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Vladimir V. Yakovlev

research@ucmt-project.net

Independent Researcher

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A Minimal Sphere Model for the Emergence of VSEPR-Like Molecular Geometries

Vladimir V. Yakovlev
Independent Researcher, Russian Federation

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Corresponding author: Vladimir V. Yakovlev
Independent Researcher, Perm, Russian Federation Correspondence to:
research@ucmt-project.net

Abstract

We present a minimal geometric model in which VSEPR-like molecular geometries emerge from the energy minimization of interacting nodes constrained to a sphere. The model uses only two node types, a control parameter governing effective repulsion, and numerical optimization, without separately introducing rules for hybridization, orbital structure, or allowed molecular forms. Within this framework, familiar small- N geometries are recovered, including the trigonal-bipyramidal reference case at $N = 5$, a soft octahedral regime at $N = 6$, and the onset of geometric degeneracy with pentagonal motifs at $N = 7$. A probe case at $N = 12$ further yields a robust icosahedral-like packing. The aim of the model is not to provide a full theory of chemical bonding, but to test how much of the familiar repertoire of molecular geometry can be recovered from a sparse and uniform set of assumptions. In this sense, the results are methodological as much as geometric: they suggest that part of the descriptive structure of molecular geometry may emerge from a single optimization principle rather than from a larger independent rule set.

Keywords: molecular geometry; VSEPR; sphere-constrained optimization; minimal model; emergent structure; geometric modeling

1 Introduction

Molecular geometry is commonly described through a combination of empirical rules and semi-empirical concepts, including electron-pair repulsion, lone-pair effects, hybridization patterns, and standard canonical forms [10, 3, 2, 5, 4]. This descriptive language is highly effective in practice, but it also raises a methodological question: how much of the familiar geometric repertoire can be recovered from a smaller and more uniform set of assumptions [9, 6, 8]?

In the present work, we study a minimal geometric model in which interacting nodes are constrained to the surface of a sphere. The model uses only two node types, denoted B and L , a control parameter α , and numerical minimization of an energy-like functional. No separate rules are introduced for tetrahedral, trigonal-bipyramidal, octahedral, or other standard molecular geometries. When such forms appear, they arise as minima of the same optimization problem. In this respect, the model is also related, at the level of geometric optimization on curved surfaces, to the broader class of sphere-packing and generalized Thomson-type problems [1, 7].

The aim of the model is deliberately limited. It is not proposed as a complete theory of chemical bonding, nor as a replacement for the established chemical description of molecular structure. Rather, it is intended as a geometric baseline: a test of how far one can go in recovering familiar structural motifs while keeping the descriptive framework sparse and uniform.

Within that limited scope, the results define a coherent sequence. At small N , the model reproduces standard VSEPR-like motifs. At $N = 6$, it enters a soft octahedral regime rather than a single rigid ideal form. At $N = 7$, geometric degeneracy appears together with pentagonal organization. Finally, a probe test at $N = 12$ yields a robust icosahedral-like packing. Taken together, these cases suggest that part of the usual descriptive rule set of molecular geometry may be reorganized in terms of a single optimization principle on the sphere, at least at the level of geometric motif formation.

2 Minimal model

2.1 Degrees of freedom

The configuration consists of N nodes constrained to the unit sphere, with

$$N = N_B + N_L,$$

where N_B is the number of bonding centres (B) and N_L is the number of lone centres (L).

Each configuration is defined by:

- the total number of nodes N ,
- the composition (N_B, N_L) ,
- the node positions on the sphere,
- the interaction parameter α .

2.2 Interaction and control parameter

The model uses a single effective parameter α controlling the relative strength of repulsion in the optimization functional. In version 1, α is treated as an external control parameter rather than a quantity derived from a deeper physical model.

2.3 Optimization

For fixed (N_B, N_L, α) , the configuration is obtained numerically by repeated restarts followed by local minimization. The best minimum found across all restarts is retained as the representative configuration.

The basic diagnostics recorded for each run are:

- best energy,
- full angle statistics,
- type-resolved angle statistics,
- Cartesian coordinates of the optimized points.

2.4 Scope of version 1

Version 1 is deliberately restricted to geometry. It does not attempt to encode orbital structure, explicit charge distributions, or a full microscopic theory of chemical bonding. Its purpose is to test how much of the standard geometric repertoire can arise from a sparse and uniform set of assumptions.

