On the Geometry of Icosahedral Viruses

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Research Questions

Goal: study natural symmetries in biological viruses.

(I) Explore geometric properties of icosahedral viruses (esp. of disymmetrons).

(II) Model and visualize viruses (esp. with Chimera).

(III) Produce 3D-printed virus puzzles to aid in teaching symmetries.

RESULTS

(I) Summarized viruses' geometric classifications and properties.

(II) Obtained a new and complete classification of symmetron arrangements involving disymmetrons.

NEXT STEPS

(III) Turn mathematical models into computer models.

(V) Design a 3D model of viruses to teach symmetries.

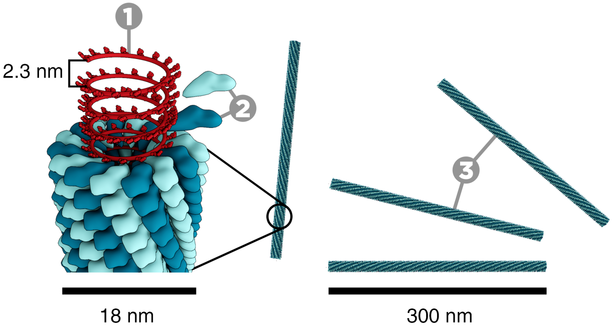
(VI) Understand constraints on irregular viruses.

Timeline of Viral History

- 1885: Pasteur suspects the existence of tiny pathogens
- 1898: Beijernick proves existence of tiny pathogens, coins term "virus"
- 1917: D'Herelle shows viruses are discrete particles
- 1931: Ruska and Knoll invent electron microscope

Components of a Virus

- Genetic material
- Protein capsid to contain genetic material—made of capsomers
- Lipid envelope around capsid (not in all viruses)



Timeline of Viral History (Continued)

- 1956: Watson and Crick suspect symmetrical capsid assembly from many proteins
- 1962: Caspar and Klug theorize about quasi-equivalence
- 1969: Wrigley finds evidence of symmetrons

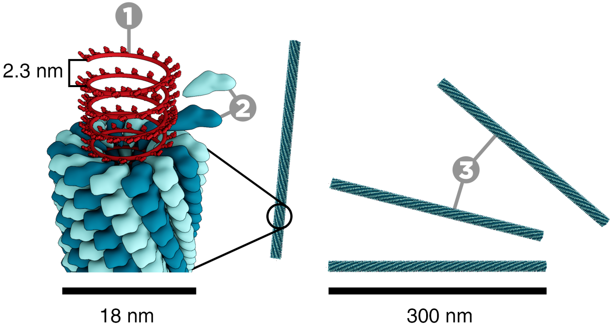
Biological Virus Classification

- Type of genetic material
- Number of strands in genetic material
- Infected cells / species
- Methods of infection / reproduction / transmission

