

σ -Aromatic Be₃ Ring as a Platform for Molecular Dinitrogen Fixation: A Combined DFT and Topological Study

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Abstract: Fixation and coordination of molecular dinitrogen (N₂) by main-group clusters offer fundamental insight into non-classical multi-centre bonding and light-metal activation pathways. Here we report a combined density-functional and ab initio study of the cyclic cluster Be₃(N₂)₃. Geometry optimization and frequency analysis establish a stable, closed-shell C_s-symmetric trimer containing an isosceles triangular Be₃ metal core coordinated end-on by three terminal N₂ ligands. Energy decomposition analysis coupled with natural orbitals for chemical valence (ETS-NOCV) shows that the Be₃... (N₂)₃ interaction is dominated by orbital contributions (≈ 60 % of attractive forces), supplemented by electrostatic attraction that together overcome Pauli repulsion. Quantum theory of atoms in molecules (QTAIM) identifies two non-nuclear attractors along the apical–basal Be–Be edges, while electron localization function (ELF) and localized orbital locator (LOL) basin analyses reveal a distinct heart-shaped trisynaptic valence basin V(Be,Be,Be) populated by ≈ 1.8 –2.0 electrons. These topological signatures establish multi-centre σ -aromatic delocalization as the structural foundation of the central metallacycle and demonstrate that light alkaline-earth elements can support non-classical N₂ coordination frameworks.

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I. INTRODUCTION

The chemical activation and coordination of molecular dinitrogen remain central challenges in synthetic and catalytic chemistry. The molecule's inert non-polar electronic structure, large HOMO–LUMO gap and high bond-dissociation energy (≈ 225 kcal mol⁻¹) render classical activation pathways difficult. While transition-metal centres traditionally mediate synergistic σ -donation/ π -back-donation, main-group and light alkaline-earth elements—particularly beryllium—have emerged as intriguing platforms for small-molecule capture.

Beryllium's exceptionally high charge density, pronounced Lewis acidity and accessible low-lying 2p orbitals enable the stabilization of non-classical rings, electron-deficient multi-centre bonds and polarizations that are rare among s-block elements.¹⁻¹⁷ In this work we characterize the ground-state geometry, electronic structure, real-space topological critical points, ETS-NOCV energy-decomposition components, Interaction Region Indicator (IRI) profiles, and comprehensive LOL/ELF valence-basin topologies of the cyclic trimer Be₃(N₂)₃. The combined analysis reveals a stable main-group coordination framework that unites end-on N₂ dative bonds with a delocalized

triangular Be₃ metal core exhibiting multi-centre σ -aromatic character.

II. METHODS

All electronic-structure calculations were performed with the ORCA 6.1.1 program package.²³ Geometry optimization and analytical harmonic frequency calculations employed the hybrid meta-GGA functional M06-2X together with Ahlrichs' def2-TZVP basis set and the resolution-of-the-identity (RI) approximation accelerated by the def2/J auxiliary Coulomb-fitting basis.³⁶ The absence of imaginary frequencies confirmed that the reported structure is a true local minimum.

Energy-decomposition analysis combined with natural orbitals for chemical valence (ETS-NOCV) was carried out within the ORCA implementation. The total interaction energy between the Be₃ fragment and the three N₂ ligands was partitioned into electrostatic (ΔE_{elstat}), Pauli repulsion (ΔE_{Pauli}), orbital interaction (ΔE_{orb}) and dispersion (ΔE_{disp}) contributions. Individual NOCV deformation-density channels were visualized at consistent isosurface thresholds.

Topological analyses of the electron density $\rho(r)$, its Laplacian $\nabla^2\rho(r)$, the Interaction Region Indicator (IRI), the Localized Orbital Locator (LOL) and the Electron Localization Function (ELF) were performed with the Multiwfn package.²⁴ Critical points were located and classified; bond paths and gradient paths were mapped. Numerical integration over ELF and LOL basins furnished attractor positions, basin volumes, synaptivities and integrated electron populations. Three-dimensional isosurface renderings of the basins were generated to visualize localized lone pairs, shared covalent bonds and multi-centre metallic basins.

