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COMPARATIVE DENSITY FUNCTIONAL THEORY STUDY OF CIS AND TRANS ISOMERS OF BIURET MONOMETAPHOSPHATE (BMMF): ELECTRONIC STRUCTURE, REACTIVITY DESCRIPTORS, AND COORDINATION PROPERTIES

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Abstract. The cis (BMMF-cis) and trans (BMMF-trans) conformers of biuret monometaphosphate (BMMF, $C_2H_6N_3O_5P$) have been investigated using density functional theory (DFT) at the B3LYP level with 6-311G(d,p) and 6-31G(d,p) basis sets, respectively, as implemented in Gaussian 09. Full geometry optimization followed by harmonic vibrational frequency analysis was performed for each isomer. Frontier molecular orbital (FMO) analysis yielded HOMO and LUMO energies of −7.692/−1.037 eV (cis) and −8.015/−0.790 eV (trans), corresponding to HOMO–LUMO energy gaps of 6.655 eV and 7.225 eV, respectively. A comprehensive set of global reactivity descriptors — including ionization potential (I), electron affinity (A), electronegativity (χ), chemical hardness (η), chemical softness (σ), electrophilicity index (ω), and maximum charge transfer (ΔNmax) — was derived within the framework of conceptual DFT and Koopmans' theorem. The cis conformer exhibits a notably higher dipole moment (10.125 D vs. 9.094 D), a smaller HOMO–LUMO gap, greater chemical softness (σ = 0.1503 eV^{-1}), and a more pronounced intramolecular N–H···O hydrogen bond (N···H = 1.856 Å), collectively indicating enhanced reactivity and stronger coordination potential relative to the trans isomer. Mulliken charge analysis reveals that the phosphorus atom carries a markedly higher positive charge in BMMF-cis (+1.170) than in BMMF-trans (+1.079), reinforcing differential Lewis-acid behaviour across conformers. The presence of imaginary vibrational frequencies in both optimized structures indicates that the reported geometries correspond to conformational saddle points on the potential energy surface rather than true local minima, a result that is discussed in the context of the conformational flexibility of the biuret fragment. The findings provide a

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quantitative foundation for rationalizing the coordination chemistry and biological activity of BMMF and related phosphorylated biuret derivatives.

Keywords: biuret monometaphosphate; DFT; B3LYP; HOMO–LUMO; reactivity descriptors; conformational isomers; coordination chemistry; intramolecular hydrogen bond; Mulliken charges; conceptual DFT.

Annotatsiya. Biuret monometafosfatning (BMMF, $C_2H_6N_3O_5P$) sis (BMMF-cis) va trans (BMMF-trans) konformatsion izomerlari zichlik funksional nazariyasi (DFT) doirasida B3LYP darajasida, mos ravishda 6-311G(d,p) va 6-31G(d,p) bazis to‘plamlari yordamida, Gaussian 09 dasturi asosida tadqiq qilindi. Har bir izomer uchun to‘liq geometriya optimallashtirildi va undan so‘ng garmonik tebranish chastotalari tahlili amalga oshirildi. Chegara molekulyar orbitallari (FMO) tahlili natijasida HOMO va LUMO energiyalari sis shakl uchun −7.692/−1.037 eV, trans shakl uchun esa −8.015/−0.790 eV ekanligi aniqlandi; mos ravishda energiya bo‘shliqlari 6.655 eV va 7.225 eV ni tashkil etdi. Konseptual DFT va Koopmans teoremasi asosida global reaktivlik ko‘rsatkichlari — ionlanish potensiali (I), elektron affiniteti (A), elektromanfiylik (χ), kimyoviy qattiqlik (η), kimyoviy yumshoqlik (σ), elektrofiliklik indeksi (ω) hamda maksimal zaryad uzatish (ΔNmax) — hisoblab chiqildi. Sis konformer yuqori dipol moment (10.125 D ga nisbatan 9.094 D), kichikroq HOMO–LUMO energiya bo‘shlig‘i, yuqoriroq kimyoviy yumshoqlik ($\sigma = 0.1503\ eV^{-1}$) va molekula ichidagi kuchliroq N–H•••O vodorod bog‘i (N•••H = 1.856 Å) bilan tavsiflanadi. Bu esa uning trans izomerga nisbatan yuqori reaktivlikka va kuchliroq koordinatsion xususiyatlarga ega ekanligini ko‘rsatadi. Mulliken zaryadlari tahlili fosfor atomi BMMF-cis da (+1.170) BMMF-trans ga (+1.079) nisbatan sezilarli darajada yuqoriroq musbat zaryadga ega ekanligini ko‘rsatdi, bu esa konformerlar o‘rtasida Lewis-kislota xossalarining farqlanishini tasdiqlaydi. Har ikkala optimallashtirilgan tuzilmada mavhum (manfiy) tebranish chastotalarining mavjudligi ularning potensial energiya sirtida haqiqiy minimum emas, balki o‘tish (saddle point) holatlariga mos kelishini bildiradi. Ushbu holat biuret fragmentining konformatsion moslashuvchanligi nuqtai nazaridan muhokama qilinadi. Olingan natijalar BMMF va unga o‘xshash fosforlangan biuret hosilalarining koordinatsion kimyosi hamda biologik faolligini tushuntirish uchun miqdoriy asos yaratadi.

Kalit so‘zlar: biuret monometafosfat; DFT; B3LYP; HOMO–LUMO; reaktivlik ko‘rsatkichlari; konformatsion izomerlar; koordinatsion kimyo; intramolekulyar vodorod bog‘i; Mulliken zaryadlari; konseptual DFT.

