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B– Teorik Bilimler

Volume/Cilt 11 Number/Sayı 2 – August / Ağustos 2023

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B- Theoretical Sciences
Eskişehir Teknik Üniversitesi Bilim ve Teknoloji Dergisi B – Teorik Bilimler

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RESEARCH ARTICLE

THE NOWICKI CONJECTURE FOR BICOMMUTATIVE ALGEBRAS

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ABSTRACT

Let K be a field of characteristic zero, and $K[X_n, Y_n]$ be the commutative associative unitary polynomial algebra of rank $2n$ generated by the set $X_n \cup Y_n = \{x_1, \dots, x_n, y_1, \dots, y_n\}$. It is well known that the algebra $K[X_n, Y_n]^\delta$ of constants of the locally nilpotent linear derivation δ of $K[X_n, Y_n]$ sending y_i to x_i, and x_i to 0, is generated by $x_1, \dots, x_n$ and the determinants of the form $x_i y_j - x_j y_i$; that was first conjectured by Nowicki in 1994, and later proved by several authors. Bicommutative algebras are nonassociative noncommutative algebras satisfying the identities $(xy)z = (xz)y$ and $x(yz) = y(xz)$. In this study, we work in the $2n$ generated free bicommutative algebra as a noncommutative nonassociative analogue of the Nowicki conjecture, and find the generators of the algebra of constants in this algebra.

Keywords: Algebra of constants, Bicommutative algebra, The Nowicki conjecture

1. INTRODUCTION

Roots of the Nowicki conjecture dates back to 1900, when the famous German mathematician David Hilbert posed 23 unsolved major questions at the Paris International Congress of Mathematicians [1]. In the fourteenth problem, he asked the finite generation of the algebra $K[X_n]^G$ of invariants of any subgroup G of the general linear group consisting of $n \times n$ invertible matrices with entries from a field K of characteristic zero, where $K[X_n]$ is the commutative associative unitary polynomial algebra of rank n.

The negative answer to the fourteenth problem was given by Nagata [2] in 1959, while many partially affirmative cases were considered by several authors. One may count the work by Noether [3] who showed that $K[X_n]^G$ finitely generated for every finite group G. Another remarkable approach was given by Weitzenböck [4] who considered algebras constants of linear nilpotent derivations δ of $K[X_n]$. He showed that the algebra $K[X_n]^\delta$ is finitely generated that is equal to the algebra $K[X_n]^{\langle \exp\delta \rangle}$ of invariants. However, no information about the explicit forms of generators were provided. Many years later in 1994, Nowicki [5] conjectured an explicit generating set for the algebra $K[X_n, Y_n]^\delta$ of constants of the Weitzenböck derivation δ sending y_i to x_i, and x_i to 0, where $K[X_n, Y_n]$ is the polynomial algebra of rank $2n$ generated by the set $X_n \cup Y_n = \{x_1, \dots, x_n, y_1, \dots, y_n\}$. He proposed that $K[X_n, Y_n]^\delta$ is generated by $x_1, \dots, x_n$ and the elements of the form $x_i y_j - x_j y_i$, where $1 \leq i < j \leq n$. Then, the conjecture was verified by many mathematicians [6, 7, 8, 9].

Noncommutative nonassociative analogues of the Nowicki conjecture have been studied, recently. See e.g. [10], in which the authors consider the free metabelian Lie algebra F_{2n} of rank $2n$ generated by $X_n \cup Y_n$. They gave a finite generating set for the algebra $(F'_{2n})^\delta$ included in the commutator ideal F'_{2n} of F_{2n} as a $K[X_n, Y_n]^\delta$-module. As a continuation of this work a finite generation set for the algebra of constants in the commutator ideal of the free metabelian associative algebra generated by $X_n \cup Y_n$ as a $K[X_n, Y_n]^\delta$-bimodule was given in [11]. In the same work, a set of finite generators was obtained for

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the free algebra in the variety of infinite dimensional Grassmann algebras. There is also the free metabelian Possion algebra analogue of the Nowicki conjecture [12].

In the current study, we consider the free algebra of rank $2n$ in the variety of bicommutative algebras and determine the generators of the algebra of constants of Weitzenböck derivation that was stated in the Nowicki conjecture.

2. PRELIMINARIES

We assume that $\boldsymbol{K}$ is a field of characteristic zero throughout the paper. Let $\boldsymbol{K}[\boldsymbol{X_n}]$, $\boldsymbol{K}[\boldsymbol{Y_n}]$, and $\boldsymbol{K}[\boldsymbol{X_n}, \boldsymbol{Y_n}]$ be the polynomial algebras generated by sets $\boldsymbol{X_n} = \{\boldsymbol{x_1}, \dots, \boldsymbol{x_n}\}$, $\boldsymbol{Y_n} = \{\boldsymbol{y_1}, \dots, \boldsymbol{y_n}\}$, and $\boldsymbol{X_n} \cup \boldsymbol{Y_n}$, respectively. We also fix notations $\boldsymbol{\omega}(\boldsymbol{K}[\boldsymbol{X_n}])$ and $\boldsymbol{\omega}(\boldsymbol{K}[\boldsymbol{X_n}])$ for augmentation ideals of $\boldsymbol{K}[\boldsymbol{X_n}]$ and $\boldsymbol{K}[\boldsymbol{Y_n}]$, respectively, consisting of the polynomials without constant terms.

We call a noncommutative nonassociative algebra over $\boldsymbol{K}$ *right symmetric* and *left symmetric* if it satisfies the identity $(\boldsymbol{xy})\boldsymbol{z} = (\boldsymbol{xz})\boldsymbol{y}$ and $\boldsymbol{x}(\boldsymbol{yz}) = \boldsymbol{y}(\boldsymbol{xz})$, respectively. An algebra over $\boldsymbol{K}$ is called *bicommutative* if it is left and right symmetric.

Let $\boldsymbol{F_{2n}}$ be the free algebra of rank $\boldsymbol{2n}$ generated by $\boldsymbol{X_n} \cup \boldsymbol{Y_n}$ in the variety of bicommutative algebras over the field $\boldsymbol{K}$, and let $\boldsymbol{a} = \boldsymbol{a_1}\boldsymbol{a_2}$, $\boldsymbol{b} = \boldsymbol{b_1}\boldsymbol{b_2}$, $\boldsymbol{c} \in \boldsymbol{F_{2n}^2}$ for some $\boldsymbol{a_1}, \boldsymbol{a_2}, \boldsymbol{b_1}, \boldsymbol{b_2} \in \boldsymbol{F_{2n}}$. Then the following straightforward computations show that the ideal $\boldsymbol{F_{2n}^2} = \boldsymbol{F_{2n}}\boldsymbol{F_{2n}}$ of $\boldsymbol{F_{2n}}$ is commutative and associative.

$$\begin{aligned}\boldsymbol{ab} = (\boldsymbol{a_1a_2})(\boldsymbol{b_1b_2}) = \big(\boldsymbol{a_1}(\boldsymbol{b_1b_2})\big)\boldsymbol{a_2} = \big(\boldsymbol{b_1}(\boldsymbol{a_1b_2})\big)\boldsymbol{a_2} = (\boldsymbol{b_1a_2})(\boldsymbol{a_1b_2}) = \boldsymbol{a_1}\big((\boldsymbol{b_1a_2})\boldsymbol{b_2}\big)\\ = \boldsymbol{a_1}\big((\boldsymbol{b_1b_2})\boldsymbol{a_2}\big) = (\boldsymbol{b_1b_2})(\boldsymbol{a_1a_2}) = \boldsymbol{ba},\end{aligned}$$

and

$$(\boldsymbol{ab})\boldsymbol{c} = \boldsymbol{c}(\boldsymbol{ab}) = \boldsymbol{a}(\boldsymbol{cb}) = \boldsymbol{a}(\boldsymbol{bc}).$$

Therefore, $\boldsymbol{F_{2n}}$ can be considered as a direct sum of the vector space $\boldsymbol{K}(\boldsymbol{X_n} \cup \boldsymbol{Y_n}) = \mathbf{Span}\{\boldsymbol{X_n} \cup \boldsymbol{Y_n}\}$ and $\boldsymbol{\omega}(\boldsymbol{K}[\boldsymbol{A_n}, \boldsymbol{B_n}])\boldsymbol{\omega}(\boldsymbol{K}[\boldsymbol{C_n}, \boldsymbol{D_n}])$, where

$$\boldsymbol{A_n} = \{\boldsymbol{a_1}, \dots, \boldsymbol{a_n}\}, \boldsymbol{B_n} = \{\boldsymbol{b_1}, \dots, \boldsymbol{b_n}\}, \boldsymbol{C_n} = \{\boldsymbol{c_1}, \dots, \boldsymbol{c_n}\}, \boldsymbol{D_n} = \{\boldsymbol{d_1}, \dots, \boldsymbol{d_n}\}$$

such that

$$\begin{aligned}\boldsymbol{x_ix_j} &= \boldsymbol{a_ic_j},\\ \boldsymbol{y_iy_j} &= \boldsymbol{b_id_j},\\ \boldsymbol{x_iy_j} &= \boldsymbol{a_id_j},\\ \boldsymbol{y_ix_j} &= \boldsymbol{b_ic_j}.\end{aligned}$$

Note that $\boldsymbol{F_{2n}^2} \cong \boldsymbol{\omega}(\boldsymbol{K}[\boldsymbol{A_n}, \boldsymbol{B_n}])\boldsymbol{\omega}(\boldsymbol{K}[\boldsymbol{C_n}, \boldsymbol{D_n}])$ contains elements as linear combinations of the form

$$\boldsymbol{a_1^{\alpha_1}} \cdots \boldsymbol{a_n^{\alpha_n}}\boldsymbol{b_1^{\beta_1}} \cdots \boldsymbol{b_n^{\beta_n}}\boldsymbol{c_1^{\gamma_1}} \cdots \boldsymbol{c_n^{\gamma_n}}\boldsymbol{d_1^{\varepsilon_1}} \cdots \boldsymbol{d_n^{\varepsilon_n}},$$

where $\alpha_1 + \cdots + \alpha_n + \beta_1 + \cdots + \beta_n > 0$, $\gamma_1 + \cdots + \gamma_n + \varepsilon_1 + \cdots + \varepsilon_n > 0$. We refer to the paper [13] for more details.

Now let $\delta: F_{2n} \to F_{2n}$ be the locally nilpotent derivation of F_{2n} acting linearly on the vector space spanned on $X_n \cup Y_n$ such that $\delta(y_i) = x_i$, $\delta(x_i) = 0$ for each $i = 1, \dots, n$. Our main result concerns with the generators of the subalgebra

$$F_{2n}^{\delta} = \{f \in F_{2n} : \delta(f) = 0\}$$

of constants of the derivation δ in the free bicommmutative algebra F_{2n}. For this purpose, we will work in the algebra

$$F_{2n} = K(X_n \cup Y_n) \oplus F_{2n}^2 \cong K(X_n \cup Y_n) \oplus \omega(K[A_n, B_n])\omega(K[C_n, D_n]).$$

An easy observation gives that

$$\begin{aligned} F_{2n}^{\delta} &\cong K(X_n \cup Y_n)^{\delta} \oplus \big(\omega(K[A_n, B_n])\omega(K[C_n, D_n])\big)^{\delta} \\ &= KX_n \oplus \big(\omega(K[A_n, B_n])\omega(K[C_n, D_n])\big)^{\delta}. \end{aligned}$$

Here, we assume that δ acts on $K(A_n \cup B_n)$ and $K(C_n \cup D_n)$ same as on $K(X_n \cup Y_n)$; i.e.,

$$\begin{aligned} \delta(b_i) = a_i \, , \, \delta(a_i) = 0 \\ \delta(d_i) = c_i \, , \, \delta(c_i) = 0 \end{aligned}$$

for each $i = 1, \dots, n$. Hence, it is sufficient to determine constants of δ in the algebra

$$(F_{2n}^2)^{\delta} = \big(\omega(K[A_n, B_n])\omega(K[C_n, D_n])\big)^{\delta}.$$

In the next section, we determine the elements of $(F_{2n}^2)^{\delta}$, and consequently describe the algebra F_{2n}^{δ}.

3. MAIN RESULTS

The following theorem and corrollary are our main results.

Theorem 1. The algebra $\big(\omega(K[A_n, B_n])\omega(K[C_n, D_n])\big)^{\delta}$ is generated by determinants

$$\begin{vmatrix} a_i & c_j \\ b_i & d_j \end{vmatrix} = a_i d_j - b_i c_j \, , \quad 1 \le i, j \le n,$$

and it is a $K\big[A_n, C_n, a_i b_j - b_i a_j, c_i d_j - d_i c_j, a_k d_l - b_k c_l : 1 \le i < j \le n, 1 \le k, l \le n\big]^{\delta}$-module.

Proof. Clearly, $\omega(K[A_n, B_n])\omega(K[C_n, D_n]) \subset K[A_n, B_n, C_n, D_n]$ is a $K[A_n, B_n, C_n, D_n]$-module, and $\big(\omega(K[A_n, B_n])\omega(K[C_n, D_n])\big)^{\delta}$ is a $K[A_n, B_n, C_n, D_n]^{\delta}$-module. It is well known, see e.g. [7], that $K[A_n, B_n, C_n, D_n]^{\delta}$ is generated by $a_1, \dots, a_n, c_1, \dots, c_n$ together with

$$\begin{vmatrix} a_i & a_j \\ b_i & b_j \end{vmatrix} = a_i b_j - b_i a_j \, , \qquad \begin{vmatrix} c_i & c_j \\ d_i & d_j \end{vmatrix} = c_i d_j - d_i c_j \, , \qquad 1 \le i < j \le n,$$

$$\begin{vmatrix} a_i & c_j \\ b_i & d_j \end{vmatrix} = a_i d_j - b_i c_j \, , \quad 1 \le i, j \le n.$$

It is straightforward to see that a polynomial $p(A_n, B_n, C_n, D_n) \in K[A_n, B_n, C_n, D_n]$ belongs to $\omega(K[A_n, B_n])\omega(K[C_n, D_n])$ if and only if

$$p(A_n, B_n, C_n, D_n) \not\equiv 0 \ (\mathrm{mod}\ K[A_n, B_n] \oplus K[C_n, D_n]).$$

Since,

$$a_1, \dots, a_n \equiv 0 \pmod{K[A_n, B_n] \oplus K[C_n, D_n]}$$
$$c_1, \dots, c_n \equiv 0 \pmod{K[A_n, B_n] \oplus K[C_n, D_n]}$$
$$a_i b_j - b_i a_j \equiv 0 \pmod{K[A_n, B_n] \oplus K[C_n, D_n]}$$
$$c_i d_j - d_i c_j \equiv 0 \pmod{K[A_n, B_n] \oplus K[C_n, D_n]}$$
$$a_i d_j - b_i c_j \not\equiv 0 \pmod{K[A_n, B_n] \oplus K[C_n, D_n]}$$

we obtain that $\left(\omega(K[A_n, B_n])\omega(K[C_n, D_n])\right)^{\delta}$ is generated by the elements of the form $a_i d_j - b_i c_j$, $1 \leq i, j \leq n$, and it is a

$$K[A_n, B_n, C_n, D_n]^{\delta} = K\left[A_n, C_n, a_i b_j - b_i a_j, c_i d_j - d_i c_j, a_k d_l - b_k c_l : 1 \leq i < j \leq n, 1 \leq k, l \leq n\right]^{\delta}$$

-module.

Corollary 2. F_{2n}^{δ} is generated by $x_1, \dots, x_n$ together with elements of the form

$$x_i y_j - y_i x_j \ , \ 1 \leq i, j \leq n.$$

Example 3. $(\boldsymbol{i})$ Let $n = 1$, and the free bicommutative algebra F_2 be generated by $x_1 = x$ and $y_1 = y$. Then the algebra F_2^{δ} is generated by $\{x, xy - yx\}$.
$(\boldsymbol{ii})$ Let $n = 2$, and the free bicommutative algebra F_4 be generated by $x_1 = x, y_1 = y, x_2 = z, y_2 = t$. Then the algebra F_4^{δ} is generated by $\{x, z, xy - yx, zt - tz, xt - yz\}$.

