry operations in a group

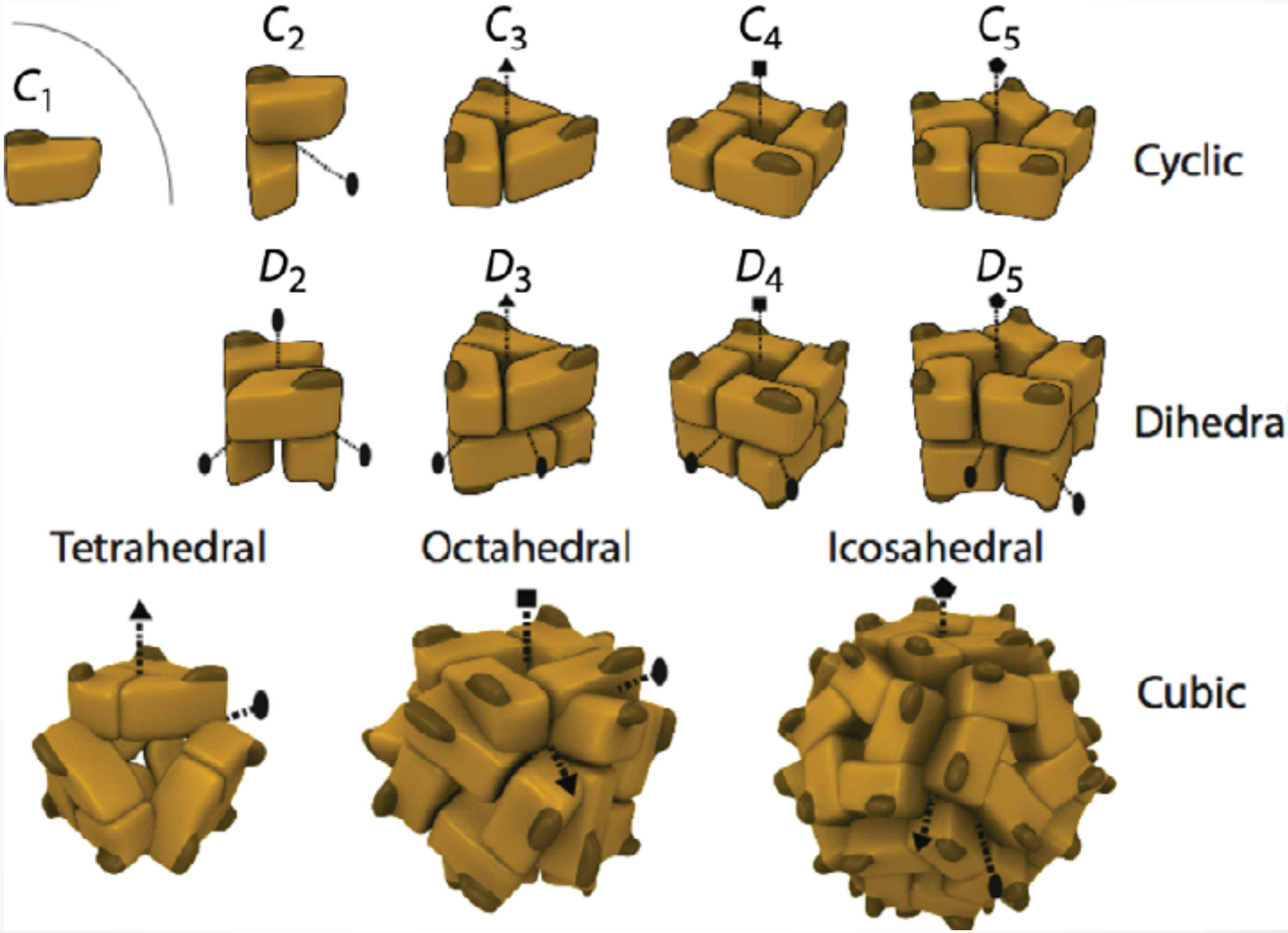
Chirality
In order to be chiral, a molecule must lack both i and σ



original copy
m
mirrored copy

Point groups of biological macromolecules

Klein, 1884: The only finite 3D symmetry groups are cyclic, dihedral, tetrahedral, octahedral, icosahedral



Janin *et al*, Quarterly Reviews of Biophysics, 2008

Cyclic pointgroups

Schonflies notation: C_n

Simplest case: $\mathbf{C_1}$

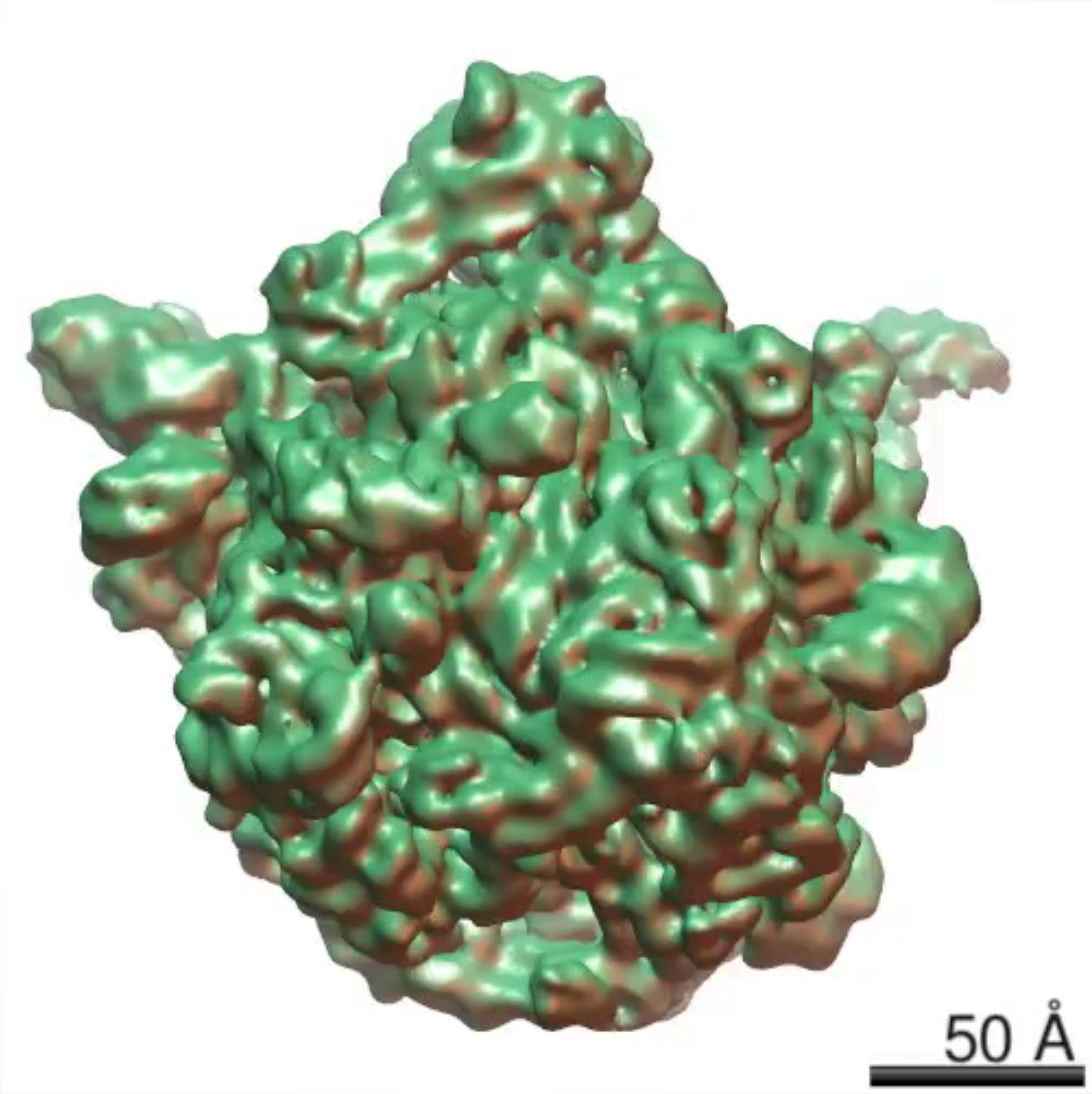
Asymmetric oligomer

Every projection is unique (does not reappear at a different combination of Euler angles)

Mirror symmetry between projection at one Euler angle and its opposite Euler angle

Asymmteric triangle = whole unit sphere

EMBD - 2605: 50S ribosome bound to ObgE



C_2

One two-fold rotational axis of symmetry

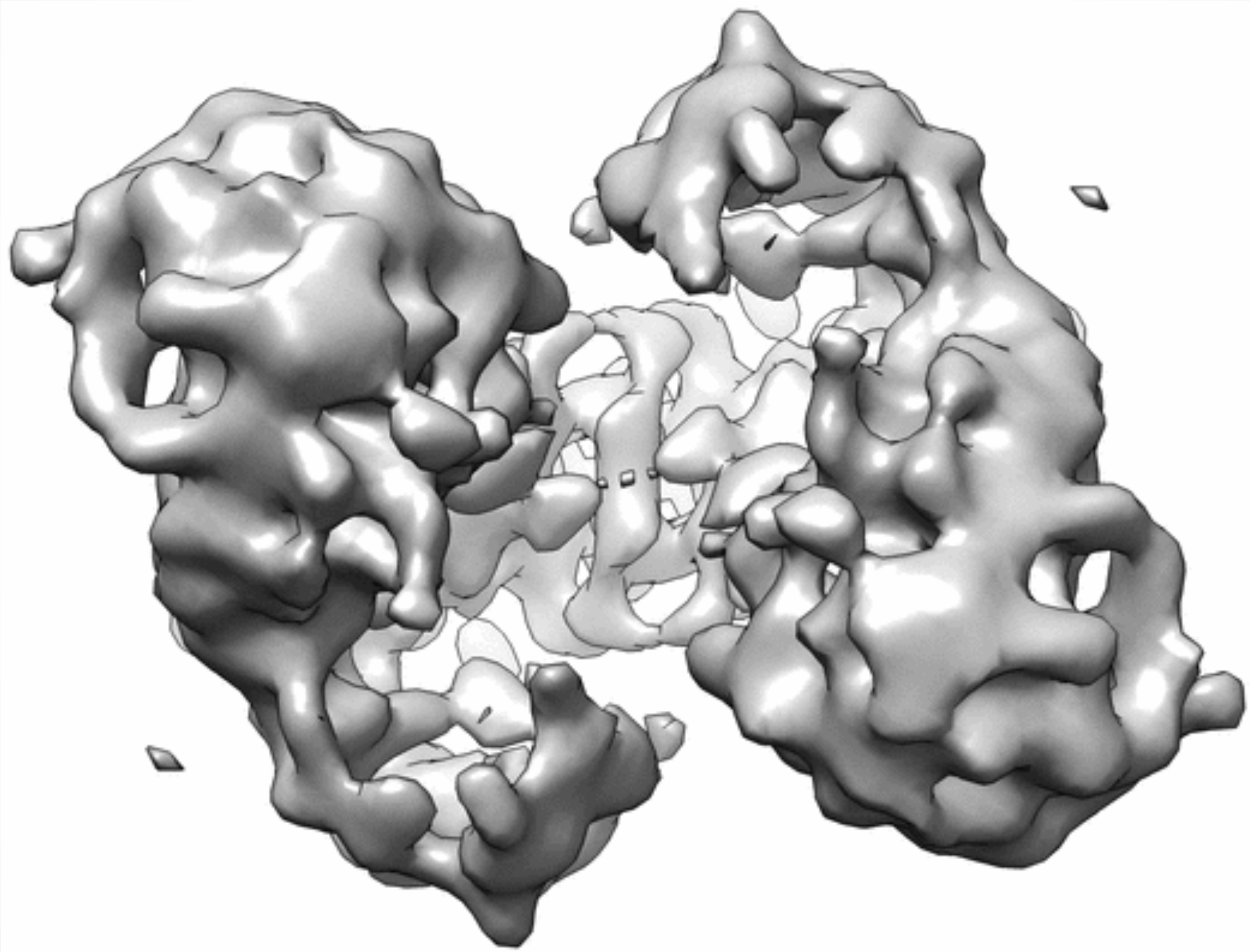
Every normal projection appears twice

Projections perpendicular to 2-fold axis will demonstrate mirror symmetry

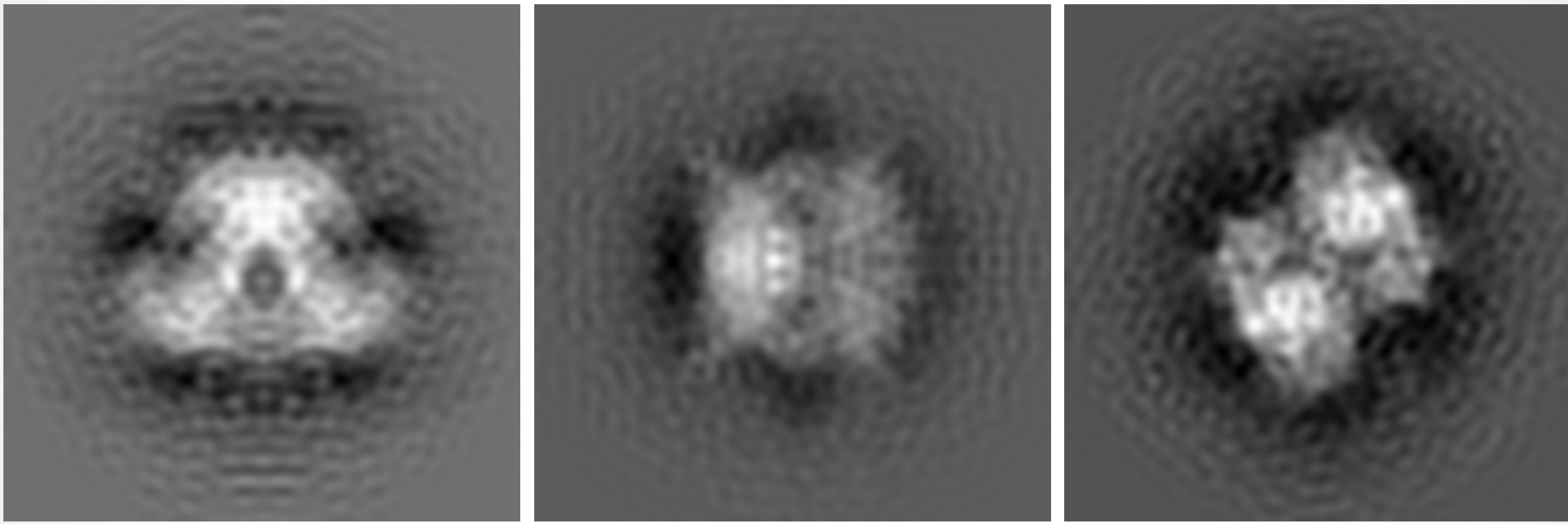
One unique projection along two-fold axis: rotates the dimer back on itself

Asymmteric triangle = half of the unit sphere

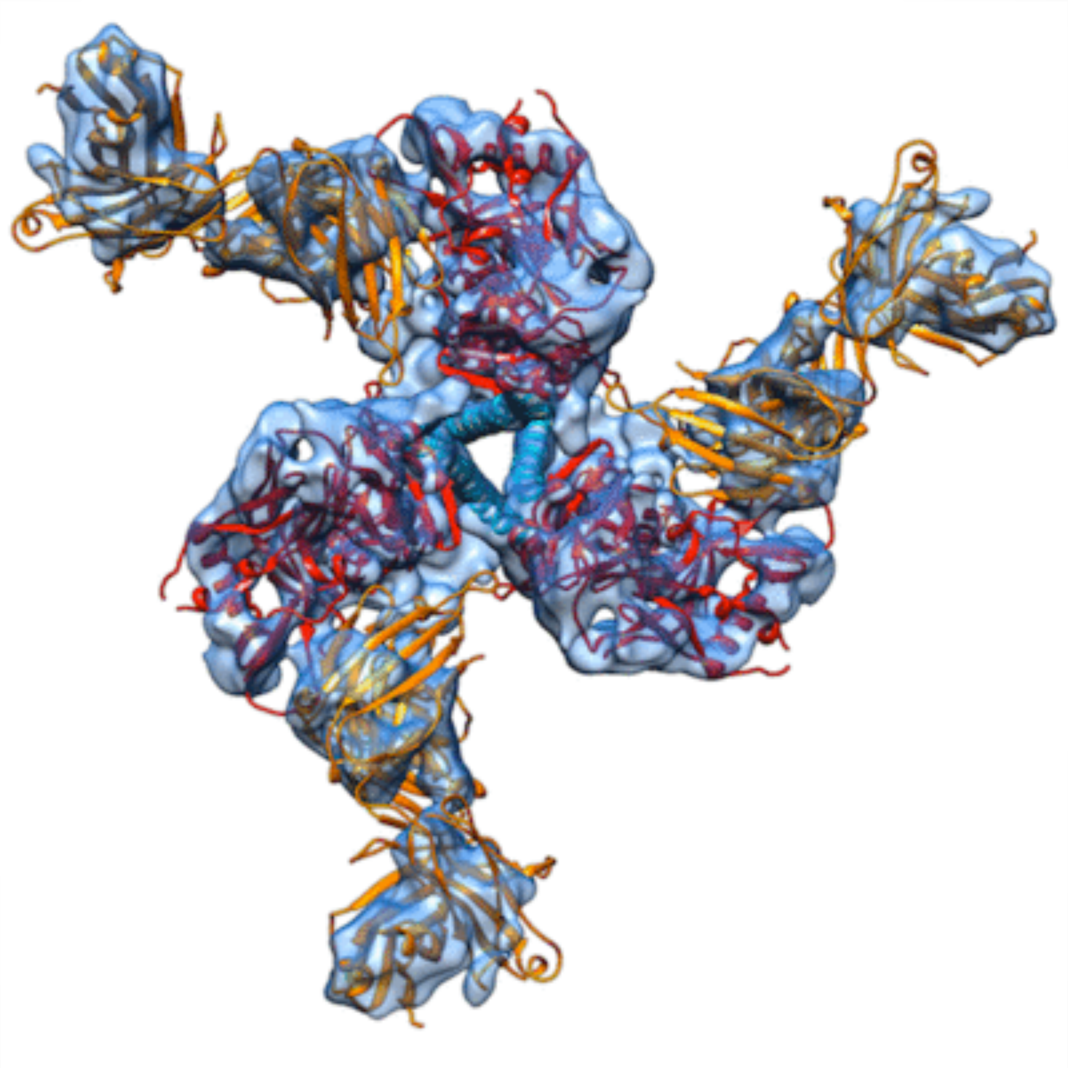
C2
Recombination activating gene (RAG): EMD6490



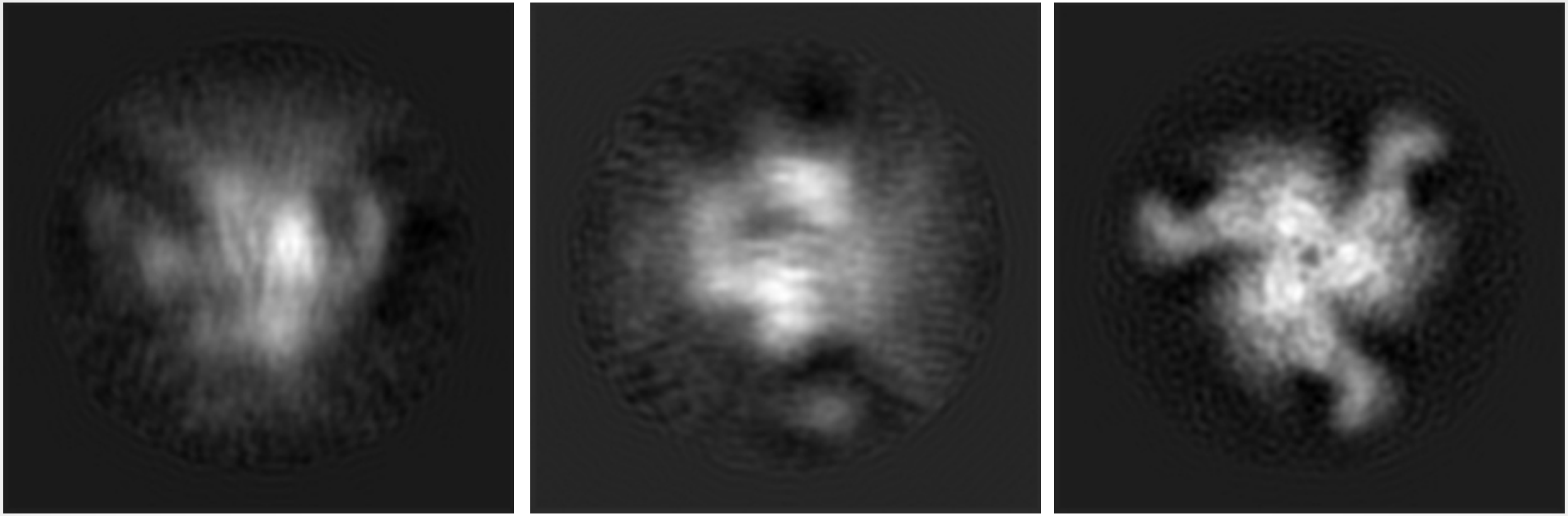
C2
Recombination activating gene (RAG): EMD6490



C3
HIV-1 envelope glycoprotein: EMD2484



C3
HIV-1 envelope glycoprotein: EMD2484



C_n: All other cyclic point groups

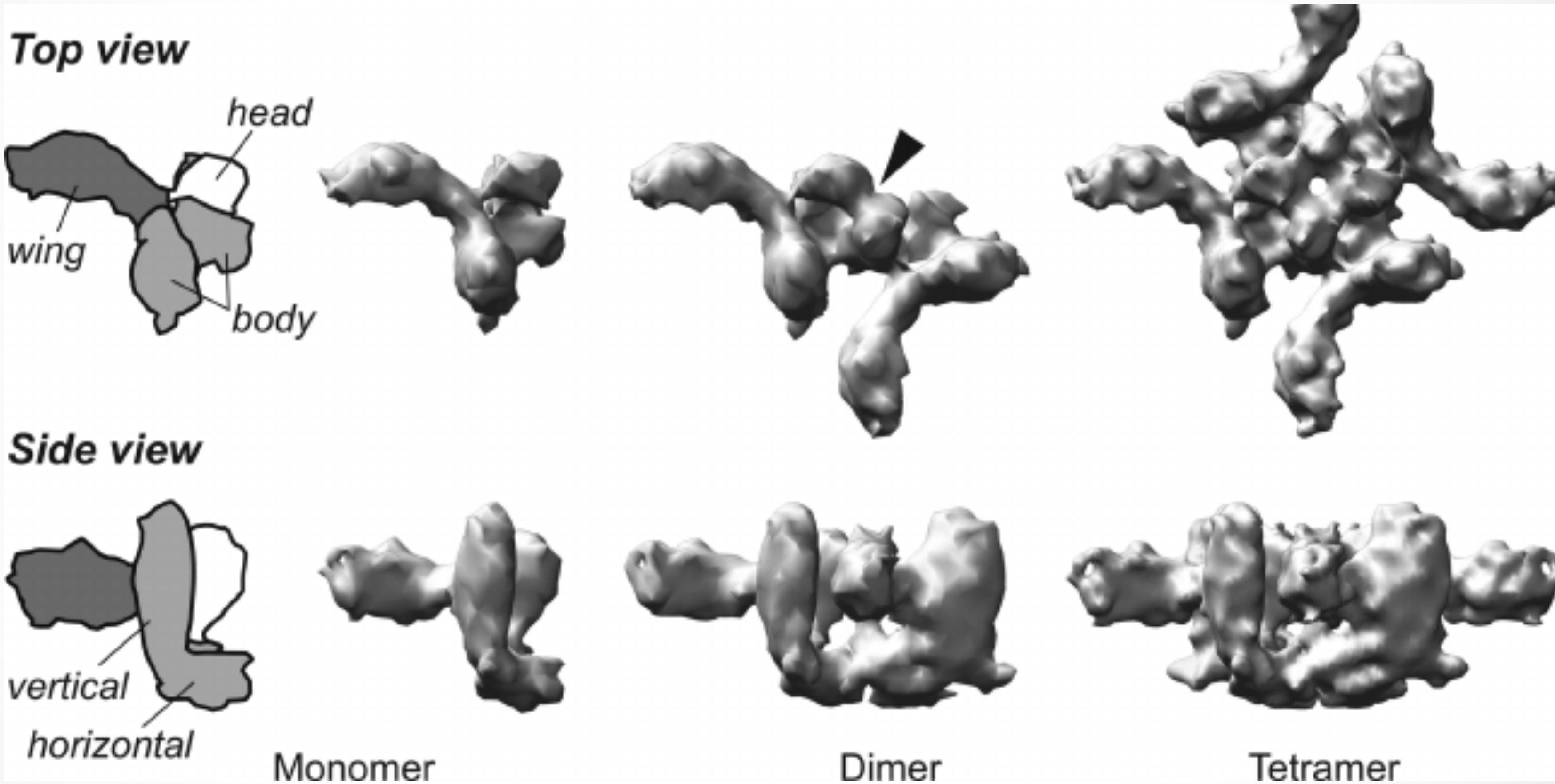
To form a C_n structure requires n identical units

"n" subunits organized in circular arrangement in head to tail fashion

Rotational axis perpendicular to the plane of arrangement of molecules

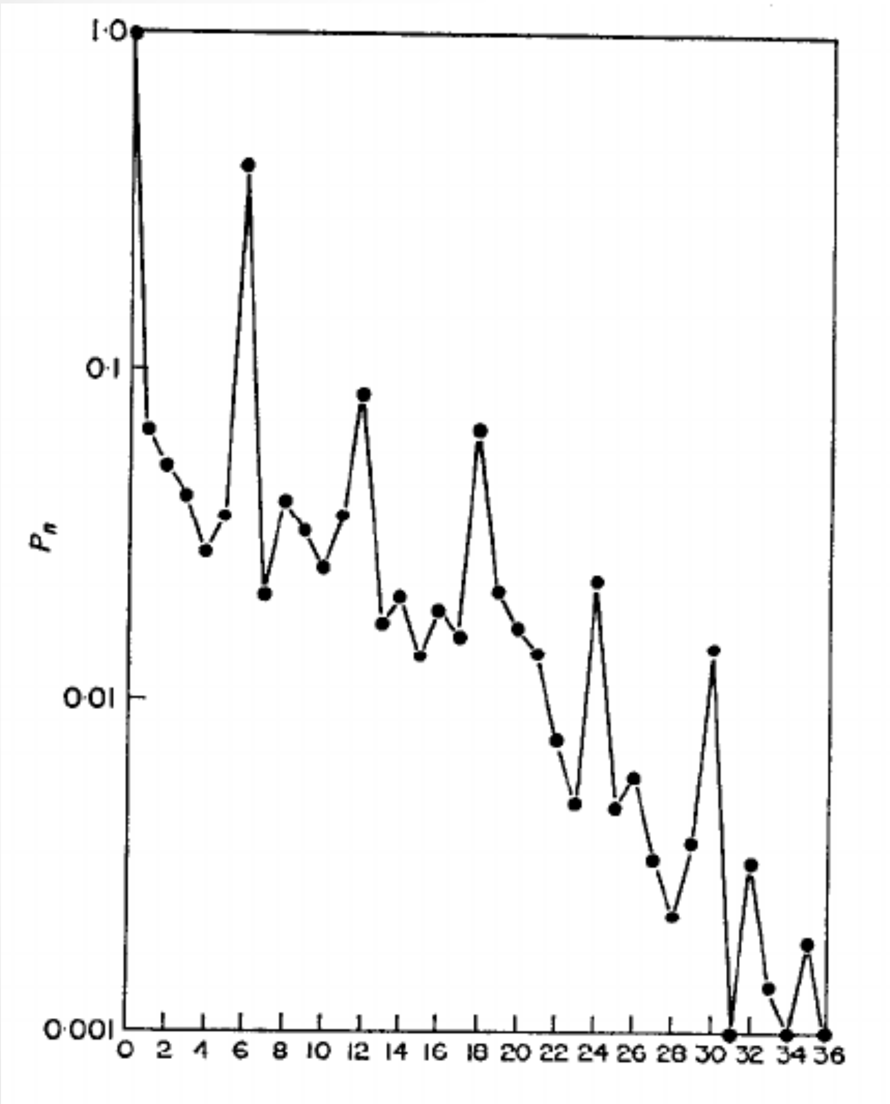
Even symmetry: projections have mirror symmetry
Odd symmetry: projections do not have mirror symmtery