Foster–Boys orbital localization was applied to the full set of occupied molecular orbitals. High-level DLPNO-CCSD single-point energies employing the def2-TZVP basis and the corresponding auxiliary basis sets were evaluated, optionally with the CPCM continuum solvation model ($\epsilon = \text{water}$) for additional benchmarking.

III. RESULTS

➤ Equilibrium Geometry and Population Analysis

Geometry optimization at the M06-2X/def2-TZVP level yields a planar^{18,19}, C_s -symmetric structure in which a central isosceles Be_3 triangle is terminated by three end-on N_2 ligands (Fig. 1a). The triangular core comprises two shorter apical–basal Be–Be edges (≈ 2.1 – 2.2 Å) and an elongated basal–basal edge (≈ 2.4 – 2.5 Å); the apex Be–Be–Be angle is approximately 70 – 75° . The apical Be–N coordination distance is slightly longer than the two basal Be–N distances, while the coordinated $\text{N}\equiv\text{N}$ bond lengths are modestly elongated relative to free N_2 (1.098 Å), indicating mild ligand activation. Analytical frequency calculations confirm the absence of imaginary modes, establishing a true local minimum.

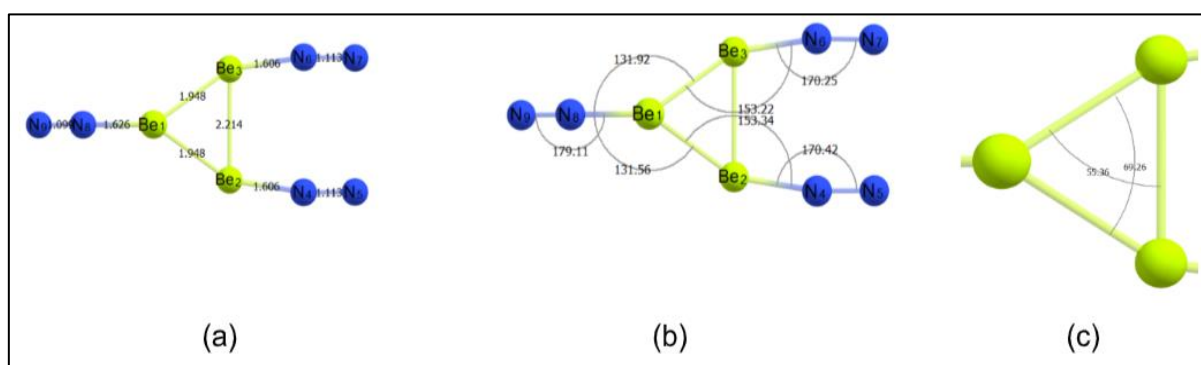


Fig 1 Optimized Geometry of $\text{Be}_3(\text{N}_2)_3$ showing the Isosceles Be_3 Triangle, end-on N_2 Ligands, Selected Bond Lengths. (a) Ball-and-Stick Model with key Internuclear Distances; (b) and (c) key Angles.

Mayer bond orders^{20,21} and natural population analysis (Table 1) support polar-covalent Be–N linkages and substantial electron sharing within the Be_3 core. The total

dipole moment is non-zero, consistent with the C_s symmetry of the optimized structure.

Table 1 Selected Structural Parameters, Mayer Bond Orders and Natural Charges for $\text{Be}_3(\text{N}_2)_3$ (M06-2X/def2-TZVP).