Remark 4. Note that in the case of commutativity the above example is compatible with the following well known results:
$(\boldsymbol{i})$ Let $n = 1$. Then $K[x, y]^{\delta}$ is generated the set $\{x\}$ in the commutative polynomial algebra generated by $x_1 = x$ and $y_1 = y$.
$(\boldsymbol{ii})$ Let $n = 2$. Then $K[x, y, z, t]^{\delta}$ is generated the set $\{x, z, xt - yz\}$ in the commutative polynomial algebra generated by $x_1 = x, y_1 = y, x_2 = z, y_2 = t$.

CONFLICT OF INTEREST

The author stated that there are no conflicts of interest regarding the publication of this article.

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ESKİŞEHİR TEKNİK ÜNİVERSİTESİ BİLİM VE TEKNOLOJİ DERGİSİ B- TEORİK BİLİMLER

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RESEARCH ARTICLE

ON THE KLEIN-4 INVARIANTS

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ABSTRACT

Let $K[X_4] = K[x_1, x_2, x_3, x_4]$ be the polynomial algebra with 4 algebraically independent commuting variables over a field K of characteristic zero. The symmetric group S_4 acts on $K[X_4]$ naturally by the action of permutations exchanging the indices of variables with respect to the corresponding permutation. It is well known that the algebra $K[X_4]^{S_4}$ of all polynomials preserved under the action of S_4 is generated by 4 algebraically independent elements called the elementary symmetric polynomials. In this study, we consider the subalgebra G of S_4 generated by the transpositions (13) and (24) which is isomorphic to the Klein-4 group, and find a free generating set for the algebra $K[X_4]^G$ of G-invariants.

Keywords: Action, Invariants, Symmetric group

1. INTRODUCTION

The initiation of study of G-invariants, where G is a subgroup of the general linear group $GL_n(K)$ for a field K of characteristic zero, dates back to the beginning of the twentieth century. The fourteenth of twenty three problems given by David Hilbert [1] is related to the algebra $K[X_n]^G$ of G-invariants of the polynomial algebra $K[X_n]$ in n commuting variables $x_1, \dots, x_n$ over the field K. Nagata [2] showed that $K[X_n]^G$ is not finitely generated in general, while it is finitely generated for finite subgroups G of $GL_n(K)$ via Noether [3].

The most interesting group in this theory is the symmetric group S_n. The algebra $K[X_n]^{S_n}$ of S_n-invariants is called the algebra of symmetric polynomials, and each polynomial in this algebra is called a symmetric polynomial. The action of each permutation $\pi \in S_n$ on a monomial is defined as follows.

$$\pi(x_{i_1} \cdots x_{i_k}) = x_{\pi(i_1)} \cdots x_{\pi(i_k)}.$$

It is well known by Cayley's Theorem that every group is a subgroup of S_n (see e.g., [4]). In this study, we realize the Klein-4 group G as a subgroup of S_4 generated by two transpositions (13) and (24), and describe the algebra $K[X_4]^G$ by providing its generators.

2. THE KLEIN-4 INVARIANTS

In this section, we investigate the algebra

$$K[X_4]^G = \{p \in K[X_4] : p(x_1, x_2, x_3, x_4) = p(x_3, x_2, x_1, x_4) = p(x_1, x_4, x_3, x_2)\},$$

where

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$$G = \langle (13), (24) \rangle = \{(1), (13), (24), (13)(24)\}$$
$$= \left\{ \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \right\},$$

that is isomorphic to the Klein-4 group. Then, we give a finite generating set for $K[X_4]^G$.

Lemma 1. $K[X_4]^G = K[\alpha_{ab}, \beta_{ab} : 0 \leq a, b]$, such that

$$\alpha_{ab} = x_1^a x_3^b + x_1^b x_3^a ,$$
$$\beta_{ab} = x_2^a x_4^b + x_2^b x_4^a ,$$

where $0 \leq a, b$.

Proof. Let $p \in K[X_4]$ be an arbitrary polynomial. One may express

$$p(x_1, x_2, x_3, x_4) = \sum_{0 \leq a,b,c,d} \varepsilon_{abcd} x_1^a x_2^b x_3^c x_4^d = \sum_{0 \leq a,b,c,d} \varepsilon_{abcd} X^{abcd} \ , \varepsilon_{abcd} \in K,$$

as $= p_1 + p_2 + p_3 + p_4$, where p_1, p_2, p_3, p_4 are of the form

$$p_1(x_1, x_2, x_3, x_4) = \sum_{0 \leq a} \varepsilon_{aaaa} X^{aaaa}$$

$$\begin{aligned} p_2(x_1, x_2, x_3, x_4) &= \sum_{0 \leq a < b} \left(\varepsilon_{abbb} X^{abbb} + \varepsilon_{bbab} X^{bbab}\right) + \left(\varepsilon_{babb} X^{babb} + \varepsilon_{bbba} X^{bbba}\right) \\ &+ \left(\varepsilon_{baaa} X^{baaa} + \varepsilon_{aaba} X^{aaba}\right) + \left(\varepsilon_{abaa} X^{abaa} + \varepsilon_{aaab} X^{aaab}\right) \\ &+ \left(\varepsilon_{aabb} X^{aabb} + \varepsilon_{baab} X^{baab} + \varepsilon_{bbaa} X^{bbaa} + \varepsilon_{abba} X^{abba}\right) + \varepsilon_{abab} X^{abab} \\ &+ \varepsilon_{baba} X^{baba} = \sum_{0 \leq a < b} p_{2,1} + \cdots + p_{2,7} \end{aligned}$$

$$\begin{aligned} p_3(x_1, x_2, x_3, x_4) &= \sum_{0 \leq a < b < c} \left(\varepsilon_{aabc} X^{aabc} + \varepsilon_{baac} X^{baac} + \varepsilon_{bcaa} X^{bcaa} + \varepsilon_{acba} X^{acba}\right) \\ &+ \left(\varepsilon_{aacb} X^{aacb} + \varepsilon_{caab} X^{caab} + \varepsilon_{cbaa} X^{cbaa} + \varepsilon_{abca} X^{abca}\right) \\ &+ \left(\varepsilon_{abac} X^{abac} + \varepsilon_{acab} X^{acab}\right) + \left(\varepsilon_{baca} X^{baca} + \varepsilon_{caba} X^{caba}\right) \\ &+ \left(\varepsilon_{bbac} X^{bbac} + \varepsilon_{abbc} X^{abbc} + \varepsilon_{acbb} X^{acbb} + \varepsilon_{bcab} X^{bcab}\right) \\ &+ \left(\varepsilon_{bbca} X^{bbca} + \varepsilon_{cbba} X^{cbba} + \varepsilon_{cabb} X^{cabb} + \varepsilon_{bacb} X^{bacb}\right) \\ &+ \left(\varepsilon_{babc} X^{babc} + \varepsilon_{bcba} X^{bcba}\right) + \left(\varepsilon_{abcb} X^{abcb} + \varepsilon_{cbab} X^{cbab}\right) \\ &+ \left(\varepsilon_{ccab} X^{ccab} + \varepsilon_{accb} X^{accb} + \varepsilon_{abcc} X^{abcc} + \varepsilon_{cbac} X^{cbac}\right) \\ &+ \left(\varepsilon_{ccba} X^{ccba} + \varepsilon_{bcca} X^{bcca} + \varepsilon_{bacc} X^{bacc} + \varepsilon_{cabc} X^{cabc}\right) \\ &+ \left(\varepsilon_{cacb} X^{cacb} + \varepsilon_{cbca} X^{cbca}\right) + \left(\varepsilon_{acbc} X^{acbc} + \varepsilon_{bcac} X^{bcac}\right) \\ &= \sum_{0 \leq a < b < c} p_{3,1} + \cdots + p_{3,12} \end{aligned}$$

$$
\begin{aligned}
p_4(x_1,x_2,x_3,x_4) &= \sum_{0\le a<b<c<d} \left(\varepsilon_{abcd}X^{abcd}+\varepsilon_{adcb}X^{adcb}+\varepsilon_{cbad}X^{cbad}+\varepsilon_{cdab}X^{cdab}\right)\\
&+\left(\varepsilon_{abdc}X^{abdc}+\varepsilon_{acdb}X^{acdb}+\varepsilon_{dbac}X^{dbac}+\varepsilon_{dcab}X^{dcab}\right)\\
&+\left(\varepsilon_{acbd}X^{acbd}+\varepsilon_{adbc}X^{adbc}+\varepsilon_{bcad}X^{bcad}+\varepsilon_{bdac}X^{bdac}\right)\\
&+\left(\varepsilon_{bacd}X^{bacd}+\varepsilon_{bdca}X^{bdca}+\varepsilon_{cabd}X^{cabd}+\varepsilon_{cdba}X^{cdba}\right)\\
&+\left(\varepsilon_{badc}X^{badc}+\varepsilon_{bcda}X^{bcda}+\varepsilon_{dabc}X^{dabc}+\varepsilon_{dcba}X^{dcba}\right)\\
&+\left(\varepsilon_{cadb}X^{cadb}+\varepsilon_{cbda}X^{cbda}+\varepsilon_{dacb}X^{dacb}+\varepsilon_{dbca}X^{dbca}\right)\\
&= \sum_{0\le a<b<c} p_{4,1}+\cdots+p_{4,6}
\end{aligned}
$$

such that $p_{i,j}$ counts the sum in the paranthesis indicated as a sum in the expression of p_i , $i = 1,2,3,4$.

Now let $p \in K[X_4]^G$. Then, clearly $p = \pi(p)$ gives that

$$p_1+p_2+p_3+p_4 = \pi(p_1+p_2+p_3+p_4) = \pi(p_1)+\pi(p_2)+\pi(p_2)+\pi(p_2)$$

and that $\pi(p_1) = p_1$, $\pi(p_2) = p_2, \pi(p_3) = p_3, \pi(p_4) = p_4$, $\pi \in G$, since the elements of the form p_i are G-invariants for each $i = 1,2,3,4$, due to the number of distinct powers of the variables in the monomials of corresponding summands.

Initially,

$$X^{aaaa} = x_1^a x_2^a x_3^a x_4^a = \left(\frac{\alpha_{11}\beta_{11}}{4}\right)^a = \sigma_4^a$$

that means

$$p_1(x_1,x_2,x_3,x_4) = \sum_{0\le a} \varepsilon_{aaaa}\sigma_4^a \in K[\sigma_4].$$

Secondly, let us consider $p_2 = \sum_{0\le a<b}\left(p_{2,1}+\cdots+p_{2,7}\right)$. Recall that

$$p_{2,1}(x_1,x_2,x_3,x_4) = \sum_{0\le a<b} \left(\varepsilon_{abbb}X^{abbb}+\varepsilon_{bbab}X^{bbab}\right).$$

The orbit of the monomial X^{abbb} is

$$X^{abbb}, X^{bbab}, X^{abbb}, X^{bbab}$$

with respect to the group G. Similarly the orbit of the monomial X^{bbab} is

$$X^{bbab}, X^{abbb}, X^{bbab}, X^{abbb}.$$

Hence,

$$\pi\left(p_{2,1}\right) \in \mathrm{span}_K\{X^{abbb}, X^{bbab}\},$$

or $\pi\left(p_{2,1}\right) = p_{2,1}$, for $\pi = (13), (24)$. This implies that

$$\varepsilon_{abbb}X^{abbb}+\varepsilon_{bbab}X^{bbab} = (13)\left(\varepsilon_{abbb}X^{abbb}+\varepsilon_{bbab}X^{bbab}\right) = \varepsilon_{abbb}X^{bbab}+\varepsilon_{bbab}X^{abbb},$$

or

$$(\varepsilon_{abbb} - \varepsilon_{bbab})X^{abbb} + (\varepsilon_{bbab} - \varepsilon_{abbb})X^{bbab} = 0,$$

for each pair (a, b). Thus, $\varepsilon_{abbb} = \varepsilon_{bbab}$, $0 \le a < b$. Therefore,

$$\begin{aligned}\varepsilon_{abbb}X^{abbb} + \varepsilon_{bbab}X^{bbab} &= \varepsilon_{abbb}\left(X^{abbb} + X^{bbab}\right)\\ &= \varepsilon_{abbb}X^{aaaa}\left(X^{0(b-a)(b-a)(b-a)} + X^{(b-a)(b-a)0(b-a)}\right)\\ &= \varepsilon_{abbb}\sigma_4^a X^{0(b-a)0(b-a)}\left(X^{00(b-a)0} + X^{(b-a)000}\right) = \varepsilon_{abbb}\sigma_4^a \frac{\beta_{(b-a)(b-a)}}{2}\alpha_{(b-a)0}\end{aligned}$$

and thus

$$p_{2,1}(x_1, x_2, x_3, x_4) = \sum_{0\le a<b} \varepsilon_{abbb}\sigma_4^a \frac{\beta_{(b-a)(b-a)}}{2}\alpha_{(b-a)0} \in K[\sigma_4, \alpha_{a0}, \beta_{aa} : 0 \le a].$$

Similar arguments gives that $\pi\left(p_{2,i}\right) = p_{2,i}$, $i = 2, \dots, 7$, $\pi\left(p_{3,j}\right) = p_{3,j}$, $j = 1, \dots, 12$, $\pi\left(p_{4,k}\right) = p_{4,k}$, $k = 1, \dots, 6$, for $\pi = (13), (24)$, and that

$$p_{2,2} = \sum_{0\le a<b} \varepsilon_{babb}\left(X^{babb} + X^{bbba}\right) = \sum_{0\le a<b} \varepsilon_{babb}\sigma_4^a \frac{\alpha_{(b-a)(b-a)}}{2}\beta_{(b-a)0} \in K[\sigma_4, \alpha_{aa}, \beta_{a0} : 0 \le a],$$

$$p_{2,3} = \sum_{0\le a<b} \varepsilon_{baaa}\left(X^{baaa} + X^{aaba}\right) = \sum_{0\le a<b} \varepsilon_{baaa}\sigma_4^a \alpha_{(b-a)0} \in K[\sigma_4, \alpha_{a0} : 0 \le a],$$

$$p_{2,4} = \sum_{0\le a<b} \varepsilon_{abaa}\left(X^{abaa} + X^{aaab}\right) = \sum_{0\le a<b} \varepsilon_{baaa}\sigma_4^a \beta_{(b-a)0} \in K[\sigma_4, \beta_{a0} : 0 \le a],$$

$$p_{2,5} = \sum_{0\le a<b} \varepsilon_{aabb}\left(X^{aabb} + X^{baab} + X^{bbaa} + X^{abba}\right) = \sum_{0\le a<b} \varepsilon_{aabb}\sigma_4^a \alpha_{(b-a)0}\beta_{(b-a)0} \in K[\sigma_4, \alpha_{a0}, \beta_{a0} : 0 \le a],$$

$$p_{2,6} = \sum_{0\le a<b} \varepsilon_{abab}X^{abab} = \sum_{0\le a<b} \varepsilon_{aabb}\sigma_4^a \frac{\beta_{(b-a)(b-a)}}{2} \in K[\sigma_4, \beta_{aa} : 0 \le a],$$

$$p_{2,7} = \sum_{0\le a<b} \varepsilon_{baba}X^{baba} = \sum_{0\le a<b} \varepsilon_{baba}\sigma_4^a \frac{\alpha_{(b-a)(b-a)}}{2} \in K[\sigma_4, \alpha_{aa} : 0 \le a],$$

$$p_{3,1} = \sum_{0\le a<b<c} \varepsilon_{aabc}\left(X^{aabc} + X^{baac} + X^{bcaa} + X^{acba}\right) = \sum_{0\le a<b<c} \varepsilon_{aabc}\sigma_4^a \alpha_{(b-a)0}\beta_{(c-a)0} \in K[\sigma_4, \alpha_{a0}, \beta_{a0} : 0 \le a],$$