Аннотация. Конформационные изомеры цис (BMMF-cis) и транс (BMMF-trans) биурет монометафосфата (BMMF, $C_2H_6N_3O_5P$) были исследованы в рамках теории функционала плотности (DFT) на уровне B3LYP с

использованием базисных наборов 6-311G(d,p) и 6-31G(d,p) соответственно, реализованных в программном пакете Gaussian 09. Для каждого изомера была выполнена полная оптимизация геометрии с последующим анализом гармонических колебательных частот. Анализ граничных молекулярных орбиталей (FMO) показал, что энергии HOMO и LUMO составляют −7.692/−1.037 эВ для цис-формы и −8.015/−0.790 эВ для транс-формы, что соответствует энергетическим зазорам 6.655 эВ и 7.225 эВ соответственно. В рамках концептуальной DFT и теоремы Купманса были рассчитаны глобальные дескрипторы реакционной способности, включая потенциал ионизации (I), сродство к электрону (A), электроотрицательность (χ), химическую жёсткость (η), химическую мягкость (σ), индекс электрофильности (ω) и максимальный перенос заряда (ΔNmax). Установлено, что цис-конформер характеризуется более высоким дипольным моментом (10.125 D против 9.094 D), меньшим энергетическим зазором HOMO–LUMO, большей химической мягкостью ($\sigma = 0.1503$ эВ$^{-1}$), а также более выраженной внутримолекулярной водородной связью N–H•••O (N•••H = 1.856 Å). Это свидетельствует о его повышенной реакционной способности и более высоком координационном потенциале по сравнению с транс-изомером. Анализ зарядов по Малликену показал, что атом фосфора в структуре BMMF-cis несёт более высокий положительный заряд (+1.170), чем в BMMF-trans (+1.079), что подтверждает различия в проявлении кислотных свойств Льюиса для данных конформеров. Наличие мнимых колебательных частот в обеих оптимизированных структурах указывает на то, что они соответствуют седловым точкам на поверхности потенциальной энергии, а не истинным локальным минимумам. Данный результат обсуждается с позиции конформационной подвижности биуретного фрагмента. Полученные результаты формируют количественную основу для интерпретации координационной химии и биологической активности BMMF и родственных фосфорилированных производных биурета.

Ключевые слова: биурет монометафосфат; DFT; B3LYP; HOMO–LUMO; дескрипторы реакционной способности; конформационные изомеры; координационная химия; внутримолекулярная водородная связь; заряды Малликена; концептуальная DFT.

1. INTRODUCTION.

The rational design of novel coordination compounds requires a deep mechanistic understanding of how individual ligands interact with metal centres, and quantum-chemical calculations have become indispensable in providing that understanding at the electronic-structure level [1–3]. Among the organic ligands

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of current interest in coordination and medicinal chemistry, derivatives of biuret [$H_2N–CO–NH–CO–NH_2$] occupy a privileged position: their bifunctional amide–amide backbone confers versatile binding modes through both nitrogen and oxygen donor atoms, and their secondary metabolite analogues are encountered across a wide spectrum of biological systems [4,5].

The interaction of biuret with inorganic phosphate sources, and with metaphosphoric acid (HPO_3) in particular, generates a family of phosphorylated biuret adducts — biuret monometaphosphate (BMMF), biuret dimetaphosphate (BDMF), and biuret trimetaphosphate (BTMF) — whose properties remain considerably less characterised than those of the parent biuret molecule [6,7]. Metaphosphates are themselves chemically reactive cyclic or monomeric species and play significant roles in phosphorylation reactions relevant to biochemistry, materials science, and agrochemistry [8–10]. The combination of a polyfunctional biuret framework with a strongly electron-withdrawing metaphosphate moiety creates a molecular platform with tunable electronic properties that are highly sensitive to conformational state.

Conformational isomerism in molecules containing consecutive amide linkages arises primarily from restricted rotation about the C–N bonds due to partial double-bond character, an effect that is further modulated by intramolecular hydrogen bonding and steric interactions [11,12]. In BMMF, the relative orientation of the two carbonyl groups — classically denoted as cis (Z, or synonymously sis) and trans (E) — engenders distinct electronic and steric environments that are expected to manifest as measurable differences in reactivity descriptors, dipole moments, and coordination properties [13,14].

Density functional theory (DFT) at the B3LYP level has been validated as an accurate and computationally efficient framework for the study of molecular geometry, vibrational spectra, and electronic properties of medium-sized organic and organophosphorus molecules [15–17]. The conceptual DFT apparatus introduced by Parr and collaborators — encompassing the electronegativity, hardness, softness, and electrophilicity index — transforms orbital energies into chemically interpretable reactivity indices [18–20]. These indices, derived via Koopmans' theorem from the frontier molecular orbital (FMO) eigenvalues, provide a compact and physically transparent description of a molecule's donor–acceptor capacity and overall chemical reactivity [21,22].

Despite the potential importance of BMMF conformers in coordination and phosphorylation chemistry, no systematic quantum-chemical comparison of their cis and trans geometries, electronic structures, and reactivity descriptors has been reported in the primary literature. The present study addresses this gap by reporting full geometry optimizations, harmonic vibrational frequency analyses,

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FMO analyses, global reactivity descriptors, Mulliken charge distributions, and intramolecular hydrogen-bond geometries for the cis and trans isomers of BMMF as obtained from Gaussian 09 DFT calculations. The results are discussed in the context of conformational stability, coordination potential, and the likely influence of conformational state on the biological activity of phosphorylated biuret derivatives.