Mathematical Virus Classification

Based on Virus Shape

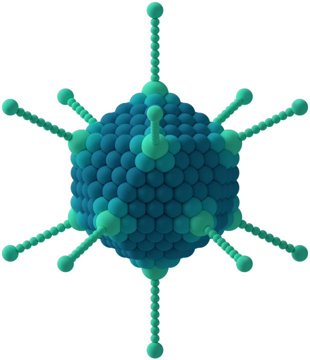
Helical



Mathematical Virus Classification

Based on Virus Shape

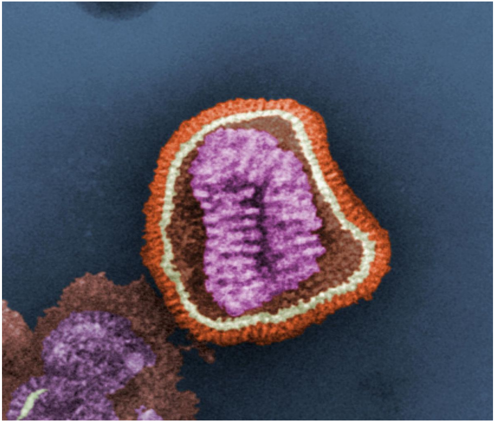
Icosahedral



MATHEMATICAL VIRUS CLASSIFICATION

BASED ON VIRUS SHAPE

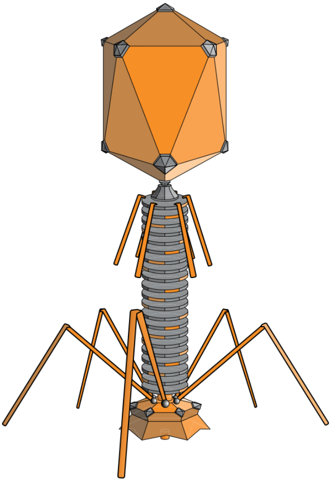
Enveloped



Mathematical Virus Classification

Based on Virus Shape

Complex

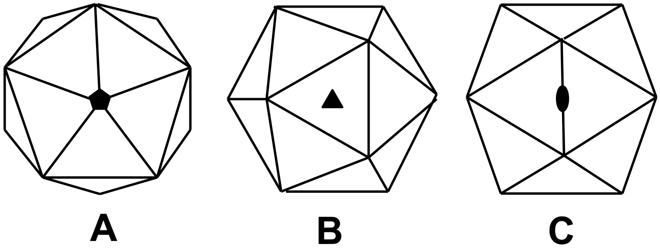


Icosahedral Virus

General properties

- Platonic solid

- High degree of symmetry: 2-fold, 3-fold, 5-fold axes

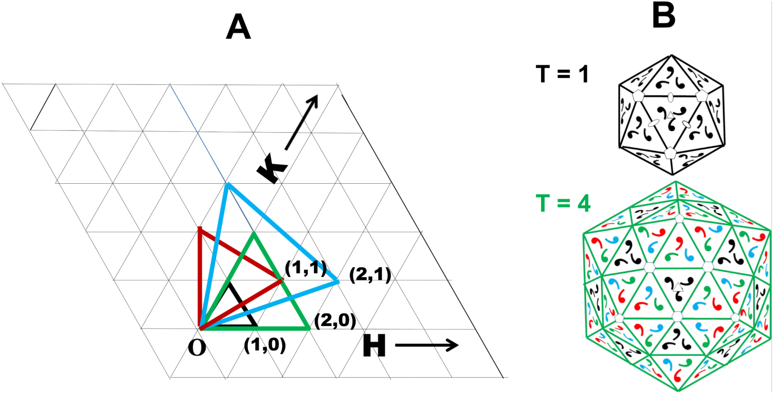


- At least 60 protein subunits

- Theories of quasi- and pseudo-equivalence

Caspar-Klug Theory of Quasi-Equivalence

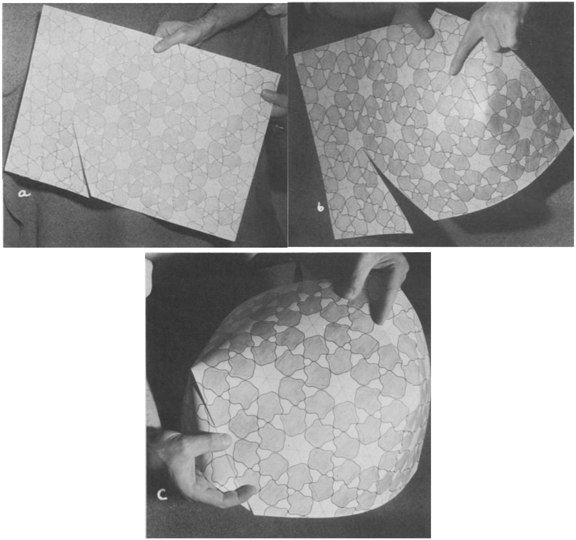
Triangulation number $T = h^2 + hk + k^2$



Pentamers and hexamers are capsomers

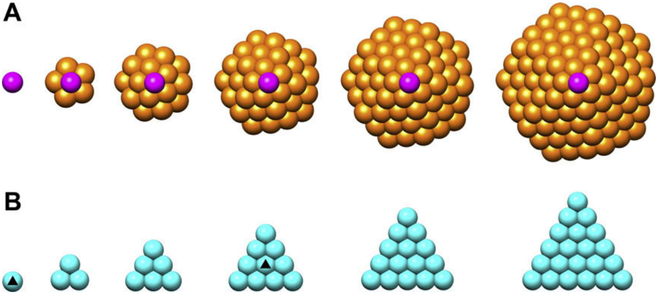
Caspar-Klug Theory of Quasi-Equivalence

2D to 3D



Wrigley's Theory of Symmetrons

Pentasymmetrons, trisymmetrons, and disymmetrons of sizes e_{PS}, e_{TS}, e_{DS}, respectively: symmetric collections of pentamers and/or hexamers