$$p_{3,2} = \sum_{0\le a<b<c} \varepsilon_{aacb}\left(X^{aacb} + X^{caab} + X^{cbaa} + X^{abca}\right) = \sum_{0\le a<b<c} \varepsilon_{aabc}\sigma_4^a \alpha_{(c-a)0}\beta_{(b-a)0} \in K[\sigma_4, \alpha_{a0}, \beta_{a0} : 0 \le a],$$

$$p_{3,3} = \sum_{0\le a<b<c} \varepsilon_{abac}\left(X^{abac} + X^{acab}\right) = \sum_{0\le a<b<c} \varepsilon_{abac}\sigma_4^a \beta_{(c-a)(b-a)} \in K[\sigma_4, \beta_{ab} : 0 \le a, b],$$

$$p_{3,4}=\sum_{0\le a<b<c}\varepsilon_{baca}\left(X^{baca}+X^{caba}\right)=\sum_{0\le a<b<c}\varepsilon_{abac}\sigma_4^a\alpha_{(c-b)(b-a)}\in K[\sigma_4,\alpha_{ab}:0\le a,b],$$

$$p_{3,5}=\sum_{0\le a<b<c}\varepsilon_{bbac}\left(X^{bbac}+X^{abbc}+X^{acbb}+X^{bcab}\right)=\sum_{0\le a<b<c}\varepsilon_{bbac}\sigma_4^a\alpha_{(b-a)0}\beta_{(c-a)(b-a)}\in K[\sigma_4,\alpha_{a0},\beta_{ab}:0\le a,b],$$

$$p_{3,6}=\sum_{0\le a<b<c}\varepsilon_{bbca}\left(X^{bbca}+X^{cbba}+X^{cabb}+X^{bacb}\right)=\sum_{0\le a<b<c}\varepsilon_{bbca}\sigma_4^a\alpha_{(c-a)(b-a)}\beta_{(b-a)0}\in K[\sigma_4,\alpha_{ab},\beta_{a0}:0\le a,b],$$

$$p_{3,7}=\sum_{0\le a<b<c}\varepsilon_{babc}\left(X^{babc}+X^{bcba}\right)=\sum_{0\le a<b<c}\varepsilon_{babc}\sigma_4^a\frac{\alpha_{(b-a)(b-a)}}{2}\beta_{(c-a)0}\in K[\sigma_4,\alpha_{aa},\beta_{a0}:0\le a],$$

$$p_{3,8}=\sum_{0\le a<b<c}\varepsilon_{abcb}\left(X^{abcb}+X^{cbab}\right)=\sum_{0\le a<b<c}\varepsilon_{abcb}\sigma_4^a\alpha_{(c-a)0}\frac{\beta_{(b-a)(b-a)}}{2}\in K[\sigma_4,\alpha_{a0},\beta_{aa}:0\le a],$$

$$p_{3,9}=\sum_{0\le a<b<c}\varepsilon_{ccab}\left(X^{ccab}+X^{accb}+X^{abcc}+X^{cbac}\right)=\sum_{0\le a<b<c}\varepsilon_{ccab}\sigma_4^a\alpha_{(c-a)0}\beta_{(c-a)(b-a)}\in K[\sigma_4,\alpha_{a0},\beta_{ab}:0\le a,b],$$

$$p_{3,10}=\sum_{0\le a<b<c}\varepsilon_{ccba}\left(X^{ccba}+X^{bcca}+X^{bacc}+X^{cabc}\right)=\sum_{0\le a<b<c}\varepsilon_{ccba}\sigma_4^a\alpha_{(c-a)(b-a)}\beta_{(c-a)0}\in K[\sigma_4,\alpha_{ab},\beta_{a0}:0\le a,b],$$

$$p_{3,11}=\sum_{0\le a<b<c}\varepsilon_{cacb}\left(X^{cacb}+X^{cbca}\right)=\sum_{0\le a<b<c}\varepsilon_{cacb}\sigma_4^a\frac{\alpha_{(c-a)(c-a)}}{2}\beta_{(b-a)0}\in K[\sigma_4,\alpha_{ab},\beta_{a0}:0\le a,b],$$

$$p_{3,12}=\sum_{0\le a<b<c}\varepsilon_{acbc}\left(X^{acbc}+X^{bcac}\right)=\sum_{0\le a<b<c}\varepsilon_{acbc}\sigma_4^a\alpha_{(b-a)0}\frac{\beta_{(c-a)(c-a)}}{2}\in K[\sigma_4,\alpha_{a0},\beta_{ab}:0\le a,b],$$

$$p_{4,1}=\sum_{0\le a<b<c<d}\varepsilon_{abcd}\left(X^{abcd}+X^{adcb}+X^{cbad}+X^{cdab}\right)=\sum_{0\le a<b<c<d}\varepsilon_{abcd}\sigma_4^a\alpha_{(c-a)0}\beta_{(d-a)(b-a)}\in K[\sigma_4,\alpha_{a0},\beta_{ab}:0\le a,b],$$

$$p_{4,2}=\sum_{0\le a<b<c<d}\varepsilon_{abdc}\left(X^{abdc}+X^{acdb}+X^{dbac}+X^{dcab}\right)=\sum_{0\le a<b<c<d}\varepsilon_{abdc}\sigma_4^a\alpha_{(d-a)0}\beta_{(c-a)(b-a)}\in K[\sigma_4,\alpha_{a0},\beta_{ab}:0\le a,b],$$

$$p_{4,3}=\sum_{0\le a<b<c<d}\varepsilon_{acbd}\left(X^{acbd}+X^{adbc}+X^{bcad}+X^{bdac}\right)=\sum_{0\le a<b<c<d}\varepsilon_{acbd}\sigma_4^a\alpha_{(b-a)0}\beta_{(d-a)(c-a)}\in K[\sigma_4,\alpha_{a0},\beta_{ab}:0\le a,b],$$

$$p_{4,4} = \sum_{0\le a<b<c<d} \varepsilon_{bacd}\left(X^{bacd} + X^{bdca} + X^{cabd} + X^{cdba}\right) = \sum_{0\le a<b<c<d} \varepsilon_{bacd}\sigma_4^a\alpha_{(c-a)(b-a)}\beta_{(d-a)0} \in K[\sigma_4, \alpha_{ab}, \beta_{a0}: 0 \le a, b],$$

$$p_{4,5} = \sum_{0\le a<b<c<d} \varepsilon_{badc}\left(X^{badc} + X^{bcda} + X^{dabc} + X^{dcba}\right) = \sum_{0\le a<b<c<d} \varepsilon_{badc}\sigma_4^a\alpha_{(d-a)(b-a)}\beta_{(c-a)0} \in K[\sigma_4, \alpha_{ab}, \beta_{a0}: 0 \le a, b],$$

$$p_{4,6} = \sum_{0\le a<b<c<d} \varepsilon_{cadb}\left(X^{cadb} + X^{cbda} + X^{dacb} + X^{dbca}\right) = \sum_{0\le a<b<c<d} \varepsilon_{cadb}\sigma_4^a\alpha_{(d-a)(c-a)}\beta_{(b-a)0} \in K[\sigma_4, \alpha_{ab}, \beta_{a0}: 0 \le a, b].$$

This yields that $K[X_4]^G \subseteq K[\alpha_{ab}, \beta_{ab}: 0 \le a, b]$. Conversely, it is straightforward to show that the elements α_{ab}, β_{ab}, $0 \le a, b$, are G-invariants, which completes the proof.

Remark 2. Note that $K[X_4]^{S_4} = K[\sigma_1, \sigma_2, \sigma_3, \sigma_4] \subseteq K[X_4]^G = K[\alpha_{ab}, \beta_{ab}: 0 \le a, b]$, where

$$\sigma_1 = x_1 + x_2 + x_3 + x_4\,,$$
$$\sigma_2 = x_1x_2 + x_1x_3 + x_1x_4 + x_2x_3 + x_2x_4 + x_3x_4\,,$$
$$\sigma_3 = x_1x_2x_3 + x_1x_2x_4 + x_1x_3x_4 + x_2x_3x_4\,,$$
$$\sigma_4 = x_1x_2x_3x_4\,,$$

which can be verified by the simple computations given below.

$$\sigma_1 = \alpha_{10} + \beta_{10}\,, \qquad \sigma_2 = \alpha_{10}\beta_{10} + \frac{\alpha_{11}}{2} + \frac{\beta_{11}}{2}\,,$$
$$\sigma_3 = \frac{\alpha_{11}\beta_{10} + \alpha_{10}\beta_{11}}{2}\,, \qquad \sigma_4 = \frac{\alpha_{11}\beta_{11}}{4}\,.$$

The next theorem is our main result.

Theorem 3. The algebra $K[X_4]^G$ is freely generated by the set $\{\alpha_{10}, \alpha_{11}, \beta_{10}, \beta_{11}\}$.

Proof. Firstly, direct computations give that

$$\alpha_{ab} = \frac{\alpha_{11}\alpha_{(a-1)(b-1)}}{2}\,, \qquad \beta_{ab} = \frac{\beta_{11}\beta_{(a-1)(b-1)}}{2}$$

for $1 \le a, b$. This yields that the elements of the form $\alpha_{ab}, \beta_{ab}, 1 \le a, b$, are included in the algebra generated by $\alpha_{11}, \beta_{11}, \alpha_{n0}, \beta_{n0}, 1 \le n$, by induction.

Let $2 \le n = 2m$ be an even positive integer. Then by binomial expansion, we have that

$$\alpha_{10}^n = \alpha_{n0} + n(x_1^{n-1}x_3 + x_1x_3^{n-1}) + \cdots + \binom{n}{m-1}(x_1^{m+1}x_3^{m-1} + x_1^{m-1}x_3^{m+1}) + \binom{n}{m}\left(\frac{\alpha_{11}}{2}\right)^m$$
$$\alpha_{n0} = \alpha_{10}^n - n\alpha_{(n-2)0}\frac{\alpha_{11}}{2} - \cdots - \binom{n}{m-1}\frac{\alpha_{11}}{2}\alpha_{m(m-2)} - \binom{n}{m}\left(\frac{\alpha_{11}}{2}\right)^m$$

and hence, $\alpha_{n0} = \alpha_{(2m)0}$ is included in the algebra generated by the elements α_{10}, α_{11} by induction.

Now let $3 \le n = 2m + 1$ be an odd positive integer. Then,

$$\alpha_{10}^{n} = \alpha_{n0} + n(x_1^{n-1}x_3 + x_1x_3^{n-1}) + \cdots + \binom{n}{m}(x_1^{m+1}x_3^{m-1} + x_1^{m-1}x_3^{m+1})$$
$$\alpha_{n0} = \alpha_{10}^{n} - n\alpha_{(n-2)0}\frac{\alpha_{11}}{2} - \cdots - \binom{n}{m}\frac{\alpha_{11}}{2}\alpha_{m(m-2)}$$

and thus, $\alpha_{n0} = \alpha_{(2m+1)0}$ is included in $K[\alpha_{10}, \alpha_{11}]$. Similarly one may show that $\beta_{n0} \in K[\beta_{10}, \beta_{11}]$ for all $2 \leq n$.

The rest is to show that the elements $\alpha_{10}, \alpha_{11}, \beta_{10}, \beta_{11}$ are algebraically independent. For this purpose, we apply the Jacobian criterion [5]. The determinant

$$\begin{vmatrix} 1 & z & 0 & 0 \\ 0 & 0 & 1 & t \\ 1 & x & 0 & 0 \\ 0 & 0 & 1 & y \end{vmatrix}$$

filled by the entries with respect to the partial derivatives of the corresponding elements is nonzero, that completes the proof.

CONFLICT OF INTEREST

The authors stated that there are no conflicts of interest regarding the publication of this article.

AUTHORSHIP CONTRIBUTIONS

The authors contributed equally to this work

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ESKİŞEHİR TEKNİK ÜNİVERSİTESİ BİLİM VE TEKNOLOJİ DERGİSİ B- TEORİK BİLİMLER

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RESEARCH ARTICLE

NUCLEAR ASYMPTOTIC NORMALIZATION COEFFICIENT FOR $^{27}Al \rightarrow ^{26}Mg+p$ REACTION

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ABSTRACT

The $^{26}Mg(p,\gamma)^{27}Al$ reaction is important in nuclear astrophysics as it play a crucial role in understanding the nucleosynthesis processes in red giants and Wolf-Rayet stars. The $^{26}Mg(p,\gamma)^{27}Al$ reaction is responsible for the production of ^{27}Al in these stars, while the $^{26}Mg(^{3}He,d)^{27}Al$ reaction provides information on the asymptotic normalization coefficient for the ground state of ^{27}Al.The asymptotic normalization coefficient (ANC) method is an indirect method that provides information on the normalization of the overlap functions for a given reaction. This information is crucial for nuclear astrophysics as it allows for the calculation of the direct component of the reaction rate at astrophysical relevant energies.In this work, the angular distribution of the $^{26}Mg(^{3}He,d)^{27}Al$ reaction have been analyzed using separate sets of optical potentials via the Distorted Wave Born Approximation which allows for a better understanding of the reaction mechanism and the determination of the ANC. Consequently,thecross section and Astrophysical S factor for $^{27}Al \rightarrow ^{26}Mg + p$ have been calculated for the direct capture.

Keywords: Direct reaction, DWBA analysis, Asymptotic normalization coefficient, Nuclear astrophysics

1. INTRODUCTION

Nuclear astrophysics is a field that seeks to understand the processes involved in the production, evolution, and distribution of chemical elements in the universe. One of the challenges in this field is to explain the origin and abundance of heavier elements, such as those beyond iron, which are formed through processes involving fusion, neutron capture, and explosive events such as supernovae[1].

One important element in this regard is Aluminum-26 (^{26}Al), half-life of^{26}Al is determined as a($t_{1/2}$=7.2*10^5 y) [2]. This isotope is produced primarily through the Mg-Al cycle [2], a series of nuclear reactions that occur in the interiors of massive stars. Understanding the production and distribution of ^{26}Al is important because its decay produces gamma rays that are observable in the galaxy.The abundance of stable aluminum-27 (^{27}Al) is also an important consideration in nuclear astrophysics. This isotope is not produced in significant quantities through nuclear fusion, but rather through the slow capture of neutrons in the s-process [3], a type of nucleosynthesis that occurs in the orduring to later stages of stellar evolution. The ratio of ^{27}Al to ^{26}Al in the galaxy can provide insights into the correspondingadditions of the s-process and the Mg-Al cycle to the production of these isotopes [2].

Another challenge in nuclear astrophysics is to realizethe galactic distribution of^{26}Al. Observations have shown that the proportion of the ground level to the isomeric level in ^{26}Al varies acrossdifferent regions of the galaxy[4]. This ratio may be influenced by the destruction of ^{26}Si [4], which can decay into ^{26}Al. This process may occur in novae, which are explosive events that can produce significant amounts of ^{26}Al. Understanding the details of these processes is important for accurately modelling the production and distribution of ^{26}Al in the galaxy.

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2. ASYMPTOTIC NORMALIZATION COEFFICIENT

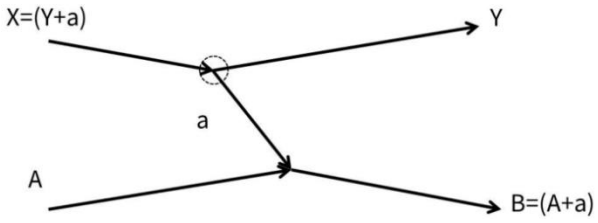

Figure 1: Sketch of a general transfer function

The ANC method, together with the DWBA formalism, permit to extract information on the nuclear structure of the initial and final states involved in the transfer reaction, and on the strength and energy dependence of the direct capture process A+a→B+γ at astrophysical energies. This information is important to understand the nucleosynthesis of heavy elements in stars and other astrophysical environments.It should be noted that the ANC method has some limitations and assumptions, such as the validity of the DWBA approximation, the neglect of higher-order effects in the transfer reaction, the assumption of a single-particle model for the bound state wave functions, and the dependence of the results on the choice of the potential model used to describe the nuclear interaction. Therefore, it is important to compare the results obtained with the ANC method with other experimental and theoretical approaches, and to carefully assess the uncertainties and systematic errors in the data analysis. In particular, the reactionA+a→B+γ can be studied via ANC in term of the radial overlap integral of a suitable one-particle transfer reaction A(X,Y)B, in which X=Y+A and B=A+a depicted in (Fig.1).This method has been carried out to a number of transfer reactions involvingα-particles [6], protons [4], neutrons [5], and indirect methods can be used to investigate nuclear reactions for astrophysics at the Gamow energies [7,8, 9].