Optimization functional and identification criteria

In version 1, the configuration is represented by N interacting nodes constrained to the unit sphere. The minimized objective is an energy-like pair functional built from effective repulsive interactions between all node pairs, with interaction weights determined by node type (B or L) and by the control parameter α . For each (N, N_B, N_L, α) case, the reported configuration is the lowest-energy solution found across repeated numerical restarts, followed by local minimization.

The purpose of the optimization is not to reproduce a chemically calibrated potential, but to test whether recognizable structural motifs emerge from a sparse and uniform rule set. A configuration is treated as VSEPR-like when its angular organization reproduces the expected canonical motif or a clear soft variant of it. In this paper, “soft” denotes a regime in which the same geometric family is retained while exact ideal-angle degeneracy is relaxed. The $N = 12$ case is included as a geometric probe of packing behaviour on the sphere rather than as a direct molecular analogue. These criteria are intentionally geometric and operational; chemically specific interpretation is left for later versions of the model.

3 Reference validation: $N = 5$

The first reference case is the configuration

$$N = 5, \quad N_B = 2, \quad N_L = 3.$$

In standard VSEPR notation, this corresponds to AX_2E_3 .

The optimized geometry reproduces the familiar trigonal bipyramidal arrangement, with the characteristic angle pattern

- $BB \approx 180^\circ$,
- $BL \approx 90^\circ$,
- $LL \approx 120^\circ$.

This case is important because no trigonal-bipyramidal rule is imposed separately. The geometry appears directly as the minimum of the same spherical optimization problem used throughout the model. It therefore serves as the reference validation for version 1.

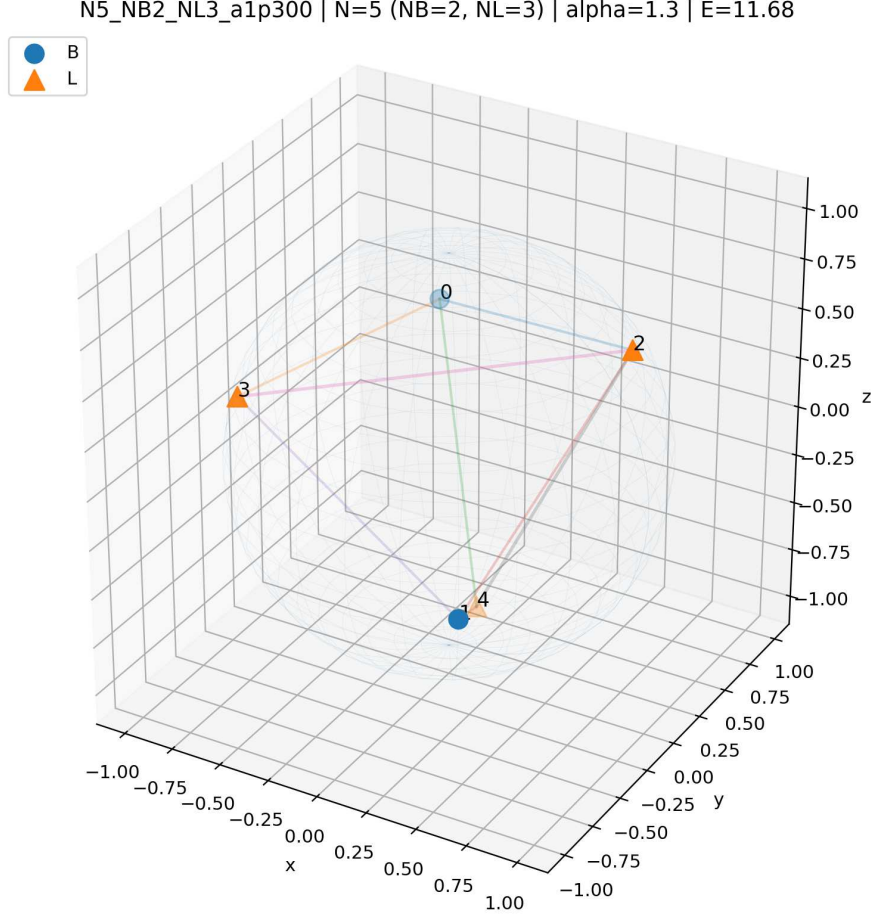


Figure 1: Reference $N = 5$ configuration for the AX_2E_3 -type case in the minimal sphere model. The optimized arrangement reproduces the expected trigonal-bipyramidal motif from energy minimization alone.