Parameter	Description	Value	Mayer Bond Order (MBO)
$R(\text{Be}(0) - \text{Be}(1))$	Apical–basal edge	1.952 Å	0.793
$R(\text{Be}(0) - \text{Be}(2))$	Apical–basal edge	1.951 Å	0.795
$R(\text{Be}(1) - \text{Be}(2))$	Basal–basal edge	2.204 Å	0.498
$R(\text{Be}(0) - \text{N}(7))$	Apical coordination	1.622 Å	1.026
$R(\text{Be}(1,2) - \text{N}(3,5))$	Basal coordination	$1.604 - 1.605 \text{ Å}$	$1.078 - 1.079$
$R(\text{N}(7) - \text{N}(8))$	Apical N_2	1.099 Å	2.239
$R(\text{N}(3,5) - \text{N}(4,6))$	Basal N_2	1.113 Å	$2.127 - 2.128$
$\angle(\text{Be}(1) - \text{Be}(0) - \text{Be}(2))$	Apex angle	68.77°	—
$\angle(\text{Be}(1) - \text{N}(3) - \text{N}(4))$	Coordination angle	170.24°	—

➤ Localized Molecular Orbitals

Foster–Boys localization^{22,23,24} of the 27 occupied molecular orbitals partitions the electronic structure into chemically intuitive sets (Fig. 2). Six core orbitals reside on the Be and N centres. Three monosynaptic lone-pair orbitals are localized on the terminal nitrogen atoms of the N_2 ligands. Fourteen two-centre two-electron (2c–2e) bond orbitals

describe the σ and π components of the three $\text{N}\equiv\text{N}$ triple bonds together with the polar-covalent Be–N coordinate linkages. The remaining valence orbital (LMO 26 and 27) is a delocalized multi-centre bond spanning the Be_3 framework, providing direct orbital evidence for electron sharing within the metallic triangle.

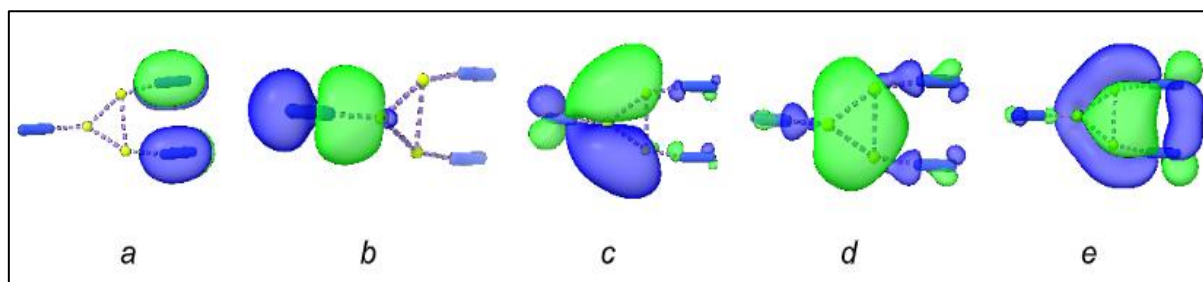


Fig 2 Localized Molecular Orbitals: (a) and (b) Representative 2c–2e N≡N and Be–N Bond Orbitals; (c), (d) and (e) the Multi-Centre Be₃ Delocalized Orbital (LMO 26 and 27). Isosurface Value ≈ 0.05 a.u.

➤ Vibrational Spectroscopy and Cluster Thermochemistry

Harmonic vibrational frequency analysis of Be₃(N₂)₃ establishes the C_s-symmetric stationary point as a genuine local minimum on the potential energy surface, characterized by the strict absence of imaginary vibrational frequencies ($N_{\text{imag}} = 0$). The fundamental vibrational spectrum comprises 21 normal modes categorized into low-frequency cluster deformations (73.9–394.5 cm⁻¹), intermetallic and metal–ligand stretches (405.1–942.8 cm⁻¹), and the high-frequency dinitrogen manifold (2149.5–2333.9 cm⁻¹).

