On the Geometry of Icosahedral Viruses

Kai-Siang Ang

Faculty Mentor: Prof. Laura Schaposnik (UIC)

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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

A

\[ N_{\text{cap}} = 12 + 10(T - 1) \]

\[ N_{PS} = 1 + \frac{5e_{PS}(e_{PS}-1)}{2} \]

\[ N_{TS} = \frac{e_{TS}(e_{TS}+1)}{2} \]

\[ N_{DS} = e_{DS} \]
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
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 PENTASYMMETRON BORDER DISYMMETRON

Disymmetrons Trisymmetrons Pentasymmetrons
CLASSIFICATION OF DISYMMETRON ARRANGEMENTS

CLASSES 6 AND 7: ONLY TRISYMMETRONS BORDER DISYMMETRONS
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

<table>
<thead>
<tr>
<th>Class #</th>
<th>$e_{DS}$ Formula</th>
<th>$e_{PS}$ Formula</th>
<th>$e_{TS}$ Formula</th>
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<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>$\frac{h+1}{2}$</td>
<td>$\frac{h+2k-1}{2}$</td>
</tr>
<tr>
<td>2</td>
<td>0</td>
<td>$\frac{k+1}{2}$</td>
<td>$\frac{2h+k-1}{2}$</td>
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<td>3</td>
<td>0</td>
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<td>$\frac{k-h-1}{2}$</td>
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<tr>
<td>4</td>
<td>$h - 1$</td>
<td>$\frac{h+k}{2}$</td>
<td>$\frac{k-h}{2} + 1$</td>
</tr>
<tr>
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<td>$h + 1$</td>
<td>$h + 1$</td>
<td>0</td>
</tr>
<tr>
<td>6</td>
<td>$h - 1$</td>
<td>$\frac{k}{2} + 1$</td>
<td>$h + \frac{k}{2} - 2$</td>
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<tr>
<td>7</td>
<td>$k - 1$</td>
<td>$\frac{h}{2} + 1$</td>
<td>$\frac{h}{2} + k - 2$</td>
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<tr>
<td>8</td>
<td>$h + k - 1$</td>
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<td>$\frac{h}{2}$</td>
<td>$\frac{h}{2} + k - 2$</td>
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<tr>
<td>11</td>
<td>$h + 1$</td>
<td>$h + 2$</td>
<td>2</td>
</tr>
<tr>
<td>12</td>
<td>$k - 3$</td>
<td>2</td>
<td>$k - 2$</td>
</tr>
</tbody>
</table>
# Classification of All Symmetron Arrangements

## Restrictions

<table>
<thead>
<tr>
<th>Class #</th>
<th>$h, k$ Restrictions</th>
<th>$T$ Restrictions</th>
</tr>
</thead>
<tbody>
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<td>$h \equiv 1 \mod 2$</td>
<td>$T \equiv 1 \mod 2$</td>
</tr>
<tr>
<td>2</td>
<td>$k \equiv 1 \mod 2$</td>
<td>$T \equiv 1 \mod 2$</td>
</tr>
<tr>
<td>3</td>
<td>$h \not\equiv k \mod 2$</td>
<td>$T \equiv 1 \mod 2$</td>
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<tr>
<td>4</td>
<td>$h \equiv k \mod 2$</td>
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<td>$k = h + 2$</td>
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<tr>
<td>6</td>
<td>$k \equiv 0 \mod 2$</td>
<td>None</td>
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<tr>
<td>7</td>
<td>$h \equiv 0 \mod 2$</td>
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<tr>
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<td>$k \equiv 0 \mod 2$</td>
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</tr>
<tr>
<td>9</td>
<td>$h \equiv k \mod 2$</td>
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<tr>
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<tr>
<td>12</td>
<td>$h = 0$</td>
<td>$T \equiv k \mod 2$</td>
</tr>
</tbody>
</table>
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

I would like to thank MIT PRIMES-USA for the opportunity to work on this project, and I would like to thank Professor Schaposnik for her dedicated mentorship and guiding counsel. I would also like to thank my teacher Mr. Spenner and the PRIMES head mentor Dr. Khovanova for their helpful suggestions and feedback.
MAIN BIBLIOGRAPHY


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.