4 Soft octahedral regime: $N = 6$

For

$$N = 6, \quad N_B = 2, \quad N_L = 4,$$

a full scan over α shows a stable regime close to the octahedral geometry. The energy remains stable across runs, the angle statistics vary smoothly with α , and no sharp phase transition is observed.

The important point is that this case is better described as a *soft octahedral regime* than as a single rigid ideal octahedron. The geometry remains organized and recognizable, but is not locked into one perfectly discrete form.

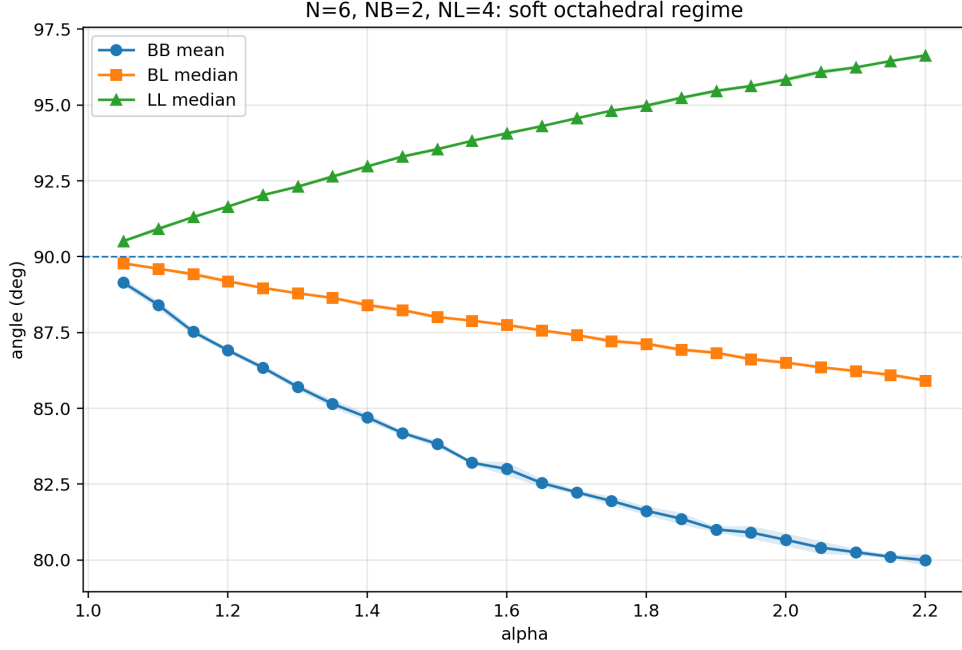


Figure 2: Angle trends across the $N = 6$, $NB = 2$, $NL = 4$ map. The characteristic angles remain close to the octahedral regime over the scanned α range, indicating a soft but persistent octahedral organization.

5 Onset of geometric degeneracy: $N = 7$

The central result of version 1 appears at $N = 7$. A dataset of 135 runs was collected for three compositions,

$$(N_B, N_L) \in \{(1, 6), (3, 4), (5, 2)\},$$

across nine values of α and five seeds per point.

The main observation is that $N = 7$ marks the onset of *soft geometric degeneracy*. The minima remain low-energy and reproducible, but the geometry is no longer captured by a single rigid symmetry class.

5.1 Case AX_1E_6

For $N_B = 1$ and $N_L = 6$, the system shows a regime change as α increases. This is visible in the type-resolved angle statistics and in the corresponding visualizations.

5.2 Case AX_3E_4

For $N_B = 3$ and $N_L = 4$, the geometry changes smoothly with α . This case illustrates continuous geometric deformation rather than abrupt restructuring.

5.3 Case AX_5E_2

For $N_B = 5$ and $N_L = 2$, the model yields the most expressive configuration in the $N = 7$ family. The characteristic angles are approximately

- $BB \approx 108^\circ$,
- $BL \approx 90^\circ$,

- $LL \approx 180^\circ$.