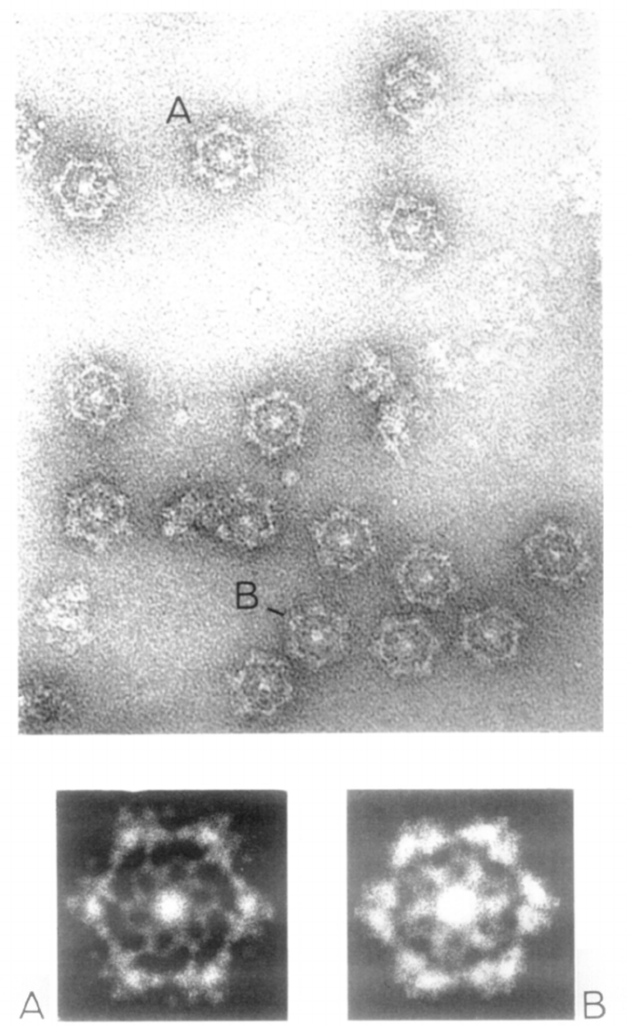
C_4: Latrotoxin



Y.A. Ushkaryov *et al*, Nat Struct Biol, 2000

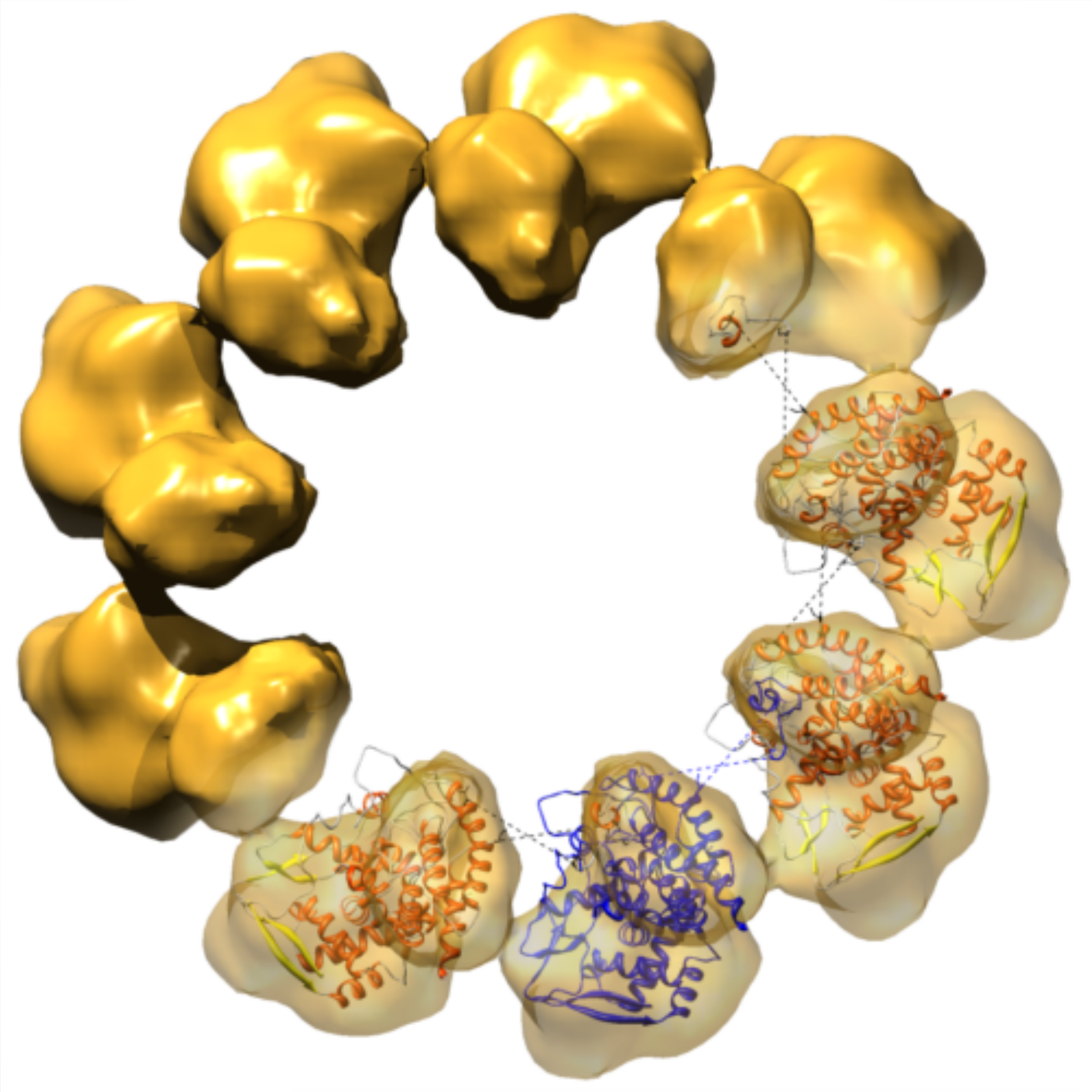
C6: Bacteriophage T4 base plates





Crowther and Amos, JMB, 1971

C9: Influenza Virus RNP (EMD1603)

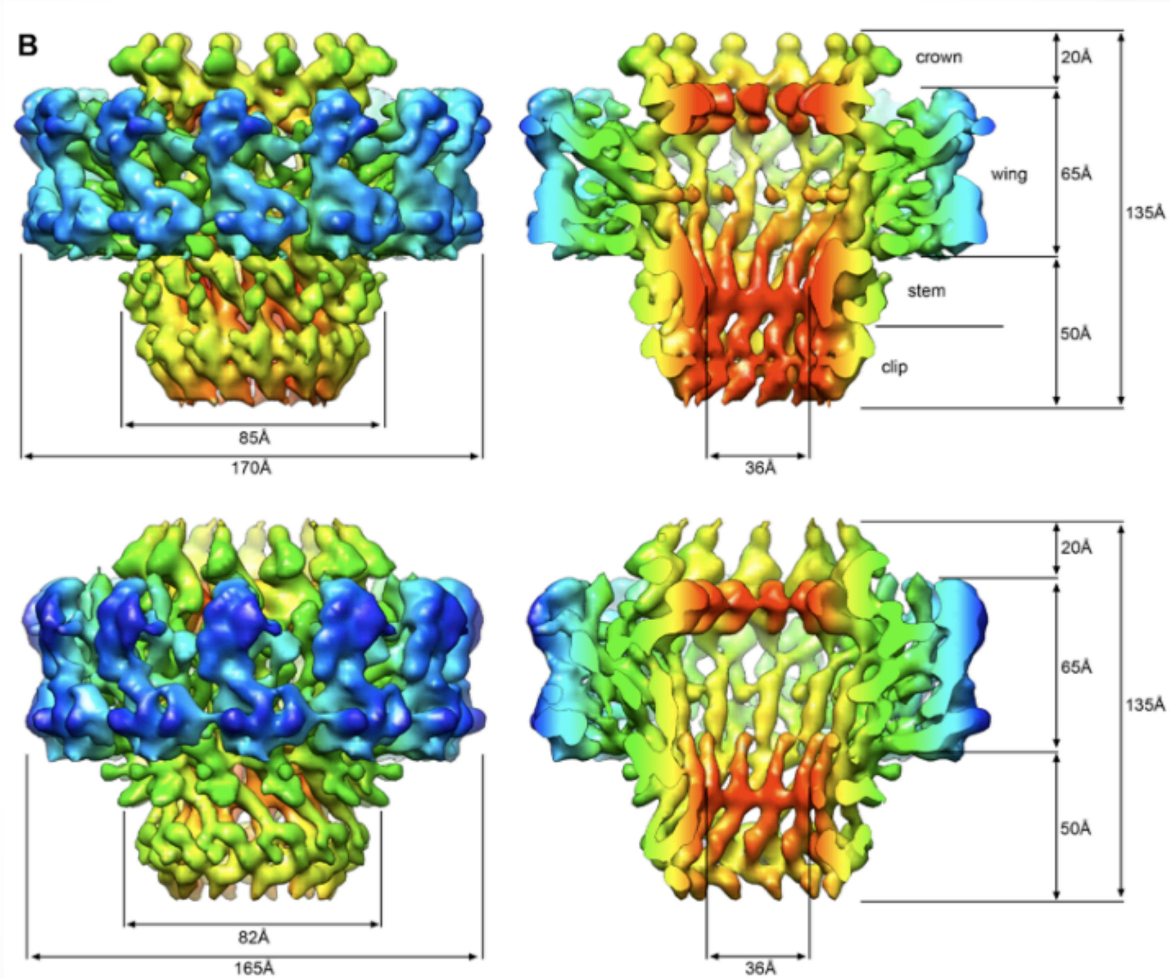


C11, 12: Bacteriophage P22 portal and tail machine

Bacteriophage P22 portal and tail machine

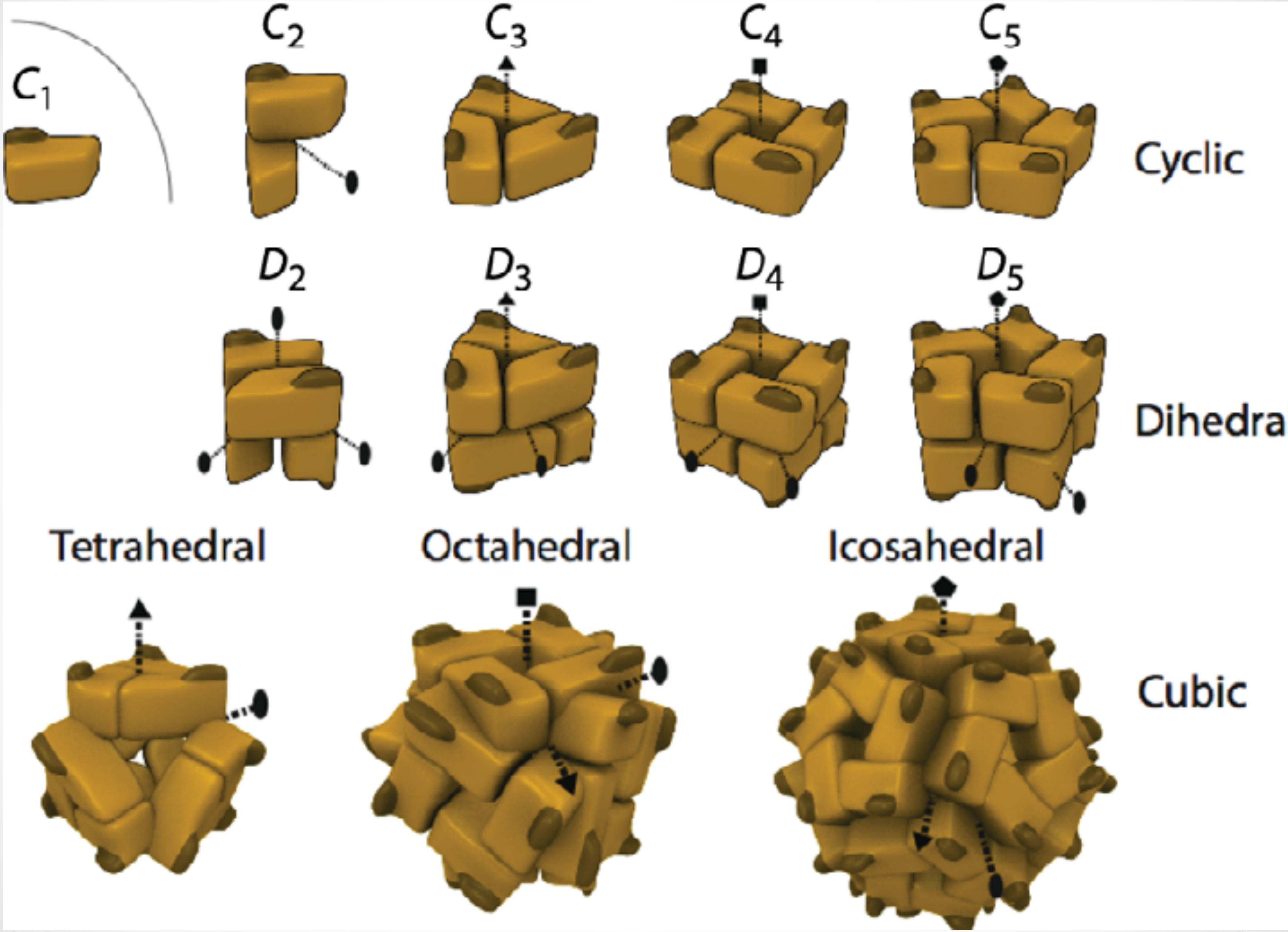
12-fold

11 fold



Lander *et al.*, Structure, 2009

Point groups of biological macromolecules



Janin *et al*, Quarterly Reviews of Biophysics, 2008

D_n: dihedral structures

n-fold rotational axis and a 2-fold axis perpendicular to it

Two C_n structures stacked top-to-top or bottom-to-bottom

$D_1 = C_2$

D_2 (222)

Three 2-fold axes, all perpendicular to each other

Minimum number of subunits required = four

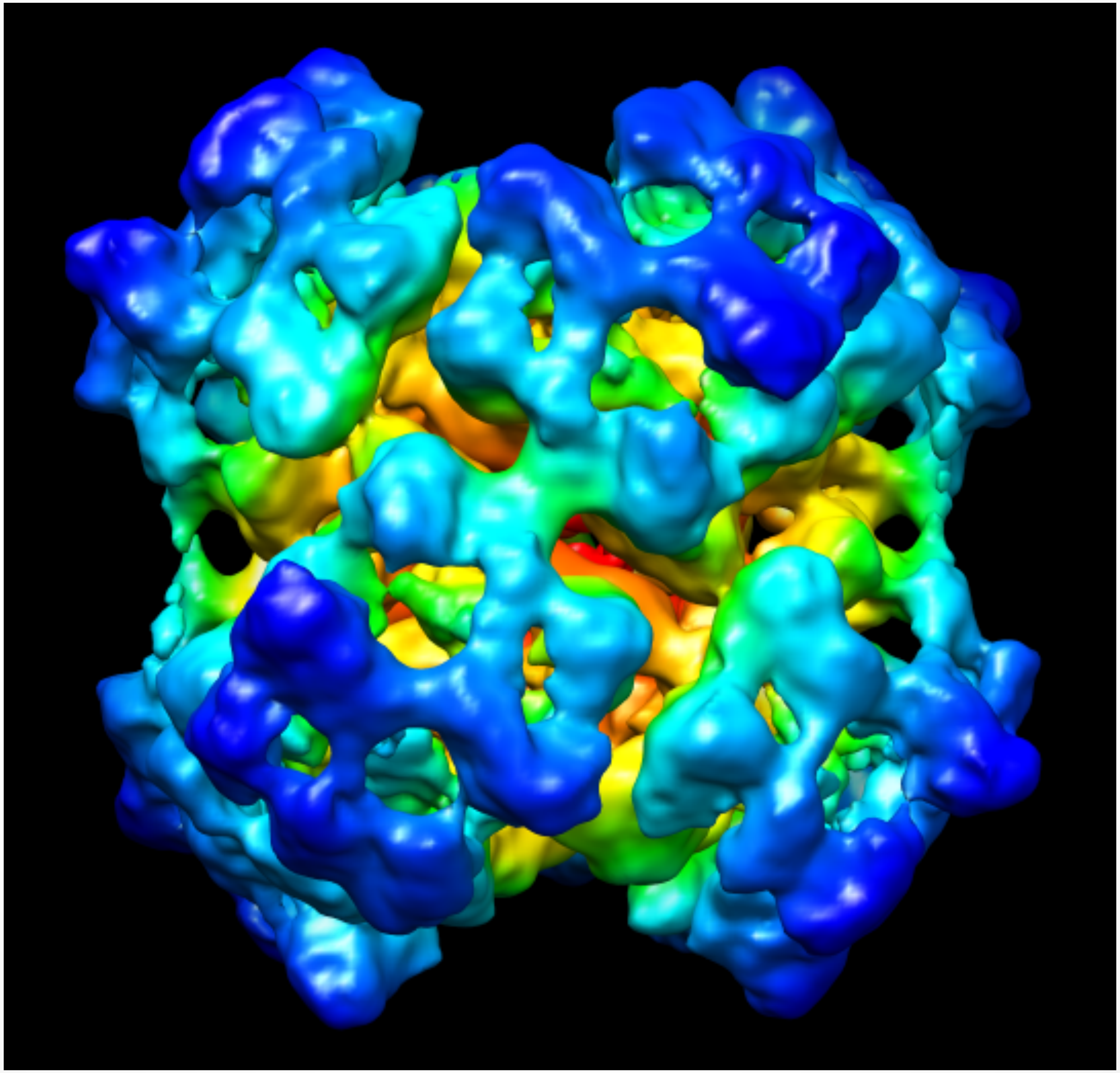
One projection equivalent to 4 different projections

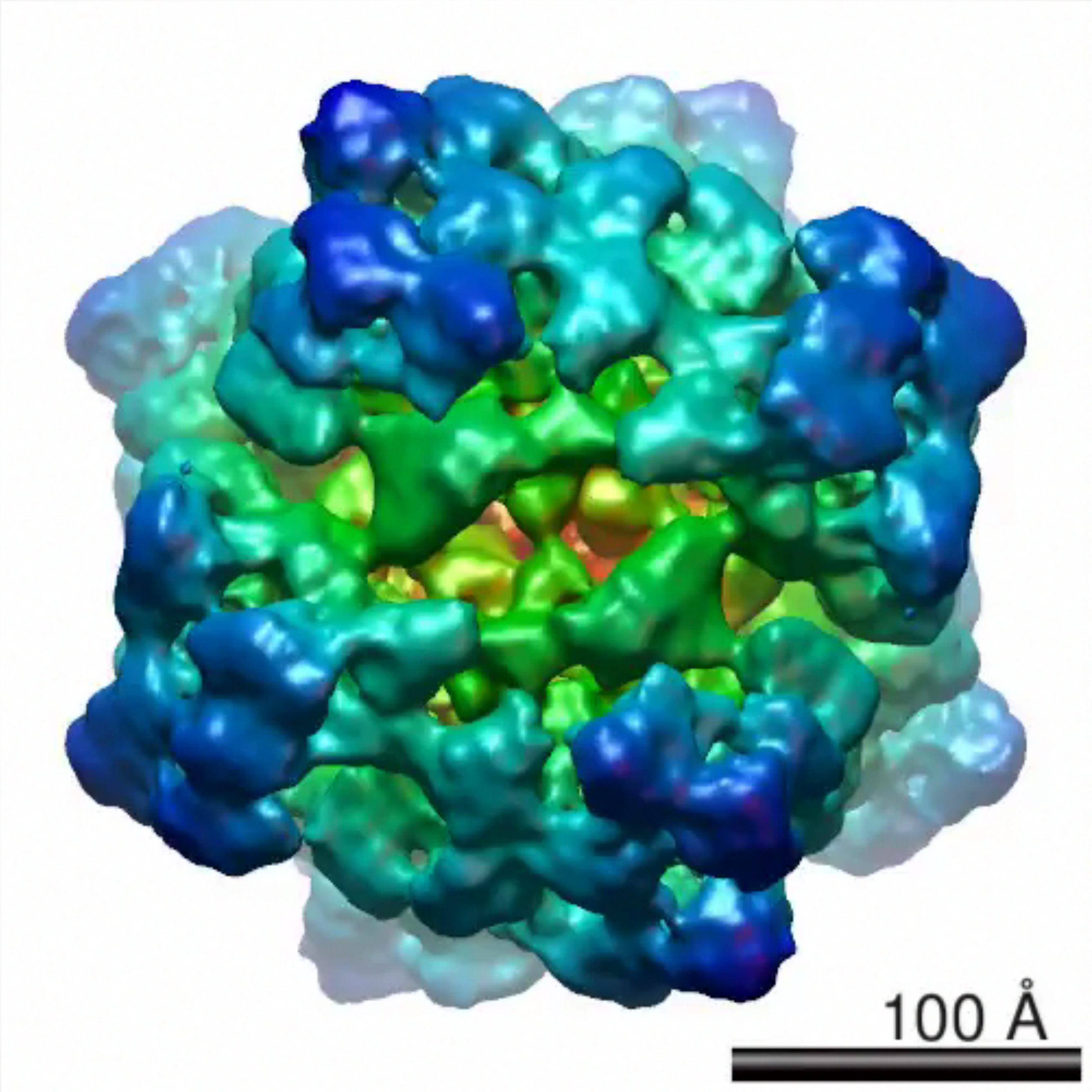
Projections along two-folds have a double mirror symmetry

Asymmetric triangle covers $1/4^{th}$ unit sphere

D_2

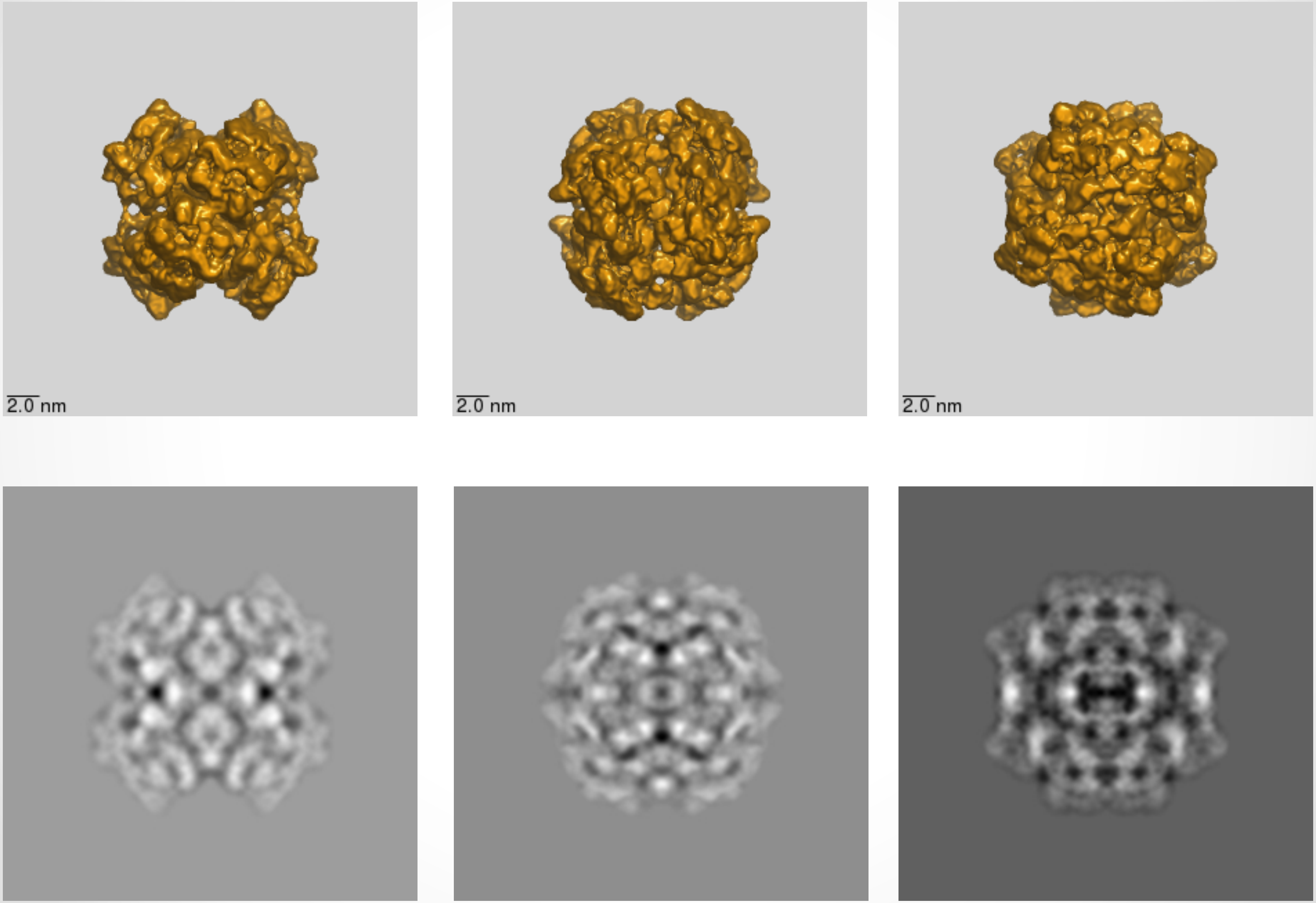
Limulus polyphemus hemocyanin EMD1304

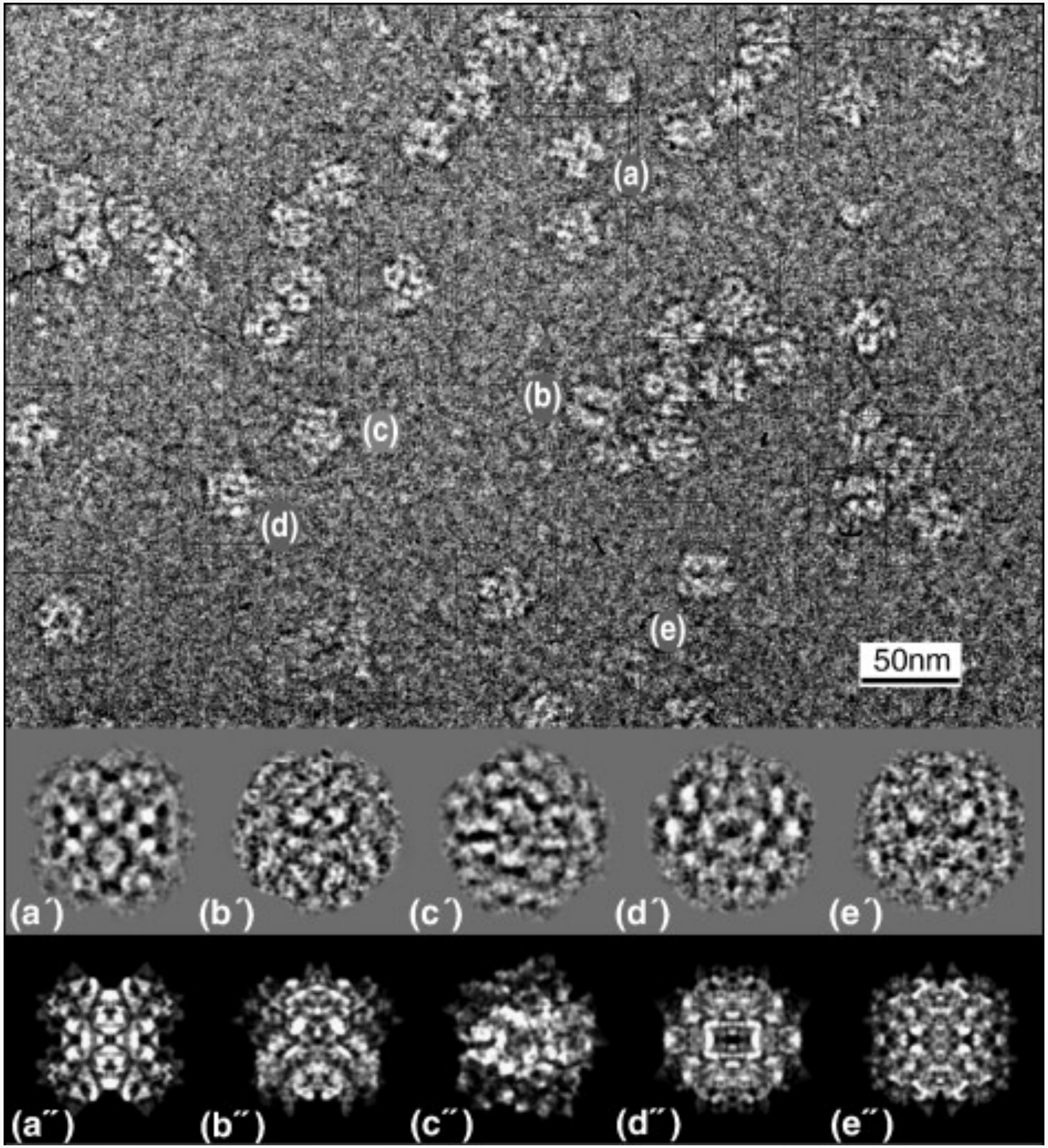



100 Å

D_2

Limulus polyphemus hemocyanin EMD1304





Martin *et al*, JMB, 2007

D_3 (32)

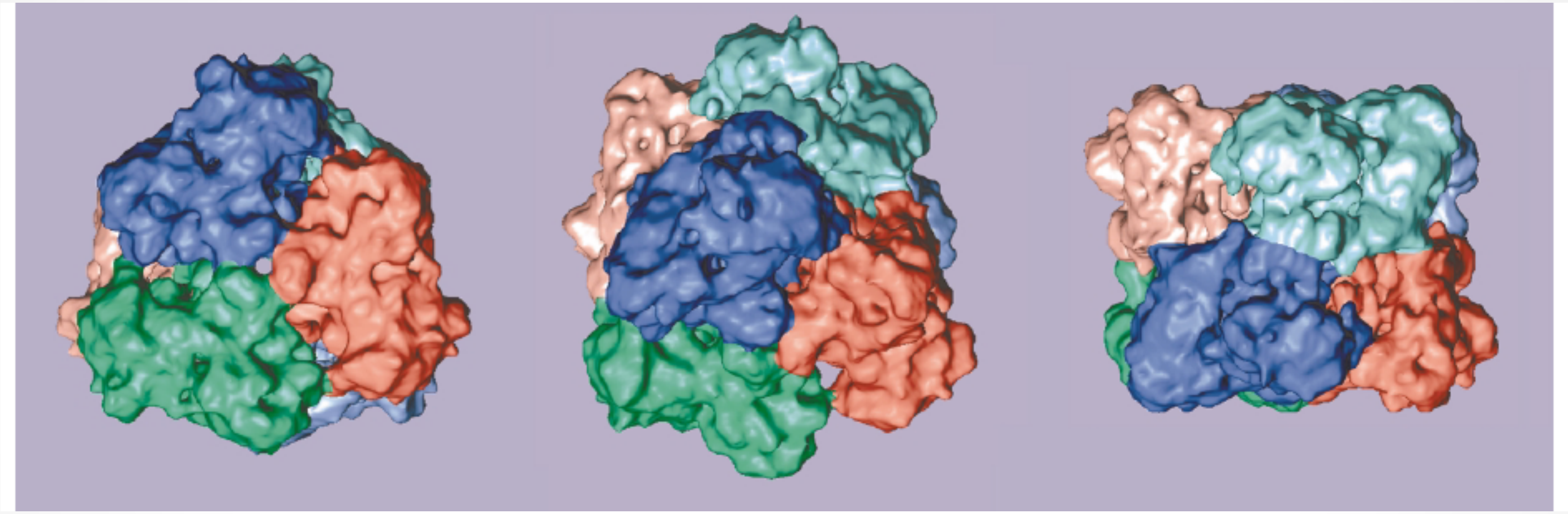
Minimum of 6 equivalent monomers required