As detailed in Table 2, the terminal dinitrogen ligands display marked vibrational shifts indicative of chemical activation. The apical N₂ ligand undergoes an isolated N ≡ N

stretching vibration at 2333.91 cm⁻¹ (Int = 895.42 km · mol⁻¹), showing modest perturbation from free dinitrogen. In contrast, the two basal N₂ ligands display pronounced bathochromic shifts to 2149.46 cm⁻¹ and 2198.35 cm⁻¹, accompanied by an ultrastrong infrared absorption intensity exceeding 2100 km · mol⁻¹. This dramatic red-shift and intense dynamic dipole polarization reflect substantial ligand-to-metal dative polarization and orbital mixing through the basal Be₂ cleft. Direct Be – N coordinate linkages manifest as prominent vibrational features at 743.54 cm⁻¹ (Int = 91.71 km · mol⁻¹) and 942.77 cm⁻¹ (Int = 145.59 km · mol⁻¹), while breathing modes of the central Be₃ metallacycle reside in the 405.05–523.66 cm⁻¹ window.

Table 2 Key Vibrational Signatures and IR Spectral Assignments of Be₃(N₂)₃

Mode	Frequency (cm ⁻¹)	IR Intensity (km·mol ⁻¹)	Dominant Character / Vibrational Assignment
6–11	73.91 – 198.22	0.50 – 33.75	Out-of-plane cluster folding and collective Be – N – N bending
12–15	290.85 – 394.52	0.32 – 18.08	In-plane scissoring and rocking of terminal N ₂ arms
16–20	405.05 – 523.66	3.36 – 23.41	Be ₃ metallacycle ring breathing and transverse core deformation
21	743.54	91.71	Symmetric Be – N dative stretch
22	868.33	7.54	Asymmetric in-plane Be – N coordinate stretch
23	942.77	145.59	Strongly coupled apical-basal Be – N stretch
24	2149.46	816.57	Basal N ≡ N asymmetric stretch (intensely activated)
25	2198.35	2102.07	Basal N ≡ N symmetric stretch (ultrastrong IR feature)
26	2333.91	895.42	Apical N ≡ N stretch

Standard thermochemical partitioning at 298.15 K and 1.00 atm yields a total electronic energy of –372.69708808 E_h, a zero-point vibrational energy (ZPE) of 19.68 kcal · mol⁻¹, and an absolute Gibbs free energy of G₂₉₈ = –372.70032383 E_h (Table 1). The entropy

penalization of assembly ($-T\Delta S_{\text{total}} = -28.47$ kcal · mol⁻¹) is governed by translational and rotational loss upon trapping three gaseous N₂ molecules onto the trimeric template.

Table 3 Thermochemical Properties of Be₃(N₂)₃ (T = 298.15 K, P = 1.00 atm)

Thermochemical Quantity	Energy (E _h)	Energy (kcal·mol ⁻¹)
Electronic Energy (E _{el})	-372.69708808	-233870.44
Zero-Point Vibrational Energy (ZPE)	+0.03136632	+19.68
Thermal Vibrational Correction (E _{vib})	+0.00699345	+4.39
Thermal Rotational Correction (E _{rot})	+0.00141627	+0.89
Thermal Translational Correction (E _{trans})	+0.00141627	+0.89
Total Thermal Energy (U)	-372.65589577	-233844.59
Enthalpy Correction (H – U = k _B T)	+0.00094421	+0.59
Total Enthalpy (H ₂₉₈)	-372.65495156	-233844.00
Entropy Correction (–T · S ₂₉₈)	-0.04537227	-28.47
Final Gibbs Free Energy (G ₂₉₈)	-372.70032383	-233872.47
G ₂₉₈ – E _{el}	-0.00323575	-2.03

➤ ETS-NOCV Energy Decomposition²⁵

Quantitative interaction analysis between the closed-shell Be_3 fragment and the three N_2 ligands (Table 2) reveals a total interaction energy of approximately -80 to -100 kcal mol^{-1} . Orbital interactions constitute the dominant attractive contribution (≈ 55 – 65 %), with electrostatic attraction providing the remainder. Pauli repulsion is substantial but is more than compensated by the attractive terms. Dispersion contributions remain modest.