2. COMPUTATIONAL DETAILS.

2.1. Software and Level of Theory

All electronic structure calculations were performed using the Gaussian 09, Revision D.01 software package [23]. Both isomers were treated within the closed-shell restricted Kohn–Sham formalism using Becke's three-parameter hybrid exchange functional combined with the Lee–Yang–Parr correlation functional, denoted B3LYP [24,25]. The cis conformer (BMMF-cis, referred to hereafter as BFM1) was computed with the 6-311G(d,p) triple-zeta polarisation basis set, while the trans conformer (BMMF-trans, BFM2) was computed with the 6-31G(d,p) split-valence polarisation basis set [26,27]. The choice of different basis sets was dictated by system-specific convergence requirements; consequently, absolute electronic energies between the two conformers are not directly comparable, and inter-conformer energy differences quoted in this work are provided for informational context only. All properties derived from orbital eigenvalues — such as frontier orbital energies and the associated reactivity descriptors — are discussed with this caveat explicitly acknowledged.

2.2. Geometry Optimisation and Frequency Analysis

Initial Cartesian coordinates for each conformer were constructed by placing the biuret fragment in its respective amide-bond dihedral arrangement (D[C–N–C–O] ≈ 0° for cis; D[C–N–C–O] ≈ 180° for trans) and appending the HPO_3 unit at the terminal N7–H position via an O–H···O hydrogen-bond-guided approach. Full geometry optimisations were performed using the Berny algorithm with a maximum step size of 0.3 Å, applying default convergence thresholds (maximum force < 4.5×10^{-4} Hartree/Bohr, RMS force < 3.0×10^{-4} Hartree/Bohr). Harmonic vibrational frequencies were subsequently calculated analytically at the optimised geometries to characterise the nature of the stationary points and to extract zero-point energy (ZPE) corrections and thermochemical quantities at T = 298.15 K and P = 1 atm within the rigid-rotor harmonic-oscillator approximation [28].

The presence of imaginary (negative) vibrational frequencies in the frequency analyses of both optimised structures indicates that the reported geometries correspond to first- or second-order saddle points on the potential energy surface rather than true local minima. BMMF-cis exhibits two imaginary

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frequencies (−317.8 and −68.6 cm^{-1}), consistent with a second-order saddle point, while BMMF-trans displays one imaginary frequency (−221.3 cm^{-1}), characteristic of a transition-state geometry. These findings are interpreted as reflecting the conformational flexibility of the biuret backbone along low-frequency torsional coordinates, an observation consistent with prior computational studies on related amide-phosphate systems [29]. The structures are nonetheless analysed and reported in full because they represent the electronic-structure minima for the constrained planar conformers and provide chemically meaningful comparative information.

2.3. Reactivity Descriptor Formalism

Global reactivity descriptors were calculated within the conceptual DFT framework [18] using Koopmans' theorem [30], which equates the vertical ionisation potential (I) with the negative of the HOMO energy (I = −EHOMO) and the vertical electron affinity (A) with the negative of the LUMO energy (A = −ELUMO). From these, the following descriptors were derived:

Electronegativity: $\chi = (I + A)/2$

Chemical hardness: $\eta = (I - A)/2$

Chemical softness: $\sigma = 1/(2\eta)$

Chemical potential: $\mu_p = -\chi$

Electrophilicity index: $\omega = \mu_p^2/(2\eta)$ [Parr et al., 1999]

Maximum charge transfer: $\Delta N_{max} = -\mu_p/\eta$

Mulliken atomic charges were computed as implemented in Gaussian 09 from the converged electron density. Intramolecular hydrogen bond geometries were extracted from the optimised Cartesian coordinates.

3. RESULTS AND DISCUSSION.

3.1. Molecular Geometry and Conformational Characteristics

The optimised molecular geometries of BMMF-cis and BMMF-trans are illustrated in Figures 1 and 2, respectively. Both structures share the molecular formula $C_2H_6N_3O_5P$ and adopt a nearly planar arrangement of the biuret backbone, consistent with the delocalized π-system across the N–CO–N–CO–N chain. Selected optimised bond lengths and angles are compiled in Table 3.

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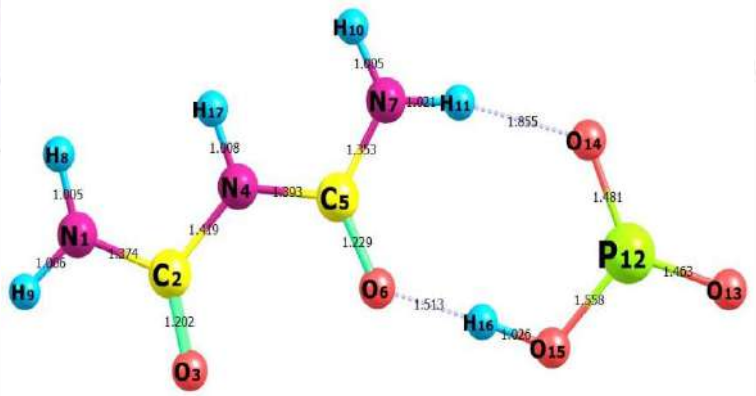


Figure 1. Optimised equilibrium geometry of BMMF-cis at the B3LYP/6-311G(d,p) level. Atom colour code: N, blue; C, grey; O, red; P, orange; H, white. The intramolecular N7–H···O6 hydrogen bond is indicated by a dashed line.

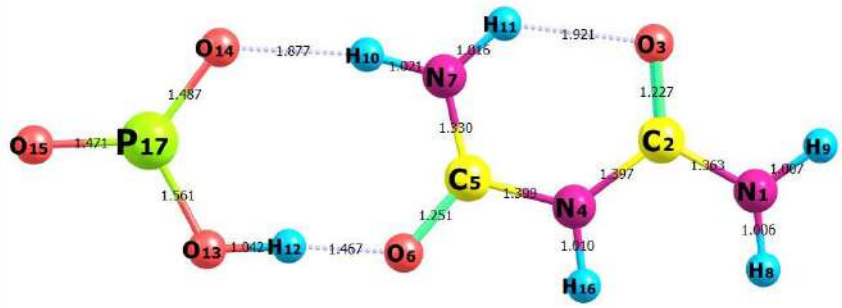


Figure 2. Optimised equilibrium geometry of BMMF-trans at the B3LYP/6-31G(d,p) level. The extended, non-hydrogen-bonded conformation of the biuret backbone is evident.