One nucleon nuclear transfer reaction could be parameterized employing the distorted wave Born approximation (DWBA)[10]. This can be made as the spectroscopic factors -S relative to the initial and final states related to a particular bound state:

$$\frac{d\sigma}{d\Omega} = \sum_{j_B,j_X} S_{Aa,l_B,j_B}\, S_{Ya,l_X,j_X} \sigma^{DWBA}_{l_B,j_B,l_X,j_X}. \qquad (1)$$

the differential cross section can be expressed as

$$\frac{d\sigma}{d\Omega} = \sum_{Aa,l_B,j_B} \left(C^{B}_{Aa,l_B,j_B} C^{X}_{Ya,l_X j_X}\right)^2 \times\times \frac{\sigma^{DWBA}_{l_B,j_B,l_X,j_X}}{b^2_{Aa,l_B,j_B} b^2_{Ya,l_X,j_X}}. \qquad (5)$$

In Equation 5, the function $\sigma^{DWBA}_{l_B,j_B,l_X,j_X}$is the cross-section and it could be used to reproduce the angular DWBA.The ANC theory, as stated in the introduction, has an extension that allows determining the ANC's for the mirror nuclei. In the case of a proton transfer, in fact, the coefficients for the process A+p→B can be extracted from its appropriatemirror partner reaction D+n→E,D and having inverted number of protons and neutrons with respect to *A* and *B* (the vice versa is also valid) [11-12]. Therefore possible to extract the ANC's for the direct capture into bound states and the and the $\Gamma_p$for the resonant ones of ^{26}Mg(p,γ)^{27}Al, applying the ANC method on data for the ^{26}Mg(^{3}He,d)^{27}Al reaction.

3. DWBA METHOD

The ^{26}Mg (^{3}He, d) ^{27}Al low energy nuclear reaction has been interpreted with the help of the DWBA, In the DWBA formalism, the scattering amplitude is obtained by multiplying the distorted wave functions

of the incoming and outgoing particles with the transition matrix element, which describes the probability of transferring a nucleon from the projectile to the target nucleus. The distorted wave functions are obtained by solving the Schrödinger equation with the appropriate optical potentials[10].The DWBA calculation also requires knowledge of the spectroscopic factor, which describes the overlap between the wave function of the initial state of the projectile and the final state of the residual nucleus[10].The full finite-range approximation takes into account the finite range of the nuclear interaction and improves the accuracy of the DWBA calculation. The DWUCK-5 and FRESCO codes are widely used for DWBA calculations in nuclear physics.In this paper, I applied full finite-range approximation using DWUCK-5[13], and FRESCO code [14] within the DWBA. The DWBA calculation with the full finite-range approximation and the appropriate optical potentials and spectroscopic factors provides a powerful tool for understanding the structure of nuclei and the mechanisms of the ^{26}Mg (^{3}He, d) ^{27}Al nuclear reactions.Here, the entrance channel optical potential parameters were taken from the experimental [15],and exit channel optical potential parameters were obtained from the experimental d+^{27}Al[15]. The optical potential model parameters could be shown in the real and imaginary part oftotal potential

$$U = V_C(r_C) - V_0\big(f(x_0)\big) + \frac{\hbar^2}{m_\pi c} V_{LS}(LS)\frac{1}{r}\frac{d}{dr} f(x_{LS}) - i\left[W_v(x_v) - 4w_D \frac{d}{dx_D}\, f(x_D)\right] \quad (6)$$

In the optical potential formula of (6), real potential is responsible for scattering and imaginer potential is responsible for absorbing. Here, V_o, $V_{LS}$and V_C (r_C) representsthe real part of potential, the spin-orbit term and the Coulomb potential, respectively. W_V and W_D are the depth of the volume term and the depth of surface term for the imaginary part of the potential, respectively. In order to calculate DWBA, the radial dependence of form of the Woods – Saxon volume potential was used. Obtained parameters for Wood- Saxon are that Real potential-V_0 = - 47.56, Coulomb radius-r_C= 1.25 and diffuseness parameter- a_C=0.65

Table 1. Optical potential parameters for of ^{26}Mg (^{3}He,d)^{27}Al reaction and corresponding to SF and ANC coefficient .

Parameter	**^{3}He**	**D-I**	**D-II**	**D-III**
V_r (MeV)	217.6	76.75	89.17	85.81
r_r	1.15	1.25	1.13	1.13
a_r	0.636	0.737	0.8	0.75
W_W	32.5	--------	-------	------
W_S	---------	13.5	12.35	12.35
r_i	1.4	1.25	1.4	1.325
a_i	0.936	0.738	0.6	0.55
V_{so}	6.2	6.2	6.2	6.2
r_{so}	1.01	1.01	1.01	1.01
a_{so}	0.75	0.75	0.75	0.75
r_c	1.25	1.25	1.25	1.25
SF	--------	0.37	0.34	0.3

Optical potential parameters for exit and entrance channel are presented in Table.1. The results of DWBA calculation compared to the different experimental data are presented in Figures 2. a,b and c. Thetheoretical astrophysical S- factor quantity in MeV has been calculated inoperating the RADCAP code [17], employing a potential model for the Woods-Saxon well of the ^{26}Mg + p compound system. The potential is adjusted to match the ANC value. This calculation shows that the S(E) is nearly constant between 0 and 2 MeV. This range was selectedtaking into account the Gamow windows and Gamow energies (E_G) for the process at the temperatures reported in [18].

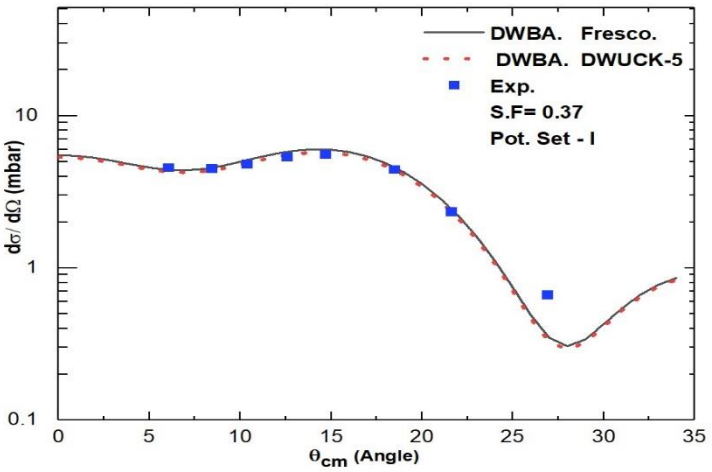

Figure 2 (a)

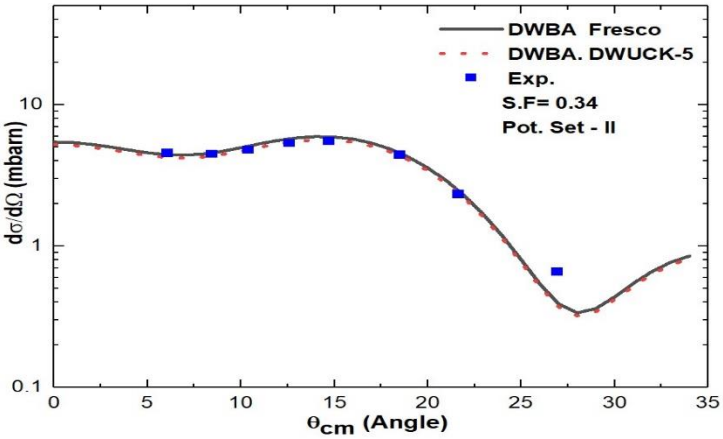

Figure 2. (b)

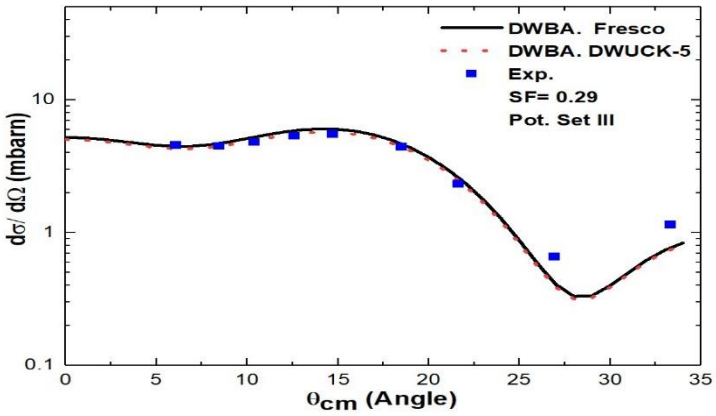

Figure 2. (c)

Figure 2. The experimental and theoretical ^{26}Mg (^{3}He,d)^{27}Al reaction differential cross sections for the transitions leading to the ground state in^{27}Al with the incident energy of 25 MeV. Blue square dots refer to experimental angular distributions from Vernotte[15]. FRESCO and DWUCK-5 codes were compared black curve and red dashed line. D-I, D-II and D-III optical potential used for producing theoretical angular distributions depicted in Figure 2. (a) and Figure 2. (b), and Figure 2. (c), respectively.

4. SUMMARY AND CONCLUSION

This paper describes a study on the one proton transfer reaction $^{26}Mg(^{3}He,d)^{27}Al$, which is important for determining nuclear asymptotic normalization coefficients (ANCs) and investigating astrophysical S-factors and cross sections. The paper reanalyses the experimental angular distribution for this reaction, leading to the ground state of ^{27}Alin $1d_{5/2}$ were shown in Figures 2. (a,b-c).

Using the extracted ANC, the $^{26}Mg(p,ɣ)$ S-factors and cross section for capture to the ground state were calculated depicted in Figune 4. And Figure 5. without the need for additional normalization constants. In order to get ANC coefficient, angular momentum transfer at low angle is crucial, one can understand that DWBA theory explain very well experimental data at low angles. DWBA method and experimental data consisted at very low angles. The squares of proton asymptotic normalization coefficient (ANC) for $^{27}Al \rightarrow {}^{26}Mg + p$ is extracted to be 8.2 ± 2 $fm^{-1}$from the angular distributions of the $^{26}Mg(^{3}He,d)^{27}Al$ reaction leading to ground state of ^{27}Al based on DWBA theory. The ANC coefficient of projectile ^{4}He interrelated to the vertex $^{3}He \rightarrow d+p$ in the channel is recognised with the high certainty and its value is also determined as a $(C_{He}{}^{4})^{2}= 3.90 \pm 0.06$ fm^{-1}. [20].This parameter used for analysis of determining ANC of ^{27}Al.

The paper also discusses the extraction of the proton ANC of $^{27}Al \rightarrow {}^{26}Mg + p$ using the wave function of ^{27}Al presented in Figure3. The calculations show that applying the FR-DWBA with the suitable optical potential angular distributions for the ground state of ^{27}Al are able to theoretically reproduce the experimental data in the locality of the first peak, which was sufficient for determining an ANC of ^{27}Al from the reaction. The theoretical angular distributions were obtained using Dwuck-5 and Fresco codes, which showed the same behaviour and results which are depicted in Figures 2. (a-b-c). We also calculated spectroscopic factor depending on different optical potential sets which is crucial for determination of ANC presented in Table-1.

However, I also note that the contribution of the reaction rate $^{27}Al \rightarrow {}^{26}Mg + p$ mainly comes not only from direct contribution but also from resonance contributions such as $J^{\Pi}=5/2^{+}$, $J^{\Pi}=1/2^{+}$, and $J^{\Pi}=3/2^{-}$. Therefore, additional computations were needed to include these other resonance contributions in the total S-factor and reaction rate calculation.

In summary, the ANC method is a useful indirect technique for studying nuclear reactions, especially direct capture, and has been successfully applied to transfer reactions involving protons, neutrons, and α-particles. The method involves determining the radial overlap integral of a suitable one-particle transfer reaction, which can be parameterized using the distorted wave Born approximation and spectroscopic factors. The radial overlap function can also be described in the asymptotic limit using the Wittaker function and Sommerfeld parameter[21]. The ANC method can be extended to determine ANC's for mirror nuclei, and can be used to extract ANC's for direct capture and resonant states in nuclear reactions which is $^{26}Mg(p,\gamma)^{27}Al$, using data from the $^{26}Mg(^{3}He,d)^{27}Al$ reaction. Because of lacking experimental data for ground state transition of $^{26}Mg(p,\gamma)^{27}Al$ reaction, i presented here just theoretical S-factor and Cross section data. Furthermore, this reaction has special interest for nuclear astrophysics and we plan to investigate experimental investigation of $^{26}Mg(p,\gamma)^{27}Al$ reaction in near future to get experimental S-factor and cross section for ground state contribution.

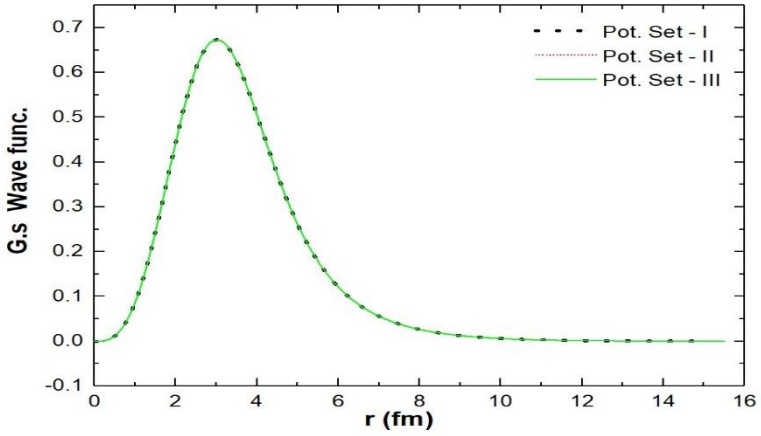

Figure 3. Extracted wave functions in terms of different optical potential parameters of Set –I, II and III.

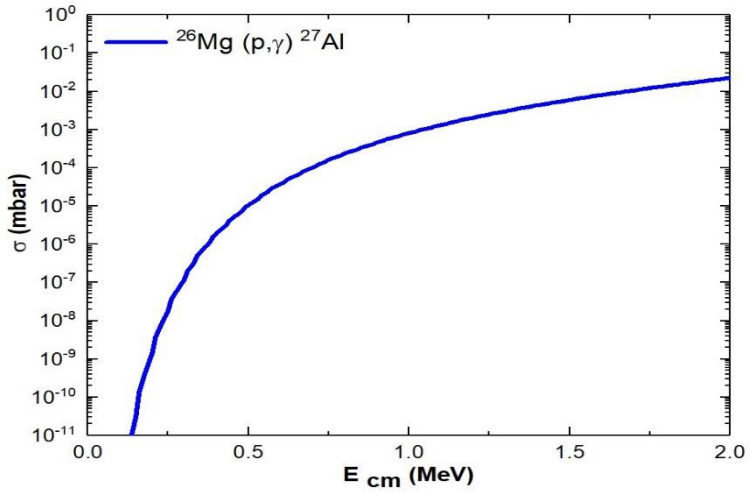

Figure 4. Direct contribution cross-section of ^{26}Mg (p, g) ^{27} Al reaction calculated using ANC method.