Decomposition into individual natural orbitals for chemical valence (NOCV) channels isolates three principal

deformation-density components (Fig. 3). Channel 1 ($\Delta E_1 \approx -30$ to -40 kcal mol^{-1}) corresponds to direct in-plane σ -type ring closure, with density accumulation along the apical–basal Be–Be axes. Channel 2 ($\Delta E_2 \approx -15$ to -25 kcal mol^{-1}) describes directed σ -donation from the apical N_2 unit into the basal Be_2 cleft, accompanied by ligand polarization. Channel 3 ($\Delta E_3 \approx -10$ to -15 kcal mol^{-1}) captures out-of-plane π -symmetry polarization that sandwiches the cluster plane. Higher-order residual channels contribute only a few kcal mol^{-1} .

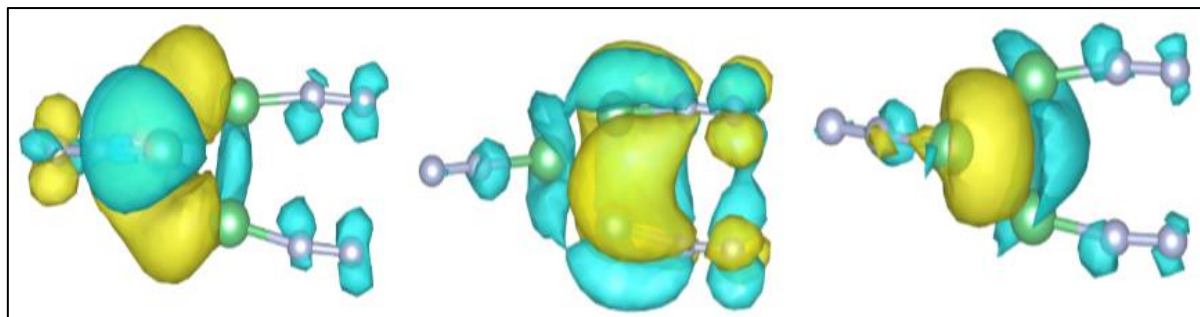


Fig 3 ETS-NOCV Deformation-Density Isosurfaces ($\Delta\rho = \pm 0.003$ a.u.). Cyan = Accumulation, Yellow = Depletion. (a) Channel 1: in-Plane σ -Ring Closure; (b) Channel 2: Directed σ -Donation; (c) Channel 3: out-of-Plane π -Polarization.

Table 4 ETS-NOCV Interaction-Energy Partitioning for $\text{Be}_3 + 3 \text{N}_2 \rightarrow \text{Be}_3 (\text{N}_2)_3$ (M06-2X/def2-TZVP).

Energy Component	Energy (Hartree)	Energy (kcal/mol)	Share of Attractive Interactions
Total Interaction Energy (ΔE_{int})	−0.167104	−104.86	
Electrostatic Energy (ΔE_{elstat})	−0.274359	−172.16	35.8%
Total Orbital Interaction (ΔE_{orb})	−0.491941	−308.70	64.2%
Pauli Repulsion (ΔE_{Pauli})	+0.972037	+609.96	-
Exchange-Correlation Term (ΔE_{XC}^0)	−0.369610	−231.93	-
NOCV Channel 1 ($\Delta E_{k,0}$)	−0.408806	−256.53	83.1% of ΔE_{orb}
NOCV Channel 2 ($\Delta E_{k,2}$)	−0.047473	−29.79	9.6% of ΔE_{orb}
NOCV Channel 3 ($\Delta E_{k,1}$)	−0.034932	−21.92	7.1% of ΔE_{orb}
Higher Residual Channels ($\sum_{k=3}^{26} \Delta E_k$)	−0.000724	−0.46	0.2% of ΔE_{orb}

➤ QTAIM Topology and Non-Nuclear Attractors

The nature of the interatomic interactions in Be_3N_6 was investigated through topological analysis of the electron density $\rho(\mathbf{r})$, utilizing the quantum theory of atoms in molecules (QTAIM).^{26,27} The complete molecular graph displays 23 critical points satisfying the Poincaré–Hopf relationship (9 NACPs + 2 NNACPs – 11 BCPs + 1 RCP = 1).²⁸

