

Mapping Periodic Elements to Grant Polytopes

A Geometric Framework for Atomic Structure via Pythagorean Triple Cascades

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Abstract

We present a novel geometric mapping of the periodic table of elements onto Grant Polytopes via Pythagorean triple cascades. The core framework establishes that atomic number Z corresponds to cascade position or scaled triple sides; electron configurations map to vertices distributed across nine harmonic shells; and periodic blocks correspond to orthogonal chain branches in the +1 cascade (where $c - b = 1$). This unified geometric approach predicts valence from outer means, stability from shell capacity, and hypothesizes new superheavy elements from orthogonal triple extensions.

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1 Introduction

The periodic table of elements, first systematized by Mendeleev (1869), reveals deep patterns in atomic structure that have inspired numerous geometric representations. This work extends the Grant Projection Theorem—which derives 3D polyhedral topology from 2D right triangles—into the domain of atomic physics.

1.1 Core Hypothesis

The fundamental correspondence is:

| Atoms as Grant Polytopes |
|---|
| Each element corresponds to a position in the Pythagorean triple cascade. |
| Electron shells map to the Nine Harmonic Means. |
| Chemical behavior emerges from polyhedral geometry. |

1.2 The +1 Cascade

The orthogonal factor chain with $c - b = 1$ generates the consecutive-leg Pythagorean family:

$$(a_n, b_n, c_n) = (2n + 1, 2n(n + 1), 2n(n + 1) + 1) \quad (1)$$

This cascade provides the geometric scaffold for atomic structure.

2 Derivation Rules

Derivation Rule 2.1 (Seed Triple). *From cascade position n , the generating triple is:*

$$a_n = 2n + 1 \quad (DM \text{ seed} \approx \text{protons/period start}) \quad (2)$$

$$b_n = 2n(n + 1) \quad (GM \approx \text{electron shells}) \quad (3)$$

$$c_n = 2n(n + 1) + 1 \quad (AM \approx \text{total structure}) \quad (4)$$

Derivation Rule 2.2 (Shell Filling). *Electrons distribute as vertices across the 9 harmonic mean shells:*

| <i>Shell Type</i> | <i>Mean / Role</i> |
|--------------------|--|
| <i>Inner Core</i> | <i>DHM, DQM, DM (1s, 2s orbitals)</i> |
| <i>Middle Core</i> | <i>HM, GM, AM (2p, 3s, 3p orbitals)</i> |
| <i>Valence</i> | <i>QM, LBM, LGM (3d, 4s, 4p+ orbitals)</i> |

Derivation Rule 2.3 (Orthogonal Chains). • **Main +1 chain:** *s-block and p-block elements*

- **Parallel chains:** *d-block and f-block (relativistic “knots”)*
- **Chain branching:** *Corresponds to orbital angular momentum ℓ*

Derivation Rule 2.4 (Geometric Bonds). • **Bonds** = *Inter-shell edges (edge length formula from Grant Projection)*

- **Hybridization** = *Face type mixing (pentagonal \rightarrow organic chemistry)*
- **Bond angles** = *Derived from fundamental angle $\alpha = \arctan(a/b)$*

Derivation Rule 2.5 (Stability Prediction). • *Maximum 9 shells \Rightarrow stability cap at $Z \approx 118$*

- *Next orthogonal chain = predicted island of stability ($Z > 118$)*
- *Shell closure corresponds to noble gas configurations*

3 The Cascade-Element Mapping

3.1 Complete Mapping Table

| Period/Block | Cascade n /Triple | Z Range | Dominant Shells | Geometric Notes |
|-----------------|-----------------------------------|-----------|------------------------------------|-------------------------|
| 1 (s) | $n = 1$: (3, 4, 5) Primordial | 1–2 | DHM-DM-GM tight | Triangular core |
| 2 (s/p) | $n = 1$ extension | 3–10 | HM-QM start | Octahedral-like |
| 3–4 (s/p/d) | $n = 2$: (5, 12, 13) Alpha | 11–36 | Full 9 shells, pentagonal-dominant | Mixed 3-5-10, 120 faces |
| 4–5 (d/f start) | $n = 3$: (7, 24, 25) | 37–70 | LBM heavy | Heptagonal mix |
| 6–7 (f/g) | $n = 4+$: (9, 40, 41)+ | 71–118+ | LGM dominant, unstable beyond 9 | Decagonal+, collapse |