One three-fold rotational axis, and three 2-fold axis perpendicular to that

Projections along 3-fold axis exhibit three mirror planes

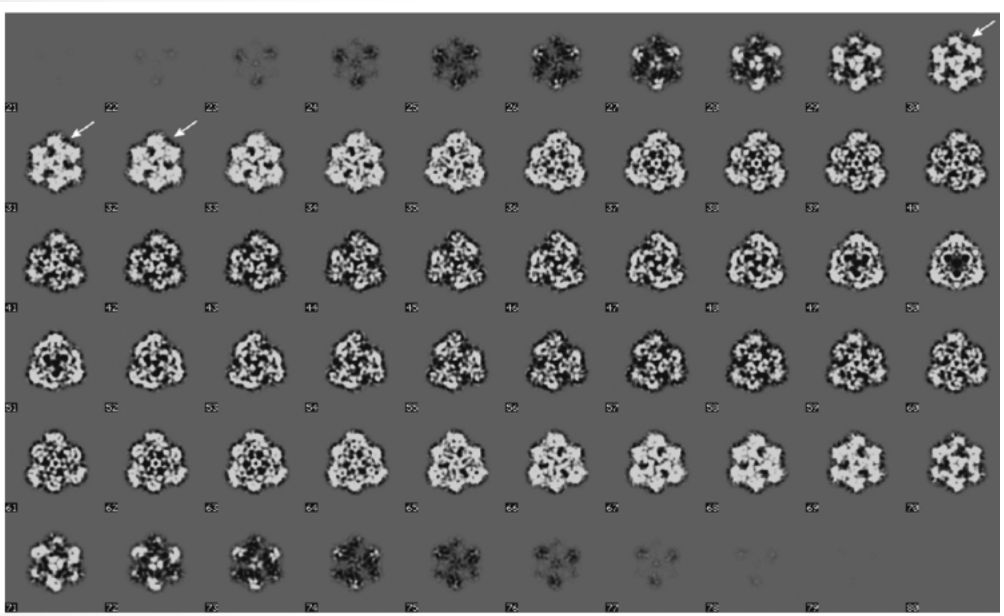
Asymmetric triangle covers 1/6th of unit sphere

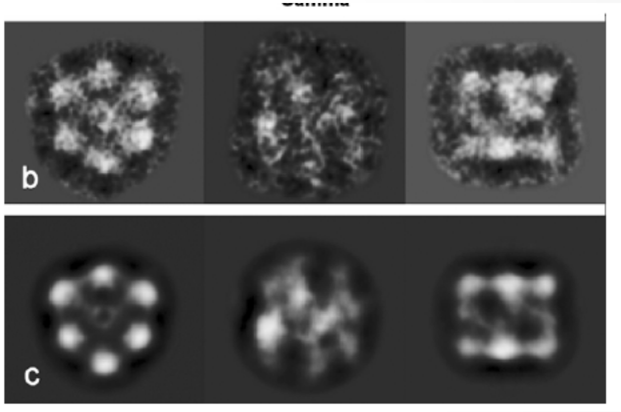
D_3
Palinurus elephas hemocyanin



Meissner *et al.*, JMB, 2003

D_3
Palinurus elephas hemocyanin





Meissner *et al.*, JMB, 2003

D_4 (422)

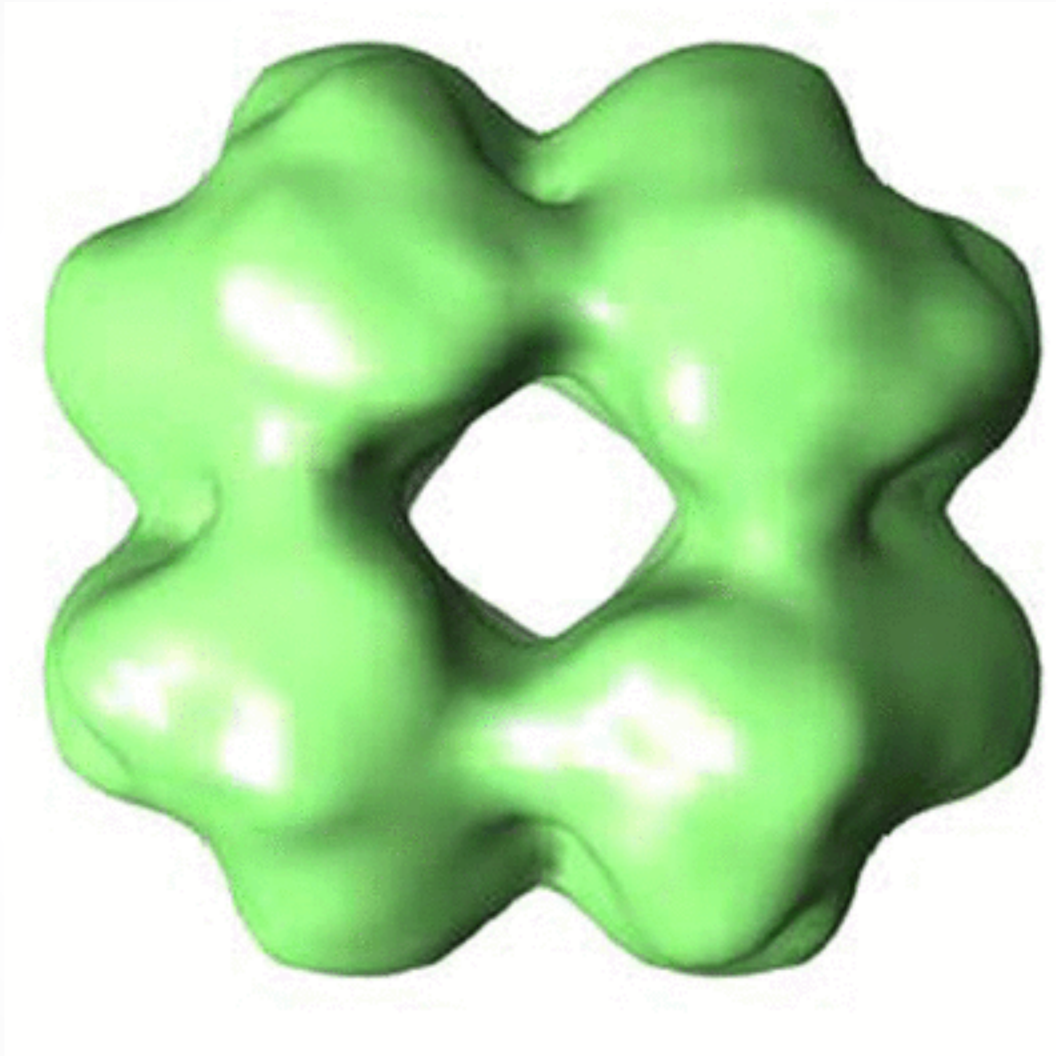
Requires 8 equivalent monomers

Two 2-fold axis, one 4-fold axis

Projections along the axis show perpendicular mirror planes

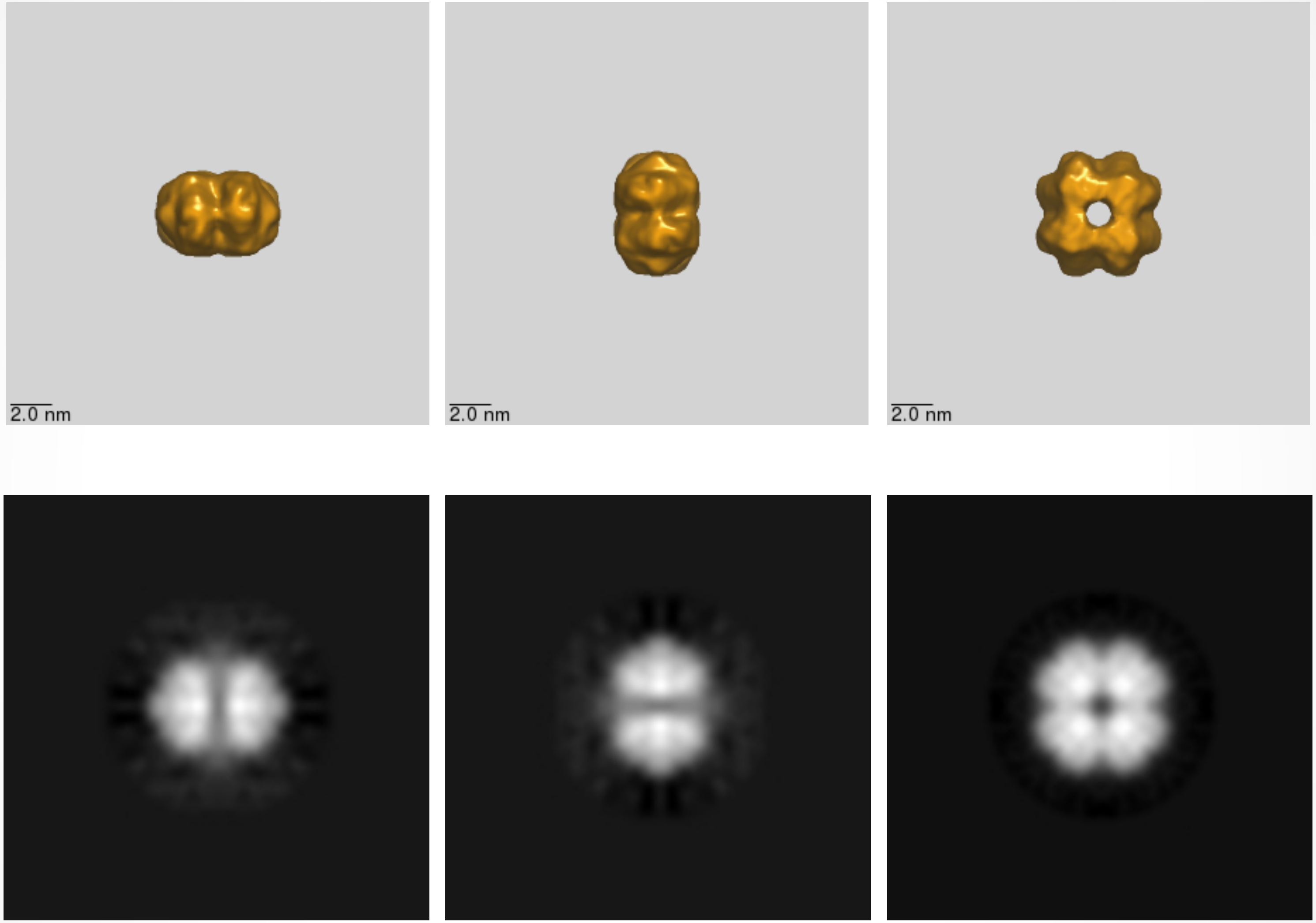
Asymmetric triangle covers 1/8th of the unit sphere

Rubisco large subunit octamer



Liu C *et al*, Nature, 2010

Rubisco large subunit octamer



D_5 (52)

Requires 10 equivalent subunits

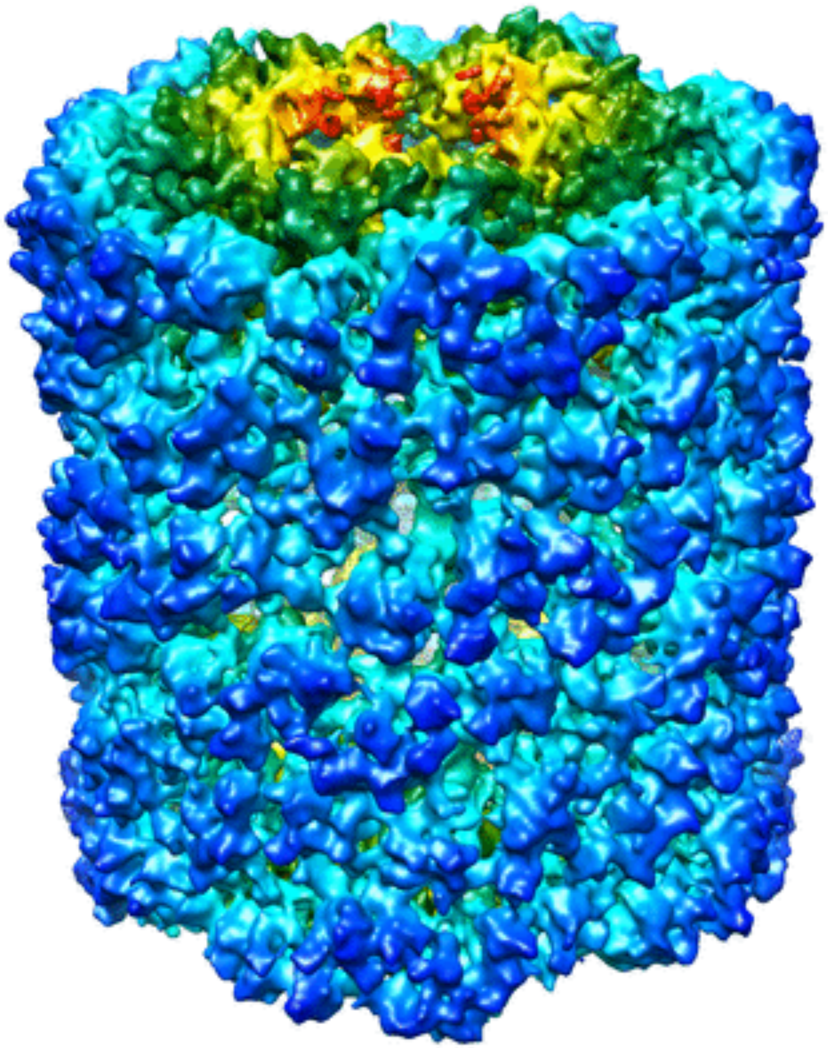
Each projection corresponds to 10 different combinations of Euler angles

Projections along 5-fold contain 5 mirror planes

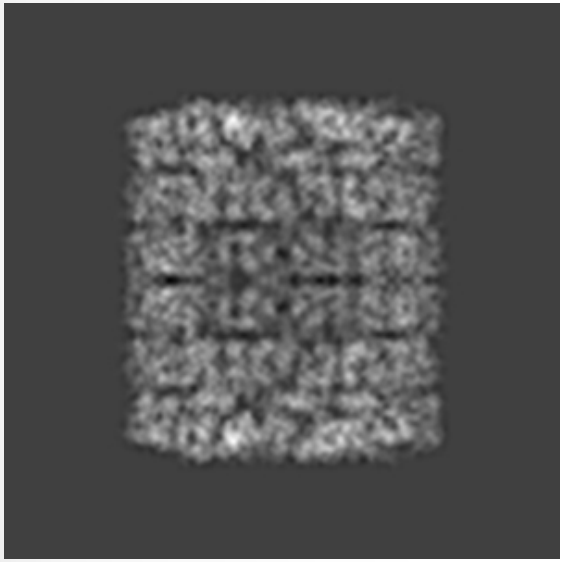
Projections along two-fold have no mirror symmetry

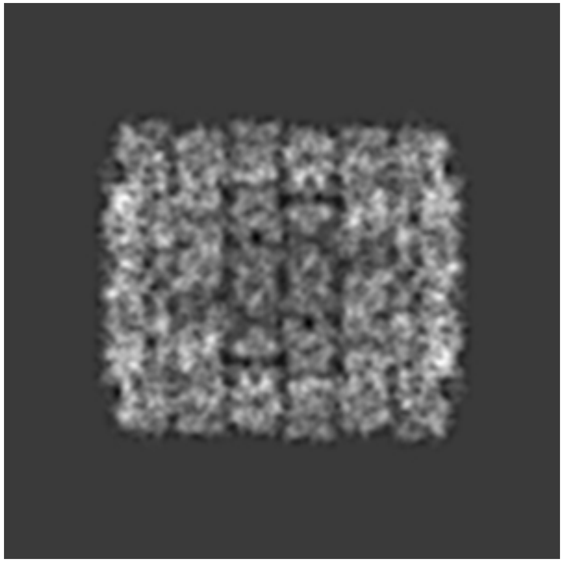
Asymmetric triangle covers $1/10^{th}$ spehere

D_5 (52)
Keyhole Limpet Hemocyanin (KLH) EMD1569

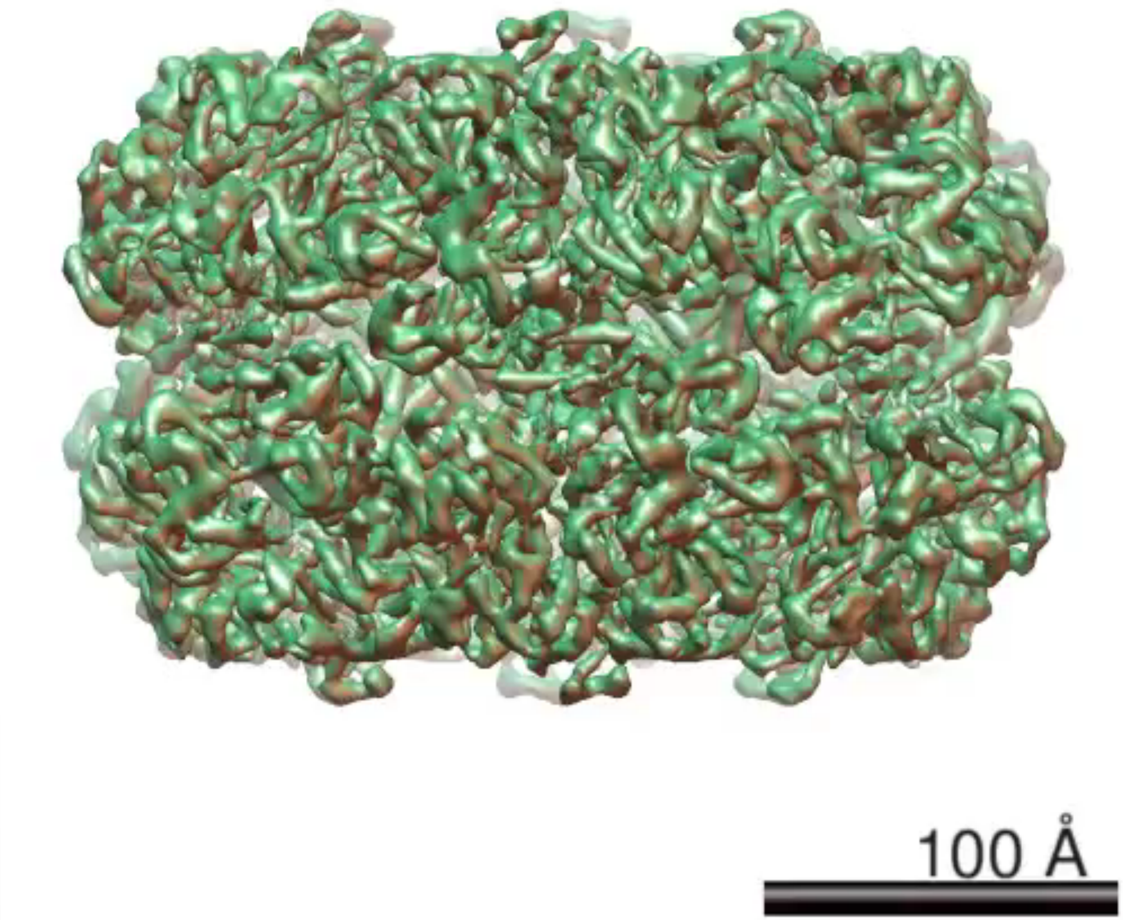


D_5 (52)
Keyhole Limpet Hemocyanin (KLH) EMD1569

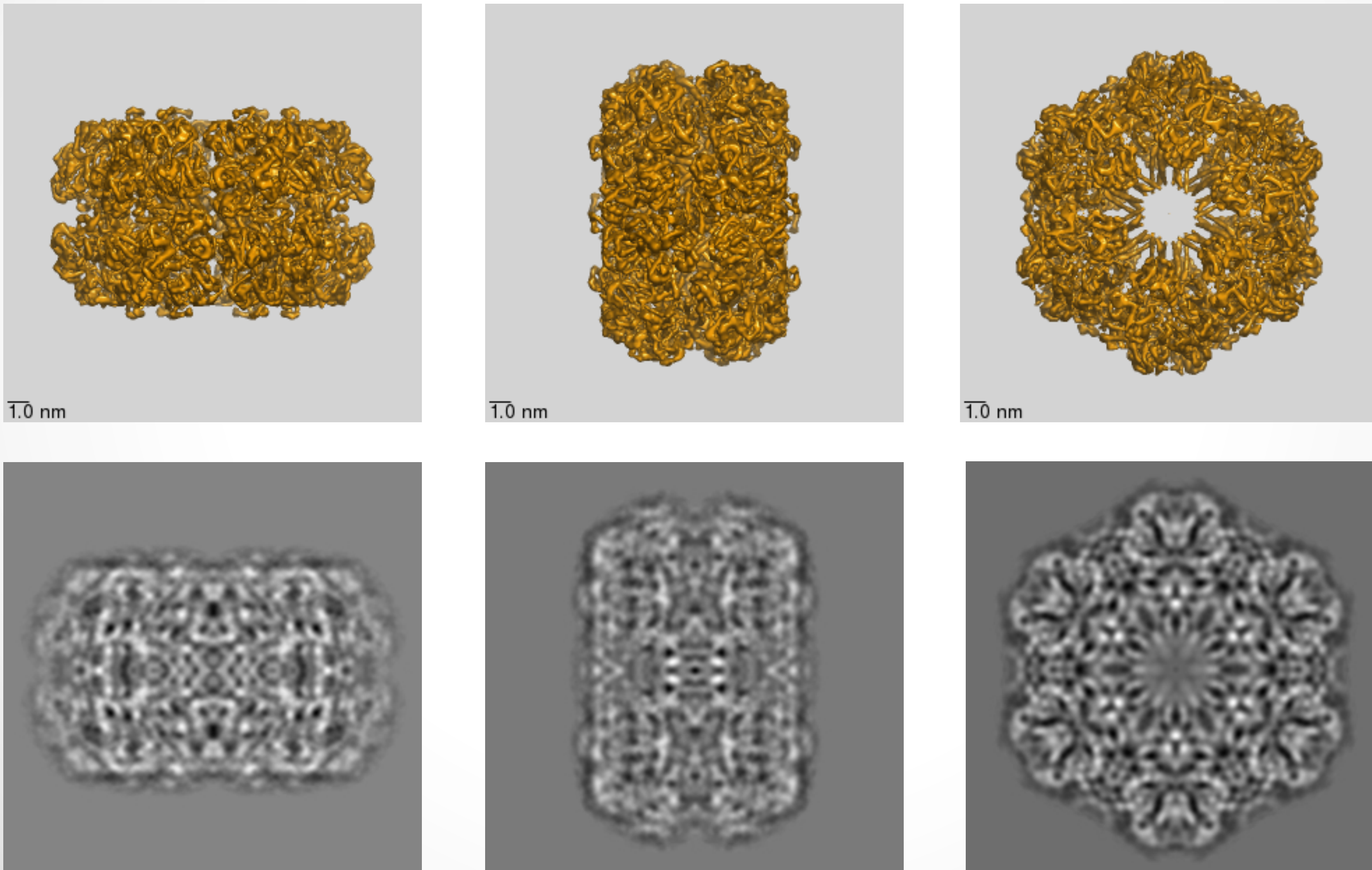




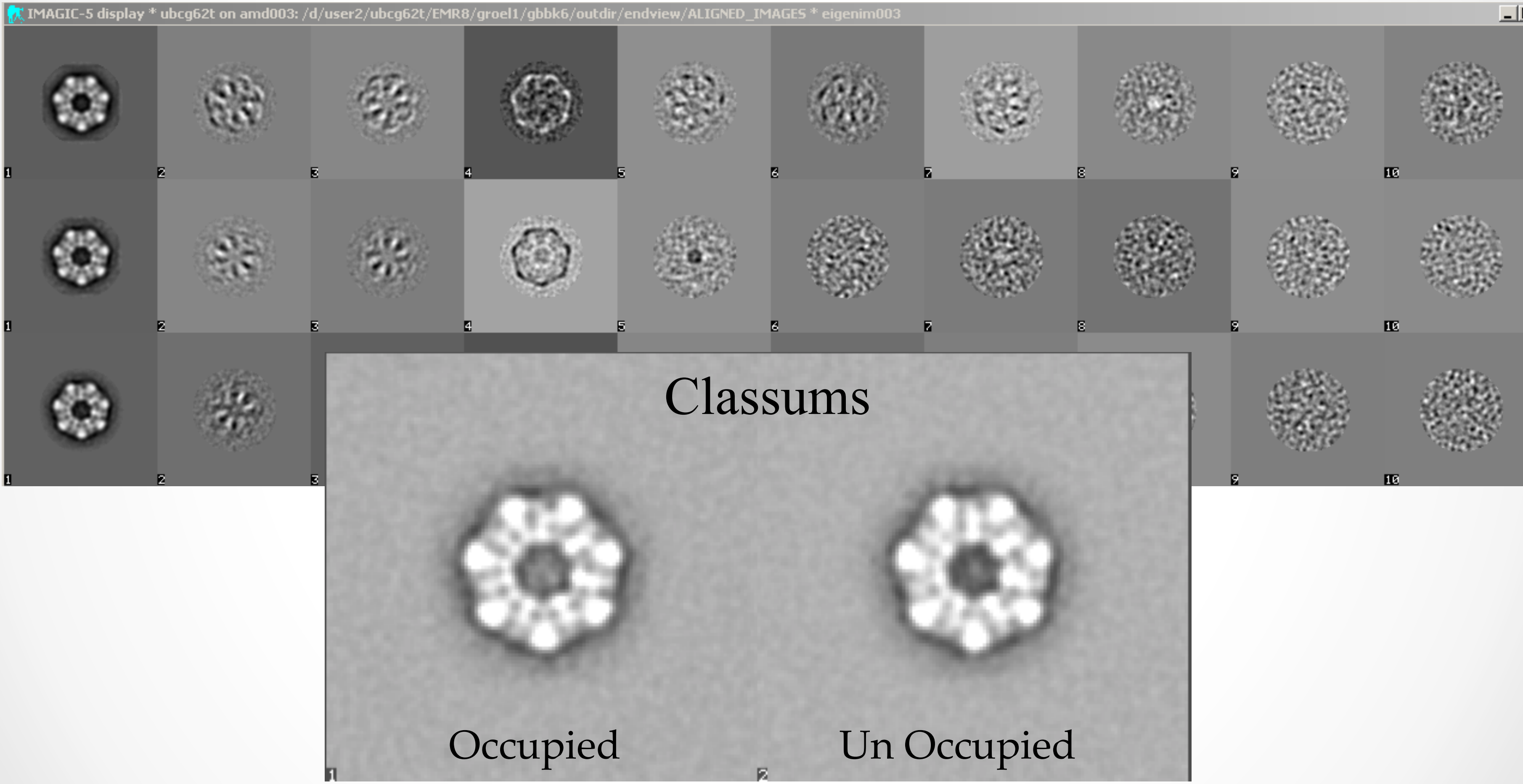
D_6 (622)
Total of 12 equivalent subunits
Worm haemoglobin, EMD2825