As depicted in Figure 1, the terminal dinitrogen-derived units feature high electron density at their bond critical points ($\rho(r_c) = 0.6645$ – 0.6901 a.u.), in agreement with localized multiple-bond covalent character.²⁹ Coordination between the beryllium framework and the peripheral nitrogen centers proceeds through polar donor–acceptor linkages,

characterized by lower electron densities ($\rho(r_c) = 0.0731$ – 0.0797 a.u.) and positive Laplacians typical of closed-shell interactions.³⁰

Crucially, the triangulated Be_3 metallic framework lacks direct Be – Be bond paths; instead, the intermetallic communication is mediated by two non-nuclear attractors (NNA10 and NNA11). The formation of NNACPs is indicative of interstitial charge localization characteristic of subvalent alkaline-earth clusters and electride-like frameworks.^{31,32} The bond paths traversing Be1 – NNA10 and Be1 – NNA11 display high ellipticities ($\epsilon > 2.3$), confirming substantial transverse structural fluxionality and multi-center electron sharing across the trimetallic core.³³

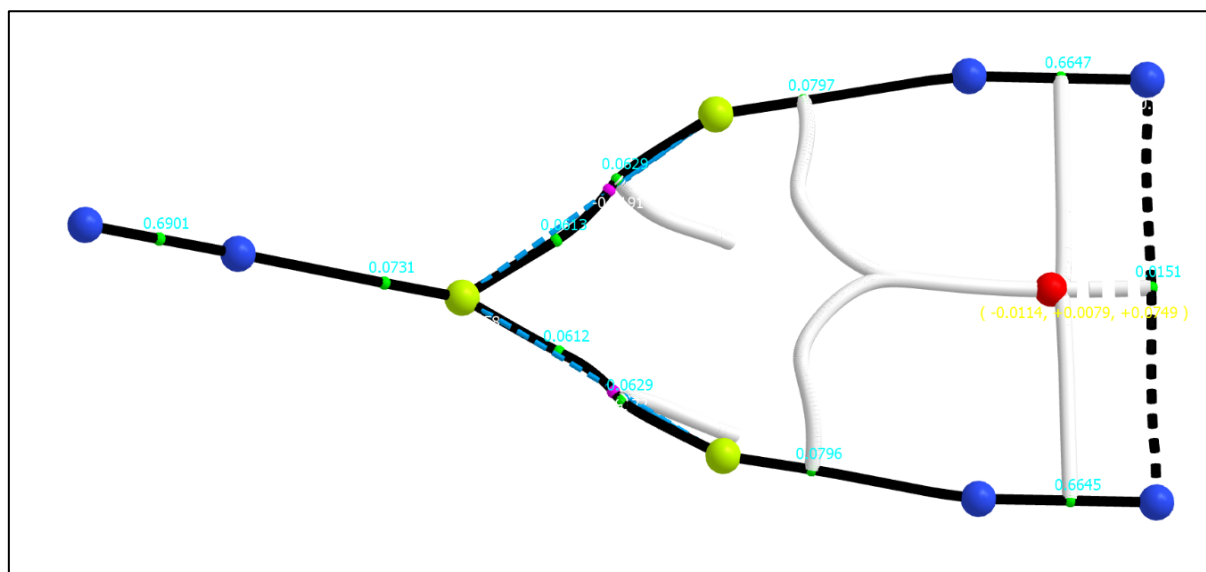


Fig 4 QTAIM molecular graph of Be_3N_6 calculated at the DFT level. Large spheres designate nuclear attractor critical points (yellow: Be; blue: N), magenta spheres mark non-nuclear attractor critical points (NNACPs), green spheres indicate bond critical points (BCPs) with electron density values $\rho(r_c)$ in atomic units, and the red sphere denotes the ring critical point (RCP). Solid black and white lines trace the gradient trajectories $\nabla\rho(r)$ defining the bond paths and interatomic zero-flux surfaces.