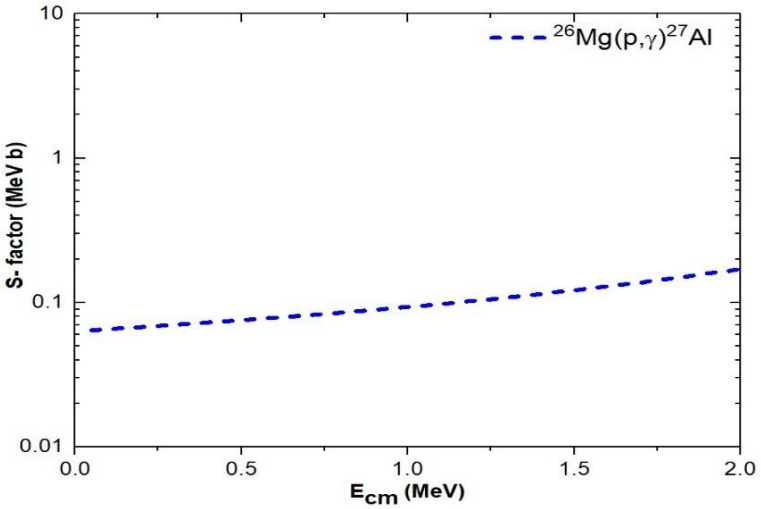

Figure 5. Direct contribution S- factor of ^{26}Mg (p, g) ^{27} Al reaction calculated using ANC method.

4. SUMMARY AND CONCLUSION

This paper describes a study on the one proton transfer reaction $^{26}Mg(^{3}He,d)^{27}Al$, which is important for determining nuclear asymptotic normalization coefficients (ANCs) and investigating astrophysical S-factors and cross sections. The paper reanalyses the experimental angular distribution for this reaction, leading to the ground state of ^{27}Alin $1d_{5/2}$ were shown in Figures 2. (a,b-c).

Using the extracted ANC, the $^{26}Mg(p,\gamma)$ S-factors and cross section for capture to the ground state were calculated depicted in Figure 4. And Figure 5. without the need for additional normalization constants. In order to get ANC coefficient, angular momentum transfer at low angle is crucial, one can understand that DWBA theory explain very well experimental data at low angles. DWBA method and experimental data consisted at very low angles. The squares of proton asymptotic normalization coefficient (ANC) for $^{27}Al \rightarrow {}^{26}Mg + p$ is extracted to be 8.2 ± 2 $fm^{-1}$from the angular distributions of the $^{26}Mg(^{3}He,d)^{27}Al$ reaction leading to ground state of ^{27}Al based on DWBA theory. The ANC coefficient of projectile ^{4}He interrelated to the vertex $^{3}He \rightarrow d+p$ in the channel is recognised with the high certainty and its value is also determined as a $(C_{He}{}^{4})^{2}= 3.90 \pm 0.06$ fm^{-1}. [20].This parameter used for analysis of determining ANC of ^{27}Al.

The paper also discusses the extraction of the proton ANC of $^{27}Al \rightarrow {}^{26}Mg + p$ using the wave function of ^{27}Al presented in Figure 3. The calculations show that applying the FR-DWBA with the suitable optical potential angular distributions for the ground state of ^{27}Al are able to theoretically reproduce the experimental data in the locality of the first peak, which was sufficient for determining an ANC of ^{27}Al from the reaction. The theoretical angular distributions were obtained using Dwuck-5 and Fresco codes, which showed the same behaviour and results which are depicted in Figures 2. (a-b-c). We also calculated spectroscopic factor depending on different optical potential sets which is crucial for determination of ANC presented in Table-1.

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In summary, the ANC method is a useful indirect technique for studying nuclear reactions, especially direct capture, and has been successfully applied to transfer reactions involving protons, neutrons, and α-particles. The method involves determining the radial overlap integral of a suitable one-particle transfer reaction, which can be parameterized using the distorted wave Born approximation and spectroscopic factors. The radial overlap function can also be described in the asymptotic limit using the Wittaker function and Sommerfeld parameter[21]. The ANC method can be extended to determine ANC's for mirror nuclei, and can be used to extract ANC's for direct capture and resonant states in nuclear reactions which is $^{26}Mg(p,\gamma)^{27}Al$, using data from the $^{26}Mg(^{3}He,d)^{27}Al$ reaction. Because of lacking experimental data for ground state transition of $^{26}Mg(p,\gamma)^{27}Al$ reaction, i presented here just theoretical S-factor and Cross section data. Furthermore, this reaction has special interest for nuclear astrophysics and we plan to investigate experimental investigation of $^{26}Mg(p,\gamma)^{27}Al$ reaction in near future to get experimental S-factor and cross section for ground state contribution.

CONFLICT OF INTEREST

The author stated that there are no conflicts of interest regarding the publication of this article.

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ESKİŞEHİR TEKNİK ÜNİVERSİTESİ BİLİM VE TEKNOLOJİ DERGİSİ B- TEORİK BİLİMLER

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RESEARCH ARTICLE

VIBRATIONAL SPECTROSCOPIC STUDY OF PYRIDINE AND PYRIMIDINE LIGANDS COORDINATED WITH ANTIMONY (III) COMPLEXES: INSIGHTS FROM DFT CALCULATIONS

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ABSTRACT

By employing the Scaled Quantum Mechanics Force Field (SQMFF) methodology, a comprehensive analysis was conducted to assign the vibrational spectra of three antimony (III) compounds, [1a-3a], that possess pyridine and pyrimidine ligands. The potential energy distribution (PED) was calculated and utilized to assign the IR spectra of the antimony (III) compounds. The theoretical frontier molecular orbital descriptors, the partial and total density of state distribution (TDOS, PDOS), molecular electronic potential surface map (MEP), nonlinear optical properties (NLO) of these complexes also were computed and investigated. The DFT/B3LYP/GEN (C, H, N, Cl: 6-31G(d,p) and Sb: LanL2DZ) level was utilized for all DFT calculations using the Gaussian 09W program. Furthermore, theoretical frontier molecular orbital descriptors, including electronegativity, chemical potential, softness, electrophilicity index, and electron affinity for six antimony (III) compounds were calculated ([1a/1b-3a/3b]). The results showed that, the ionization potential energy value of the [3a], which had the lowest experimental Leishmania activity, was also found to be the lowest among the others.

Keywords: Antimony (III) compounds, Scaled Quantum Mechanical Force Field, Nonlinear Optics, Infrared Spectra, Density Functional Theory

1. INTRODUCTION

Although antimony is known to be poisonous and carcinogenic, it has been used in medicine for several centuries [1]. The use of antimony complexes ranges from cosmetics to medicine to ancient Egypt [2,3]. The use of antimony in medicine has been widely reported in publications since ancient times [4,5]. Antimony compounds against microbes and parasites are widely used in many applications in medicine [6–9]. Strong antiproliferative activity is shown by antimony(III) complexes against human cancer cells. Some pentavalent antimony compounds are now used effectively in medicine to treat leishmaniasis [10]. Medical practice studies on the use of antimony compounds for anti-leishmania disease have already been published [11–13]. The use of antimony compounds as anthelminthic [10], antitrypanosomal [13,14], antibacterial [15,16], antifungal [17], and anticancer [18–21] agents is just one of the many possible applications for these compounds in the fields of medicine and pharmacy. Additionally, antimony compounds are widely used as catalysts in organic synthesis [14–16].

In 2007, Khalil et al., in their study with antimony complexes of planar tridentate pyridine ligands, showed that 2-acetylpyridine and tridentate Schiff base ligands derived from various acid hydrazides and Sb complexes are soluble in water. It has been concluded that it can be useful in the treatment of various health problems as it is water soluble [17]. Six new $SbBr_3$-Py (Py: Pyridine) crystalline complexes were obtained and structurally characterized in the literature [18]. The structural characteristics of two novel $SbCl_3$-Py crystalline complexes were obtained by Dovydova et al. [19].

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To investigate vibrational and electronic properties, Density functional theory (DFT) evaluation of complicated inorganic molecules such as Antimony (III) coordination compounds before experimentation can save valuable resources and time, and increase the probability of obtaining meaningful results. Antimony (III) containing complexes have been found to exhibit greater efficacy in treating when compared to free ligands. Theoretical studies with antimony complexes are very few in the literature. Theoretical DFT-based QSAR research and glutathione reductase inhibitory action of the title complexes were reported by Tunç et al [20–22]. Tunç et al. synthesized and studied several novel antimony(III) complexes, and they looked into the compounds' anti-leishmanial properties [21,22]. In vitro, research was done on the inhibitory effects of promastigote and glutathione reductase. They describe the antibacterial, DNA-cleaving, and glutathione reductase inhibitory activities of fourteen novel antimony(III) complexes [20]. The vibrational harmonic frequencies of the antimony (III) compounds [1a-3a] were calculated in this study using the DFT/B3LYP/GEN (C, H, N, Cl: 6-31G(d,p) and Sb: LanL2DZ) level and the Gaussian 09W program. To acquire a satisfactory assignment for the observed IR spectra of the complexes in the solid phase, the calculated frequency was refined using the Scaled Quantum Mechanical (SQM) approach and Total Energy Distribution (TED). Electronic properties (partial density of states, molecular electrostatic potential and nonlinear optical effect) of the bis($L^{1,2,3}$)trichloroantimony(III) and bis($L^{1,2,3}$)tribromoantimony(III) complexes (*L^1:2-aminopyridine, L^2: 2-amino-5-methylpyridine and L^3: 2-aminopyrimidine* [1a/1b-3a/3b]) have not been done yet. The same level was used to determine the frontier molecular orbital descriptors, total and partial density of state distribution (TDOS, PDOS), molecular electronic potential surface map (MEP), and nonlinear optical properties (NLO) hyper-polarizability effects of six antimony (III) compounds [1a/1b-3a/3b].

2. MATERIALS and METHODS

2.1. Theoretical Calculations

Utilizing the advanced analytical tool Gaussian 09W quantum chemical software [27] and the Lee-Yang-Parr correlation functional (B3LYP) [28–30] approaches with the C, H, N, Cl: 6-31G(d,p) and Sb: LanL2DZ basis set [31–33], the molecular structure of the title compounds was optimized. Gaussian 09W quantum chemical software was used in all simulated calculations with B3LYP/GEN (C, H, N, Cl: 6-31G(d,p) and Sb: LanL2DZ) [23]. The total and partial density of states (TDOS and PDOS) have been determined to estimate the moieties' contributions to frontier orbitals. Gauss Sum 2.2.1 program generated TDOS and PDOS data are used to determine the contribution of groups to molecular orbitals [24].

The visual technique known as molecular electrostatic potential (MEP) enables us to identify the position of the electron density. A well-known instrument for displaying the reactive behaviors of molecules is the electrical potential: V(r)

$$\mathrm{V(r)} = \sum_A \frac{Z_A}{(R_A - r)} - \int \frac{\rho(r')}{(r' - r)} \mathrm{d}(r') \quad (1)$$

Where $\rho(r')$ is the electronic density function, the nucleus A's charge, called Z_A, is situated at R_A [25–27]. Using theoretical calculations, the map of molecular electrostatic potential was examined to observe and gather information about the molecule's variable-charged areas.

Based on the finite field technique [28], the first static hyperpolarizability (β) and related properties (dipole moment, mean polarizability, and anisotropy of polarizability) have been estimated at the DFT/ B3LYP method and GEN (C, H, N, Cl: 6-31G(d,p) and Sb: LanL2DZ) level.

For the relevant optimized structure, the cartesian coordinates force fields were translated to the internal coordinates [29,30]. Scaled factors were used to scale the elements of the internal force constant matrix (Fij(scaled)) (si and sj).

$$F_{ij}(\text{scaled})=(s_i)^{1/2}F_{ij}(s_j)^{1/2} \quad (2)$$

The scaling factor is required to align each theoretical vibrational frequency with the experimental data. The scaling factors were used from the Computational Chemistry Comparison and Benchmark Database (CCCBDB) and subsequently applied to the obtained vibrational frequencies. The Scaled Quantum Mechanic (SQM) [31] tool was used to scale the quantum mechanical force fields to obtain these internal coordinate forces (Table 1).

For fitting the calculated fundamental wavenumbers to the appropriate experimental, scaled the F=[Fij] matrix was used.

Table 1. Scale factors (si)

Vibrations		Bonds	Final Scale factor
Stretching	1	X-X	1.073
	2	C-H	0.794
	3	Cl-Sb	0.964
	4	N-H	1.043
Bending	5	C-C-H	0.961
	6	C-X-X	1.001
	7	C-N-Sb	1.072
Torsion	8	X-X-X-X	0.887

The merit function χ^2 defines the scaling factor optimization strategy;

$$\chi^2(s_i) = \sum\{[v_i^{exp} - v_i^{theor}(s_i)]w_i\}^2 \quad (3)$$

The percentages of stretching, bending, or torsion that contribute to a specific normal mode were determined by the potential energy distribution (PED).

2.2. Experimental studies

Sigma-Aldrich (USA) was used to purchase all reagents, compounds, and solvents. The synthesis of chlorine and bromine-linked antimony was obtained in this study, as it was synthesized by Tunç et al. in 2016, according to the procedure in previous studies [22]. Synthesis of the complex compounds were done as in the literature [20–22]. In this study, Antimony(III) chloride was dissolved in the same solvent at a mole ratio of 2:1 in hydrochloric acid, and 25 mL of the ligand solution was added. After being refluxed for two days at 60 C, the mixture was concentrated to a third of its original volume and left to stand at room temperature for crystallization. Filters were used to create colorless, yellow, and pink crystals, which were then dried in the air. The syntheses of [1a-3a] complexes were obtained experimentally. The Perkin Elmer Spectrum Two with U-ATR spectrometer was used to observe the Fourier Transform-Infrared Spectra (FT-IR).

3. RESULTS and DISCUSSION

3.1. General Remarks on Geometry

Pyridine and pyrimidine ligands with the formation of SbX_3L_2 (X: Cl and Br, *L^1:2-aminopyridine*, *L^2: 2-amino-5-methylpyridine and L^3: 2-aminopyrimidine*) complexes given in the list below.

[1a]: *[Sb(2-aminopyridine)$_2$Cl$_3$]*
[1b]: *[Sb(2-aminopyridine)$_2$Br$_3$]*
[2a]: *[Sb(5-methyl-2-aminopyridine)$_2$Cl$_3$]*
[2b]: *[Sb(5-methyl-2-aminopyridine)$_2$Br$_3$]*
[3a]: *[Sb(2-aminopyrimidine)$_2$Cl$_3$]*
[3b]: *[Sb(2-aminopyrimidine)$_2$Cl$_3$]*

The geometrical characteristics of Sb-L_2 and Sb-X_3 fragments in the complexes are similar. The atom labelling scheme is shown in Figure 1 and the calculated geometric parameters (bond lengths and angles) are summarized in Table 2. The density functional theory at B3LYP/GEN (C, H, N, Cl: 6-31G(d,p) and Sb: LanL2DZ) was used to thoroughly optimize the ground state structures**.**

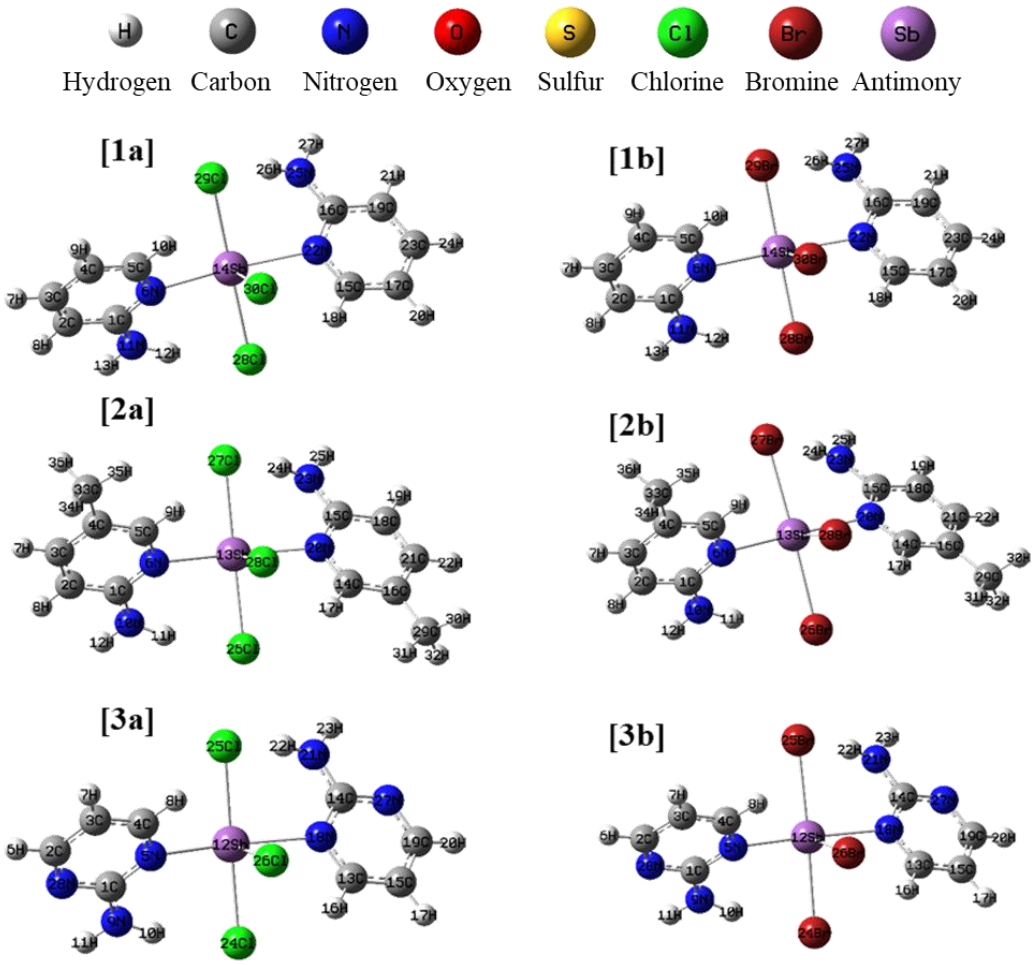

Figure 1. The ground state optimized structure of the complexes.