D_6 (622)
Total of 12 equivalent subunits
Worm haemoglobin, EMD2825



D_7: GroEL

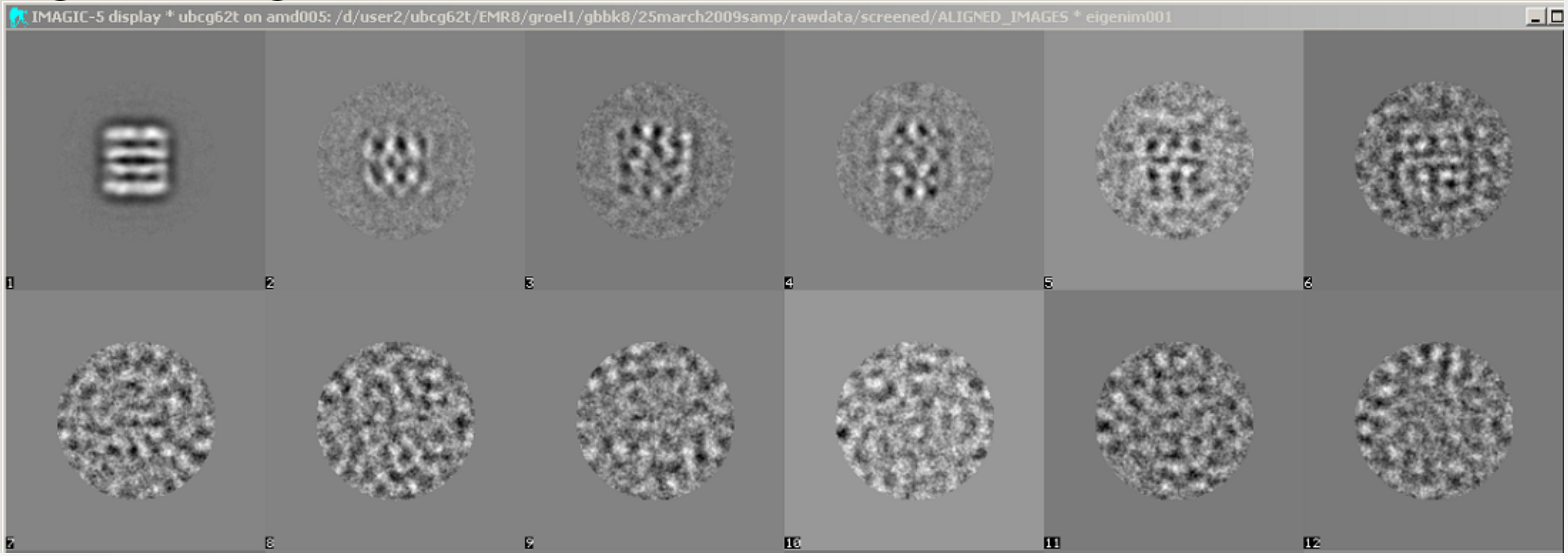


999

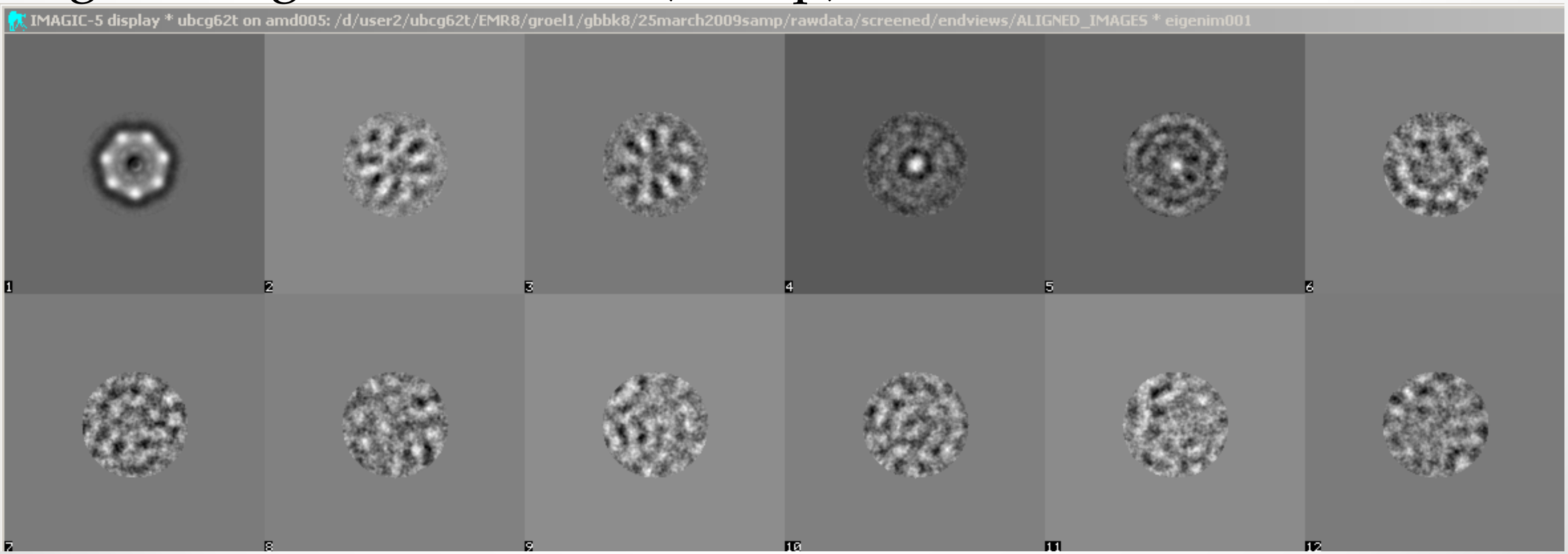
1201

Natesh *et al.*, Unpublished

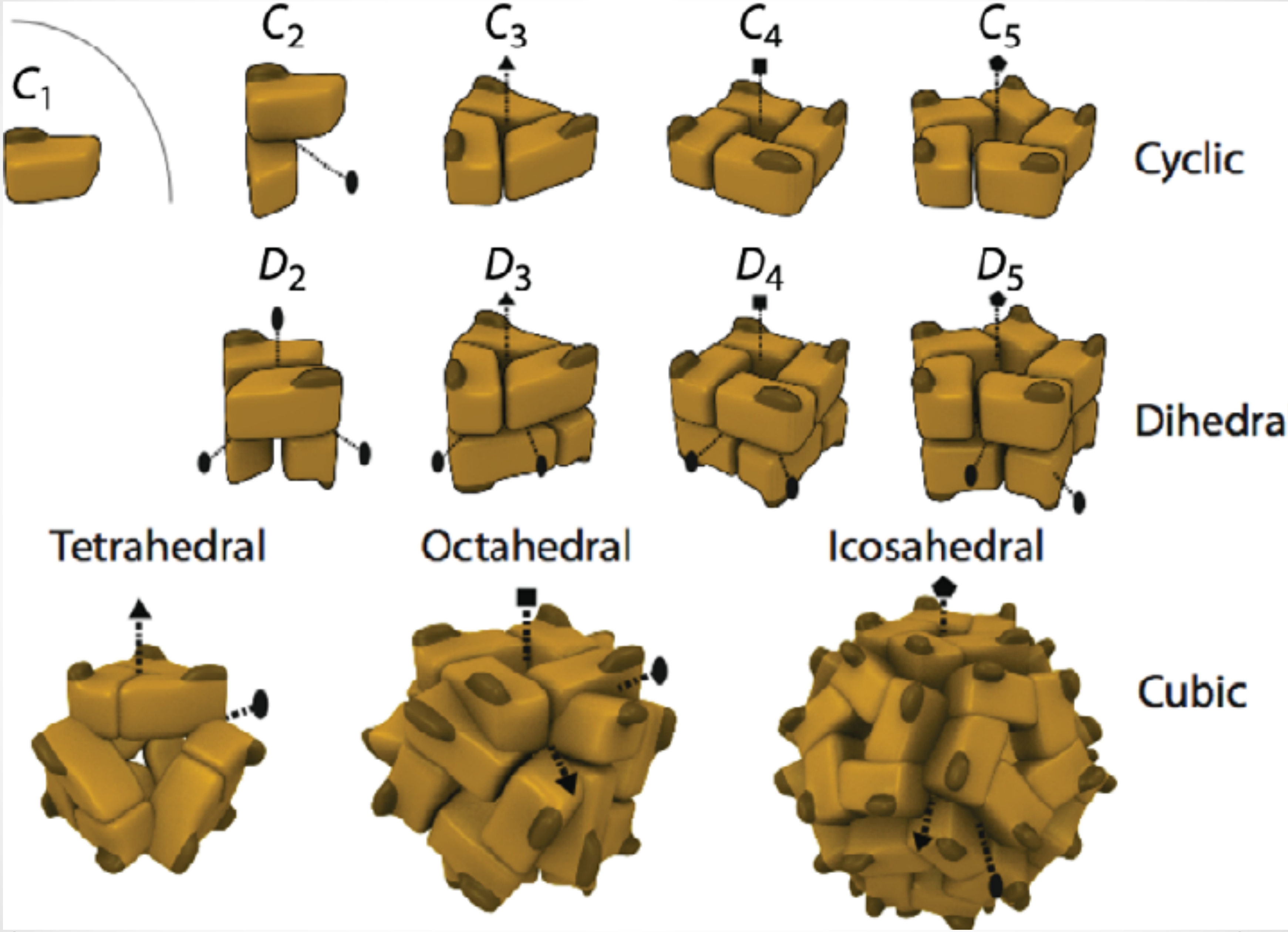
Eigen images of 4782 side views.



Eigen images of 3161 end(or top) views.

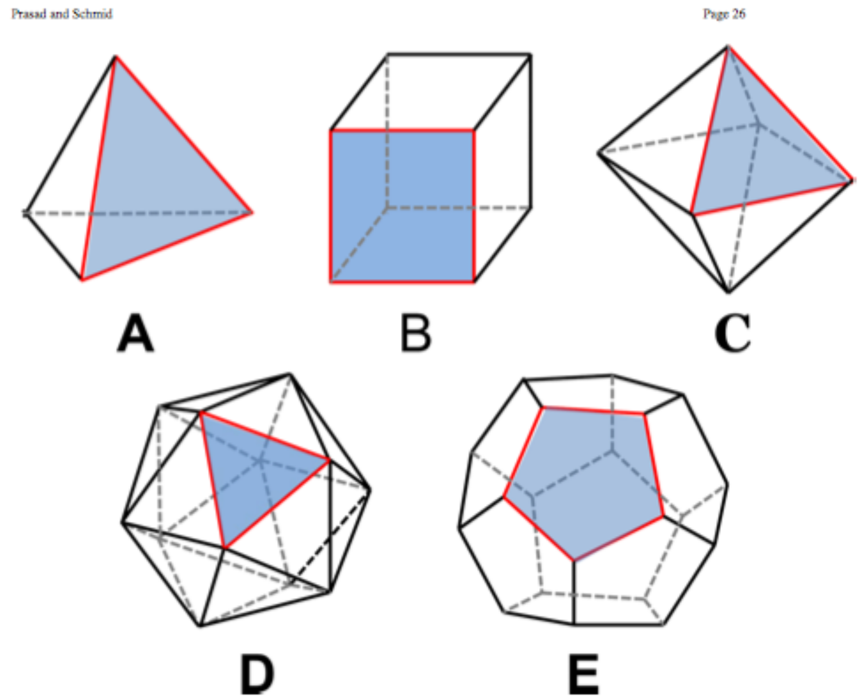


Point groups of biological macromolecules



Janin *et al*, Quarterly Reviews of Biophysics, 2008

Platonic solids (all have cubic symmetry) tetrahedron, cube, octahedron, dodecahedron and Icosahedron



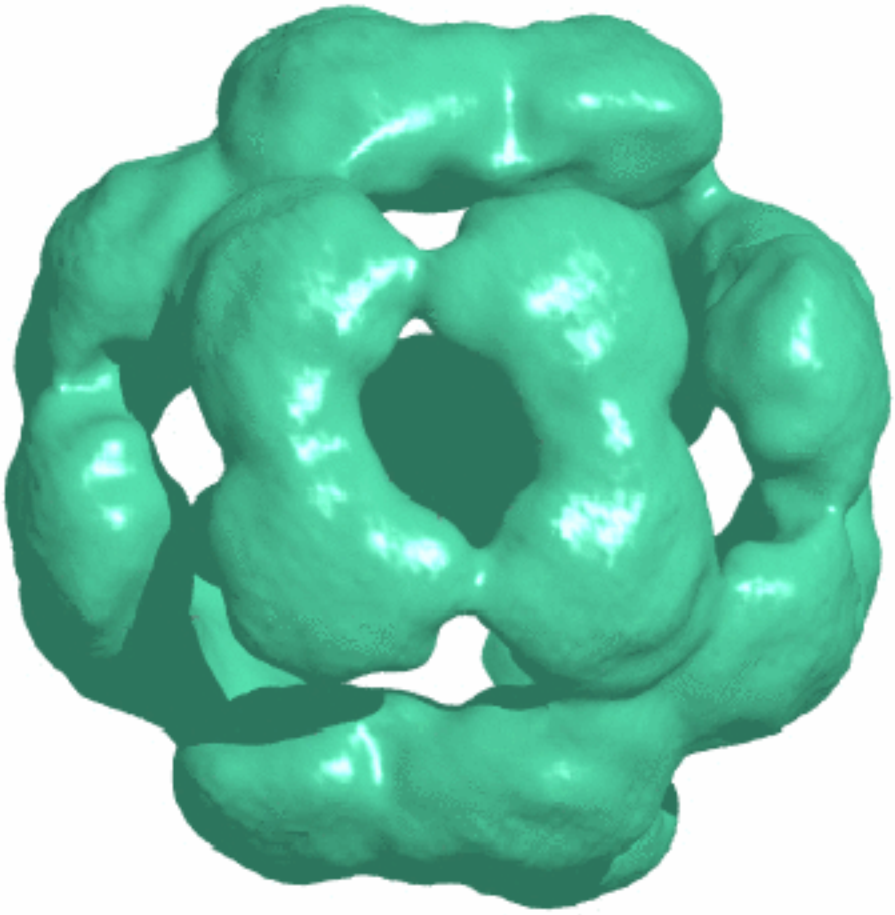
The number of vertices (V), faces (F), and edges (E) follow Euler formula, F +V=E+2

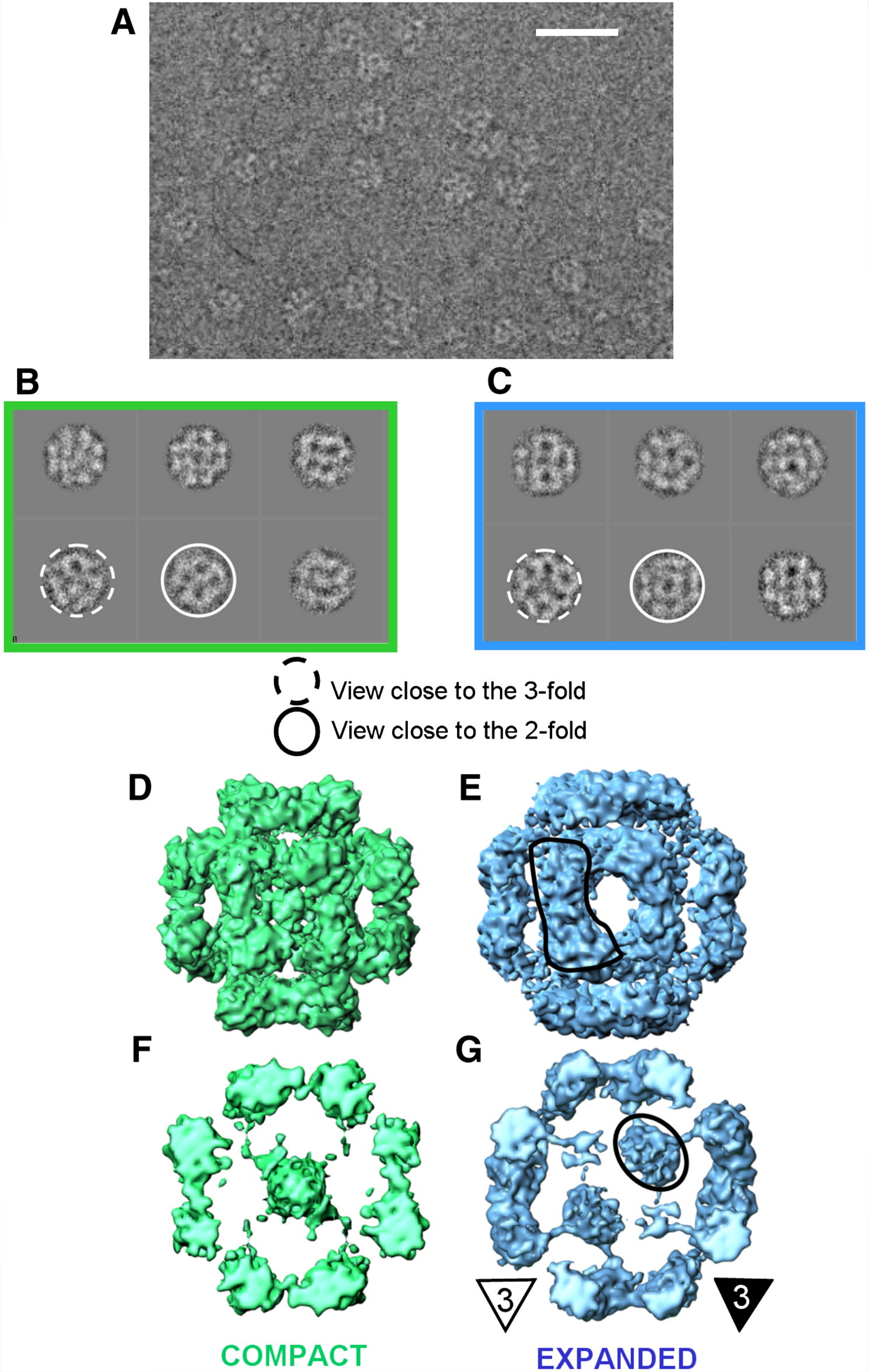
Principles of Virus Structural Organization (2012) B.V. Venkataram Prasad and Michael F Schmid

Tetrahedron (T or 23)

Four 3-fold axes and six 2-fold axes

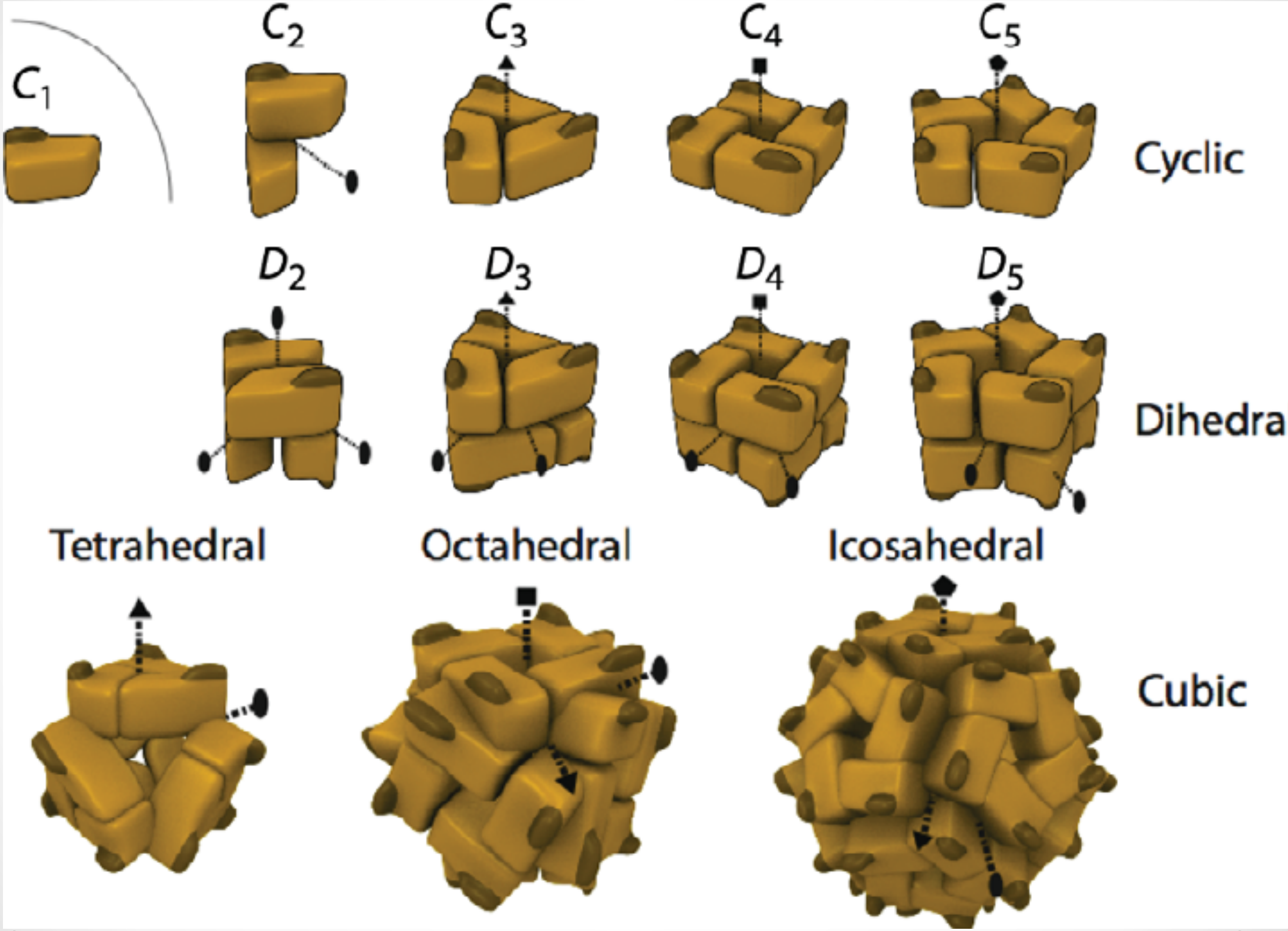
Heat shock protein HSP26: EMD1226





White et al., Structure, 2006

Point groups of biological macromolecules

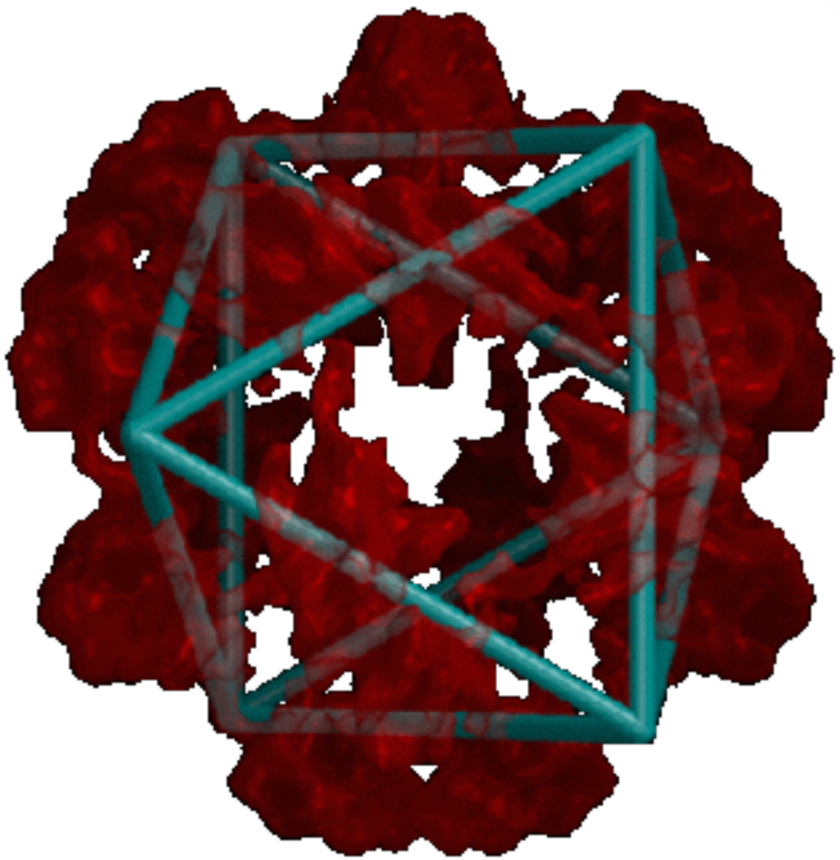


Janin et al, Quarterly Reviews of Biophysics, 2008

O (432)

Six 4-folds, eight 3-folds, 12 2-folds

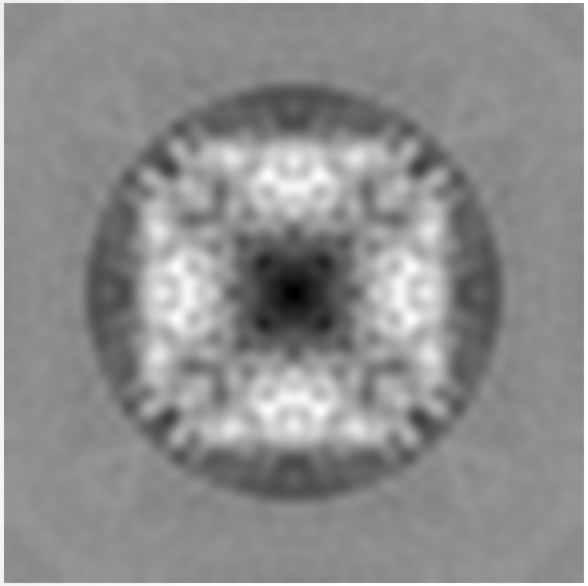
HBV small surface antigen particles: EMD1159

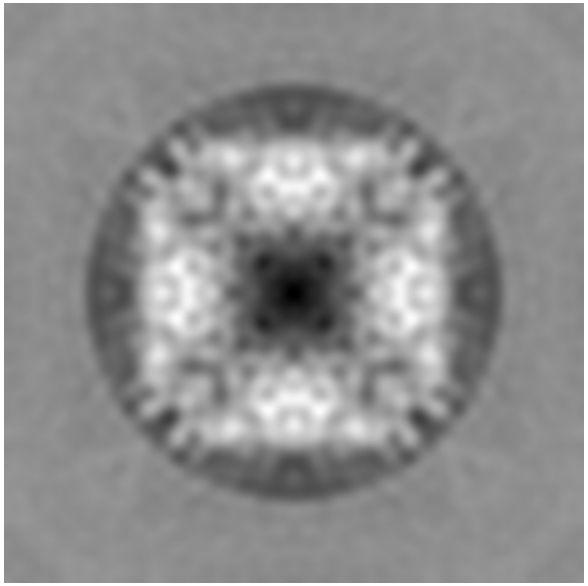


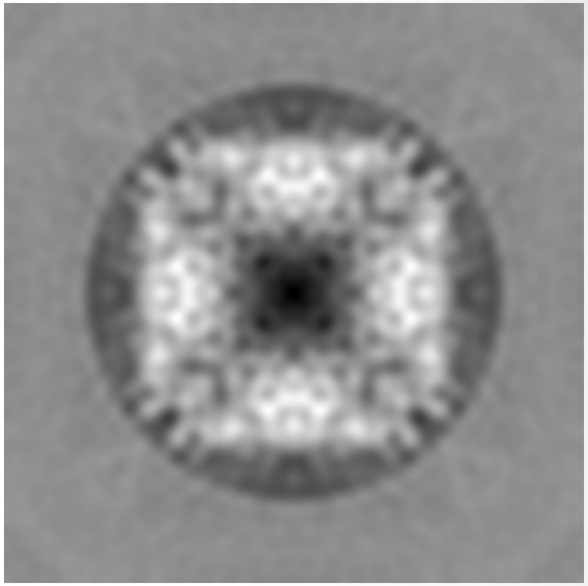
O (432)

Six 4-folds, eight 3-folds, 12 2-folds

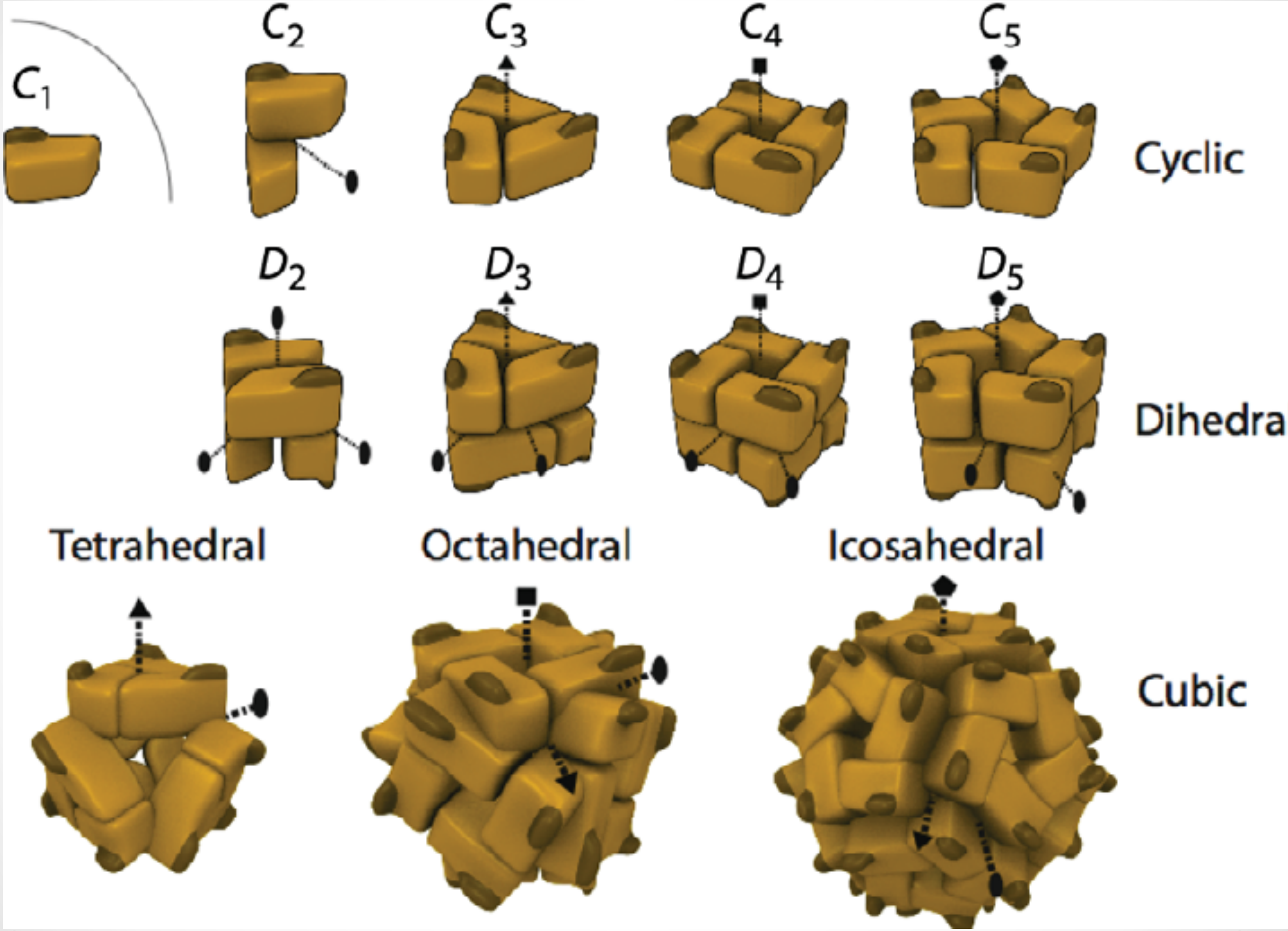
HBV small surface antigen particles: EMD1159