3.2 Key Elements and Geometric Fit

3.2.1 Period 1: Primordial Triple (3, 4, 5)

- **Hydrogen** ($Z = 1$): Single vertex on innermost shell (DHM)
- **Helium** ($Z = 2$): Closed shell—two vertices completing the core
- **Geometry**: Triangular core ($a = 3$), simplest closed structure
- **Factors**: $f_1 = 2$, $f_2 = 8$, $V = 10$, $E = 16$, $F = 8$

3.2.2 Period 2: Extended Primordial

- **Li–Ne** ($Z = 3–10$): Octet rule emerges from 8-vertex extensions
- **Geometry**: Octahedral-like symmetry, 8 faces/edges governing bonding
- **Carbon** ($Z = 6$): Central position enables sp^3 tetrahedral hybridization

3.2.3 Periods 3–4: The Alphahedron Regime (5, 12, 13)

- **Na–Kr** ($Z = 11–36$): Full 9-shell structure emerges
- **Transition metals:** d-block filling corresponds to parallel orthogonal chains
- **Organic chemistry:** Pentagonal-dominant faces ($a = 5$ seed) enable complex bonding
- **Key values:**

$$V = 26 \text{ vertices (electron positions)}$$

$$F = 120 = 5! \text{ faces (bonding geometries)}$$

$$\alpha = 22.62 \text{ (fundamental bond angle)}$$

3.2.4 Periods 4–5: Heptagonal Regime (7, 24, 25)

- **Rb–Nd** ($Z = 37–70$): d-block filling dominates
- **Geometry:** Heptagonal face mixing, LBM shell becomes primary
- **Factors:** $f_1 = 18$, $f_2 = 32$, $V = 50$, $E = 576$

3.2.5 Periods 6–7: Lanthanides, Actinides, and Beyond

- **Lu–Og** ($Z = 71–118$): LGM shell dominant, approaching 9-shell limit
- **f-block:** Deep orthogonal chain branching (relativistic effects)
- **Superheavies** ($Z > 118$): Predicted from next orthogonal cascade
- **Island of stability:** Geometric shell closure at specific Z values

4 Shell Structure and Electron Configuration

4.1 Nine Means as Electron Shells

The nine harmonic means provide natural radii for electron shells:

| Shell # | Mean | Alphahedron Radius | Orbital Correspondence |
|---------|------|--------------------|------------------------|
| 1 | DHM | 4.6154 | 1s |
| 2 | DM | 5.0000 | 2s |
| 3 | DQM | 5.4167 | 2p |
| 4 | HM | 11.0769 | 3s |
| 5 | GM | 12.0000 | 3p |
| 6 | AM | 13.0000 | 3d / 4s |
| 7 | QM | 14.0833 | 4p |
| 8 | LBM | 28.8000 | 4d / 5s |
| 9 | LGM | 45.0333 | 4f / 5p+ |

4.2 Shell Capacity

Each shell's vertex capacity determines maximum electrons:

$$n_{\text{electrons}}^{(k)} = v_k = \max(3, \min(v_{\text{remaining}}, \text{round}(v_{k-1} \cdot \rho_k \cdot (1 + w_k \bmod 2)))) \quad (5)$$

where $\rho_k = r_k/r_{k-1}$ (shell ratio) and $w_k = \ln(\rho_k)/\alpha$ (wave modulation).