When we look at the structural parameters of metal halide, Sb-Cl bond length is about 2.66 Å, while Sb-Br bond length is 2.80-2.90 Å. is in the range. All three molecules have a similar structure and trans geometry. The equatorial angles (N-Sb-N) are in varied from 167-172°. Cl-Sb-Cl angle is in the range of 176-179°, planar.

Table 2. Selected calculated structural parameters of the complexes (X = Cl, Br)

R	**[1a]**	**[1b]**	**R**	**[2a]**	**[2b]**	**R**	**[3a]**	**[3b]**
C_1-C_2	1.41	1.42	C_1-C_2	1.42	1.42	C_1-N_5	1.36	1.36
C_1-N_6	1.36	1.35	C_1-N_6	1.37	1.37	C_1-N_9	1.35	1.35
C_1-N_{10}	1.37	1.37	C_1-N_{10}	1.37	1.37	C_1-N_{28}	1.35	1.35
C_2-C_3	1.38	1.38	C_2-C_3	1.39	1.39	C_2-C_3	1.40	1.40
C_2-H_8	1.09	1.09	C_2-H_8	1.09	1.09	C_2-H_6	1.09	1.09
C_3-C_4	1.40	1.42	C_3-C_4	1.42	1.42	C_2-N_{28}	1.33	1.33
N_6-Sb_{14}	2.47	2.49	N_6-Sb_{13}	2.47	2.48	N_5-Sb_{12}	2.47	2.49
Sb_{14}-X_{28}	2.66	2.80	Sb_{13}-X_{26}	2.66	2.91	Sb_{12}- X_{24}	2.65	2.80
Sb_{14}-X_{29}	2.66	2.80	Sb_{13}-X_{27}	2.66	2.91	Sb_{12}-X_{25}	2.65	2.80
Sb_{14}-X_{30}	2.43	2.57	Sb_{13}-X_{28}	2.50	2.68	Sb_{12}-X_{26}	2.43	2.57
(°)	**[1a]**	**[1b]**	**(°)**	**[2a]**	**[2b]**	**(°)**	**[3a]**	**[3b]**
C_7-C_1-N_6	120	120	C_7-C_1-N_6	120	120	N_5-C_1-N_9	119	119
N_6-C_1-N_{11}	119	119	N_6-C_1-N_{10}	119	119	N_9-C_1-N_{28}	117	117
C_1-C_2-C_3	120	120	C_1-C_2-C_3	120	120	C_1-C_2-H_6	121	121
C_5-C_4-H_9	120	120	C_5-C_4-C_{33}	121	121	N_5-C_4-H_8	116	117
C_4-C_5-N_6	123	123	C_4-C_5-N_6	124	124	C_1-N_5-C_4	118	118
N_6-Sb_{14}-X_{28}	92	94	N_6-Sb_{13}-X_{26}	92	93	N_5-Sb_{12}-X_{26}	83	86
N_6-Sb_{14}-X_{29}	87	87	N_6-Sb_{13}-X_{27}	88	87	N_{18}-Sb_{12}-X_{24}	87	94
N_6-Sb_{14}-X_{30}	84	86	N_6-Sb_{13}-X_{28}	84	86	N_{18}-Sb_{12}-X_{25}	93	85
N_{22}-Sb_{14}-X_{28}	88	88	N_{20}-Sb_{13}-X_{26}	88	87	$N_{18}Sb_{12}$-X_{26}	83	92
N_{22}-Sb_{14}-X_{29}	92	92	N_{20}-Sb_{13}-X_{27}	92	93	N_{24}-Sb_{12}-X_{26}	89	92
N-Sb-N	168	172	N-Sb-N	167	172	N-Sb-N	166	170
X-Sb-X	177	179	X-Sb-X	178	176	X-Sb-X	178	179

3.1. Frontier Molecular Orbital Parameters and PDOS

In this section, Frontier molecular orbital parameters and the partial density of state results are given. The highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO), sometimes known as frontier molecular orbitals, are particularly well-liked quantum chemical characteristics. They determine a molecule's light-absorbing capacity and molecular reactivity. According to Koopmans theorem equations, these descriptors can be expressed as chemical potential $\mu=(E_{HOMO}+E_{LUMO})/2$, chemical hardness $\eta=(E_{HOMO}-E_{LUMO})/2$, global softness $S=1/\eta$ and electrophilicity index $\omega= \mu^2/2\eta$ from the orbital energy gap [32,33].

Table 3 contains a list of descriptors for the antimony (III) compounds [1-3a/b]. Additionally, the table includes information on the anti-leishmanial activity of these compounds. Notably, [3a] exhibits the strongest anti-leishmanial activity among the tested compounds, as evidenced by its highest HOMO value, lowest energy gap, and lowest chemical hardness. The global hardness value is directly related to the stability of the chemical system. [3b] has the highest electrophilicity index (ω).

Table 3. Global reactivity properties and antileishmanial activity

Molecular Properties (eV)	**[1a]**	**[2a]**	**[3a]**	**[1b]**	**[2b]**	**[3b]**
E_{LUMO}	-1.69	-1.62	-2.05	-1.76	-1.69	-2.07
E_{HOMO}	-6.43	-6.23	-6.69	-6.04	-5.97	-6.28
$\Delta E_{HOMO-LUMO}$	-4.74	-4.61	***-4.64***	-4.28	-4.28	-4.21
Ionisation Potential (IP)	6.43	6.23	6.69	6.04	5.97	6.28
Electron Affinity (EA)	1.69	1.62	2.05	1.76	1.69	2.07
Chemical Hardness (η)	2.37	2.31	2.32	2.14	2.14	2.11
Electronegativity (χ)	4.06	3.93	4.37	3.90	3.83	4.18
Chemical Potential (μ)	-4.06	-3.93	-4.37	-3.90	-3.83	-4.18
Softness (S) ev^{-1}	0.42	0.43	0.43	0.47	0.47	0.48
Electrophilicity index (ω)	3.48	3.34	4.12	3.55	3.43	***4.14***
LC_{50} (M)*	$2.19x10^{-5}$	$1.40x10^{-4}$	$1.47x10^{-5}$			

*Antileishmanial activity [34]

The population analysis was calculated and presented in Figure 2. In PDOS plots and the structure of fragment orbitals that are a part of molecular orbitals–demonstrated. Where, the groupings of N-Sb-Cl/Br, Ring, N-H, and other atoms have been divided at the PDOS. A bonding interaction supported the PDOS's positive value, whereas an anti-bonding interaction contends that are negative values and non-binding interactions imply values very near to zero.

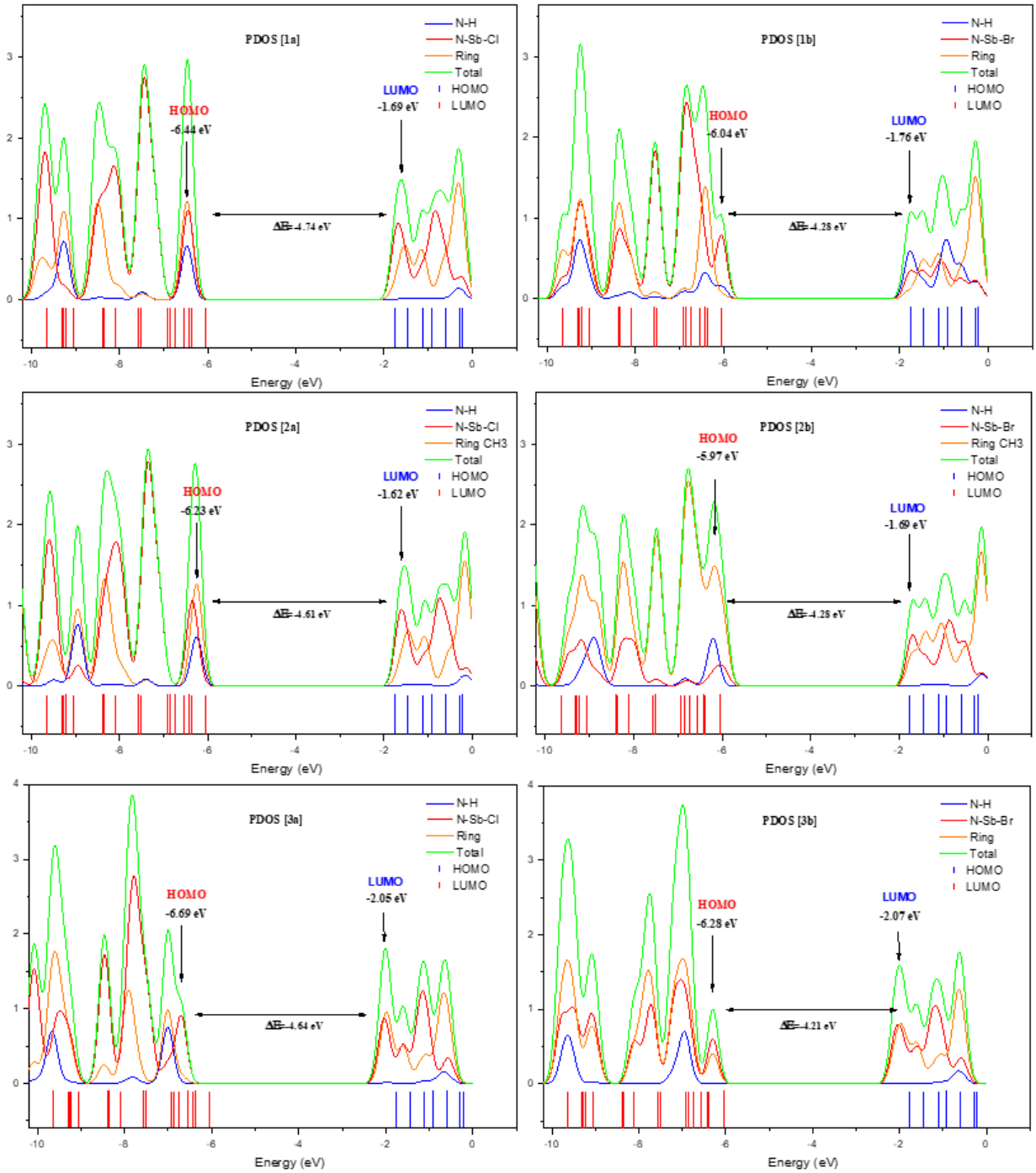

Figure 2. The partial density of state diagrams

As shown in Figure 2, the partial density of state plot (PDOS) primarily illustrates the structure of the fragment orbitals that contribute to the molecular orbitals. The HOMO LUMO orbital distributions of each compound are shown in the graph Figure 2. Table 4 shows the calculated contribution percentages

of the molecular orbitals. The partial density of state plot (PDOS) mainly presents the composition of the fragment orbitals contributing to the molecular orbitals which is seen from Figure 2. The calculated contribution percentage of the structures are listed in Table 4. As seen in the Table 4, HOMO-LUMO orbitals are localized on the N-Sb-X (X=Cl, Br) and their contributions are about 59-90 %.

Table 4. The calculated contribution percentage of the complexes from PDOS

		The contribution percentage			
		eV	N-Sb-Cl	Ring	N-H
[1a]	LUMO	-1.69	81	18	0
	HOMO	-6.43	89	8	3
			N-Sb-Br	Ring	N-H
[1b]	LUMO	-1.76	75	20	5
	HOMO	-6.04	68	26	6
			N-Sb-Cl	Ring CH_3	N-H
[2a]	LUMO	-1.62	81	18	0
	HOMO	-6.23	62	30	8
			N-Sb-Br	Ring CH_3	N-H
[2b]	LUMO	-1.69	61	38	0
	HOMO	-5.97	59	41	0
			N-Sb-Cl	Ring	N-H
[3a]	LUMO	-2.05	65	35	0
	HOMO	-6.69	90	9	1
			N-Sb-Br	Ring	N-H
[3b]	LUMO	-2.07	78	12	0
	HOMO	-6.28	60	40	0

3.2. Molecular Electronic Potential Surface

A method for illustrating the distribution of electrostatic potential is the molecular electrostatic potential (MEP) surface. Different colours are used to represent the various electrostatic potential levels at the surface. Potential increases from red-orange-yellow-green-blue, with blue denoting the highest electrostatic potential energy and red denoting the lowest. Molecular electrostatic potential (MEP) provide the distribution, molecular structure, size, and dipole moments of the complexes, and allowing the reader to comprehend electrophilic attack and nucleophilic interactions. In Figure 3, the negative (red) portions of MEP were linked to electrophilic reactivity, whereas the positive (blue) regions were linked to nucleophilic reactivity. The negative (red) and positive (blue) regions of MEP were connected to electrophilic and nucleophilic reactivity, respectively. According to Figure 3, there are two possible targets for electrophilic attack on complex compounds, negative areas are mostly around N-Sb-X (X: Cl, Br), while the positive ones around the nitrogen atoms.