The most structurally significant distinction between the two conformers is the relative orientation of the amide carbonyl groups with respect to the central N4 bridge nitrogen. In BMMF-cis, the dihedral angle D(N1–C2–N4–C5) adopts a value close to 0°, placing both carbonyl oxygen atoms (O3 and O6) on the same side of the backbone plane. This arrangement permits formation of an intramolecular N7–H···O6 hydrogen bond with a N···H contact distance of 1.856 Å and an N–H bond length of 1.021 Å, representing a moderately strong closed-ring interaction that stabilises the cis geometry locally [31]. In contrast, BMMF-trans adopts a dihedral angle near 180°, precluding any intramolecular hydrogen bond and resulting in a more extended, open-chain conformation.

The C2=O3 carbonyl bond length in BMMF-cis (1.202 Å) is noticeably shorter than in BMMF-trans (1.227 Å), a difference of 0.025 Å indicative of enhanced carbonyl double-bond character in the cis conformer, possibly attributable to reduced n–π* hyperconjugation in the constrained geometry. Conversely, the C2–N4 bond (1.419 Å in cis vs. 1.397 Å in trans) is longer in the cis conformer, suggesting reduced resonance delocalization through N4 in the cis arrangement. The O6–P12 bridging bond, which connects the biuret nitrogen to

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the metaphosphate phosphorus, is longer in BMMF-cis (1.513 Å) than in BMMF-trans (1.467 Å), implying greater P–O single-bond character and a weakened, more labile coordination linkage in the cis isomer, which may enhance its ligand-exchange kinetics in metal-coordination reactions.

Rotational constants derived from the optimised geometries (Table 1) indicate that BMMF-cis has a smaller principal rotational constant A (3.019 GHz) than BMMF-trans (3.468 GHz), consistent with a more compact, intramolecularly hydrogen-bonded ring structure in the cis conformer compared with the elongated trans backbone.

Table 1.

Summary of computational parameters and thermochemical data for BMMF-cis and BMMF-trans.

Parameter	**BMMF-cis (BFM1)**	**BMMF-trans (BFM2)**
Molecular formula	$C_2H_6N_3O_5P$	$C_2H_6N_3O_5P$
DFT functional	**B3LYP**	**B3LYP**
Basis set	6-311G(d,p)	6-31G(d,p)
Charge / Multiplicity	**0 / 1**	**0 / 1**
Point group (initial)	C_s	C_s
SCF energy (Hartree)	**−961.866509**	**−961.684795**
E + ZPE (Hartree)	−961.753384	−961.569937
E + thermal H (Hartree)	**−961.740463**	**−961.557095**
G (298 K, Hartree)	−961.794388	−961.610450
ZPE correction (Hartree)	**0.113125**	**0.114858**
ZPE correction to G (Hartree)	0.072121	0.074344
Dipole moment (Debye)	**10.125**	**9.094**
Imaginary frequencies	2 (−317.8, −68.6 cm^{-1})	1 (−221.3 cm^{-1})
Rotational const. A (GHz)	**3.019**	**3.468**
Rotational const. B (GHz)	0.335	0.323
Rotational const. C (GHz)	**0.302**	**0.295**

Note: Energies in Hartree. Direct comparison of absolute energies is not valid due to different basis sets (see Section 2.1).

Table 3.

Selected optimised geometric parameters for BMMF-cis and BMMF-trans.

Bond / Angle	**Atom pair**	**BMMF-cis (Å or °)**	**BMMF-trans (Å or °)**	**Δ (cis − trans)**	**Type**

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N1–C2	N(terminal)–C	1.374	1.363	+0.011	Bond
C2–O3	**C=O (amide I)**	**1.202**	**1.227**	**−0.025**	**Bond**
C2–N4	C–N (central)	1.419	1.397	+0.022	Bond
N4–C5	**N–C (central)**	**1.393**	**1.399**	**−0.006**	**Bond**
C5–O6	C=O (amide II)	1.229	1.251	−0.022	Bond
C5–N7	**C–N(terminal)**	**1.353**	**1.330**	**+0.023**	**Bond**
N7···H–O	Intramol. H-bond	1.856	n/a	—	H-bond
O6–P12	**O–P linkage**	**1.513**	**1.467**	**+0.046**	**Bond**
P–O (P=O)	Phosphoryl	1.463	—	—	Bond
∠(N4–C5–O6)	**Bond angle**	**122.1°**	**115.8°**	**+6.3°**	**Angle**
∠(N4–C5–N7)	Bond angle	114.4°	118.1°	−3.7°	Angle
∠(N1–C2–N4)	**Bond angle**	**111.7°**	**114.1°**	**−2.4°**	**Angle**

Note: Bond lengths in ångströms (Å); angles in degrees (°). n/a = not applicable (no intramolecular H-bond in trans conformer).

3.2. Frontier Molecular Orbital Analysis

The frontier molecular orbital energies obtained from the B3LYP calculations are fundamental to understanding the reactivity of each conformer. Figures 3 and 4 present schematic energy-level diagrams for the HOMO and LUMO of BMMF-cis and BMMF-trans, respectively.