This corresponds to a pentagonal belt of B -nodes together with two nearly antipodal L -nodes. In visual form, this case provides the clearest demonstration that the model develops a genuine pentagonal motif at $N = 7$.

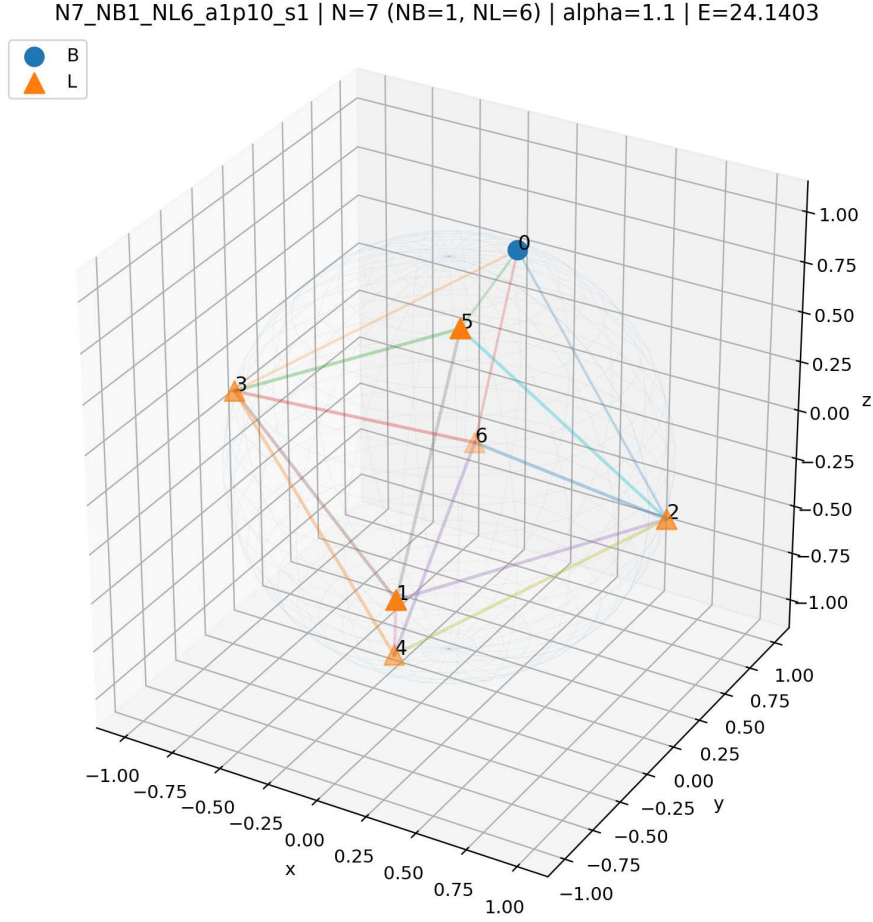


Figure 3: Representative $N = 7$, AX_1E_6 -type configuration. This case illustrates the onset of geometric softening: the arrangement remains structured, but no longer locks into a single rigid canonical form.