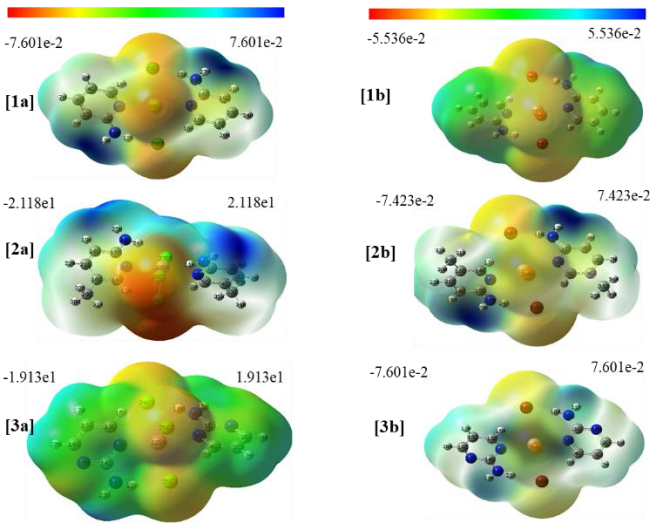

Figure 3. Molecular electronic potential surface of the complexes

3.3. First Hyperpolarizability

For emerging technologies in fields like communication, signal processing, and optical interconnections, such as frequency shifting, optical modulation, switching, and logic, nonlinear optical (NLO) activity provides essential functions [35,36]. The first hyperpolarizability of a system in the presence of an applied electric field is a third-rank tensor that may be characterized by a 3x3x3 matrix, and the energy of a system is a function of the electric field. Using the x, y, and z components, the total static dipole moment (μ), mean polarizability ($<\alpha_{tot}>$), anisotropy of polarizability (Δα), and first-order hyperpolarizability (β_{tot}) can be determined as follows:

$$\mu = (\mu_x^2 + \mu_y^2 + \mu_z^2)^{1/2} \quad (4)$$

$$<\alpha_{tot}> = 1/3\ (\alpha_{xx} + \alpha_{yy} + \alpha_{zz}) \quad (5)$$

$$\Delta\alpha = 2^{-1/2}[(\alpha ii-\alpha jj)^2+(\alpha ii-\alpha kk)^2+(\alpha jj-\alpha kk)^2+6\alpha xx^2]^{1/2} \quad (6)$$

$$\beta_i = (\beta_{iii} + \beta_{ijj} + \beta_{ikk}) \text{ and } i, j, k = x, y, z \quad (7)$$

$$\beta_{tot} = (\beta_x+\beta_y+\beta_z)^{1/2} \quad (8)$$

With the calculating by using the schemes of the B3LYP/GEN value of electric dipole moment, polarizabilities and first hyperpolarizabilities for the title complexes were tabulated in Table 5 ($\Delta\alpha_{tot}\times10^{-23}$ esu and $\beta_{tot}\times10^{-31}$ esu). αi, β_{ikk} components of the polarizability and first hyperpolarizability can be seen in Table S1 (Supplementary Information). Since the polarizabilities and hyperpolarizabilities of the Gaussian 03 outputs are presented in atomic units (a.u.), the predicted values have been transformed into electrostatic units by using α: 1a.u. = 0.1482×10^{-24} esu and β; 1a.u. = 8.6393×10^{-33} esu, respectively. Along the z-axis, the highest dipole moment was identified for all complexes. Among the complexes, the largest dipole moment is μ=10.77 Debye [2b] and the lowest molecular dipole moment is μ=0.25 Debye [3b]. At the same time [3b] complex has β_{tot}=241.85 a.u. and it has a relatively higher average polarizability Δα (a.u.) value than the others. x, y, and z components of dipole (μ), polarizability (α), and first-order hyperpolarizability (β) were given in the Table S1 (Supplementary information).

Table 5. The calculated dipole moment, polarizabilities and first-order hyperpolarizabilities of the complexes

μ&α	**[1a]**	**[2a]**	**[3a]**	**[1b]**	**[2b]**	**[3b]**
μ (Debye)	1.24	1.02	0.64	1.13	10.77	0.25
<α> (a.u.)	216.33	243.56	207.36	240.49	473.20	231.43
Δα (×10^{-23} esu)	7.73	8.60	7.40	8.19	21.40	7.86
βx	6.03	2.15	-0.63	-3.22	2.84	-7.37
βy	-8.12	-10.79	-5.01	-3.99	-0.07	-0.39
βz	15.76	24.63	115.98	105.06	-1851.43	241.73
β_{tot} (a.u.)	18.73	26.98	116.09	105.19	1851.44	241.85
βtot (×10^{-31} esu)	1.62	2.33	10.03	9.09	159.95	20.89

α (1 a.u.) = 0.1482×10^{-24} esu; β (1 a.u.) = 8.6393×10^{-33} esu

Table S1. x, y, and z components for dipole (μ), polarizability (α), and first-order hyperpolarizability (β)

μαβ	**[1a]**	**[2a]**	**[3a]**	**[1b]**	**[2b]**	**[3b]**
μx	1.00E-07	-1.90E-06	2.20E-06	1.48E-05	2.79E-05	1.19E-05
μy	4.30E-06	7.70E-06	-5.10E-06	-1.16E-05	8.19E-05	3.00E-06
μz	-1.24	-1.02	-0.45	-1.13	-10.77	-0.25
αxx	292.32	326.24	279.32	311.69	786.73	298.55
αxy	-16.48	-16.98	-19.28	-18.80	70.06	-22.13
αyy	207.55	228.73	206.32	235.56	362.80	233.35
αxz	0.00	0.00	0.00	0.00	0.00	0.00
αyz	0.00	0.00	0.00	0.00	0.00	0.00

αzz	149.11	175.70	136.44	174.23	270.07	162.39
βxxx	0.67	-0.78	-0.38	-2.81	0.93	-0.94
βxxy	-2.15	-3.12	-2.89	-0.34	0.49	0.09
βxyy	3.14	4.80	-1.92	0.18	0.67	-2.74
βyyy	-7.06	-6.89	-1.58	-2.49	0.65	1.07
βxxz	-2.72	28.97	86.18	46.61	512.11	153.95
βxyz	135.92	-119.45	-111.91	-139.97	-829.97	-115.28
βyyz	136.47	76.27	148.80	181.00	-1592.29	193.04
βxzz	2.22	-1.87	1.67	-0.59	1.24	-3.69
βyzz	1.08	-0.77	-0.54	-1.16	-1.21	-1.56
βzzz	-117.99	-80.61	-118.99	-122.55	-771.25	-105.25

3.4. Vibrational Spectral Analysis

The title compound's vibrational frequencies were made, and the calculated results were contrasted with experimental FT-IR spectra in this section. The scaled quantum mechanical force field (SQM-FF) methodology has been applied to the theoretically anticipated wavenumbers using the SQM program. Depending on the type of Hessian calculations, it is expected that the harmonic wavenumbers estimated for a molecule will greatly exceed the corresponding actual wavenumbers. The SQM-FF method, which applies an effective empirical scaling process to the calculated harmonic wavenumbers or, more preferably, to the calculated harmonic force constants, can successfully correct these overestimations even though they are not completely systematic [27, 28]. These findings suggest that the calculated expected frequencies match the observed infrared values quite well. According to the SQMFF technique, the average percentage error RMS was found to be 11.09, 12.64, and 14.26 for the [1a-3a] complexes, respectively (see Table 6).

Table 6. RMS values of SQM calculation

	[1a]	**[2a]**	**[3a]**
RMS error	11.09	12.64	14.26
Pre-fingerprint region	4.51	1.59	12.71
Fingerprint region (500-2500 cm^{-1})	12.60	11.69	15.62
Post-fingerprint region	2.35	16.55	11.30

Total Energy Distribution (TED), which is produced by the SQMFF technique, was used to create characterized normal mode descriptions and interpret them. The TED components quantify the contribution of each internal coordinate to the external coordinates. The descriptions of the internal coordinates utilized in the TED computations are provided in Table S2-S4. Experimental and calculated-SQM infrared spectrums of the complexes [1a-3a] shown in the Figure 4, 5 and 6.

Table S2. The vibrational wavenumbers, harmonic and scaled (SQM) frequencies (cm−1), IR intensities, TED and assignments of [1a]

		B3LYP		SQM		Exp.	
No		$Freq^{Har}$	I_{IR}	$Freq^{SQM}$	I_{IR}^{SQM}	IR^{Exp}	Mode Description and TED>%5
1	A	27	1.25	26	1.4		τHClClH(52)+τSbClHN(28)+δClSbN(12)+δClHN(12)
2	A	28	4.08	28	4.1		τSbClHN(36)+τHClClH(71)
3	A	40	2.28	40	2.3		τSbClHN(242)+τHNCC(16)
4	A	46	0.28	46	0.3		τSbClHN(135)+δClHN(28)+δHNC(11)
5	A	71	1.15	70	1.1		τHClSbCl(60)+τSbClHN(58)+δSbClH(16)
6	A	85	1.20	84	1.1		τClHNC(78)+tClHNH(145)+tHNCN(88)
7	A	97	3.31	97	3.4		δHNCl(52)+δSbClH(14)+τSbClHN(50)
8	A	113	4.14	112	3.5		δHClSb(52)+τClHNC(50)+τClHNH(32)+τHClSbCl(20)
9	A	123	39.13	121	0.4		δSbClH(65)+τHNCN(26)
10	A	125	0.66	123	44.6		νClH(64)+δHClSb(30)+δClSbCl(13)+τSbClNH(27)
11	A	135	18.12	133	13.8		δClHN(76)+τClSbCl(27)
12	A	136	0.42	135	0.2		νClH(83)+νHSb(11)+τClHNC(62)+τClHNH(40)
13	A	141	14.31	143	14.5		νClH(83)+νHSb(11)+τClHNC(62)+τClHNH(40)
14	A	171	0.11	170	101.8		νSbCl(17)+νSbH(15)+τHClSbCl(25)+τClHNC(12)+τClHNH(11)
15	A	172	108.82	171	0.4		δClHN(27)+τClHNC(164)+τClHNH(119)+τHCLCLH(9)
16	A	216	43.30	210	29.7		νClSb(11)+τCCCN(18)+τCNCN(10)+τClHNC(15)

17	A	220	2.84	216	2.8			νClSb(30)+τCCCN(14)+τSbClHN(30)
18	A	235	0.55	233	0.0			νClSb(31)+νClH(15)+τSbClHN(26)
19	A	241	88.27	240	104.9			νClSb(69)+νClH(11)
20	A	313	30.63	318	28.7			νClSb(95)
21	A	430	16.98	405	17.0			δCCN(36)
22	A	433	10.09	409	5.4			δCCC(16)+δCCN(16)+τSbClHN(16)
23	A	437	26.99	432	22.0			δNCC(62)+τClHNH(13)
24	A	438	2.37	434	10.9			δCCN(30)+δCNC(25)+τClHNH(36)
25	A	475	26.42	458	32.5			τHNCN(22)+τHNCN(20)+τClHNH(36)+τClHNC(11)
26	A	479	88.01	461	96.5			δNCC(11)+τHNCC(21)+τHNCN(21)
27	A	529	7.90	501	8.7	496	m	τRing(54)
28	A	529	29.63	501	24.0			τRing(54)
29	A	571	0.28	558	2.3	549	w	δCCN(22)
30	A	572	13.14	559	16.8			δCCN(22)+τClHNC(25)+τClHNH(15)
31	A	652	73.29	646	145.4	626	m	τSbClHN(100)
32	A	653	33.11	648	199.3			τSbClHN(100)
33	A	659	78.11	654	1.0	653	m	τClHNC(22)
34	A	663	250.82	656	72.6			βCCC(13)+τClHNC(28)+τSbClHN(76)
35	A	755	10.70	720	13.3	719	w	τRing(44)+τSbClHN(13)
36	A	756	0.07	721	8.1			τCCCH(15)+τCNCC(15)+tHCCN(14)+tSbClHN(13)
37	A	781	39.69	749	37.2			τCCCH(48)+τHCCN(25)
38	A	782	77.09	749	74.0	763	m	τCCCH(48)+τHCCN(25)
39	A	862	22.09	824	45.0			νCN(53)+νCC(8)+δCCC(13)
40	A	864	1.11	827	0.0			νCN(53)+νCC(8)+δCCC(13)
41	A	864	6.35	831	2.8			τCCCH(14)+τHCCH(13)+τHCCN(18)
42	A	864	4.51	831	8.4			τCCCH(14)+τHCCH(13)+τHCCN(18)
43	A	973	0.04	916	0.0			τHCCH(46)+τHCCC(18)+τHCCC(16)
44	A	974	0.25	917	0.4			τHCCH(46)+τHCCC(18)+τHCCC(16)
45	A	1004	0.52	949	0.1			τHCCH(74)
46	A	1004	0.12	949	0.4			τCCCH(25)+τHCCH(48)
47	A	1016	75.62	987	116.5			δCNC(34)+νCN(29)
48	A	1018	0.68	991	1.2	993	w	δCNC(34)+νCN(29)
49	A	1081	29.26	1082	7.0			δHNC(36)+νCC(17)
50	A	1082	0.33	1083	0.0			δHNC(33)+νCC(17)
51	A	1085	1.46	1096	0.3			νCC(50)ring
52	A	1085	0.00	1097	0.0	1119	w	νCC(50)ring
53	A	1166	1.72	1150	13.8			νCN(25)+δHCC(25)
54	A	1167	2.20	1151	0.0	1164	w	νCN(15)+δHCC(28)
55	A	1190	17.33	1193	16.2			δHCC(76)
56	A	1190	8.78	1193	11.8	1190	w	δHCC(76)
57	A	1320	71.61	1252	55.5	1234	w	νCN(29)+νCC(23)
58	A	1322	1.95	1254	0.0			νCN(29)+νCC(23)
59	A	1371	42.30	1318	55.1			νCN(54)+νCC(12)
60	A	1371	10.59	1318	27.8	1321	m	νCN(54)+νCC(12)
61	A	1382	1.08	1370	31.0			δNCH(22)+δHCC(15)+δHNC(15)
62	A	1383	0.08	1370	5.8	1382	m	δNCH(22)+δHCC(15)+δHNC(15)
63	A	1494	60.56	1483	85.7	1472	m	δCCH(27)+νCC(15)
64	A	1495	37.61	1483	58.3			δCCH(28)+νCC(14)
65	A	1539	97.31	1525	84.7			δHCN(28)+δHCC(18)
66	A	1541	68.43	1527	58.1	1544	m	δHCN(28)+δHCC(18)
67	A	1621	74.78	1632	57.7	1621	s	νCC(54)
68	A	1621	25.26	1632	16.4			νCC(54)
69	A	1667	136.36	1674	122.2	1661	s	δHCH(49)+δHCH(17)
70	A	1668	0.65	1675	25.7			δHCH(49)+δHCH(17)
71	A	1697	259.89	1697	37.3			νCC(36)+νCN(21)
72	A	1698	88.21	1698	205.1			νCC(36)+νCN(21)
73	A	3195	8.76	3138	9.3			νHC(98)
74	A	3195	2.78	3138	2.4			νHC(98)
75	A	3210	23.61	3153	23.5			νHC(95)
76	A	3210	4.04	3153	4.0			νHC(94)
77	A	3228	0.43	3170	0.4	3169	m	νHC(95)
78	A	3228	1.80	3170	1.6			νHC(95)
79	A	3241	0.75	3183	0.7			νHC(97)
80	A	3241	15.21	3183	14.7	3184	m	νHC(97)
81	A	3416	722.76	3346	722.0	3343	s	νHN(96)
82	A	3416	11.43	3347	11.6			νHN(96)
83	A	3670	104.88	3597	104.8			νHN(95)

84	A	3671	33.51	3597	33.3	3600	m	νHN(95)

[Har] Harmonic vibrational frequencies. Freq[SQM], Calculated from SQM frequencies, I[IR] Infrared intensities
ν, stretching; δ, bending; τ, torsion.