Point groups of biological macromolecules



Janin *et al*, Quarterly Reviews of Biophysics, 2008

I (532) point group

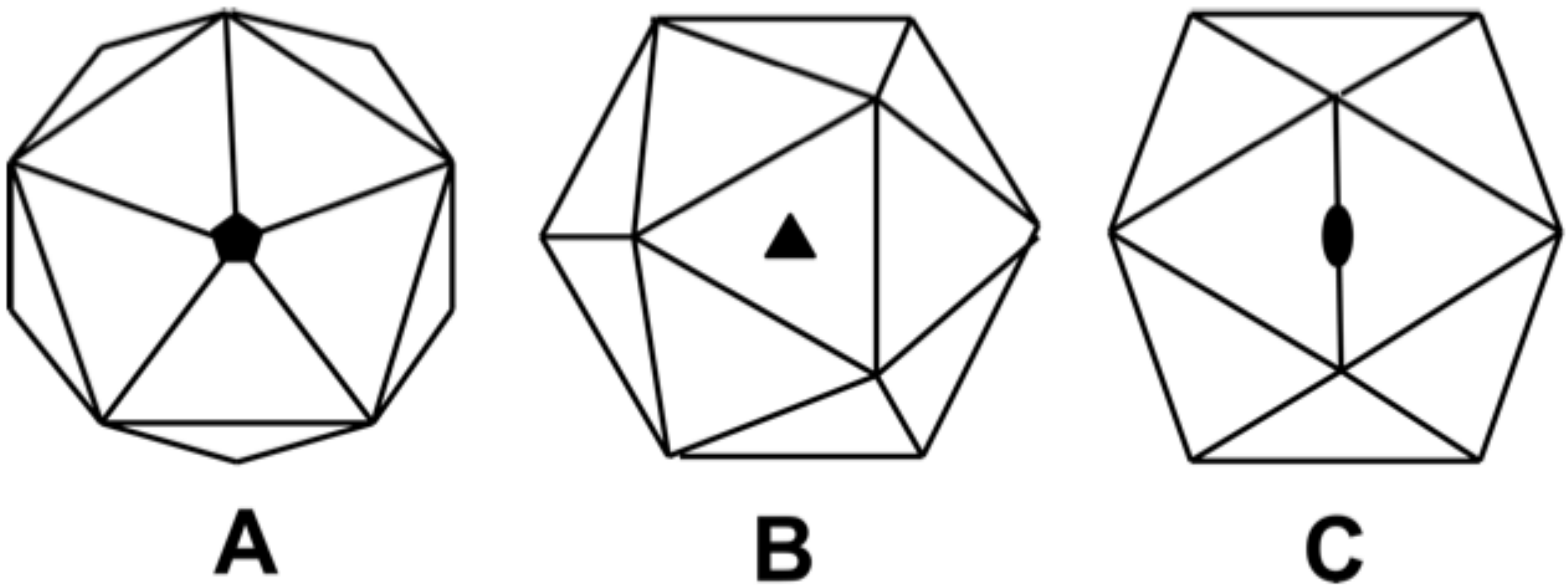
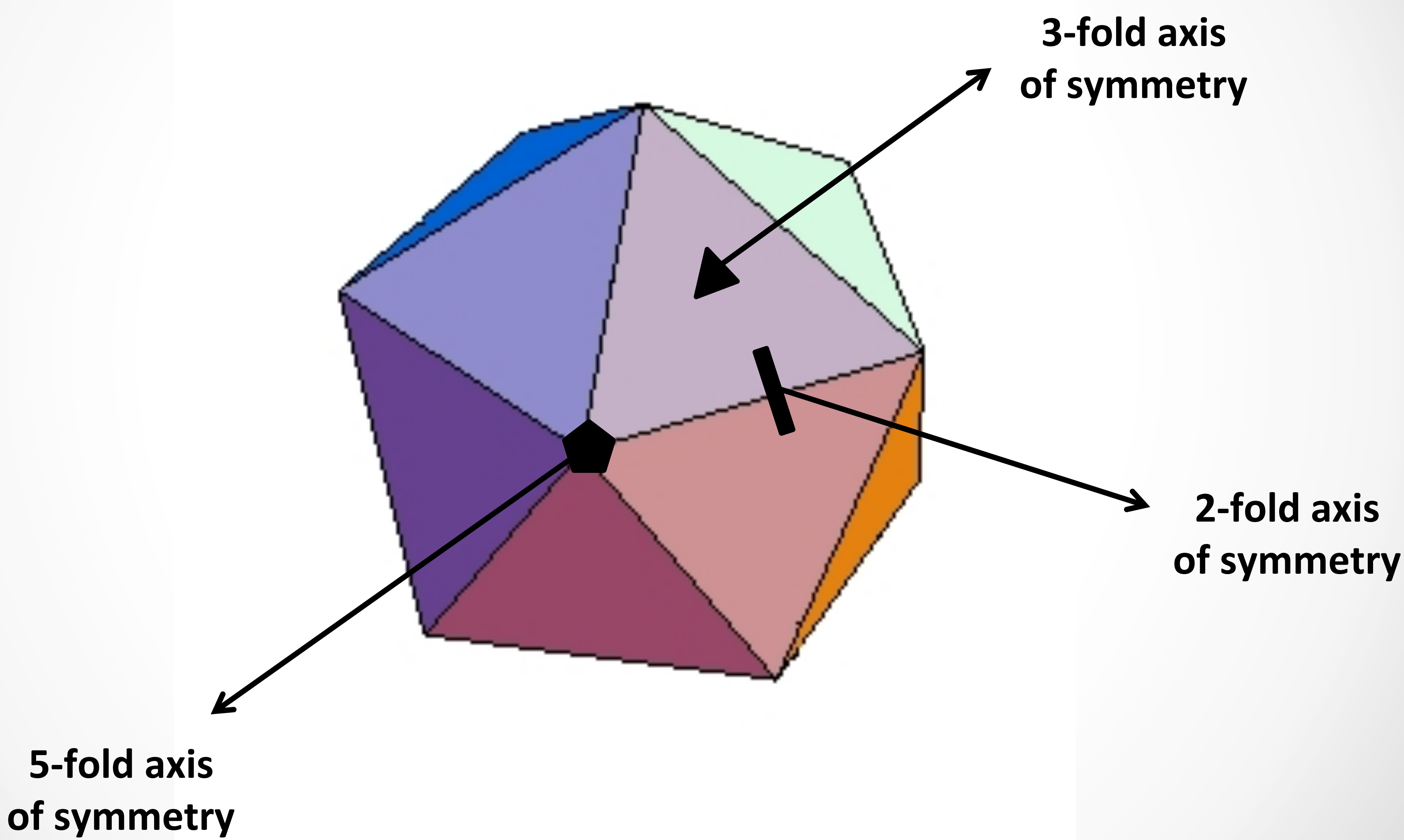


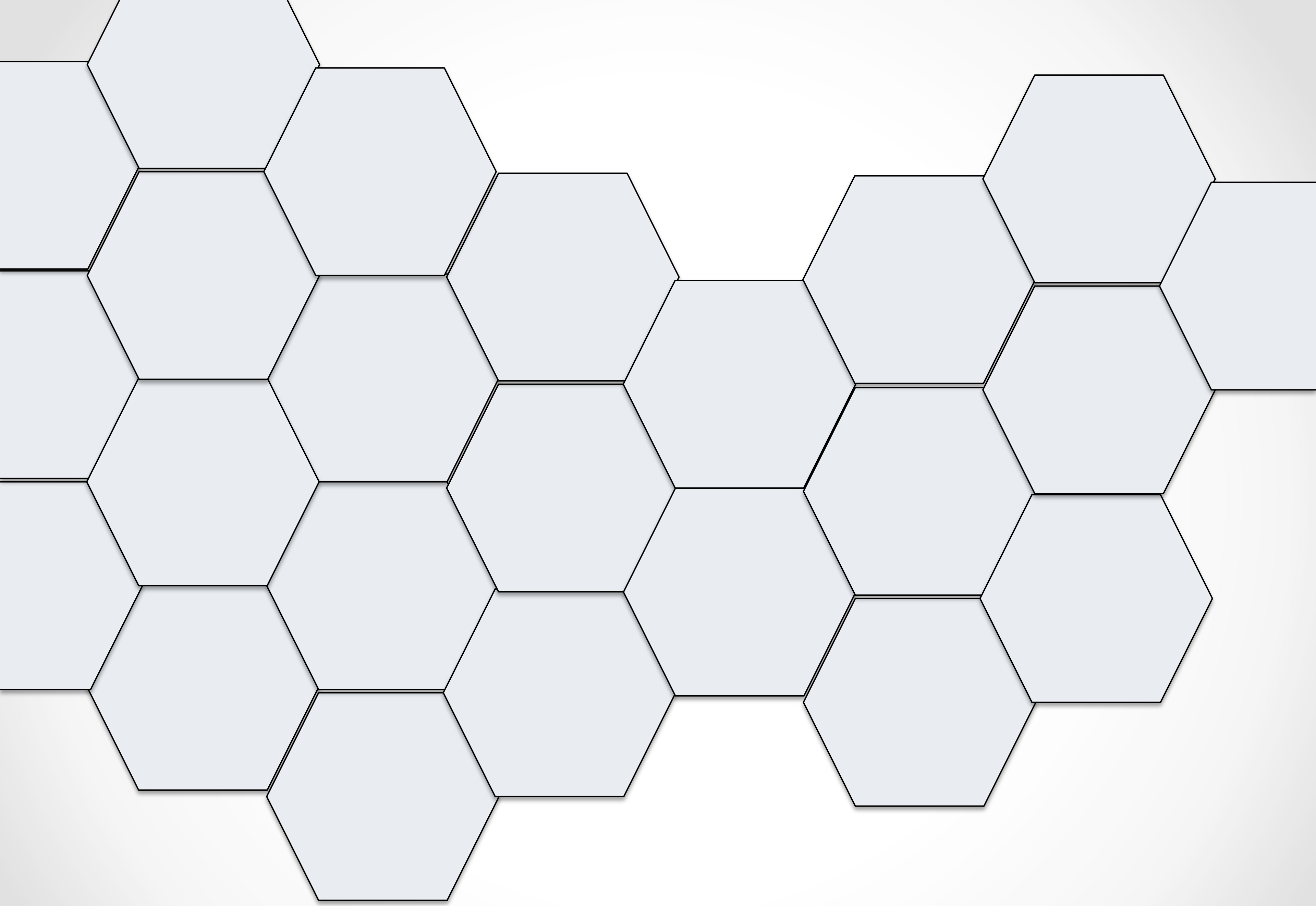
Figure 2.
Icosahedral axes of symmetry. An icosahedron displayed along the (**A**) 5-, (**B**) 3-, and (**C**) 2-fold symmetry axes. The 5-fold rotation axis passes through the vertices of the icosahedron; the 3-fold axis passes through the middle of each triangular face; and the 2-fold axis through the center of each edge.

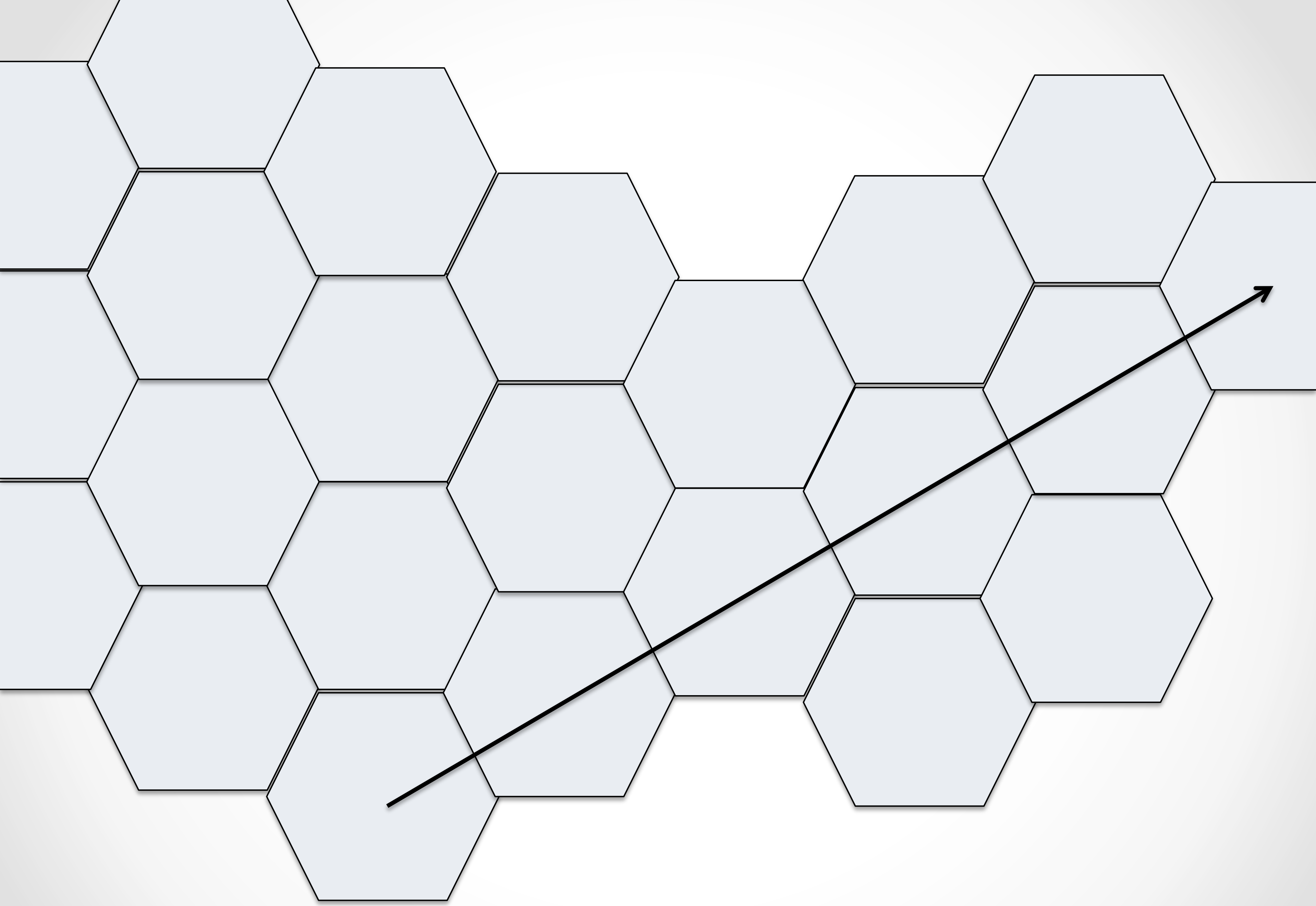
Prasad and Schmid, Adv Exp Med Biol, 2012