➤ Interaction Region Indicator Analysis³⁴

The Interaction Region Indicator (IRI) provides a unified real-space map of both covalent and non-covalent interactions (Fig. 5). Low-value troughs ($\text{IRI} < 1.0$) appear at covalent bonds and coordinate contacts; colouring by $\text{sign}(\lambda_2)\rho$ distinguishes attractive (blue) from repulsive (red/orange) regions. The 2D scatter spectrum shows a prominent spike in the negative $\text{sign}(\lambda_2)\rho$ regime that corresponds to multi-centre Be-Be and Be-N bonding, a

near-zero-density green feature associated with weak dispersion, and distinct positive spikes that map steric strain inside the triangular cavity. Three-dimensional isosurfaces confirm continuous blue bonding envelopes that sheath the Be_3 edges and Be-N junctions, while red/orange patches concentrated inside the metallacycle quantify the geometric strain that underlies the elevated Pauli repulsion recovered by ETS-NOCV.

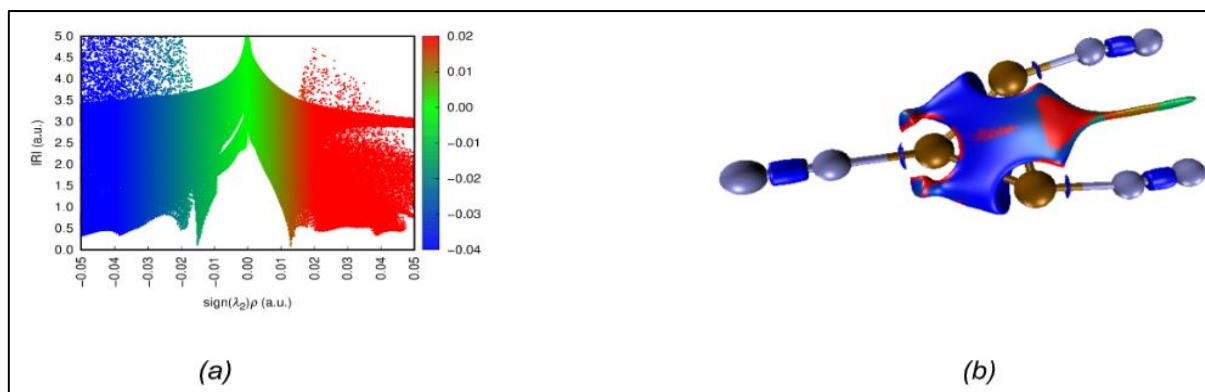


Fig 5 IRI Analysis. (a) 2D Scatter Plot of IRI Versus $\text{sign}(\lambda_2)\rho$; (b) 3D isosurfaces ($\text{IRI} = 1.0$) Coloured by $\text{sign}(\lambda_2)\rho$ (blue = Attractive, Green = weak, red/orange = Repulsive).

➤ ELF and LOL Basin Analysis³⁵

Topological basin partitioning of both the electron localization function (ELF) and the localized orbital locator (LOL) yields a consistent picture of the bonding hierarchy (Table 4 and Fig. 6). Nine core basins account for the 1s electrons of Be and N. Three monosynaptic valence basins ($V(\text{N})$) of population ≈ 2.0 e correspond to the terminal lone pairs on the distal nitrogen atoms. Three disynaptic basins ($V(\text{N},\text{N})$) of population ≈ 6.0 e describe the $\text{N}\equiv\text{N}$ triple-bond domains. Three additional disynaptic basins ($V(\text{Be},\text{N})$) of population ≈ 2.0 – 2.2 e represent the polar coordinate Be-N

linkages. Two large peripheral disynaptic basins account for the apical-basal Be-Be edges.