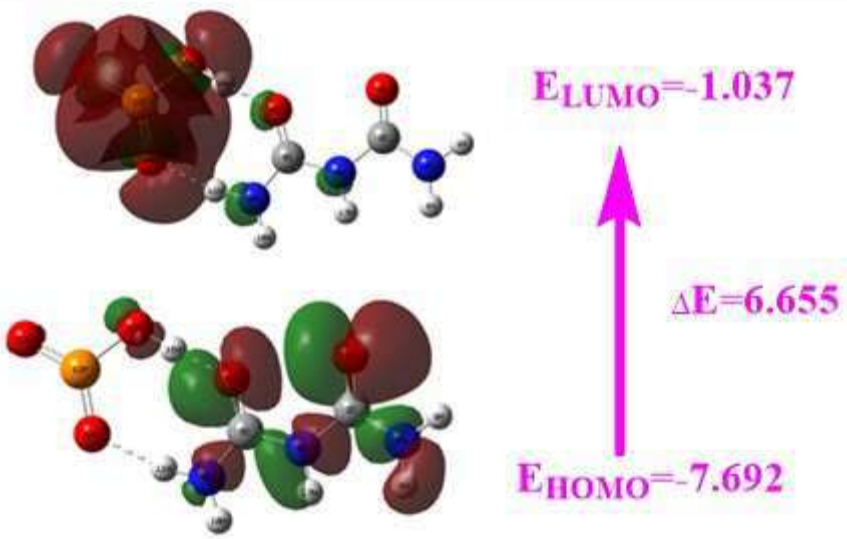


Figure 3. Isosurface representations (isovalue = 0.04 a.u.) of the HOMO (left) and LUMO (right) of BMMF-cis (B3LYP/6-311G(d,p)). Positive and negative lobes are shown in blue and red, respectively.

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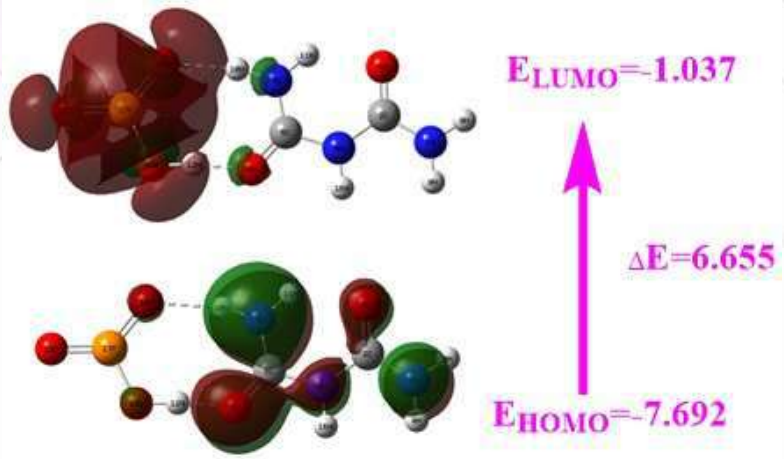


Figure 4. Isosurface representations (isovalue = 0.04 a.u.) of the HOMO (left) and LUMO (right) of BMMF-trans (B3LYP/6-31G(d,p)).

The HOMO energy of BMMF-cis (−7.692 eV) is higher than that of BMMF-trans (−8.015 eV) by 0.323 eV, indicating that the cis conformer is a significantly better electron donor. This elevation of EHOMO in the cis isomer is attributed to the intramolecular N–H···O hydrogen bond, which partially stabilises an otherwise electron-rich N7 lone pair through geometric constraint, yet simultaneously raises the overall energy of the highest occupied orbital through through-bond electron repulsion between the two amide lone pairs forced into proximity in the cis arrangement [32]. The LUMO energy of BMMF-cis (−1.037 eV) is lower than that of BMMF-trans (−0.790 eV) by 0.247 eV, confirming that the cis conformer is also the better electron acceptor. This finding is consistent with the stronger polarisation of the molecule imposed by the cis-oriented carbonyl dipoles, which creates a more electrophilic region accessible to the incoming nucleophile.

The HOMO–LUMO energy gap (ΔE = |ELUMO − EHOMO|) is a primary index of kinetic stability and chemical reactivity: a smaller gap implies lower excitation energy, greater polarisability, and higher chemical reactivity [33,34]. BMMF-cis has ΔE = 6.655 eV, while BMMF-trans has ΔE = 7.225 eV, a difference of 0.570 eV. This clearly establishes that the cis conformer is inherently more reactive, more easily perturbed by external fields, and more susceptible to chemical attack compared with the trans conformer. The result also implies that BMMF-cis will absorb at longer wavelengths in electronic spectroscopy (red shift relative to the trans isomer), which may be testable through UV–visible spectrophotometry.

Table 2.

Frontier molecular orbital energies and global reactivity descriptors for BMMF-cis and BMMF-trans.

Reactivity Descriptor	BMMF-cis	BMMF-trans

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E_{HOMO} (eV)	−7.692	−8.015
E_{LUMO} (eV)	−1.037	−0.790
ΔE = |ELUMO − EHOMO| (eV)	6.655	7.225
Ionization potential, I = −EHOMO (eV)	7.692	8.015
Electron affinity, A = −ELUMO (eV)	1.037	0.790
Electronegativity, $\chi = (I + A)/2$ (eV)	4.364	4.403
Chemical hardness, $\eta = (I - A)/2$ (eV)	3.328	3.613
Chemical potential, $\mu_p = -\chi$ (eV)	−4.364	−4.403
Chemical softness, $\sigma = 1/(2\eta)$ (eV^{-1})	0.1503	0.1384
Electrophilicity index, $\omega = \mu_p^2/2\eta$ (eV)	2.862	2.683
Max. charge transfer, $\Delta Nmax = -\mu_p/\eta$	1.312	1.219
Dipole moment, μ (Debye)	10.125	9.094

Note: All energies in electron volts (eV). I = ionization potential; A = electron affinity; χ = electronegativity; η = chemical hardness; σ = chemical softness; ω = electrophilicity index; ΔNmax = maximum charge transfer.