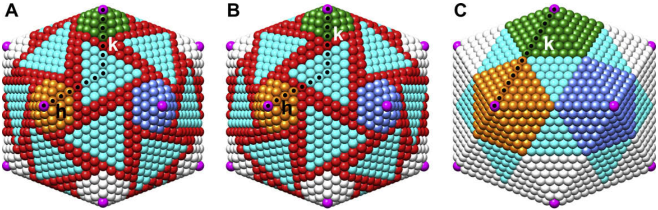


$$N_{cap} = 12 + 10(T-1)$$

$$N_{PS} = 1 + \frac{5e_{PS}(e_{PS}-1)}{2} \qquad N_{TS} = \frac{e_{TS}(e_{TS}+1)}{2} \qquad N_{DS} = e_{DS}$$

SINKOVITS-BAKER'S CLASSIFICATIONS

Penta- and trisymmetrons only



Classification of Disymmetron Arrangements

Basic Ideas

- Symmetry of overlapping arguments
- Rotations in the h, k coordinate system
- Bordering and casework

Classification of Disymmetron Arrangements

Main Result

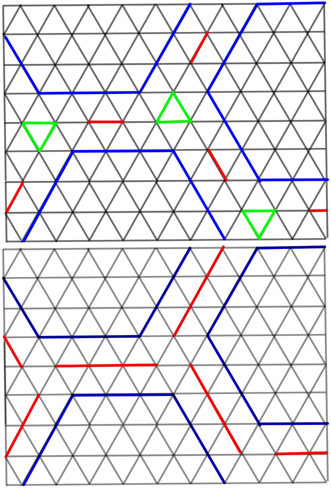
Theorem

All possible configurations of regular symmetrons to compose an icosahedral surface fit into the Classes described by Sinkovits-Baker or depicted in the following figures. Furthermore, these Classes are subject to the formulas and restrictions later shown in two tables.

Classification of Disymmetron Arrangements

Classes 4 and 5: Only Pentasymmetrons Border Disymmetrons

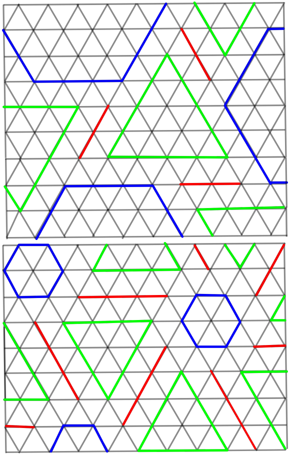
Disymmetrons Trisymmetrons Pentasymmetrons



Classification of Disymmetron Arrangements

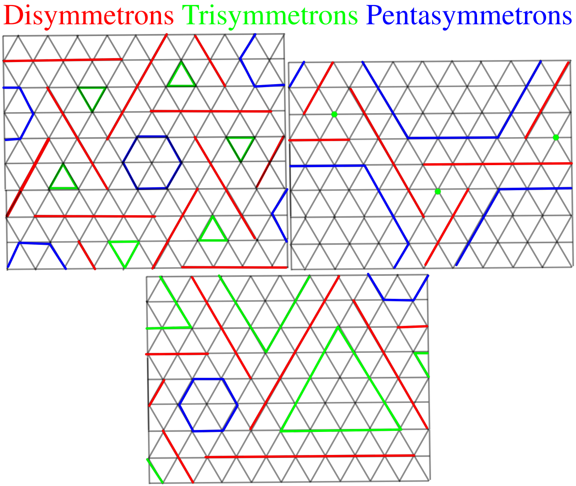
Classes 6 and 7: Only Trisymmetrons Border Disymmetrons

Disymmetrons Trisymmetrons Pentasymmetrons



Classification of Disymmetron Arrangements

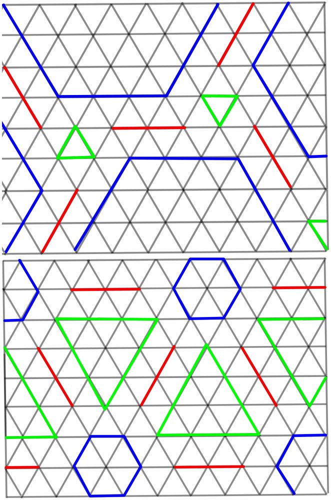
Classes 8, 9, and 10: Both Penta- and Trisymmetrons Border Disymmetrons