N7_NB3_NL4_a1p60_s1 | N=7 (NB=3, NL=4) | alpha=1.6 | E=36.0065

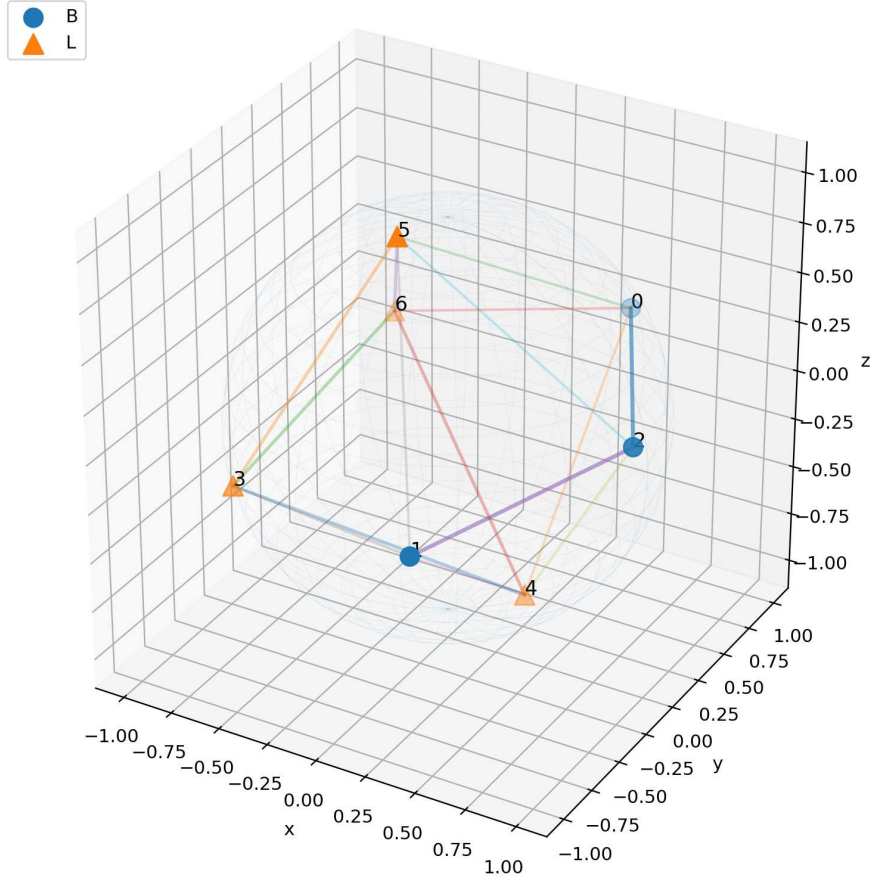


Figure 4: Representative $N = 7$, AX_3E_4 -type configuration. The optimized structure shows visible deformation relative to lower- N rigid motifs, consistent with the emergence of soft geometric degeneracy.

N7_NB5_NL2_a1,10_s1 | N=7 (NB=5, NL=2) | alpha=1.1 | E=21.6052

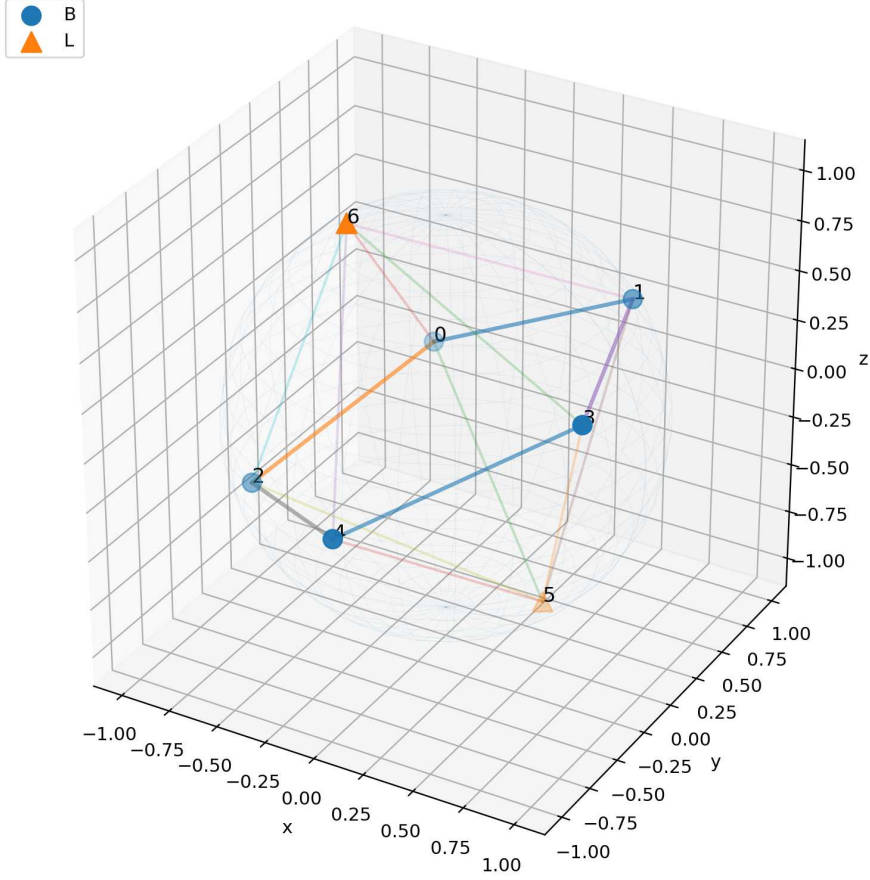


Figure 5: Representative $N = 7$, AX_5E_2 -type configuration with a pronounced pentagonal motif. This case highlights the appearance of a pentagonal belt structure within the same minimal optimization framework.