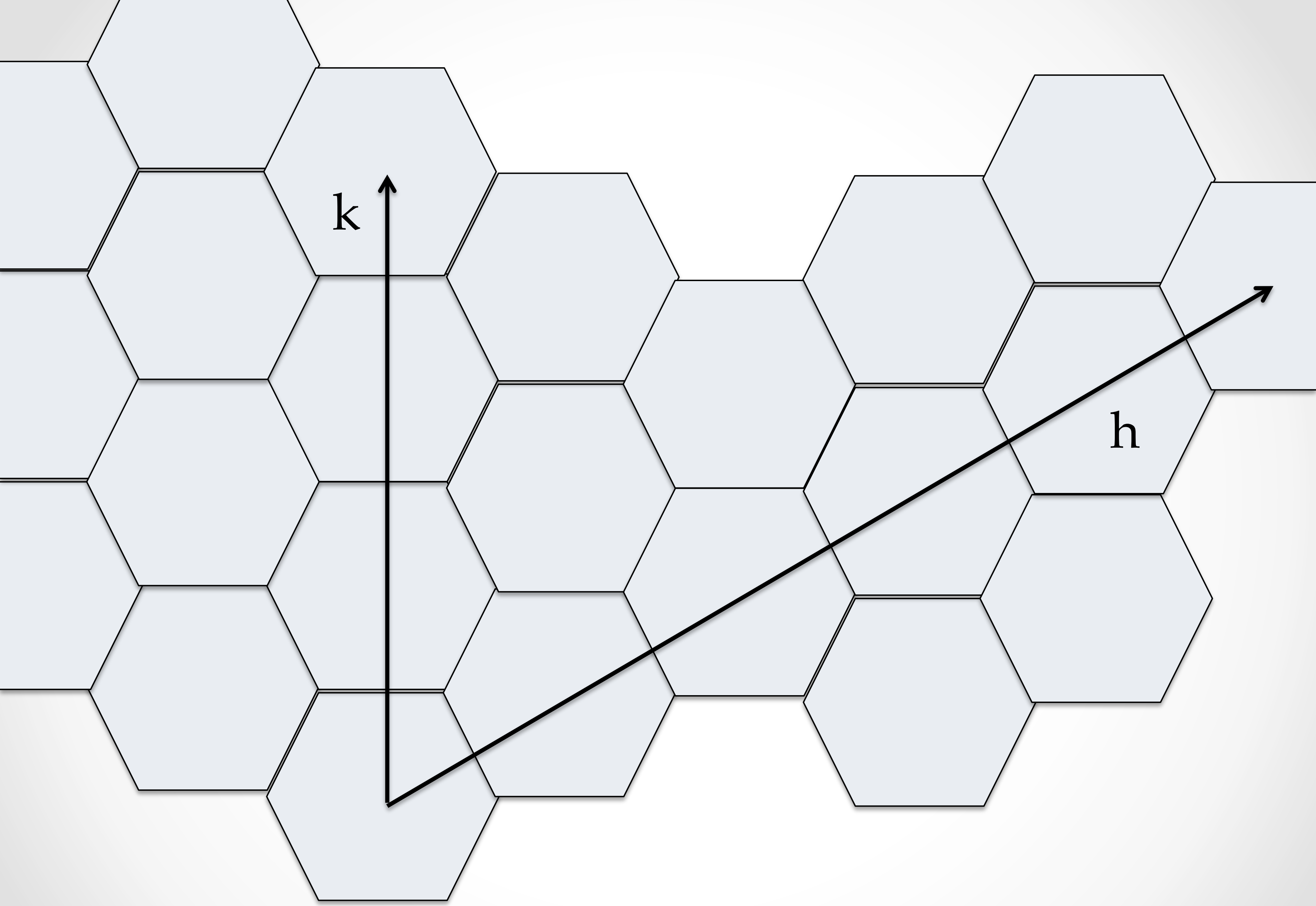
Symmetry of an icosahedron

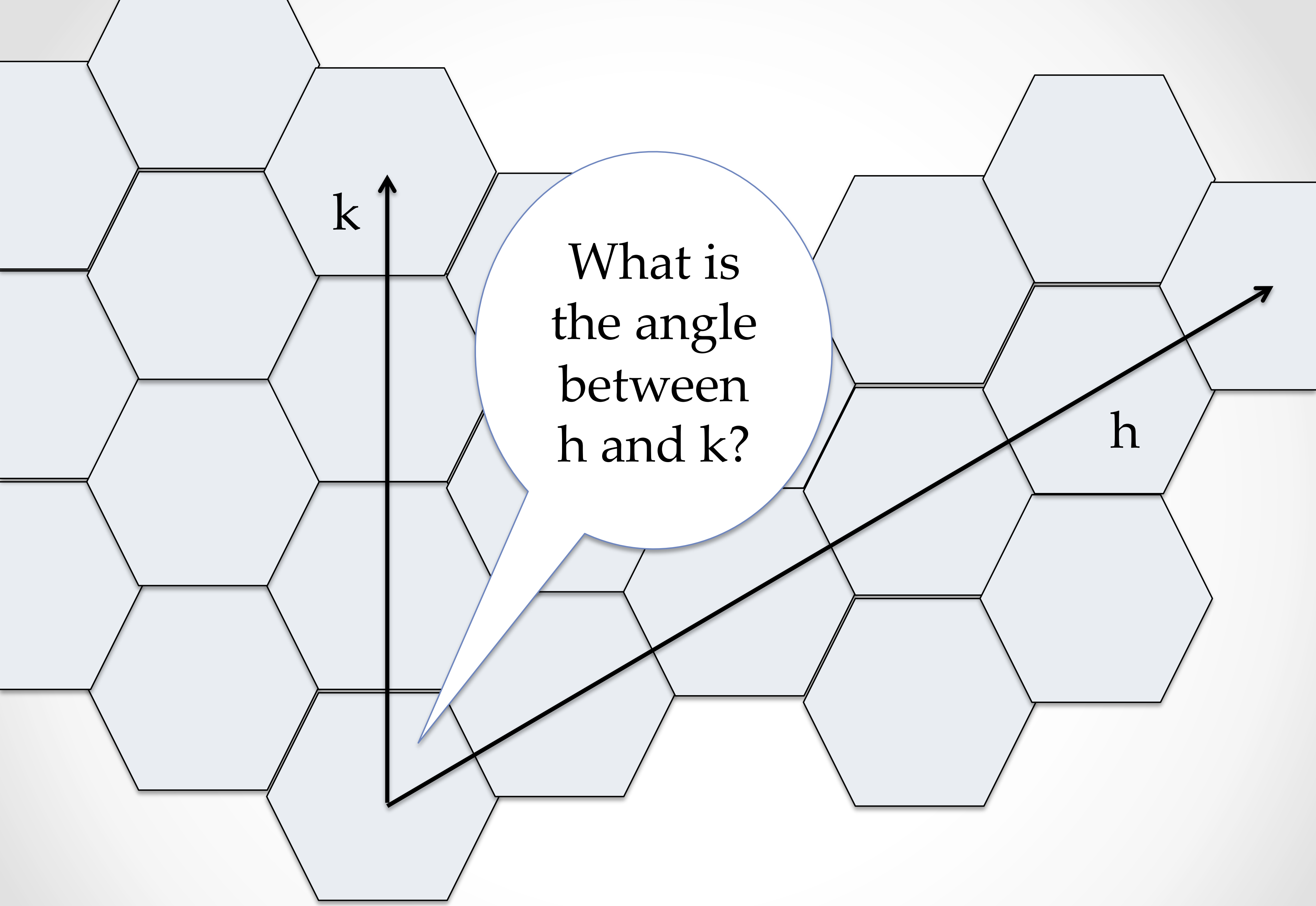


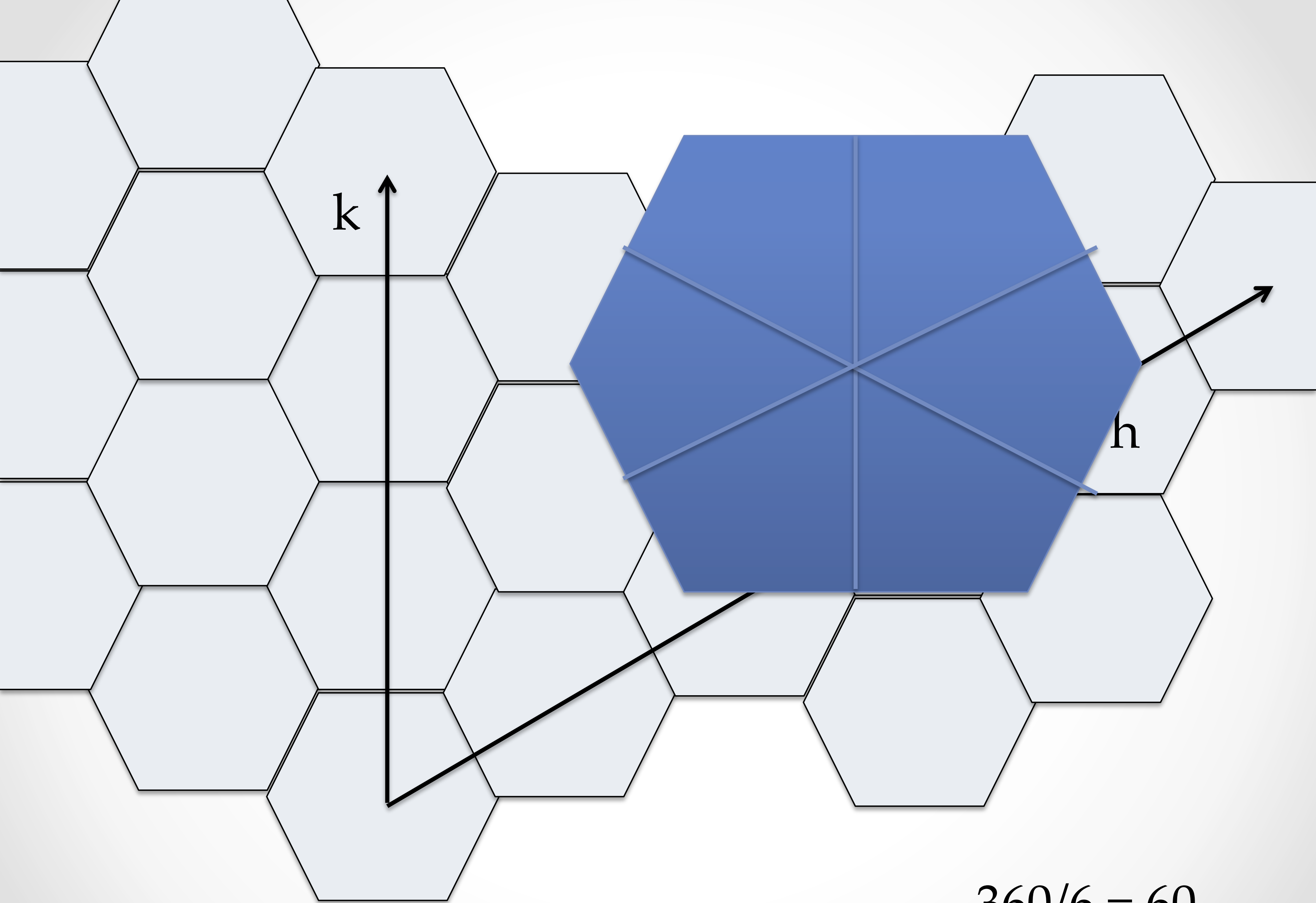
12 5-folds, 20 3-folds and 30 2-folds



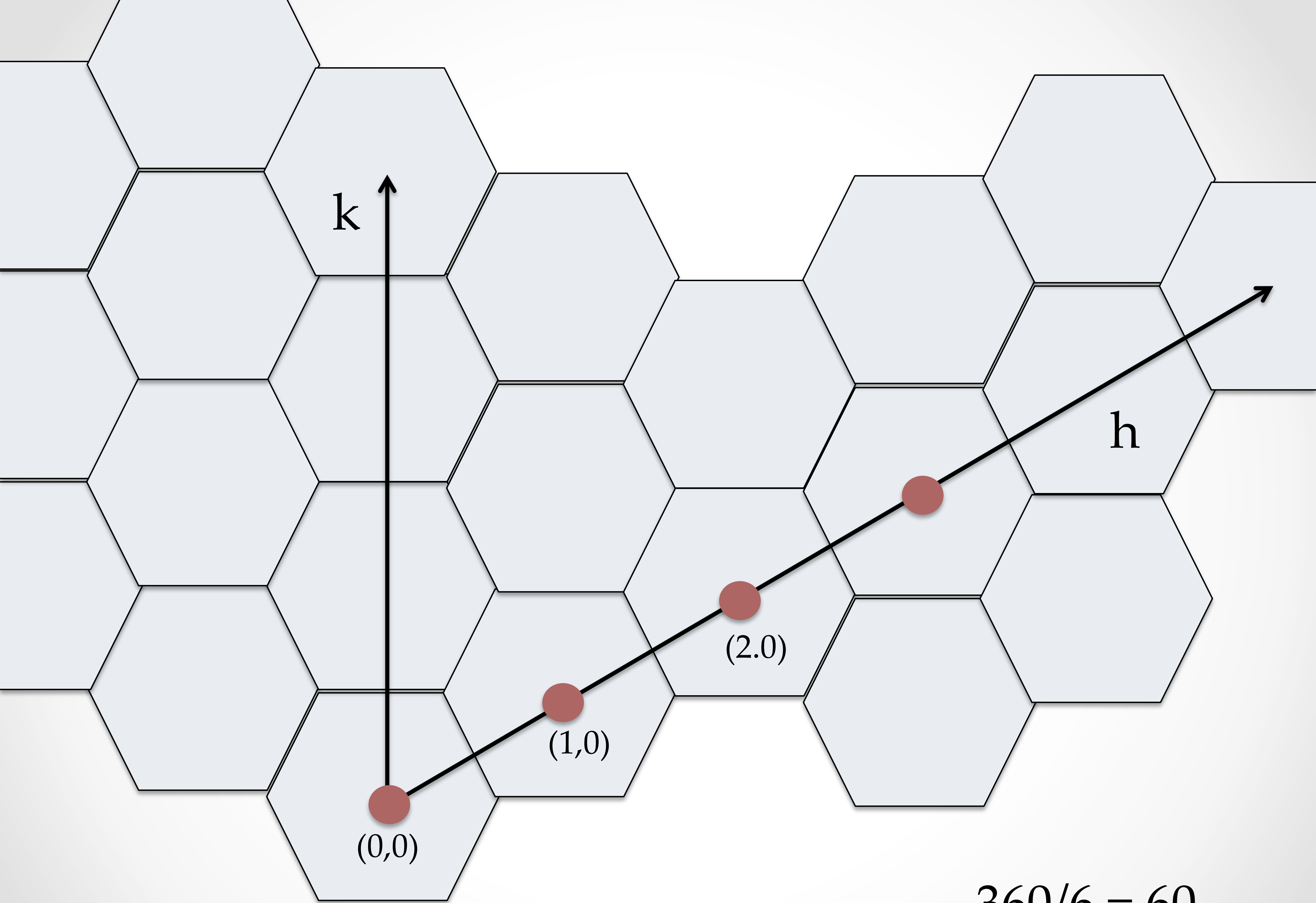



k
h

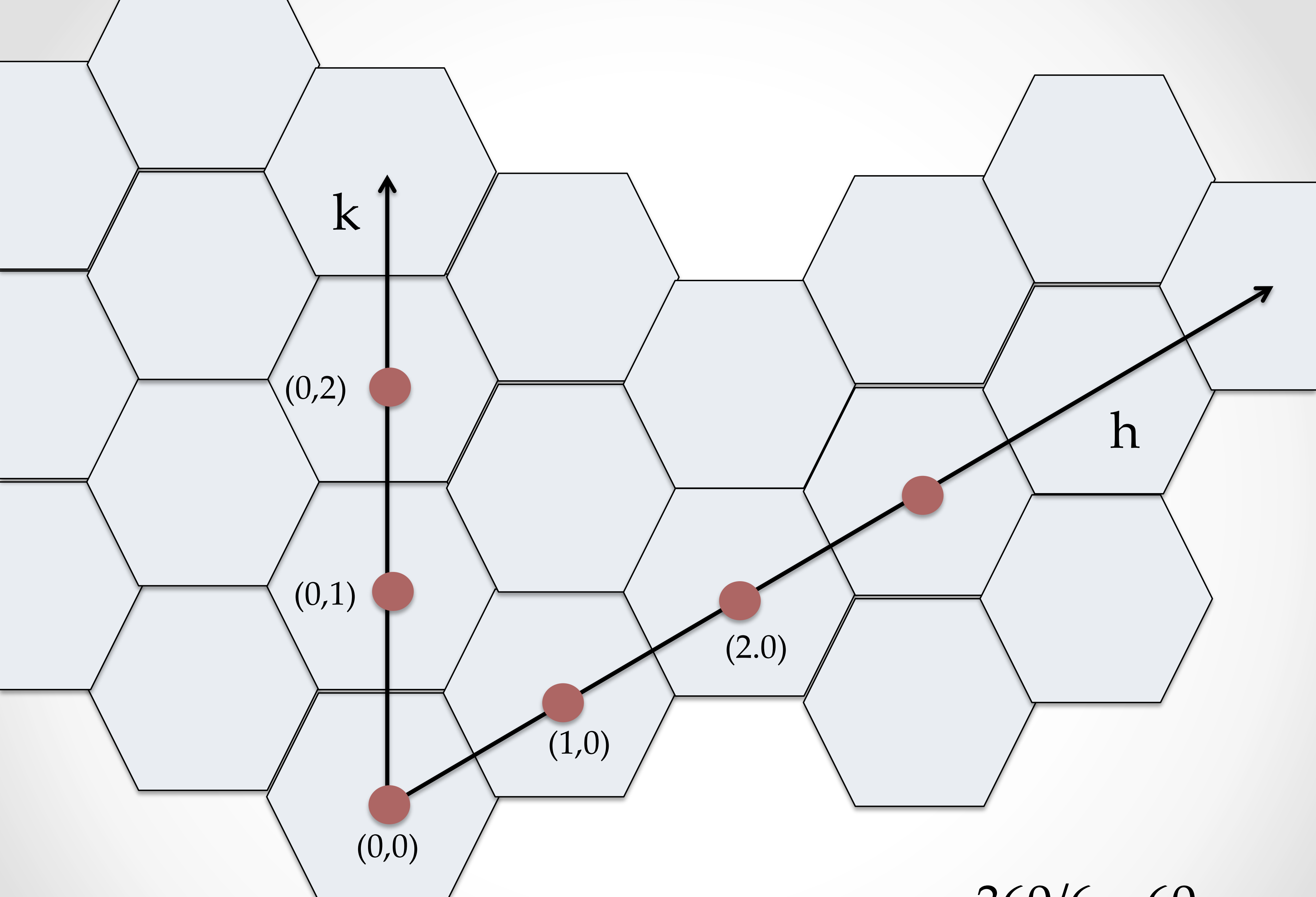

k
What is the angle between h and k?
h



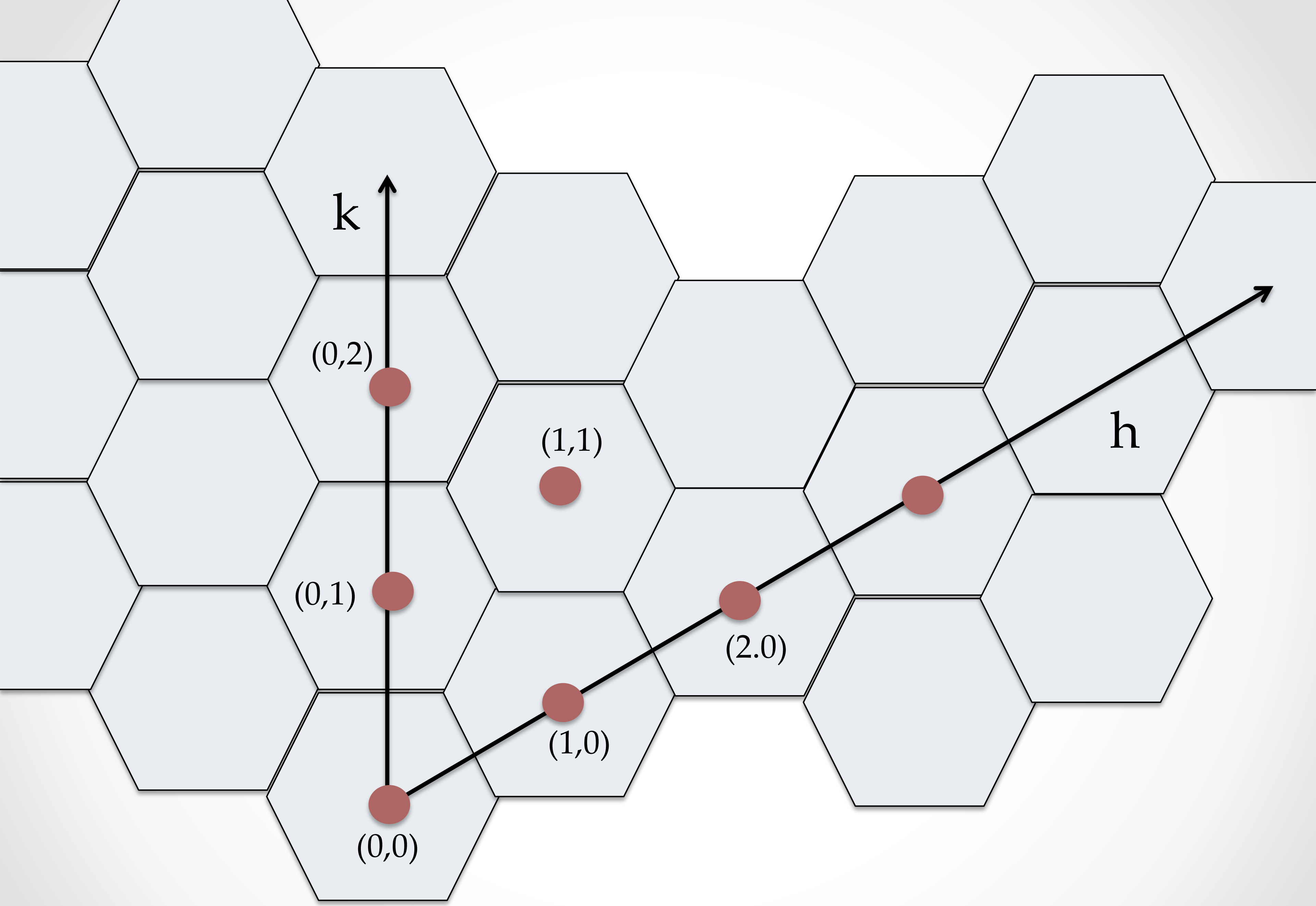
360/6 = 60

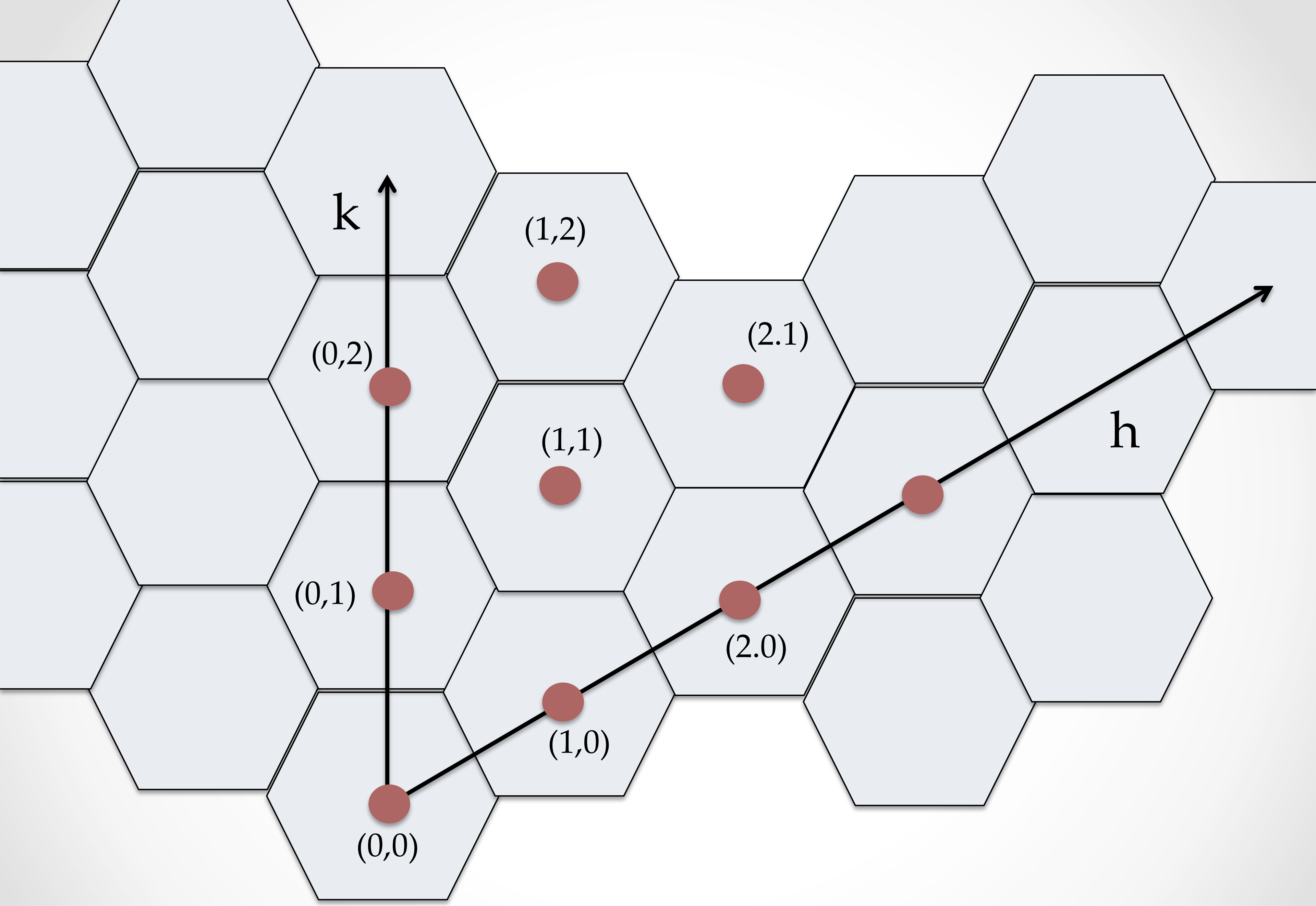


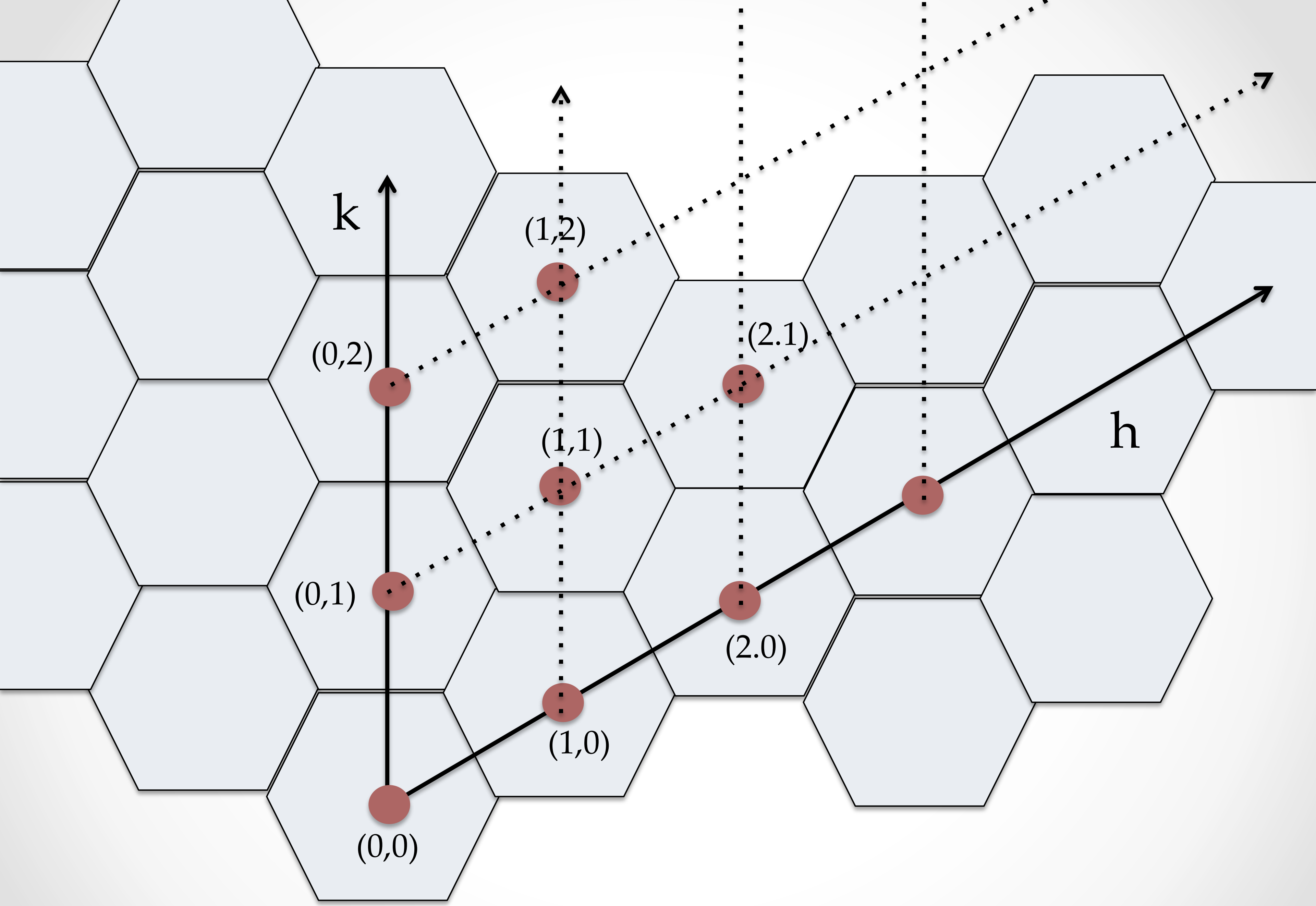
360/6 = 60



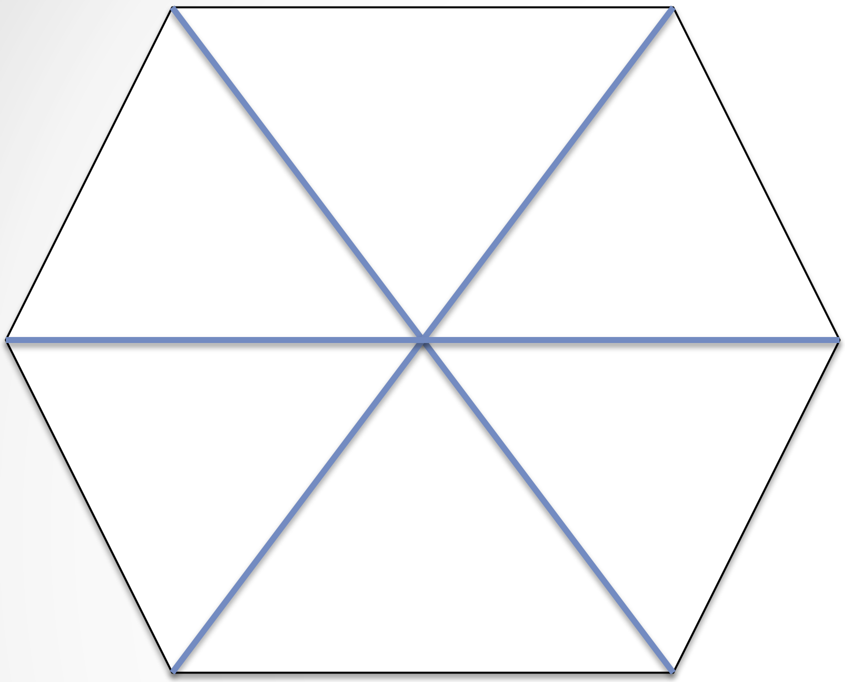
360/6 = 60


k
(0,2)
(1,1)
h
(0,1)
(2.0)
(1,0)
(0,0)


k
(1,2)
(2.1)
(0,2)
(1,1)
h
(0,1)
(2.0)
(1,0)
(0,0)



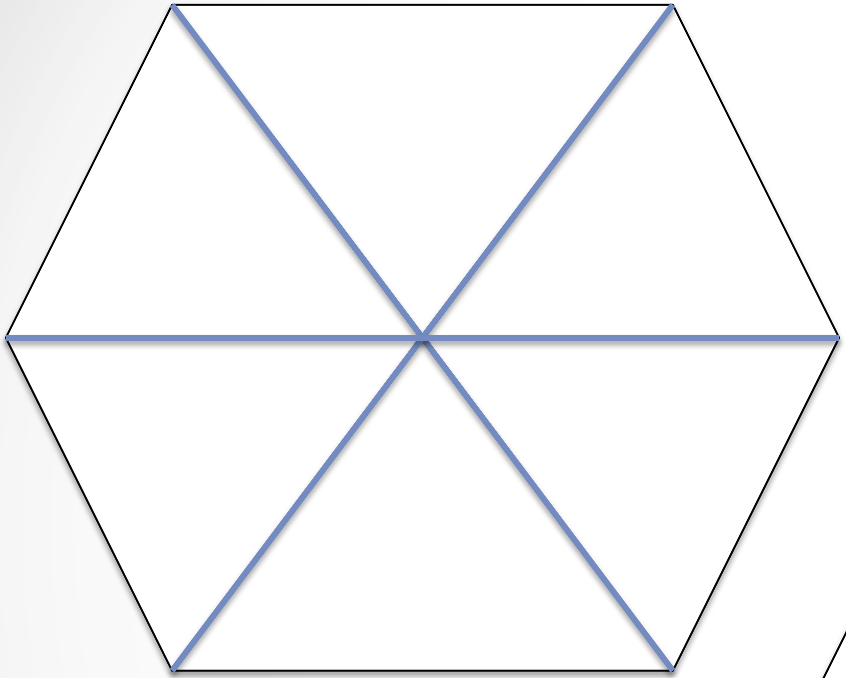
k
h
(0,0)
(0,1)
(0,2)
(1,0)
(1,1)
(1,2)
(2.0)
(2.1)

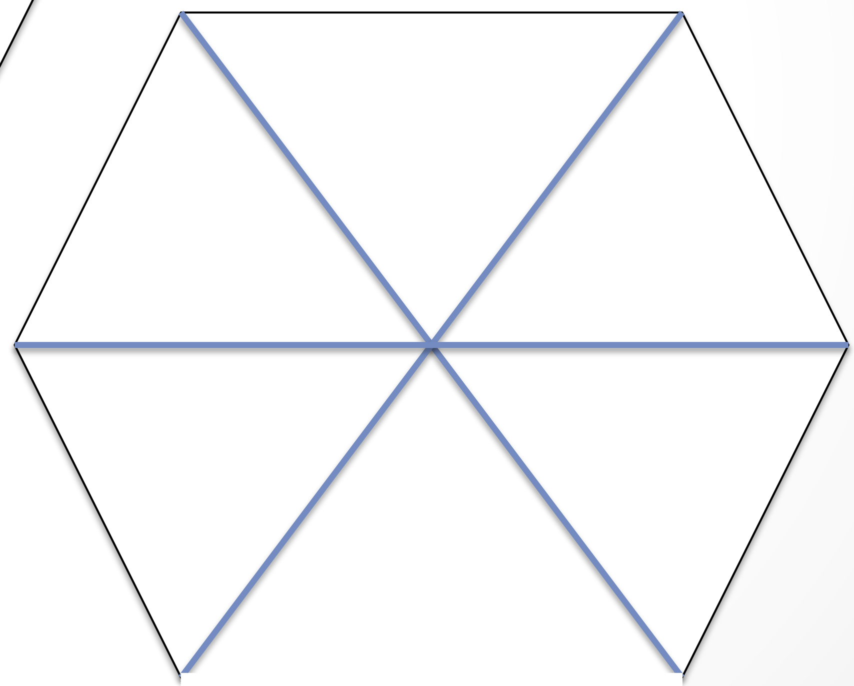


Each hexagon can be decomposed into 6 equilateral triangles

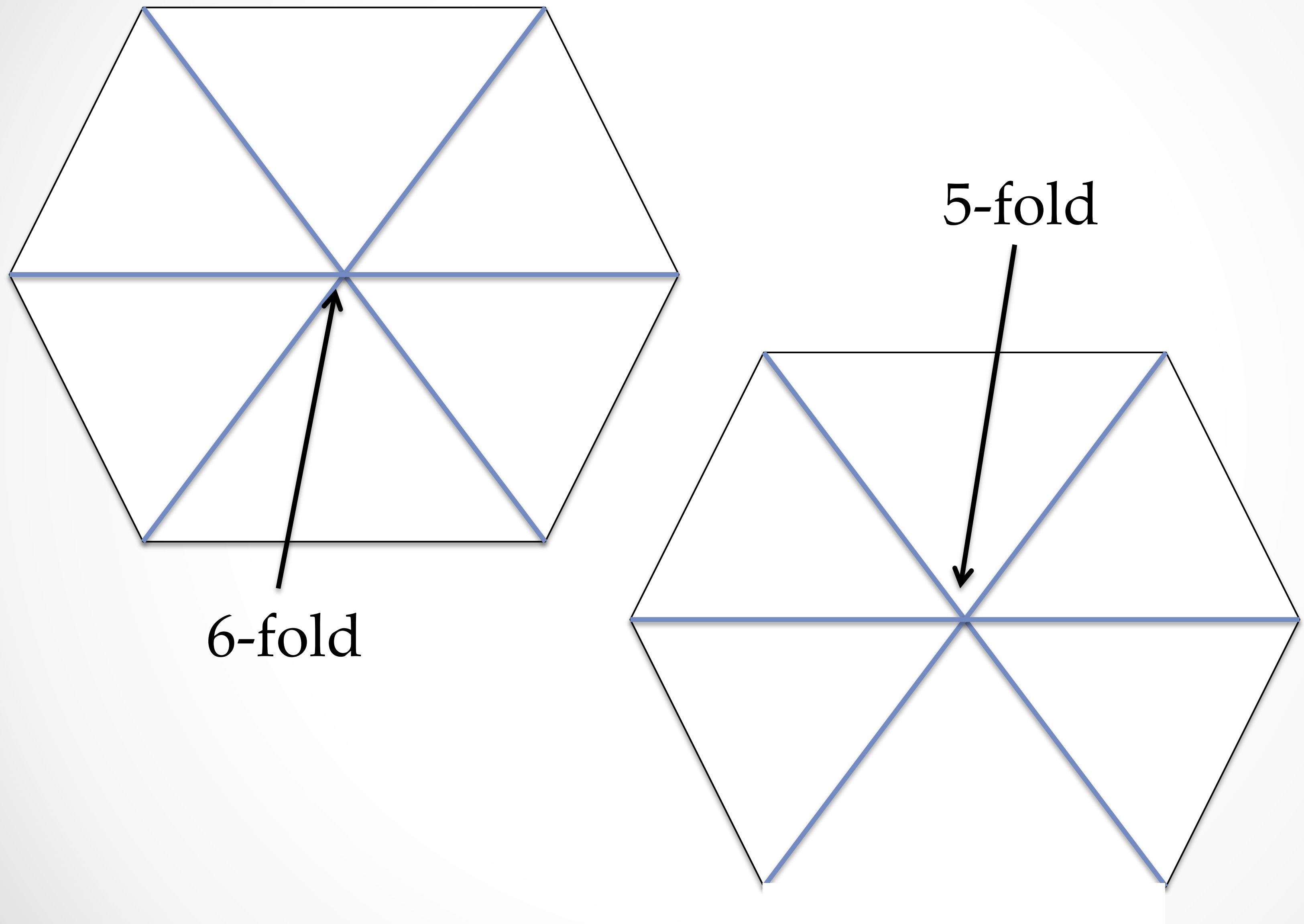
http://www.virology.wisc.edu/virusworld/tri_number.php

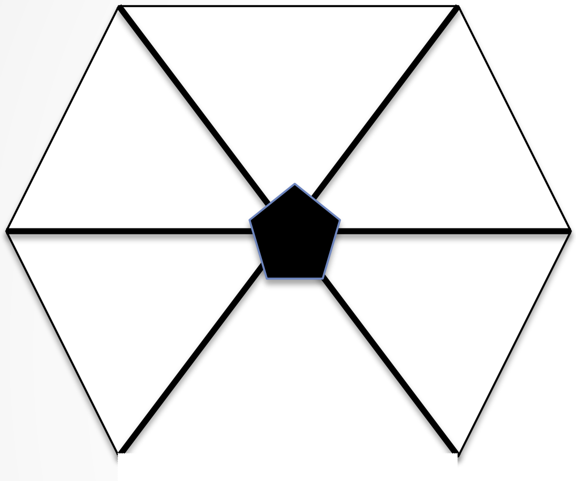
One hexagon is flat. If you remove one of the triangles you need to be in 3 dimensions to connect the 2 free edges, constructing a pentamer.