CLASSIFICATION OF DISYMMETRON ARRANGEMENTS

CLASSES 11 AND 12: EXCEPTIONAL CASES

Disymmetrons Trisymmetrons Pentasymmetrons



CLASSIFICATION OF ALL SYMMETRON ARRANGEMENTS

FORMULAS

Class #	e_{DS} Formula	e_{PS} Formula	e_{TS} Formula
1	0	$\frac{h+1}{2}$	$\frac{h+2k-1}{2}$
2	0	$\frac{k+1}{2}$	$\frac{2h+k-1}{2}$
3	0	$\frac{h+k+1}{2}$	$\frac{k-h-1}{2}$
4	$h-1$	$\frac{h+k}{2}$	$\frac{k-h}{2}+1$
5	$h+1$	$h+1$	0
6	$h-1$	$\frac{k}{2}+1$	$h+\frac{k}{2}-2$
7	$k-1$	$\frac{h}{2}+1$	$\frac{h}{2}+k-2$
8	$h+k-1$	$\frac{k}{2}$	$h+\frac{k}{2}-2$
9	$k-1$	$\frac{h+k}{2}$	$\frac{k-h}{2}-2$
10	$h+k-1$	$\frac{h}{2}$	$\frac{h}{2}+k-2$
11	$h+1$	$h+2$	2
12	$k-3$	2	$k-2$

CLASSIFICATION OF ALL SYMMETRON ARRANGEMENTS

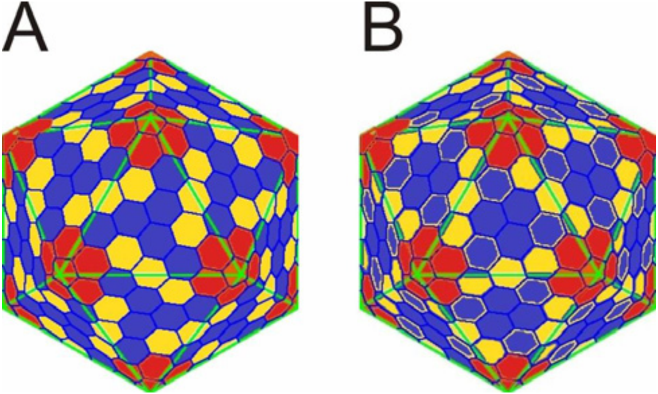
RESTRICTIONS

Class #	h,k Restrictions	T Restrictions
1	$h \equiv 1 \mod 2$	$T \equiv 1 \mod 2$
2	$k \equiv 1 \mod 2$	$T \equiv 1 \mod 2$
3	$h \not\equiv k \mod 2$	$T \equiv 1 \mod 2$
4	$h \equiv k \mod 2$	None
5	$k = h + 2$	$T \equiv h \mod 2$
6	$k \equiv 0 \mod 2$	None
7	$h \equiv 0 \mod 2$	None
8	$k \equiv 0 \mod 2$	None
9	$h \equiv k \mod 2$	None
10	$h \equiv 0 \mod 2$	None
11	$k = h + 4$	$T \equiv h \mod 2$
12	$h = 0$	$T \equiv k \mod 2$

QUESTION FROM NATURE

Only structure observed in nature containing disymmetrons:

Notice strange shape of trisymmetron.



Summary and Future Questions

- 3 Main Ideas
- Complete Classification of Symmetron Arrangements
- What conditions should be relaxed?
- What physical rules should we take into account? More broadly, why are certain arrangements favored?

Thank you for listening.

Questions?

Acknowledgments

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Main Bibliography

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2 A. Klug and D. L. D. Caspar. Physical principles in the construction of regular viruses. *Cold Spring Harbor Symposia on Quantitative Biology*, 27:1–24, 1962.

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5 N. G. Wrigley. An electron microscope study of the structure of sericesthis iridescent virus. *Journal of General Virology*, 5(1):123–134, March 1969.

Note About Pictures

Most of these images were taken from previous papers.

The original pictures are those depicting arrangements with disymmetrons. Thanks to Professor Schaposnik for her help in digitalizing these images.