6 Probe toward icosahedral packing: $N = 12$

As a closing probe, the pure- B case

$$N = 12, \quad N_B = 12, \quad N_L = 0$$

was tested for several values of α and multiple seeds.

Across all probe runs, the optimized configurations converge to essentially the same angular structure. The characteristic angle distribution is centered around values close to

- 63.5° ,
- 116° ,
- 180° ,

with only minor variations between seeds.

This is consistent with a robust icosahedral-like packing on the sphere. In the logic of the present paper, the $N = 12$ result is not introduced as a separate main chapter, but as a final probe showing that the same minimal model extends from small VSEPR-like forms to deeper spherical packing structures.

PURE_N12_a1p10_s1 | N=12 (NB=12, NL=0) | alpha=1.1 | E=78.003

● B

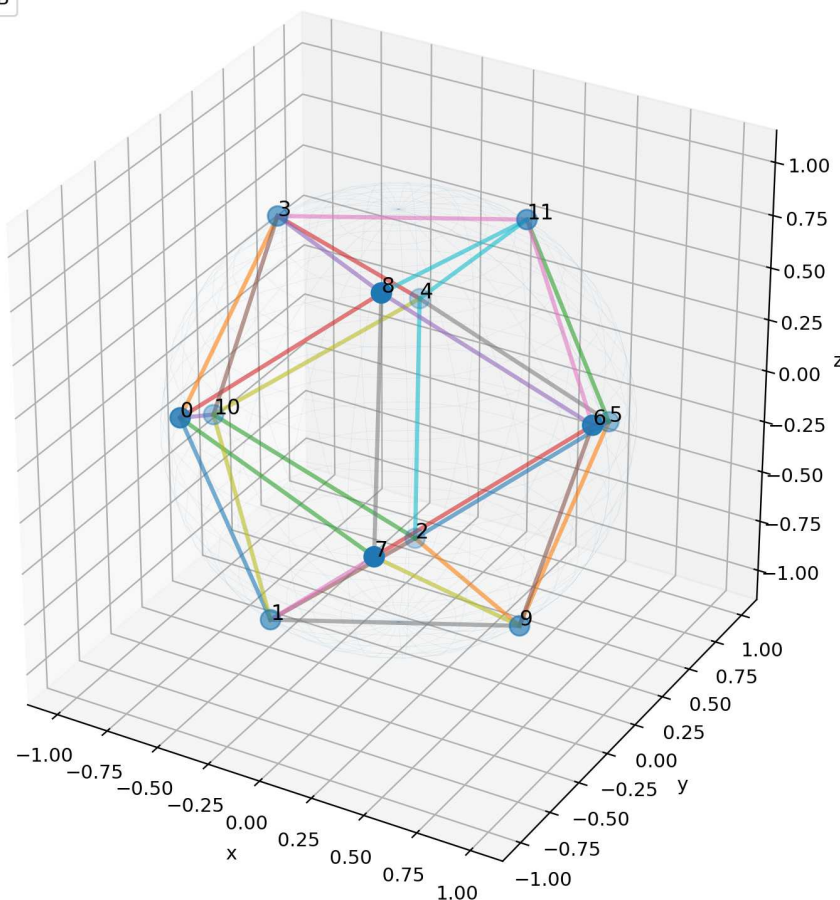


Figure 6: Pure- B probe for $N = 12$. The optimized arrangement is consistent with an icosahedral-like packing and remains stable across the tested α values and seeds.

7 Interpretation

Taken together, the results define a coherent geometric sequence:

- small- N baseline includes the tetrahedral form,
- $N = 5$: trigonal bipyramidal form,
- $N = 6$: soft octahedral regime,
- $N = 7$: onset of geometric degeneracy and pentagonal motifs,
- $N = 12$: stable icosahedral-like packing.