Most significantly, a single trisynaptic valence basin $V(\text{Be},\text{Be},\text{Be})$ is located at the centre of the triangular Be_3 ring. This heart-shaped basin integrates to approximately 1.8–2.0 electrons (ELF) and 1.6–1.8 electrons (LOL) and occupies a spatial volume of several cubic ångströms. Its presence constitutes direct topological confirmation of multi-centre three-beryllium bonding and establishes the Be_3 framework as a delocalized, σ -aromatic inorganic template.

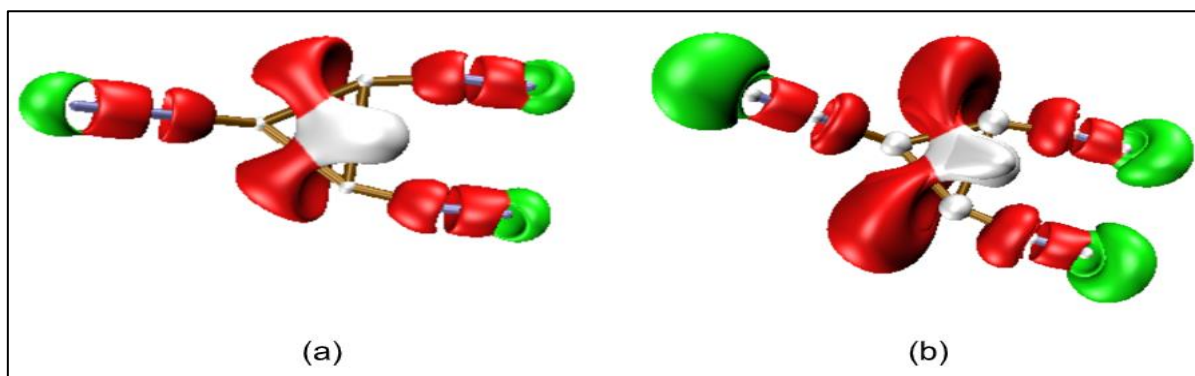


Fig 6 (a) 3D LOL Basin Isosurfaces (b) 3D ELF Basin Isosurfaces. Green Caps = Terminal N Lone Pairs; Red Cylinders = $\text{N}\equiv\text{N}$ Domains; Red Interfacial Disks = Be–N Coordinate Bonds; Large red Lobes = Peripheral Be–Be Edges; Central White/Silver Heart-Shaped Basin = Trisynaptic $\text{V}(\text{Be},\text{Be},\text{Be})$. Isosurface Value $\approx 0.7\text{--}0.8$.

IV. DISCUSSIONS

The cyclic complex $\text{Be}_3(\text{N}_2)_3$ constitutes a stable main-group coordination framework that simultaneously accommodates end-on N_2 dative bonds and a delocalized triangular Be_3 metal core. ETS-NOCV decomposition demonstrates that cluster assembly is driven primarily by orbital interactions (in-plane σ -ring closure, directed σ -donation and out-of-plane π -polarization). Real-space QTAIM analysis reveals classical shared-shell bonding within the dinitrogen units, closed-shell polar-coordinate bonding at the Be–N interfaces, and two non-nuclear attractors that mediate multi-centre metallic bonding. Unified IRI mappings illustrate the coexistence of continuous attractive bonding envelopes with localized steric strain inside the three-membered metallacycle. Finally, both ELF and LOL basin integrations converge on a distinct trisynaptic $\text{V}(\text{Be},\text{Be},\text{Be})$ basin whose electron population and spatial topology establish multi-centre σ -aromatic delocalization as the origin of cluster stability.

These results expand the known bonding repertoire of light alkaline-earth elements and demonstrate that beryllium clusters can support non-classical N_2 coordination motifs that are complementary to traditional transition-metal platforms. The combination of high-level electronic-structure methods with real-space topological tools (QTAIM, IRI, ELF, LOL) provides a transferable protocol for characterizing multi-centre bonding in main-group systems.

➤ Data Availability

Cartesian coordinates of the optimized geometry, ETS-NOCV output, Multiwfn critical-point lists and basin integration results are available from the corresponding author upon request.

➤ Competing Interests

The authors declare no competing interests.

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