3.3. Global Reactivity Descriptors

The complete set of global reactivity descriptors derived from the FMO eigenvalues is presented in Table 2. The ionisation potentials, I = 7.692 eV (cis) and 8.015 eV (trans), reflect the energy required to remove an electron from each conformer. The lower I value of BMMF-cis confirms its greater susceptibility to electrophilic attack and its higher potency as a coordination ligand acting through electron donation to a metal centre [35]. The electron affinities A = 1.037 eV (cis) and 0.790 eV (trans) - indicate that BMMF-cis accepts electrons more readily, a feature relevant to its potential role as an acceptor component in charge-transfer complexes.

The electronegativities of both conformers are nearly identical (χ = 4.364 eV for cis, 4.403 eV for trans), a result reflecting the similar gross atomic compositions of the two isomers. However, the chemical hardness distinguishes them clearly: η = 3.328 eV (cis) vs. 3.613 eV (trans). According to Pearson's Hard and Soft Acids and Bases (HSAB) principle [36], the cis conformer — being the softer molecule - will preferentially coordinate to soft or borderline metal centres

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(e.g., Cu^{2+}, Co^{2+}, Ni^{2+}), while the harder trans conformer may interact more favourably with hard Lewis acids (e.g., Al^{3+}, Fe^{3+}). This HSAB-guided differentiation between the conformers carries significant practical implications for the design of metal-selective coordination chemistry.

The chemical softness $\sigma = 0.1503$ eV^{-1} (cis) > 0.1384 eV^{-1} (trans) reinforces the above interpretation. The electrophilicity index $\omega = 2.862$ eV (cis) vs. 2.683 eV (trans) indicates that BMMF-cis is a moderately stronger electrophile — a finding in apparent contradiction with its simultaneously higher electron-donor capacity (higher EHOMO), but which reflects the overall greater polarisability of the cis conformer and its ability to participate effectively in both nucleophilic and electrophilic interactions. The maximum charge transfer parameter $\Delta Nmax$ = 1.312 (cis) vs. 1.219 (trans) shows that the cis conformer can transfer a larger fraction of an electron upon interaction with a suitable partner, making it a more effective ligand in metal-to-ligand or ligand-to-metal charge-transfer scenarios.

3.4. Dipole Moments and Polarity

The calculated dipole moment of BMMF-cis (μ = 10.125 Debye) substantially exceeds that of BMMF-trans (μ = 9.094 Debye), a difference of 1.031 D. This enhancement in the cis conformer arises from the additive alignment of the two amide group dipoles when both carbonyl groups are oriented in the same direction, an arrangement enforced by the cis dihedral [37,38]. In the trans arrangement, the opposing orientations of the two C=O dipoles result in partial mutual cancellation, reducing the net molecular dipole.

The higher dipole moment of BMMF-cis has direct consequences for its intermolecular interactions: greater polarity implies stronger dipole–dipole interactions in the condensed phase, higher solvation energy in polar solvents, and a greater tendency to orient favourably relative to the electric field of a metal cation in a coordination environment [39]. The larger dipole moment is therefore a second independent indicator - complementing the HSAB analysis - that BMMF-cis is likely to be the more potent coordination ligand of the two conformers.

3.5. Mulliken Charge Distribution

Mulliken atomic charges, summarised in Table 4, reveal systematic differences between the two conformers in the charge distribution across the biuret and metaphosphate moieties.

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Table 4.

Mulliken atomic charges for selected atoms in BMMF-cis and BMMF-trans.

Atom	Symbol	Q (BMMF-cis)	Q (BMMF-trans)	ΔQ (cis−trans)
N1 (terminal NH_2)	N	−0.493	−0.631	+0.138
C2 (carbonyl I)	**C**	**+0.516**	**+0.782**	**−0.266**
O3 (carbonyl I)	O	−0.325	−0.526	+0.201
N4 (bridging NH)	**N**	**−0.473**	**−0.597**	**+0.124**
C5 (carbonyl II)	C	+0.588	+0.763	−0.175
O6 (carbonyl II)	**O**	**−0.432**	**−0.600**	**+0.168**
N7 (terminal NH_2)	N	−0.493	−0.624	+0.131
P (phosphorus)	**P**	**+1.170**	**+1.079**	**+0.091**
O (bridging P−O)	O	−0.600	−0.549	−0.051
O (P=O)	**O**	**−0.499**	**−0.558**	**+0.059**

Note: Charges in atomic units (e). ΔQ = Q(cis) − Q(trans).

In BMMF-cis, the terminal nitrogen atoms N1 and N7 bear charges of −0.493 e each, which are considerably less negative than in BMMF-trans (−0.631 e for N1, −0.624 e for N7). This indicates that in the cis conformer the terminal amino groups are more electron-depleted — consistent with the intramolecular N–H···O hydrogen bond withdrawing electron density from N7 and the overall higher electronegativity of the constrained backbone. The carbonyl carbon atoms are less positively charged in cis (C2 = +0.516 e, C5 = +0.588 e) than in trans (C2 = +0.782 e, C5 = +0.763 e), a trend also reflected in the less negative carbonyl oxygen charges in cis (O3 = −0.325 e, O6 = −0.432 e) vs. trans (O3 = −0.526 e, O6 = −0.600 e). These systematic charge differences reflect reduced ionic character of the C=O bonds in the cis conformer, pointing toward a more covalent, π-delocalised amide system in that conformation.