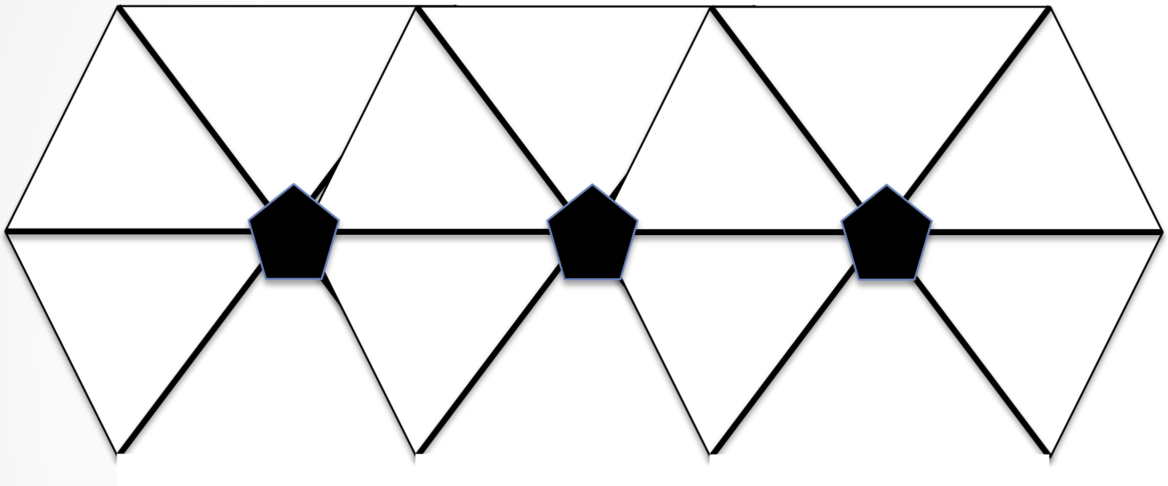


http://www.virology.wisc.edu/virusworld/tri_number.php


5-fold
6-fold



If the hexagon is not isolated but part of a gigantic net, the net will now have a curvature and be in 3 dimensions. If this folding is repeated 12 times on 12 contiguous hexagons an regular icosadeltahedron is obtained



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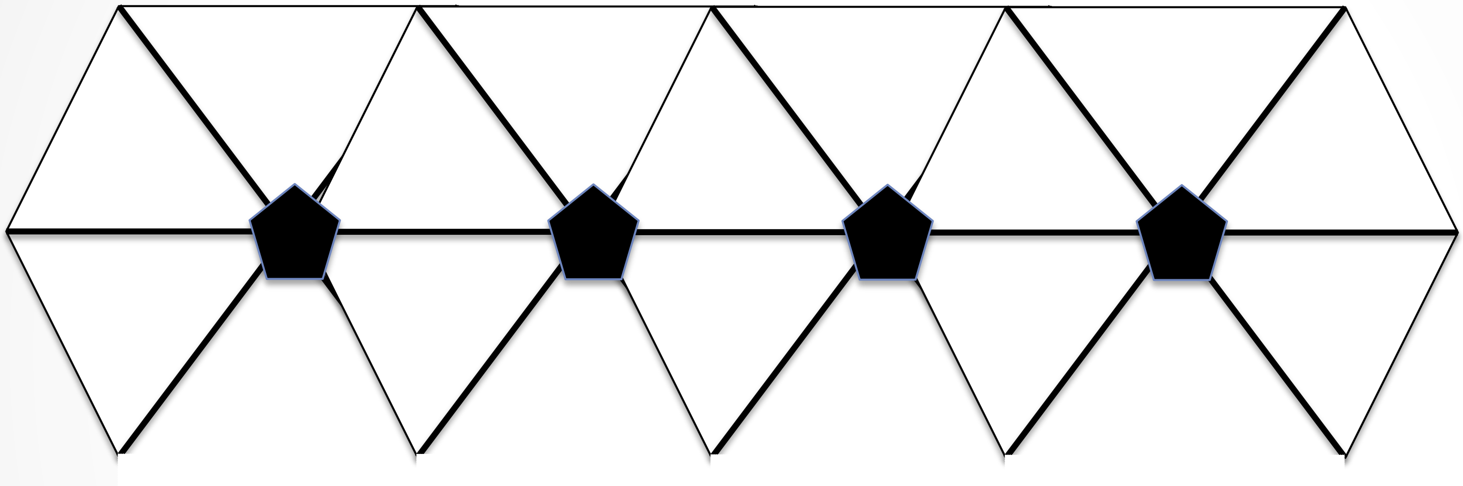

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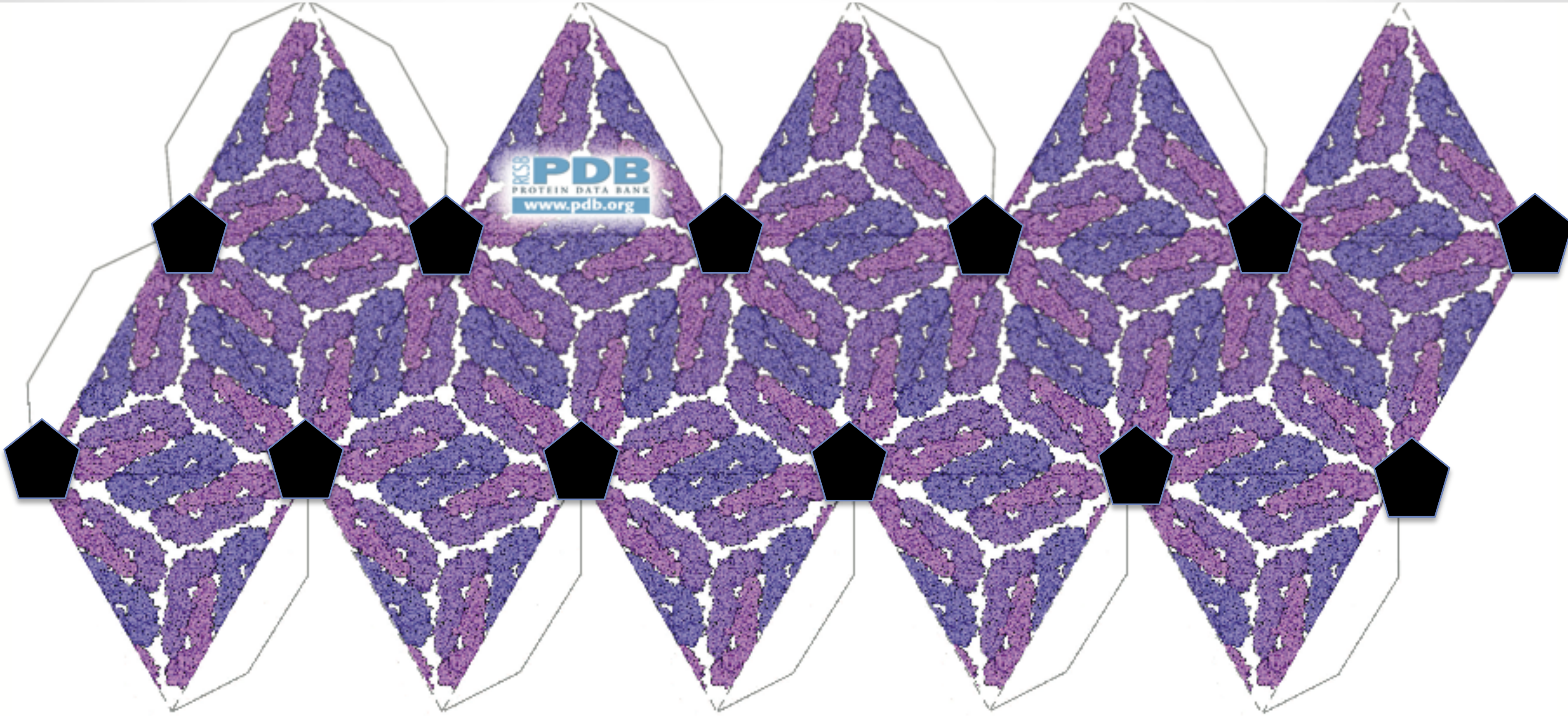
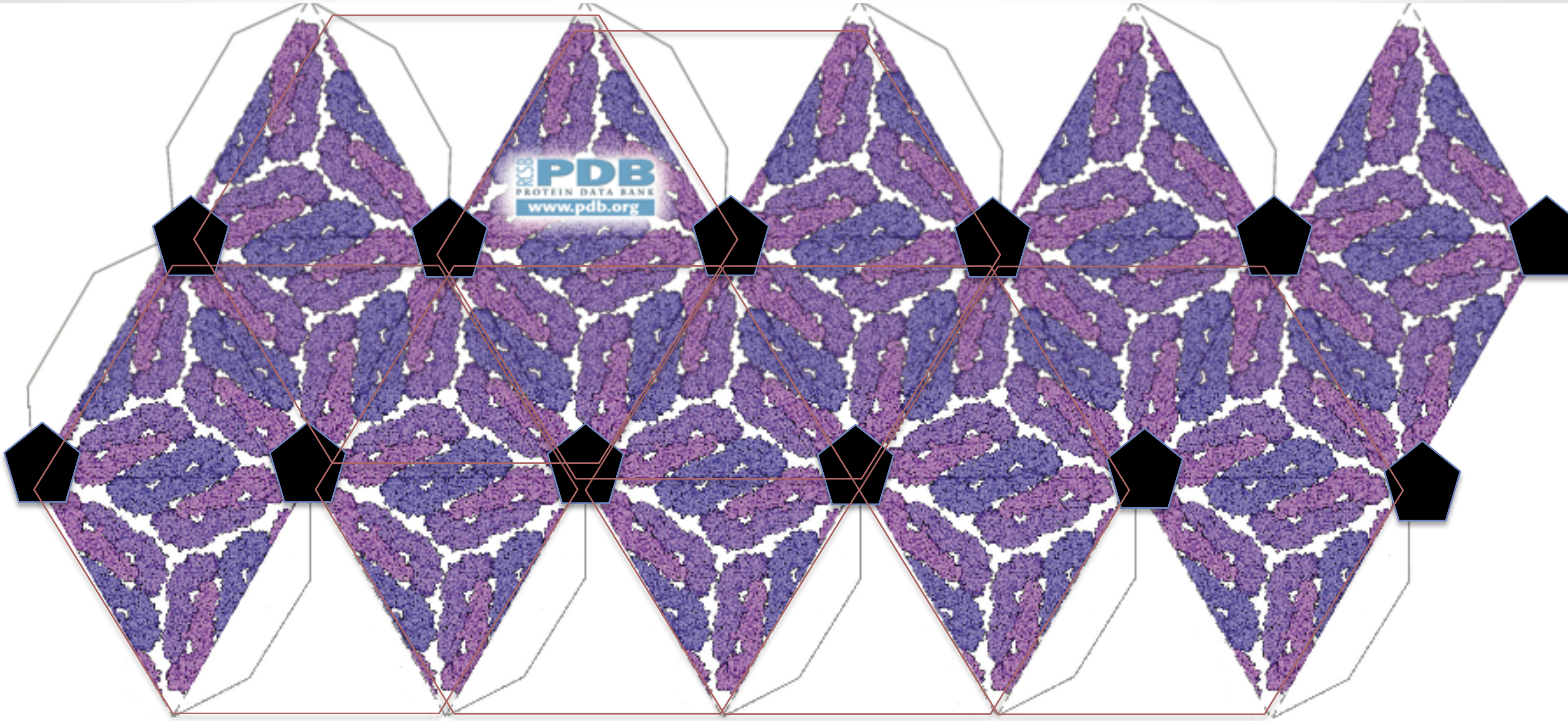


If the hexagon is not isolated but part of a gigantic net, the net will now have a curvature and be in 3 dimensions. If this folding is repeated 12 times on 12 contiguous hexagons an regular icosadeltahedron is obtained

Each of the 12 vertices is at the center of a pentagone.
60 identical units


RCSB PDB
PROTEIN DATA BANK
www.pdb.org

Construction of complex viruses

What if we want to build a bigger virus?

How to regularly arrange > 60 subunits??

geosodic dome by Buckminster Fuller

Construction of complex viruses

What if we want to build a bigger virus?

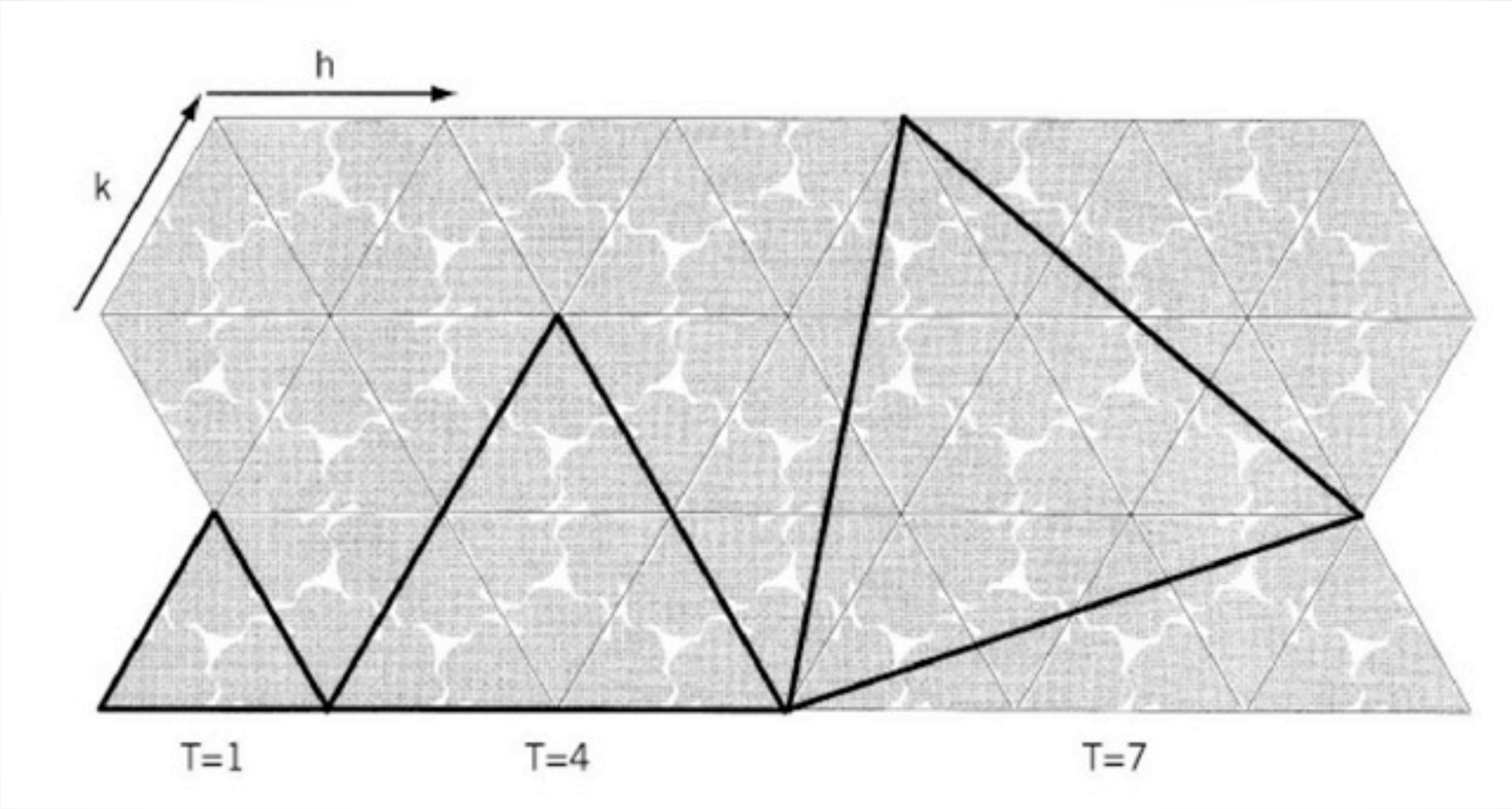
How to regularly arrange > 60 subunits??

The basic triangular facet of the icosahedron has to be first enlarged and then subdivided into smaller triangles.

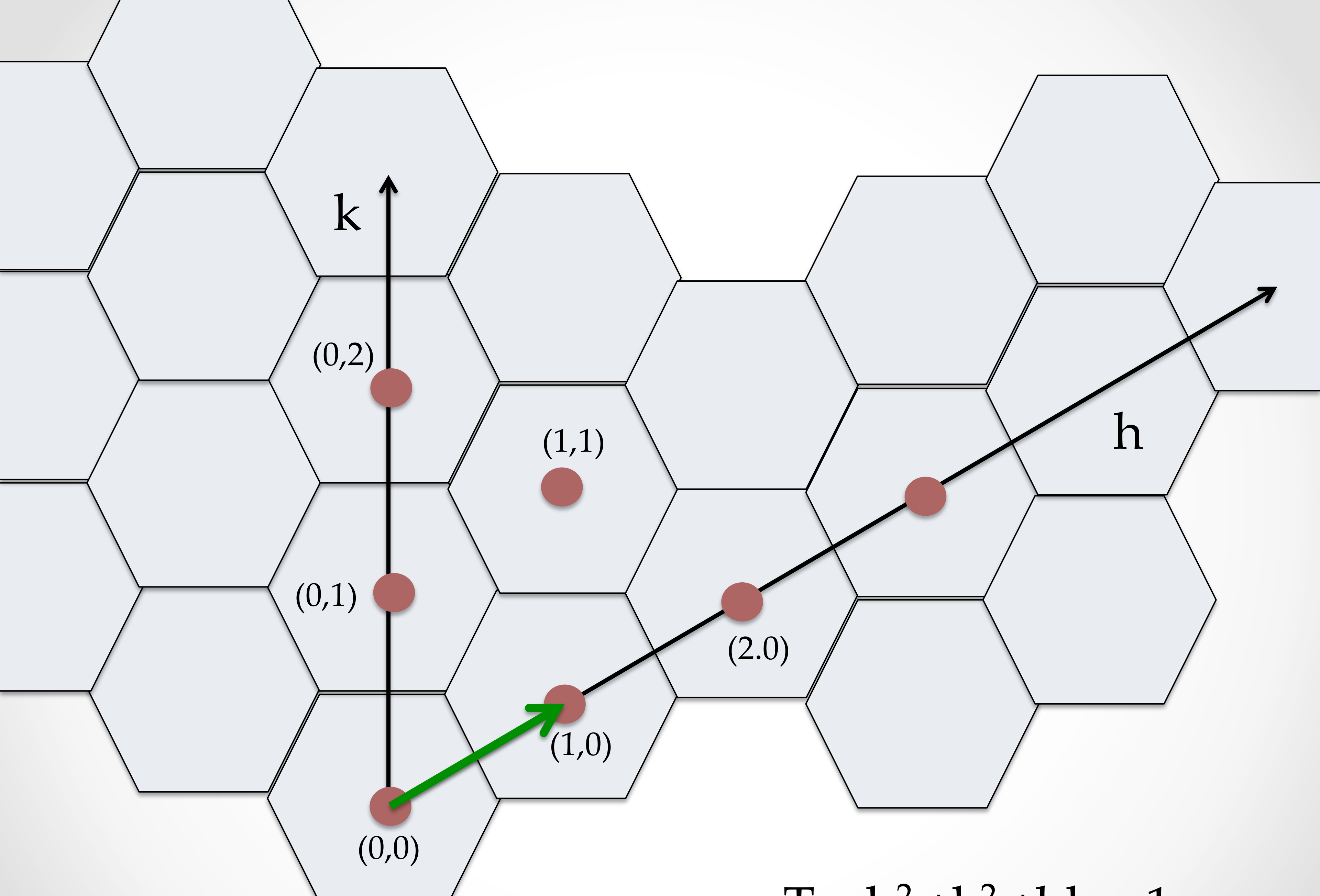
Triangulation dictated by the equation:

$\underline{T=h^2+hk+k^2}$

where T is **the triangulation number**, and h and k are 0 or positive integers

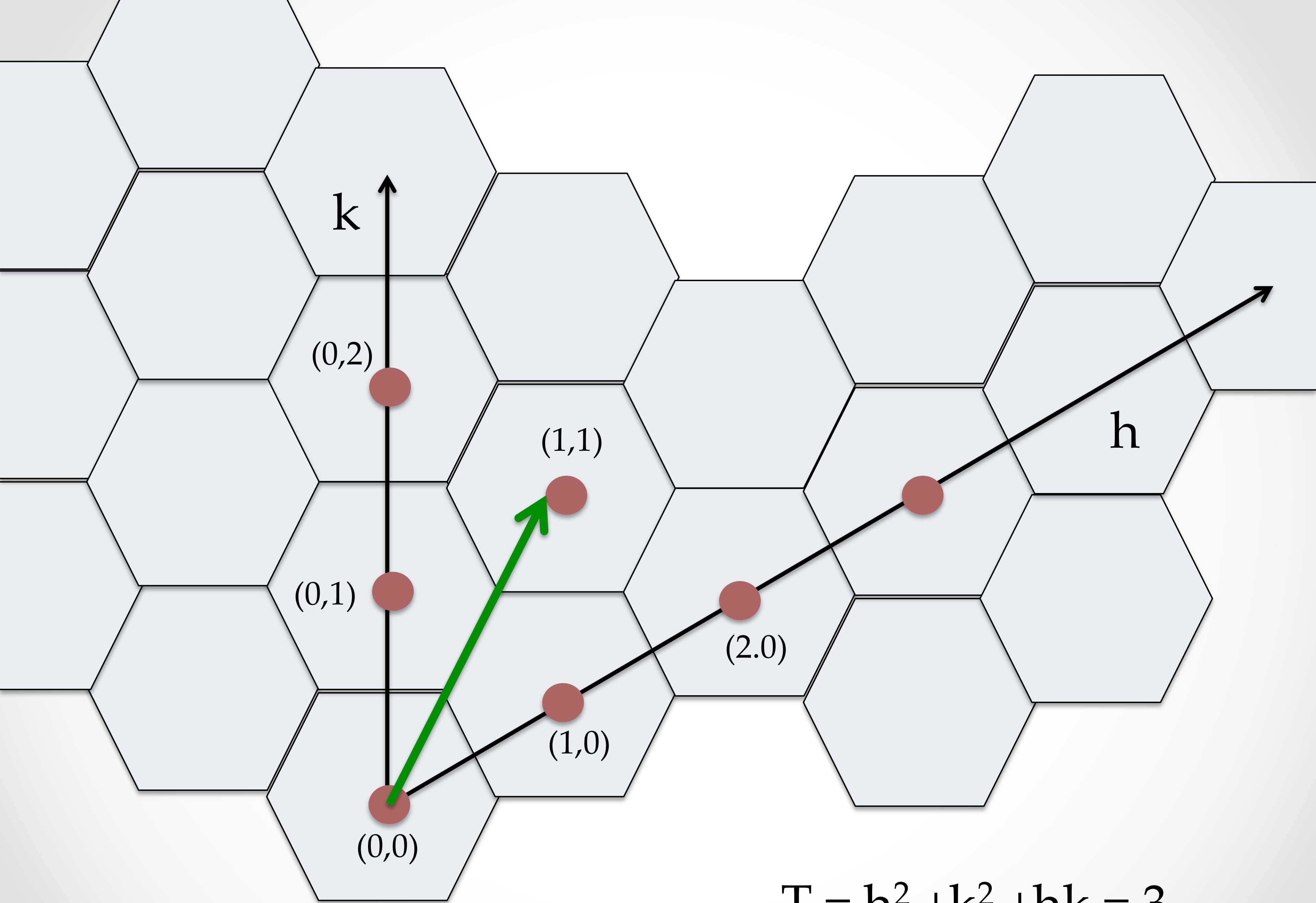


http://what-when-how.com/molecular-biology/capsids-viral-molecular-biology/



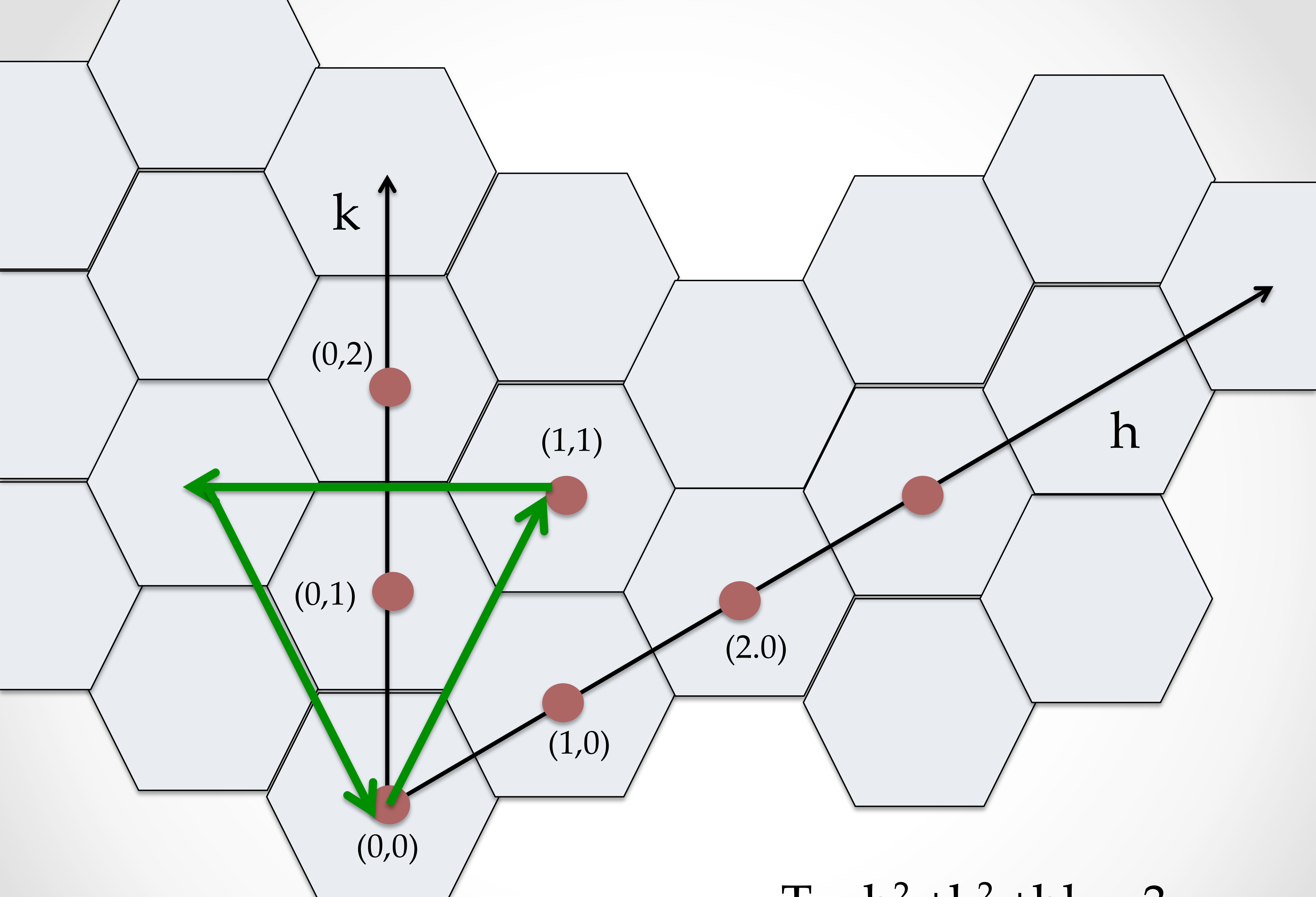
$$T = h^2 + k^2 + hk = 1,$$

$h=1, k=0$



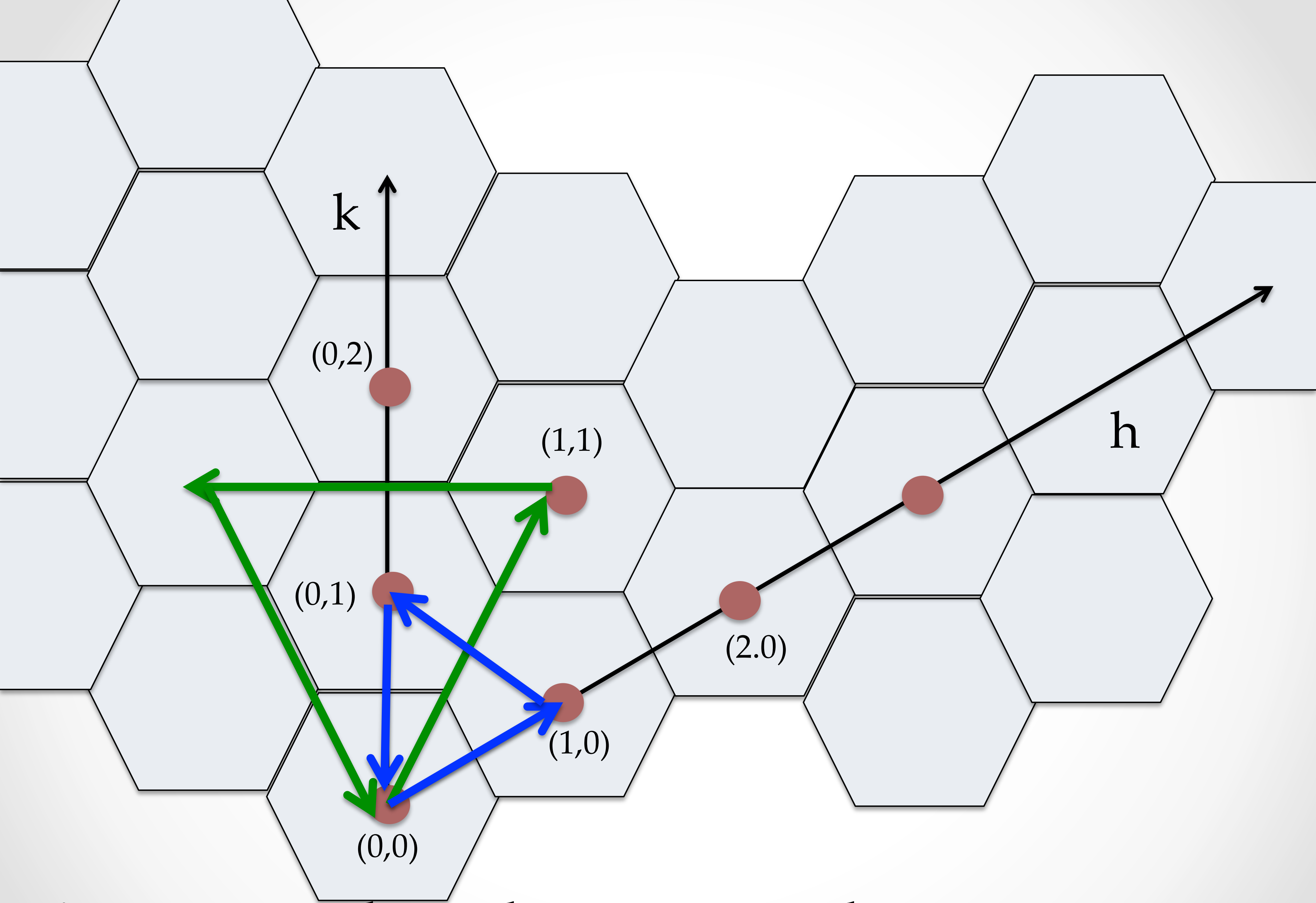
$T = h^2 + k^2 + hk = 3,$

$h=1, k=1$

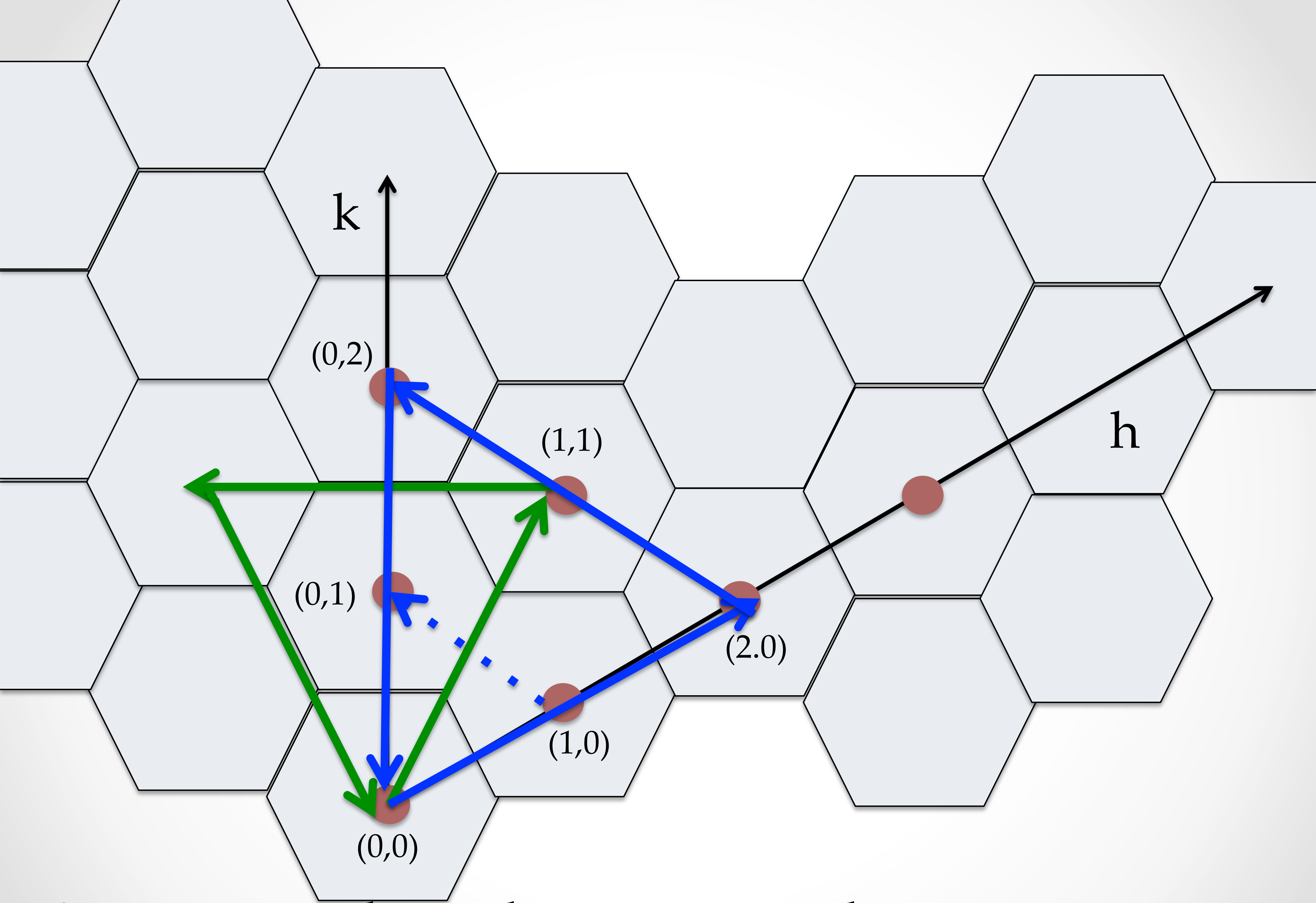


A T=3 triangle

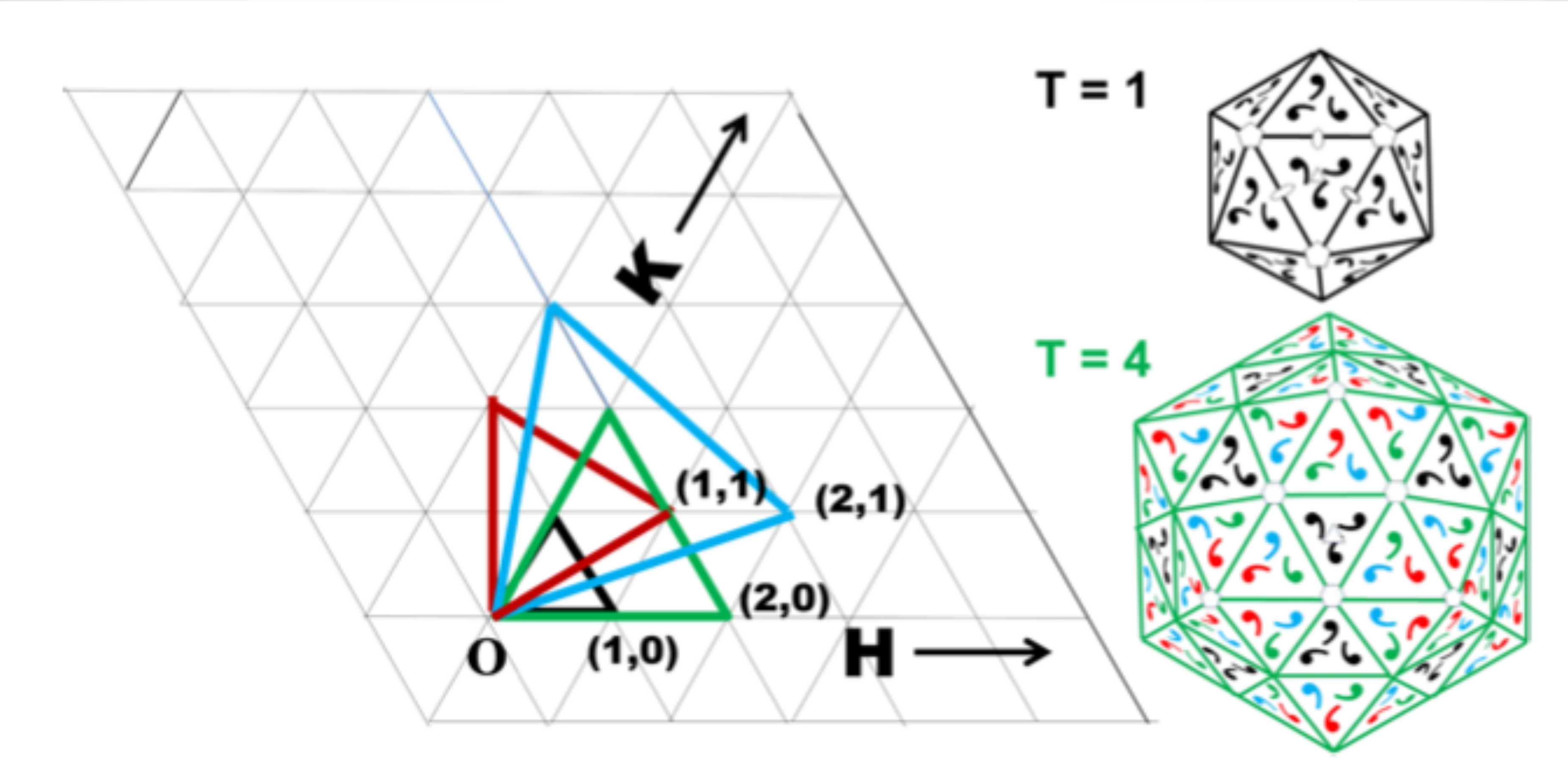
$T = h^2 + k^2 + hk = 3$,
$h=1, k=1$



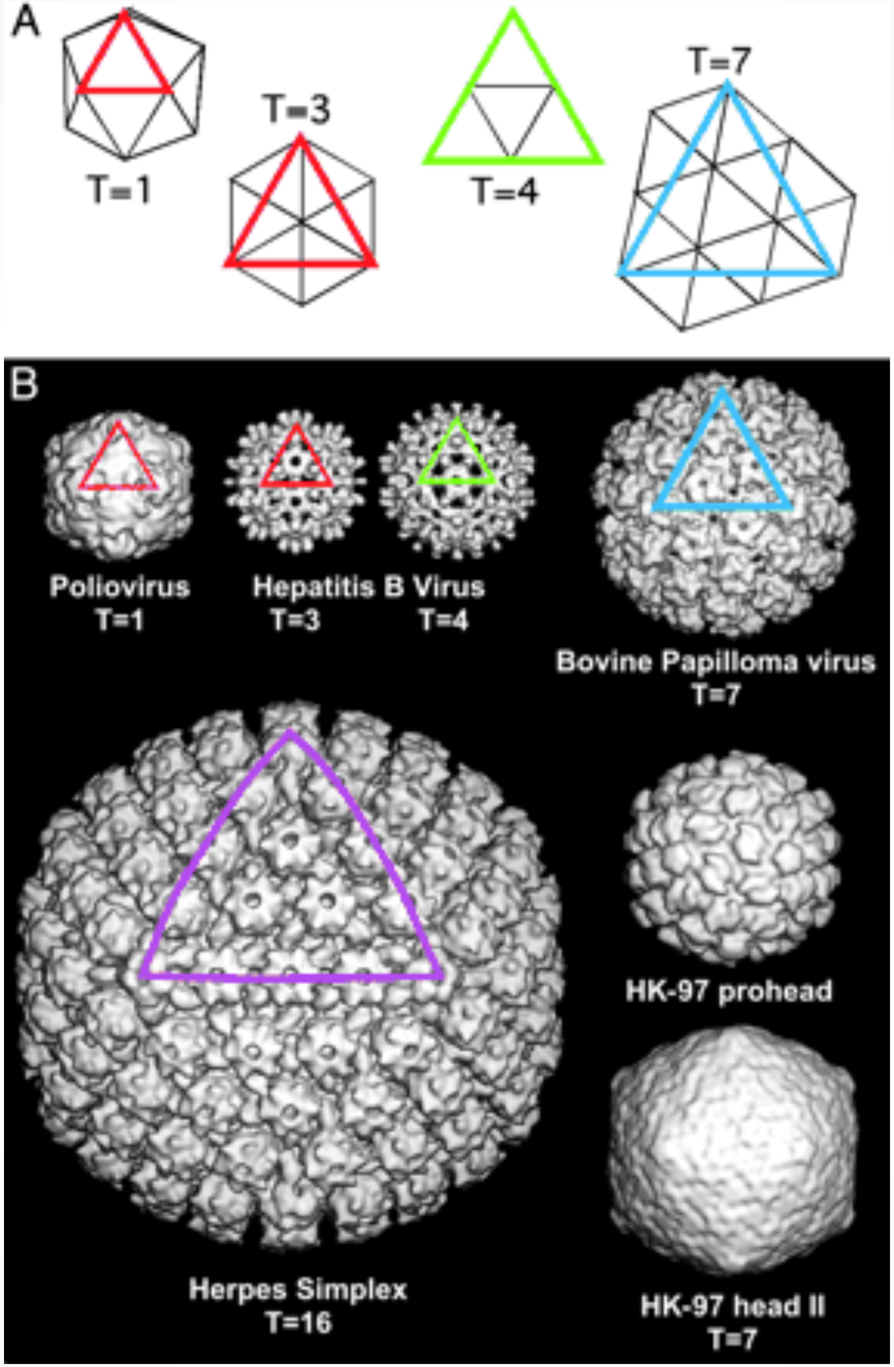
A T=3 triangle and a T=1 triangle



A T=3 triangle and a T=4 triangle

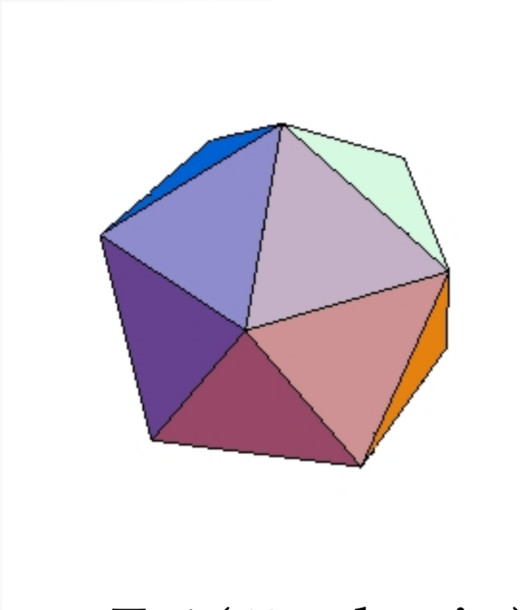


Prasad and Schmid, Adv Exp Med Biol, 2012

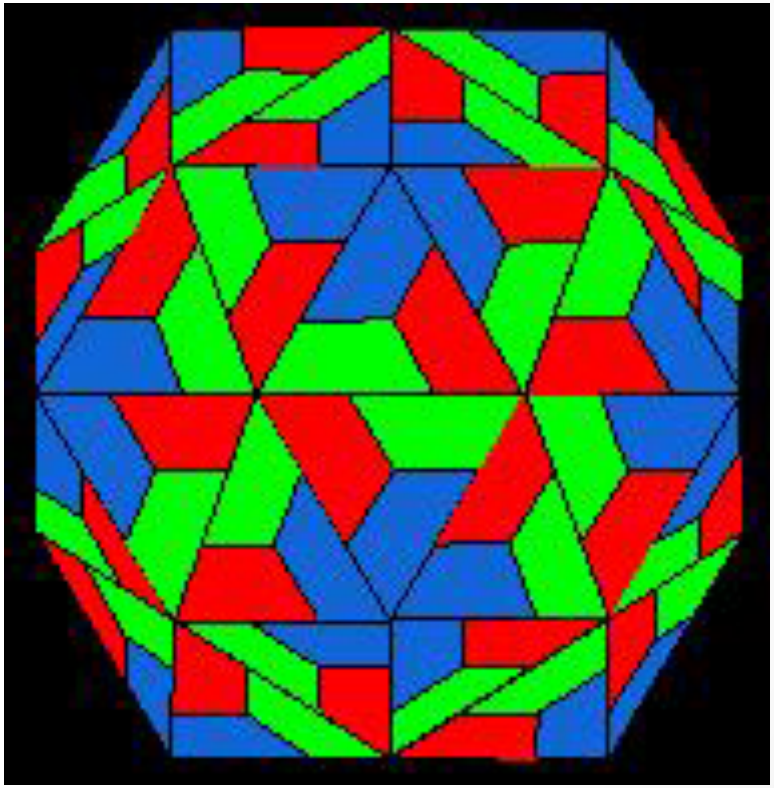


http://www.pnas.org/cgi/content-nw/full/101/44/15549/FIG1

Construction of complex viruses



T=1 (60 subunits)

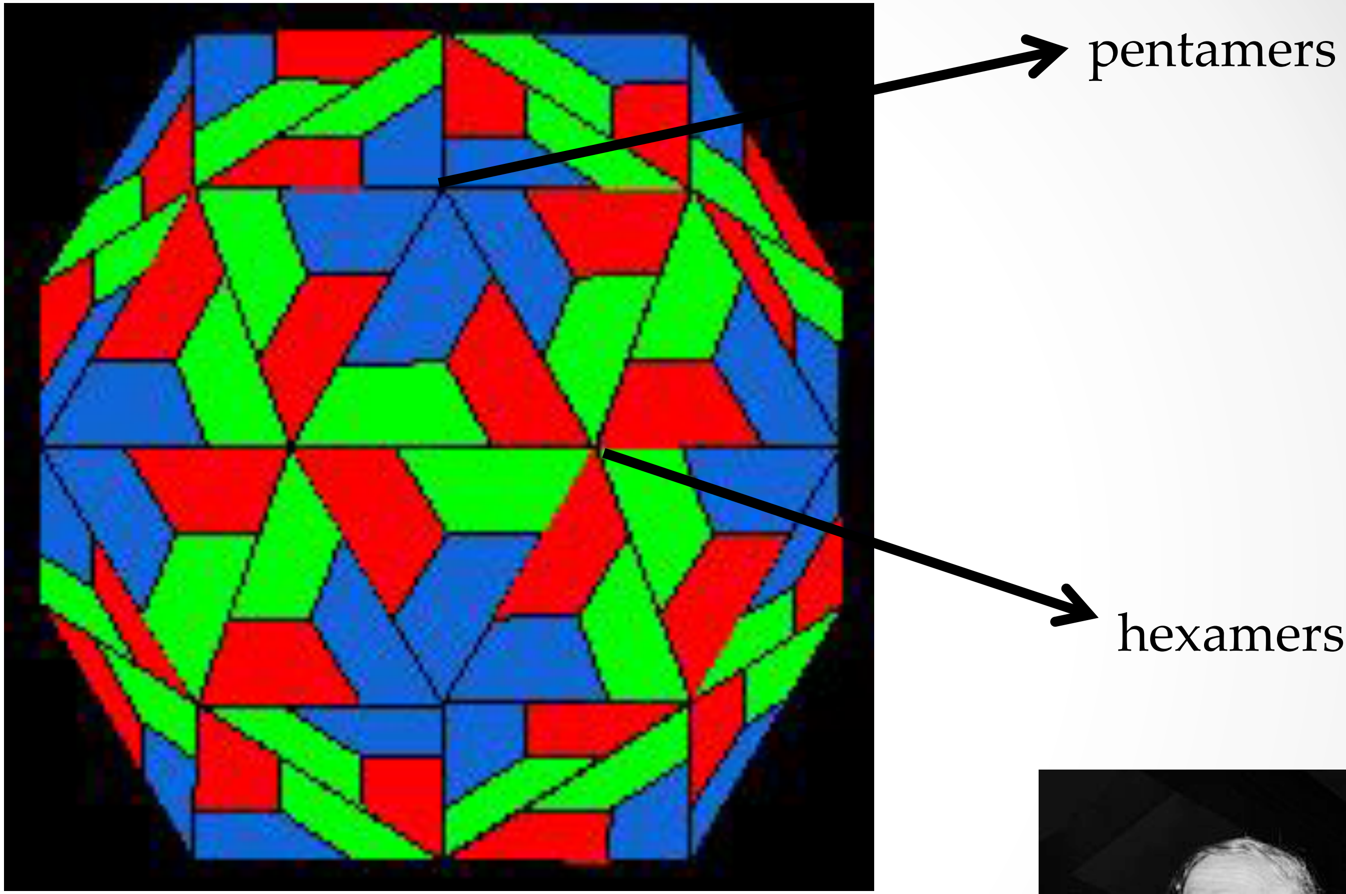


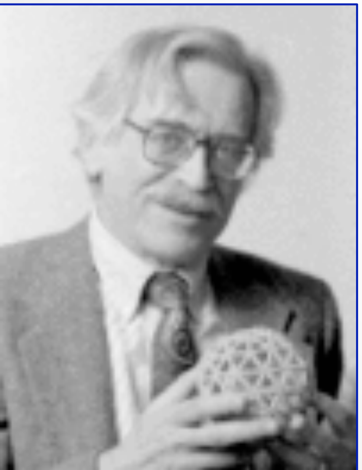
T=3 (180 subunits)

Some examples

P	f	T	No. of subunits (60T)	Example
1	1	1	60	Satellite tobacco necrosis virus
3	1	3	180	picornavirus
1	2	4	240	Sindbis Virus
1	3	9	540	Reovirus
1	4	16	960	Herpesvirus
1	5	25	1500	Adenovirus

Quasi-equivalence in virus structures





Casper and Klug

The Icosahedral Server

Main | Paradigm | Paper Template | Icos. Gallery | Swelling of CCMV

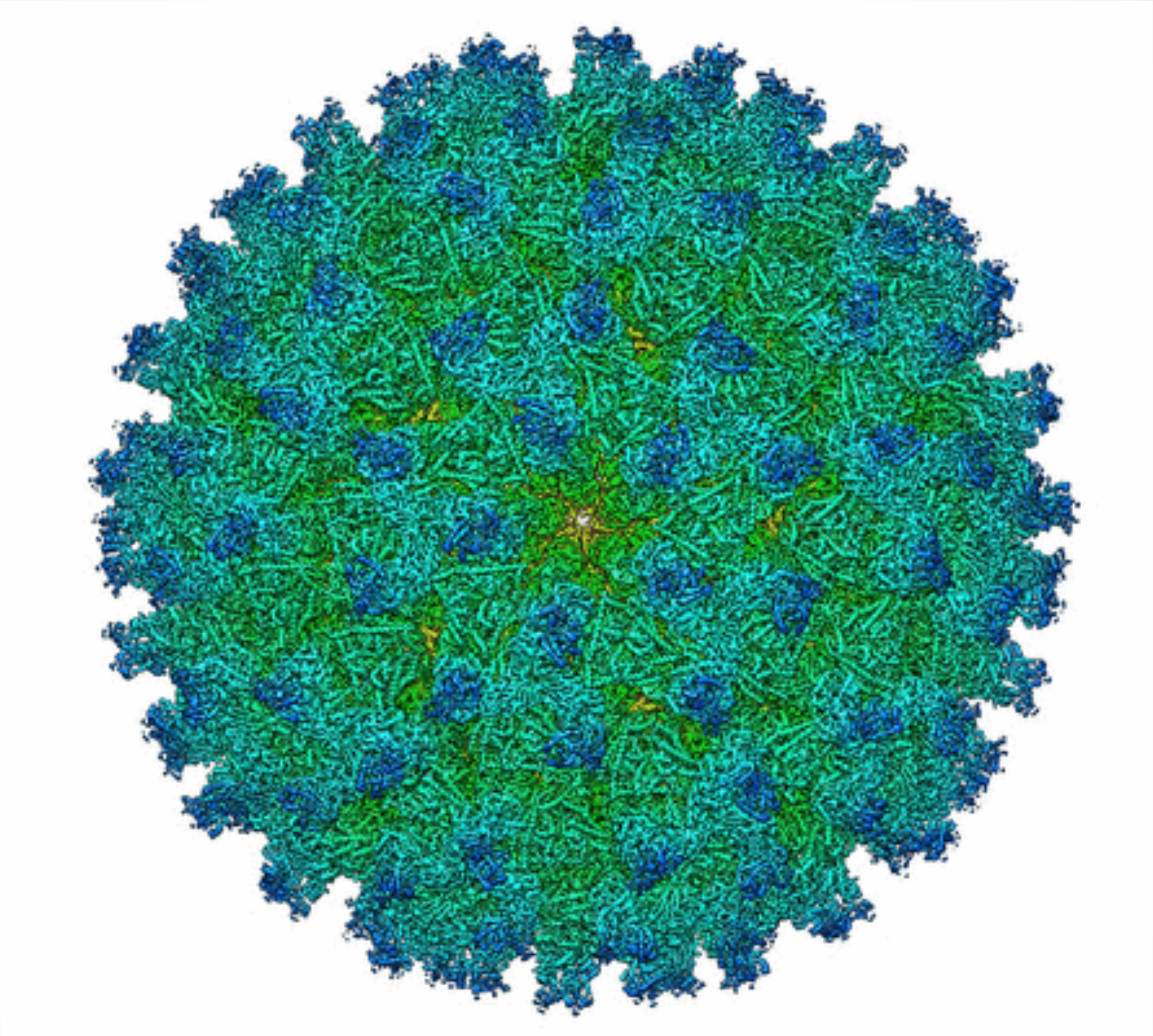
Paper Model Templates

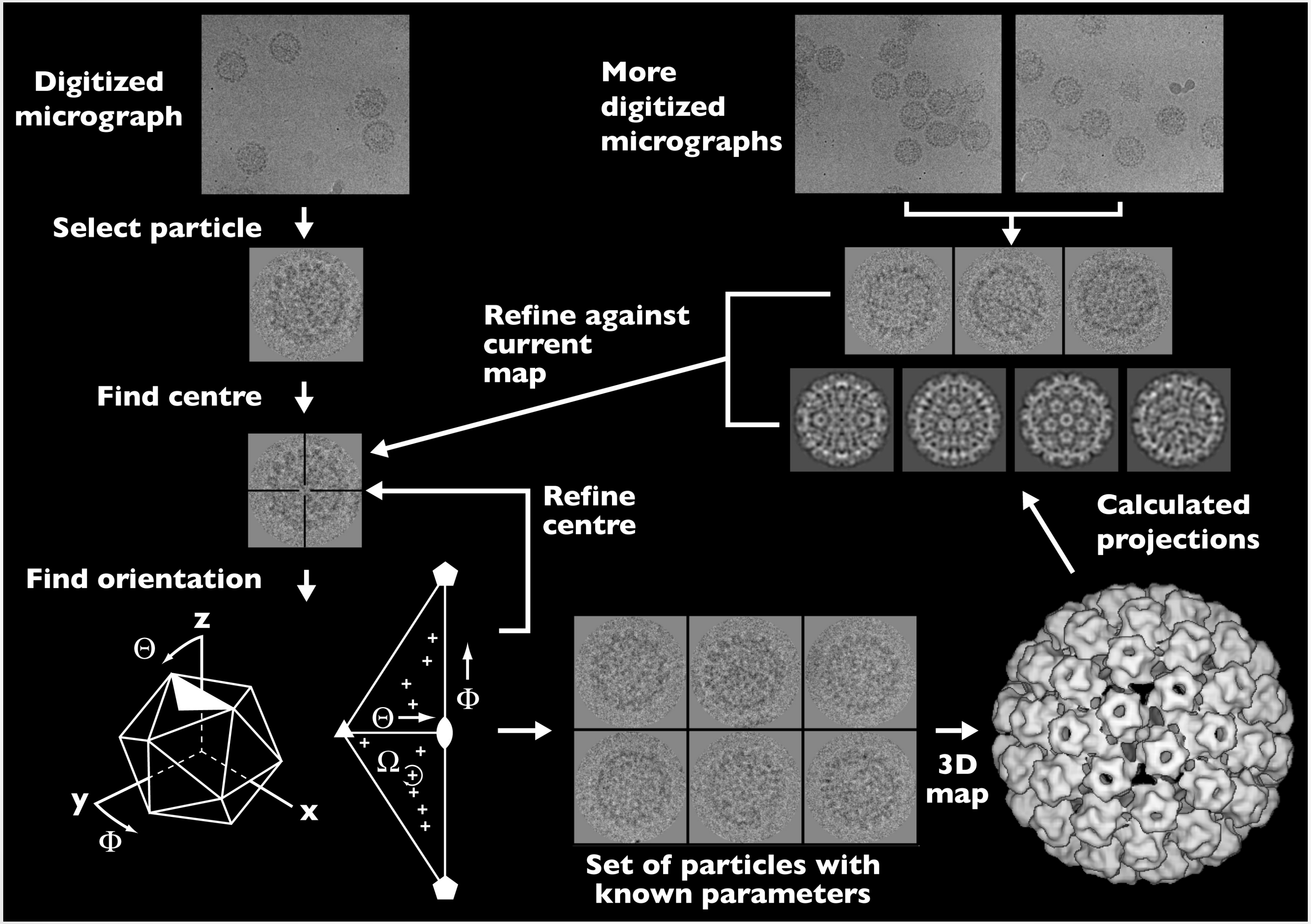
Download the original postscript files

Paper hexagonal template sheet

T=1 (h,k) = (1,0)
T=3 (h,k) = (1,1)
T=4 (h,k) = (2,0)
T=7 (h,k) = (2,1) / (h,k) = (1,2)
T=9 (h,k) = (3,0)
T=12 (h,k) = (2,2)
T=13 (h,k) = (3,1) / (h,k) = (1,3)
T=16 (h,k) = (4,0)
T=19 (h,k) = (3,2) / (h,k) = (2,3)
T=21 (h,k) = (4,1) / (h,k) = (1,4)
T=25 (h,k) = (5,0)
T=27 (h,k) = (3,3)
T=28 (h,k) = (4,2) / (h,k) = (2,4)
T=31 (h,k) = (5,1) / (h,k) = (1,5)

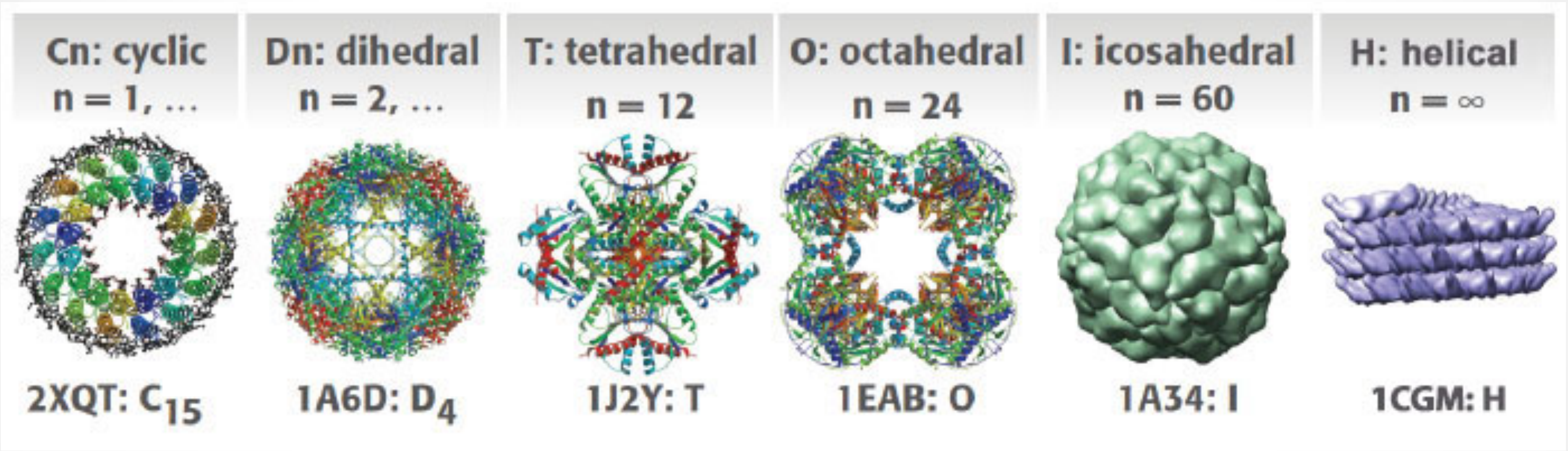
Bluetongue virus (EMD6444)





Crowther, 1971

Some examples from PDB/EMDB



Point Group Chart

See only cyclic C_n? Symmetries are C_n.

See cyclic C_n and C_2? D_n

See C_3 and C_2? T

See C_4, C_3, C_2? O

See C_5, C_3, C_2? I

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Principles of Virus Structural Organization. B.V. Venkataram Prasad and Michael F Schmid. Adv Exp Med Biol. 2012 ; 726: 17–47

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Personal communication, Barnali Chaudhuri, CSIR-IMTECH, India
EMDB
Internet Sources