The significance of this sequence is methodological. Molecular-like geometries are not entered as a table of allowed forms. They arise from a single optimization principle acting on nodes constrained to a sphere.

The model therefore suggests that part of the standard geometric repertoire may be recoverable from fewer assumptions than are usually introduced at the descriptive level, and thus belongs to the broader question of how chemical structure is represented, idealized, and formalized in theoretical chemistry [9, 6, 8].

Table 1: Compact summary of representative configurations in v.1 of the minimal sphere model.

Case	Representative setting	Emergent motif	Interpretation
$N = 5$	AX_2E_3	trigonal bipyramidal	reference rigid case
$N = 6$	AX_2E_4	soft octahedral regime	stable but not perfectly rigid
$N = 7$	AX_1E_6	shifted soft arrangement	onset of degeneracy
$N = 7$	AX_3E_4	deformed structured form	soft geometric competition
$N = 7$	AX_5E_2	pentagonal belt motif	strong pentagonal tendency
$N = 12$	pure- B probe	icosahedral-like packing	robust high-symmetry packing

8 Conclusion

The present study was intended as a minimal geometric test rather than as a complete account of chemical bonding. Within that limited scope, the model shows that several familiar VSEPR-like geometries can be recovered from a single optimization framework based on interacting nodes constrained to a sphere. The results also indicate that this framework naturally extends beyond rigid canonical forms, producing soft octahedral behaviour at $N = 6$, geometric degeneracy at $N = 7$, and an icosahedral-like packing probe at $N = 12$.

The main significance of the model is therefore methodological. It suggests that part of the standard descriptive repertoire of molecular geometry may be reorganized in terms of a smaller number of assumptions, without reproducing each form through a separate rule. Whether this minimal language can be connected more directly to chemically specific structure is a question for later versions. In its present form, the model is best understood as a geometric baseline for further development. The present results should therefore be read as evidence of geometric generative capacity, not as a chemically complete account of molecular structure.

Declarations

Ethics approval and consent to participate

Not applicable.

Consent for publication

Consent to Publish declaration: not applicable.

Authors’ contributions

The sole author conceived the study, carried out the modeling and analysis, and wrote the manuscript.

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Competing interests

The author declares no competing interests.

Reproducibility note

A compact reproducibility bundle accompanies this paper, including representative JSON outputs, the $N = 6$ map series, figure-generation scripts, summary data, and the LaTeX source. The bundle is archived at Zenodo [11].

References

- [1] Mark Bowick, Angelo Cacciuto, David R. Nelson, and Alex Travasset. Crystalline order on a sphere and the generalized thomson problem. *Physical Review Letters*, 89(18):185502, 2002.
- [2] R. J. Gillespie. The VSEPR model revisited. *Chemical Society Reviews*, 21(1):59–69, 1992.
- [3] R. J. Gillespie and R. S. Nyholm. Inorganic stereochemistry. *Quarterly Reviews, Chemical Society*, 11:339–380, 1957.
- [4] Ronald J. Gillespie and Paul L. A. Popelier. *Chemical Bonding and Molecular Geometry: From Lewis to Electron Densities*. Oxford University Press, New York, 2001.
- [5] Ronald J. Gillespie and Edward A. Robinson. Models of molecular geometry. *Chemical Society Reviews*, 34(5):396–407, 2005.
- [6] Savino Longo. Hints for a formal language inspired by lewis structures. *Foundations of Chemistry*, 24(3):315–330, 2022.
- [7] W. L. Miller and A. Cacciuto. Two-dimensional packing of soft particles and the soft generalized thomson problem. *Soft Matter*, 7(16):7552–7559, 2011.
- [8] Valeria A. Seifert. The role of idealisations in describing an isolated molecule. *Foundations of Chemistry*, 22:1–15, 2020.
- [9] Shant Shahbazian and Mansour Zahedi. The role of observables and non-observables in chemistry: A critique of chemical language. *Foundations of Chemistry*, 8(1):37–52, 2006.
- [10] N. V. Sidgwick and H. M. Powell. Bakerian lecture. stereochemical types and valency groups. *Proceedings of the Royal Society A*, 176(965):153–180, 1940.
- [11] Vladimir V. Yakovlev. UCM-T chem / VSEPR sphere v.1: minimal sphere model and reproducibility bundle, 2026.