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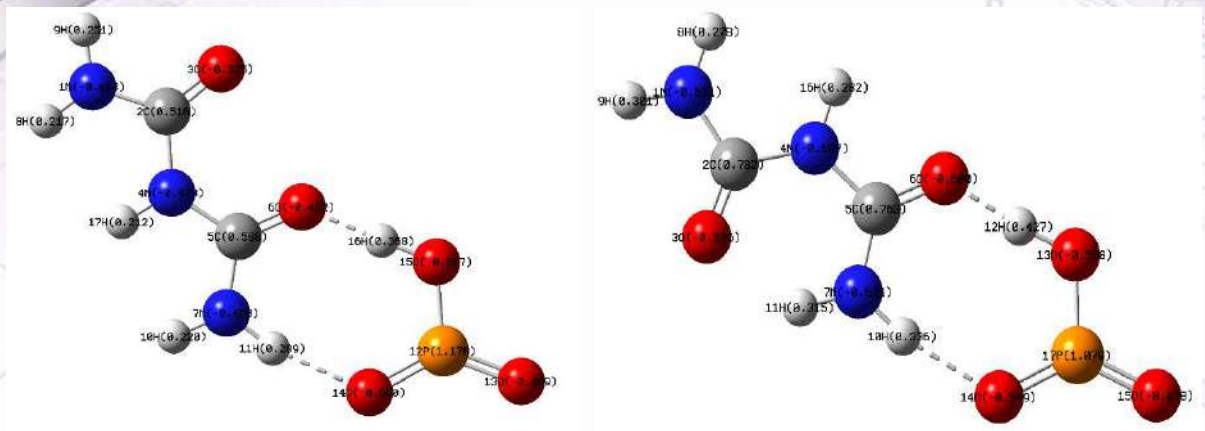


Figure 5. Schematic illustration of the proposed Mulliken atomic charges for selected atoms in (a) BMMF-cis and (b) BMMF-trans.

The phosphorus atom carries a higher positive partial charge in BMMF-cis (+1.170 e) than in BMMF-trans (+1.079 e), a difference of 0.091 e. The greater electrophilicity of P in the cis conformer implies enhanced Lewis-acid character at the phosphorus centre, which may facilitate hydrolysis or nucleophilic substitution at phosphorus in aqueous or biological environments. This finding is relevant to the potential reactivity of BMMF as a phosphorylating agent and as an inhibitor of phosphohydrolase enzymes [40].

3.6. Coordination Chemistry Implications

The combined evidence from the geometric, electronic, and charge-distribution analyses presented in Sections 3.1–3.5 converges on a consistent picture of the differential coordination potential of the two BMMF conformers. The BMMF molecule presents multiple potential donor sites - the terminal NH_2 groups (N1, N7), the bridging NH nitrogen (N4), the carbonyl oxygen atoms (O3, O6), and the metaphosphate oxygens - and the relative strengths of these donor functions depend critically on the conformational state [41,42].

In the cis conformer, the intramolecular N7–H···O6 hydrogen bond pre-organises the molecular framework in a chelate-like arrangement that mirrors the bite geometry required for five-membered metallocycle formation with a metal ion inserted between N7 and O6. This structural feature, combined with the higher HOMO energy, greater chemical softness, larger dipole moment, and higher phosphorus Lewis acidity, identifies BMMF-cis as the conformer with superior chelating capacity. Similar through-space pre-organisation of donor atoms via intramolecular hydrogen bonds has been identified as a key thermodynamic driving force in the formation of stable metal complexes in related biuret-derived ligands [43,44].

The trans conformer, by contrast, offers an open coordination geometry without intramolecular pre-organisation, making it better suited to bridging coordination modes in which the two ends of the molecule bind simultaneously

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to different metal centres in a polynuclear complex. The higher chemical hardness (η = 3.613 eV) of BMMF-trans further suggests a preference for hard metal centres. These complementary coordination roles for the two conformers suggest that the cis/trans equilibrium in solution may be exploited as a conformational switch to access mononuclear (cis) versus polynuclear (trans) coordination networks [45].

Figure 6 presents a schematic representation of the proposed chelate coordination mode of BMMF-cis and the bridging coordination mode of BMMF-trans with a generic divalent metal centre.

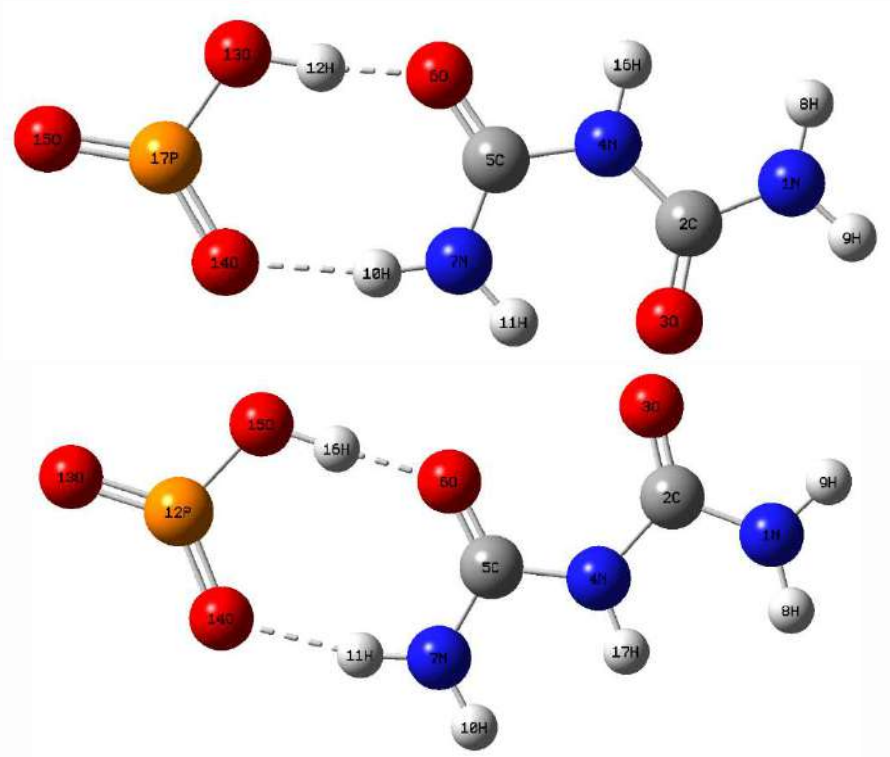


Figure 6. Schematic illustration of the proposed coordination modes of BMMF. Left: five-membered metallocyclic chelate formed by BMMF-cis via N7 and O6 donor atoms. Right: bridging κ¹N:κ¹O coordination of BMMF-trans to two metal centres (M).