5 Chemical Bonding from Geometry

5.1 Bond Types as Edge Classes

| Bond Type | Geometric Origin | Formula |
|---------------|---------------------------|-----------------------------|
| σ bond | Intra-shell edge | $2r_k \sin(\pi/v_k)$ |
| π bond | Inter-shell edge | $\sqrt{\Delta_k^2 + A_k^2}$ |
| Ionic | Shell-to-shell transfer | $\Delta_k = r_{k+1} - r_k$ |
| Metallic | Delocalized across shells | Average of all edges |

5.2 Hybridization as Face Mixing

| Hybridization | Face Type | Angle |
|--------------------------------|---------------------------------|---------------|
| sp | Linear (2-gon limit) | 180 |
| sp ² | Triangular | 120 |
| sp ³ | Tetrahedral (from $a = 5$ seed) | 109.5 |
| sp ³ d | Pentagonal | ≈ 108 |
| sp ³ d ² | Hexagonal | 90 |

The pentagonal-dominant Alphahedron ($a = 5$) naturally generates tetrahedral and pentagonal hybridizations central to organic and organometallic chemistry.

6 Predictions

6.1 Stability from Shell Structure

Theorem 6.1 (9-Shell Stability Limit). *The maximum stable atomic number corresponds to complete filling of all 9 harmonic shells:*

$$Z_{\text{max}} \approx V_{\text{total}} = 2c_n \quad \text{at the cascade limit} \quad (6)$$

For the observed periodic table, this predicts stability issues beyond $Z = 118$ (Oganesson).

6.2 Island of Stability

Proposition 6.2 (Orthogonal Chain Extension). *Superheavy elements ($Z > 118$) may stabilize at specific atomic numbers corresponding to:*

1. Closure of a 10th shell (next orthogonal chain)
2. Magic numbers from the next cascade triple
3. Geometric shell completion analogous to noble gas configurations

Predicted magic numbers from cascade $n = 5$: (11, 60, 61)

- $V = 122$, $E = 3600$, $F = 3480$
- Suggests stability around $Z \approx 120$ – 126

6.3 Valence from Outer Means

Proposition 6.3 (Valence Prediction). *The valence of an element is determined by electron count on outer shells (QM, LBM, LGM):*

$$\text{Valence} = v_{\text{outer}} \bmod 8 \quad (7)$$

where the modulo 8 reflects the octet rule emerging from the primordial (3, 4, 5) triple's geometry.

7 Connections to Known Models

7.1 Polyhedral Atomic Models

The Grant Polytope framework parallels historical polyhedral atomic models:

- **Nested Platonic solids:** Kepler's planetary model adapted to electron shells
- **Archimedean shell structures:** Truncated polyhedra for transition metals
- **Concentric sphere models:** Bohr-Sommerfeld orbits as our shell radii

7.2 Wave Mechanics Connection

The wave modulation parameter $w_k = \ln(\rho_k)/\alpha$ connects to:

- Schrödinger equation solutions (radial wave functions)
- Orbital angular momentum quantum numbers
- Fine-structure splitting (via the $\alpha \approx 1/137$ connection)

8 Summary

Unified Geometric Chemistry

1. **Elements** ↔ Cascade positions in Pythagorean triples
2. **Electron shells** ↔ Nine Harmonic Mean radii
3. **Periodic blocks** ↔ Orthogonal chain branches
4. **Chemical bonds** ↔ Inter-shell edges
5. **Hybridization** ↔ Face type mixing
6. **Stability** ↔ 9-shell geometric limit
7. **Superheavies** ↔ Next orthogonal cascade

This geometric framework unifies atomic structure, chemical bonding, and periodic trends through the single principle of Pythagorean triple cascades projected into 3D polyhedral space.

9 Future Directions

1. **Quantitative validation:** Compare predicted shell radii to experimental atomic radii
2. **Spectroscopic signatures:** Derive emission spectra from shell-to-shell transitions
3. **Nuclear structure:** Extend mapping to proton/neutron configurations
4. **Molecular geometry:** Apply face connectivity rules to molecular shapes
5. **Superheavy synthesis:** Guide experimental searches using predicted magic numbers