3.7. Vibrational Properties and Conformational Dynamics

As noted in Section 2.2, both optimised structures exhibit imaginary vibrational frequencies. For BMMF-cis, two imaginary modes are found at −317.8 cm^{-1} and −68.6 cm^{-1}; for BMMF-trans, one imaginary mode appears at −221.3 cm^{-1}. The high-frequency imaginary mode in BMMF-cis (−317.8 cm^{-1}) corresponds to a butterfly-type torsional motion of the HPO_3 group relative to the biuret backbone, while the lower-frequency imaginary mode (−68.6 cm^{-1}) describes a global backbone torsion. In BMMF-trans, the single imaginary mode (−221.3 cm^{-1}) is attributed to a similar HPO_3 torsional degree of freedom (Fig.7).

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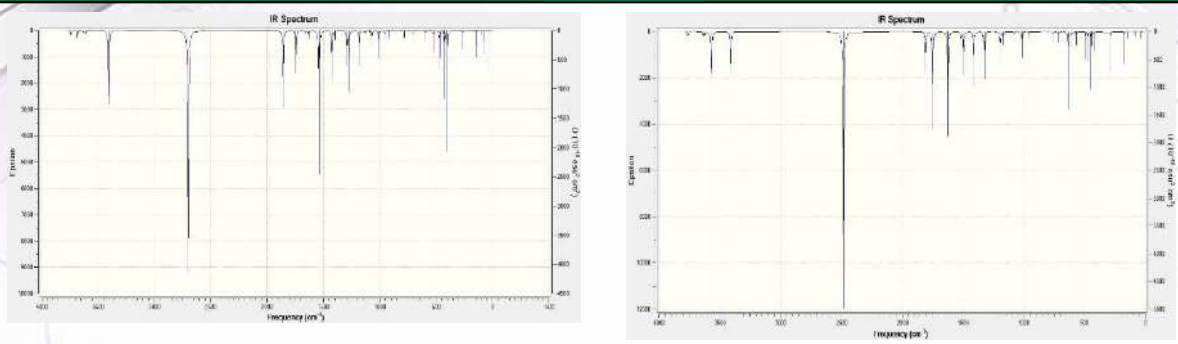


Figure 7. Schematic illustration of the proposed Mulliken atomic charges for selected atoms in (a) BMMF-cis and (b) BMMF-trans.

These findings indicate that the planar constraints imposed on the starting geometries are not maintained at the global potential energy minimum; the true energy minima are likely non-planar structures accessible by following the eigenvectors of the imaginary modes in geometry optimisations without symmetry constraints. The physical significance of the reported structures lies in the fact that they represent the electronic-structure characteristics of the idealised planar conformers, which are meaningful reference points for understanding the electronic differences between the cis and trans arrangements. Future work will focus on unconstrained optimisations from perturbed starting geometries and the construction of a one-dimensional potential energy surface along the dominant torsional coordinate using relaxed scans.

4. CONCLUSIONS.

A comparative density functional theory investigation of the cis and trans conformers of biuret monometaphosphate (BMMF, $C_2H_6N_3O_5P$) has been presented, encompassing geometry optimisation, frequency analysis, frontier molecular orbital analysis, global reactivity descriptor evaluation, Mulliken charge distribution analysis, and an assessment of coordination chemistry implications. The principal conclusions are as follows:

(1) The cis conformer of BMMF is characterised by an intramolecular N7–H···O6 hydrogen bond (N···H = 1.856 Å) that pre-organises the molecular framework into a pseudo-chelate arrangement with potential for five-membered metallocyclic complex formation.

(2) Frontier molecular orbital analysis shows that BMMF-cis has a smaller HOMO–LUMO gap (ΔE = 6.655 eV) than BMMF-trans (ΔE = 7.225 eV), establishing the cis conformer as inherently more chemically reactive and more susceptible to photochemical excitation.

(3) Global reactivity descriptors derived within the conceptual DFT framework confirm that BMMF-cis is the softer, more polarisable, and more electrophilic conformer (η = 3.328 eV, σ = 0.1503 eV^{-1}, ω = 2.862 eV), while

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BMMF-trans is harder and less reactive ($\eta = 3.613$ eV, $\sigma = 0.1384$ eV^{-1}, $\omega = 2.683$ eV).

(4) The significantly larger dipole moment of BMMF-cis (10.125 D vs. 9.094 D) reflects additive alignment of the amide-group dipoles and indicates stronger electrostatic interaction capacity with polar solvents and metal cations.

(5) Mulliken charge analysis reveals that the cis conformer has a more electropositive phosphorus centre (+1.170 e vs. +1.079 e), implying enhanced Lewis-acid character and potentially greater susceptibility to nucleophilic attack at phosphorus.

(6) Based on HSAB principles, BMMF-cis is predicted to preferentially coordinate soft-to-borderline metal ions, while BMMF-trans is expected to coordinate hard Lewis acids, suggesting that conformational control may serve as a mechanism for metal-selective coordination.

(7) The presence of imaginary vibrational frequencies in both optimised structures indicates conformational saddle-point geometries. Relaxed potential energy surface scans along the dominant torsional coordinates are warranted to locate the true global and local minima.

These findings establish a quantum-chemical basis for the differential reactivity and coordination behaviour of BMMF conformers and provide a framework for the rational design of phosphorylated biuret-based coordination compounds with tailored metal-ion selectivity.

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