Table S3. The vibrational wavenumbers, harmonic and scaled (SQM) frequencies (cm^{-1}), IR intensities, TED and assignments of [2a]

		B3LYP		SQM		Exp.		
No		Freq[Ha]	I_{IR}	Freq[SQ]	I_{IR}^{SQM}	IR[Exp]		Mode Description and TED>%5
1	A	26	0.85	24	0.86			τSbClHN(84)
2	A	29	4.10	28	4.10			τSbClHN(100)
3	A	34	0.00	34	0.00			τSbClHN(81)+δHClSb(23)+δClHN(23)
4	A	35	2.60	35	2.57			τSbClHN(217)+δHClSb(17)
5	A	70	0.53	69	0.44			τSbClHN(95)+τHClSbCl(11)+δHClSb(17)
6	A	79	0.40	78	0.33			τClHNC(170)+τClHNH(151)
7	A	88	0.04	85	0.08			τHCCC(62)+τClHNH(27)+τClHNC(32)
8	A	88	0.58	85	0.32			τHCCC(84)
9	A	91	3.49	90	3.87			δClHN(68)+τSbClHN(29)+τClHNH(28)
10	A	106	3.51	105	3.29			νClH(14)+δSbClH(31)+τClHNC(29)+τHClSbCl(26)
11	A	116	18.12	114	16.23			δClHN(22)+τHClSbCl(20)
12	A	118	0.04	116	0.02			δHClSb(79)+τHNCN(13)
13	A	122	0.14	121	0.05			τClHNC(82)+τClHNH(62)+νClH(22)+δClHN(20)
14	A	125	42.10	125	46.43			νClH(41)+δSbClH(25)+δClHN(12)+τSbClHN(39)
15	A	140	18.68	142	17.74			δClSbCl(61)+δHClSb(22)
16	A	152	0.21	151	0.31			νClH(64)+τClHNC(46)+τClHNH(41)
17	A	154	9.64	153	6.34			νClH(14)+νSbCl(11)+δClSbCl(18)+τSbClHN(15)
18	A	168	3.47	166	2.86			τClHNC(69)+τClHNH(40)
19	A	175	93.96	174	91.88			δClH(11)+τClHNC(18)+τHClSbCl(43)
20	A	224	123.19	226	122.14			νClSb(84)
21	A	224	0.63	227	0.76			νClSb(88)
22	A	309	25.23	310	11.54			νClSb(39)+δCCC(29)
23	A	319	27.76	312	25.80			δCCC(48)+τClHNC(19)+τClHNH(17)
24	A	321	3.63	315	1.27			δCCC(10)+τCCCC(12)+τCCCN(5)
25	A	324	0.82	315	4.41			τCCCC(12)+τCCCN(13)
26	A	325	0.78	320	15.68			νClSb(53)+δCCC(10)+tClHNC(44)+τClHNH(32)
27	A	438	12.91	424	14.40	422	w	τCC/NCC(18)+τSbClHN(11)
28	A	442	9.91	428	3.30			τCCCC(13)+τCNCC(17)+τSbClHN(30)
29	A	450	5.05	439	7.56			δCCN(40)+τHNCC(10)+τClHNH(14)
30	A	451	12.86	440	19.49			δCCN(21)+δNCN(15)+τClHNH(35)
31	A	469	39.97	458	32.59			δCCN(13)+τHNCC(17)+tHNCN(14)
32	A	472	67.53	460	69.58			δCCN(13)+τHNCC(17)+tHNCN(14)
33	A	490	5.21	475	9.67			νCC(10)+δNCN(15)+δCCC(13)+δCCC(11)
34	A	490	2.61	476	6.67	477	m	νCC(10)+δNCN(15)+δCCC(24)
35	A	531	6.53	515	6.76	512	m	τRing(33)
36	A	531	30.57	516	26.50			τRing(33)
37	A	656	144.92	647	146.98	645	w	τSbClHN(149)
38	A	660	290.84	650	233.11			τSbClHN(163)
39	A	676	5.27	660	1.08			τRing(45)+τSbClHC(33)
40	A	678	30.79	662	84.91			τClHNC(69)+τClHNH(10)
41	A	754	4.65	732	3.29			νCC(21)+δCCN(14)
42	A	754	8.57	732	6.76	740	w	νCC(21)+δCCN(14)
43	A	787	29.97	763	29.76	757	w	SbClHN(45)
44	A	789	6.81	764	14.93	789	w	τSbClHN(64)
45	A	834	22.97	817	22.16			τHCCN(60)
46	A	834	49.00	817	49.18	829	w	τHCCN(57)
47	A	874	42.42	835	59.77			νCC(29)+νCN(27)
48	A	877	0.09	838	0.00			νCC(29)+νCN(27)
49	A	923	1.17	895	0.90			τHCCC(60)
50	A	924	0.80	896	0.54			τHCCH(45)
51	A	990	0.03	961	0.01			τHCCH(61)
52	A	990	0.29	961	0.46			τHCCH(55)
53	A	1014	1.00	984	2.54			δHCC(31)
54	A	1014	0.00	984	0.01			δHCC(31)
55	A	1060	44.25	1030	59.36			δNCC(11)
56	A	1060	0.35	1030	0.41	1030	w	δNCC(11)
57	A	1073	2.34	1043	2.40			δHCC(62)
58	A	1073	3.57	1043	3.55	1054	w	δHCC(62)

59	A	1107	60.37	1082	49.28			δHNC(40)
60	A	1109	0.02	1084	0.01			δHNC(42)
61	A	1179	23.41	1147	31.10			δCCH(57)
62	A	1180	11.10	1148	11.99	1148	m	δCCH(56)
63	A	1253	19.79	1204	41.51	1212	w	νCC(38)
64	A	1254	0.12	1206	0.01	1230	w	νCN(30)+νCC(27)
65	A	1325	52.91	1258	26.01			νNC(48)+νCC(22)
66	A	1326	6.37	1259	1.29			νNC(48)+νCC(26)
67	A	1369	15.23	1311	19.42			νNC(40)+νCC(25)
68	A	1370	2.09	1312	5.91	1319	w	νNC(40)+νCC(25)
69	A	1377	32.19	1344	31.59	1342	m	δHNC(47)+δHCC(15)
70	A	1379	4.39	1345	4.59			δHNC(36)+δHCC(15)+δHNC(11)
71	A	1435	10.80	1397	95.73	1385	m	δHCH(48)
72	A	1435	2.35	1397	59.90			δCC(26)
73	A	1448	55.81	1418	2.16	1414	m	δCCC(95)
74	A	1448	29.74	1418	0.35			δCCC(95)
75	A	1499	4.06	1480	3.88	1455	m	δHCH(56)+δHCC(16)
76	A	1499	6.15	1480	5.94			δHCH(56)+δHCC(16)
77	A	1512	14.82	1490	18.64			δHCH(31)+δHCC(17)
78	A	1512	14.95	1490	18.09			δHCH(31)+δHCC(17)
79	A	1555	143.26	1500	137.26			νNC(22)
80	A	1557	104.17	1502	97.81			νNC(23)
81	A	1617	90.49	1566	85.16	1550	s	νCC(27)
82	A	1618	13.58	1567	6.70			νCC(27)
83	A	1675	83.45	1630	2.12	1624	s	νCC(25)
84	A	1675	3.23	1631	84.24			νCC(25)
85	A	1699	223.89	1658	174.43			δHNH(54)
86	A	1700	81.27	1660	60.88	1667	s	δHNH(52)
87	A	3044	53.54	3027	54.05			νHC_3(81)svm
88	A	3044	17.24	3028	17.24	3040	w	νHC_3(81)svm
89	A	3099	14.90	3082	17.01			νHC_3(100)assym
90	A	3099	16.53	3082	14.42	3090	w	νHC_3(100)assym
91	A	3136	12.88	3119	14.10			νHC_3(82)assym
92	A	3136	4.98	3119	3.82			νHC_3(81)assym
93	A	3184	21.17	3167	23.19	3155	m	νHC(93)
94	A	3184	1.25	3167	1.19			νHC(92)
95	A	3206	18.74	3188	18.03	3181	m	νHC(99)
96	A	3206	5.95	3188	5.86			νHC(99)
97	A	3222	0.22	3204	0.25			νHC(99)
98	A	3222	19.04	3205	17.06	3261	m	νNH(99)
99	A	3418	725.81	3265	726.33	3296	m	νHN(94)
10	A	3418	8.39	3266	8.58	3414	m	νHN(93)
10	A	3668	98.66	3506	98.19	3482	m	νHN(93)
10	A	3669	32.74	3506	32.70			νHN(93)

[Har] Harmonic vibrational frequencies. $Freq^{SQM}$, Calculated from SQM frequencies, I^{IR} Infrared intensities
ν, stretching; δ, bending; τ, torsion.vw, very weak; w, weak; m, medium; s, strong; vs, very strong.

Table S4. The vibrational wavenumbers, harmonic and scaled (SQM) frequencies (cm^{-1}), IR intensities, TED and assignments of [3a]

		B3LYP		SQM		Exp.	
No		$Freq^{Har}$	I_{IR}	$Freq^{SQM}$	I_{IR}^{SQM}	IR^{Exp}	Mode Description and TED>%10
1	A	21	1.03	19	1.10		τSbClHN(26)+τHClSbCl(34)+τHClClH(71)
2	A	26	0.93	26	0.95		δClHN(24)
3	A	43	0.98	42	0.99		δClHN(34)+τSbClHN(120)
4	A	43	1.31	43	1.34		τSbClHN(203)
5	A	73	1.95	72	1.83		τHClClH(17)
6	A	84	2.44	84	2.51		δHClSb(31)+τClHNC(62)+τClHNH(80)
7	A	96	2.49	96	2.56		τSbClHN(56)
8	A	112	4.01	111	3.48		δHClSb(104)+τClHNC(46)
9	A	120	0.11	118	0.05		δHClSb(89)+τClHNC(27)+τClHNH(48)
10	A	124	39.74	124	43.56		δClSbCl(72)
11	A	129	14.48	128	14.11		δClHN(47)
12	A	134	0.01	134	0.00		νClH(58)+δHClSb(28)
13	A	141	19.81	143	18.22		νClH(48)+δClHN(48)+τClHNC(24)
14	A	167	81.19	167	71.23		νClH(20)

15	A	170	1.90	169	2.42			νClH(45)
16	A	207	39.04	203	42.11			τSbClHN(109)
17	A	215	4.29	211	3.50			τSbClHN(109)
18	A	230	0.00	232	0.26			νClSb(84)+τSbClHN(38)
19	A	238	112.46	240	114.63			νClSb(92)
20	A	315	28.94	319	27.56			νClSb(94)
21	A	427	8.47	413	9.85			τCNCC(36)
22	A	430	6.35	417	5.29			τCNCC(89)
23	A	453	80.42	450	80.22	433	w	δNCN(60)+δClHN(30)
24	A	455	3.63	452	4.11	458	m	δNCN(44)+δClHN(50)
25	A	521	5.38	503	5.77	503	m	τNCCC(33)+τHCCC(14)
26	A	522	49.56	503	45.12			τNCCC(26)+τHCCC(26)
27	A	560	0.24	544	0.01	547	w	τHNCN(67)
28	A	563	195.89	546	179.02			τHNCN(68)
29	A	596	6.51	589	9.35			τClHNC(31)+τClHNH(16)
30	A	596	4.65	589	13.46	582	w	τClHNC(33)+τClHNH(18)
31	A	634	83.35	627	80.80			τSbClHN(187)+τHNCN(33)
32	A	637	165.50	629	177.70	640	m	τSbClHN(184)
33	A	662	49.28	657	43.25			δCNC(66)
34	A	664	1.50	659	1.25			δCNC(65)
35	A	802	28.47	778	32.20	777	m	τCNCN(28)
36	A	803	54.61	779	63.56			τHNCN(28)
37	A	813	7.15	798	3.60	792	m	τNCCC(23)+τNCNC(14)
38	A	814	11.06	798	3.52			τNCCC(23)+τNCNC(14)
39	A	890	38.12	864	41.44			νNC(65)
40	A	892	0.06	867	0.04	870	vw	νNC(65)
41	A	988	0.11	952	0.08			τHCCH(21)+τCCCH(22)
42	A	988	0.29	952	0.19			τHCCH(22)+τCCCH(22)
43	A	1009	3.18	973	0.60			τCCCH(35)+τHCCH(22)+tCNCH(20)
44	A	1009	0.15	973	0.13			τCCCH(35)+τHCCH(22)+tCNCH(20)
45	A	1014	8.63	994	8.53	988	m	νCC(6)+δCCC(10)
46	A	1015	0.46	995	0.06			νCC(6)
47	A	1062	32.97	1039	22.96			δHNC(26)+νNC(18)+νCC(15)
48	A	1063	0.15	1040	0.03	1045	vw	δHNC(26)+νNC(18)+νCC(15)
49	A	1113	7.66	1065	6.73			νCC(46)+νCN(10)
50	A	1114	1.76	1066	1.60	1067	vw	νCC(46)+νCN(10)
51	A	1162	3.47	1141	19.82	1115	m	δHCC(42)+νCC(14)
52	A	1163	0.25	1142	1.69	1196	w	δHCC(42)+νCC(13)
53	A	1283	78.79	1235	99.91	1213	m	νNC(67)+νCC(12)
54	A	1284	5.79	1236	7.90			νNC(66)+νCC(12)
55	A	1348	45.49	1338	49.82			δHNC(59)
56	A	1349	0.00	1339	0.00	1344	m	δHNC(57)
57	A	1402	61.87	1375	55.21			νCN(49)+δHCN(17)
58	A	1403	12.21	1376	11.71	1386	m	νCN(46)+δHCN(17)
59	A	1489	7.04	1468	10.06	1450	m	δHCC(53)+νCN(11)
60	A	1491	0.66	1470	0.01			δHCC(52)+νCN(11)
61	A	1526	172.25	1494	214.63			νNC(45)
62	A	1526	90.24	1494	109.55	1509	m	νNC(43)
63	A	1608	279.23	1547	301.71	1540	s	νCC(31)+νCN(15)
64	A	1609	59.69	1548	52.63			νCC(31)+νCN(15)
65	A	1653	188.38	1607	24.33			νCN(39)+νCC(14)
66	A	1654	0.03	1607	227.65	1620	s	νCN(39)+νCC(14)
67	A	1689	500.18	1667	372.02			δHNH(59)+νNH(13)
68	A	1689	160.76	1669	122.90	1660	vs	δHNH(59)+νNH(13)
69	A	3174	54.43	3127	54.51			νHC(99)
70	A	3174	0.35	3127	0.40	3145	m	νHC(99)
71	A	3225	0.00	3177	0.00	3160	m	νHC(93)
72	A	3225	9.31	3177	9.51			νHC(92)
73	A	3248	5.35	3199	4.80	3198	m	νHC(97)
74	A	3248	0.48	3199	0.68			νHC(97)
75	A	3442	205.37	3350	666.03	3347	m	νHN(94)
76	A	3442	462.15	3350	2.56			νHN(94)
77	A	3684	224.00	3586	223.57			νHN(93)
78	A	3684	50.95	3586	50.99	3589	w	νHN(93)

[Har] Harmonic vibrational frequencies. Freq[SQM], Calculated from SQM frequencies, I[IR] Infrared intensities
ν, stretching; δ, bending; τ, torsion.vw, very weak; w, weak; m, medium; s, strong; vs, very strong.

3.4.1. NH_2 Group Vibrations

The N–H stretches of primary aliphatic amines in the region of 3450-3160 cm^{-1}, give rise to two asymmetric and one symmetric stretching vibration. The νNH_2 vibration medium band was assigned at 3600 cm^{-1} and 3343 cm^{-1} [1a]. The corresponding calculated asymmetric and symmetric νNH_2 vibrations were found at 3597 cm^{-1}, 3346 cm^{-1} , and 3296 cm^{-1} in [1a] compound. In compound [2a], NH stretching vibration were observed as 3482 cm^{-1}, 3414 cm^{-1} and 3296 cm^{-1}, calculated 3506 cm^{-1}, 3266 cm^{-1} and 3265 cm^{-1}. In compound [3a], νNH_2 bands were observed at 3589 cm^{-1} and 3347 cm^{-1} and were calculated at 3589 cm^{-1} and 3350 cm^{-1}.

3.4.2. Aromatic C-H and CH_3 Group Vibrations

The characteristic aromatic and heteroaromatic C-H stretching vibrations are expected to appear in the wavenumber range 3000–3200 cm^{-1} [37,38]. The C-H stretching vibrations of the [1a] were observed at 3184, 3169 cm^{-1} in the FT-IR spectrum and calculated as 3183 cm^{-1} and 3170 cm^{-1}. C-H bands were [1] assigned 3181 3155 3090 3040 cm^{-1} assigned of number [2a] compounds. νHC vibrations were assigned experimental at 3198 cm^{-1}, 3145 cm^{-1} and calculation at 3199 cm^{-1}, 3177 cm^{-1} in [3a].
Fundamental $\nu(CH_3)$ stretching symmetric and asymmetric bands appear in the range 3090, 3040 cm^{-1} corresponding to the SQM frequencies 3119 cm^{-1}, 3082 cm^{-1}, and 3028 cm^{-1} respectively for the [2a]th compound because only [2a] has CH_3 group.

3.4.3. Sb-Cl Vibrations

Sb-Cl vibrations were calculated 216, 233, 240, and 318 cm^{-1} for [1a], 226, 227, and 310 cm^{-1} for [2a] and 232, 240 and 319 cm^{-1} for [3a]. 280 cm^{-1} and 308 cm^{-1} for νSbCl in the literature [39].

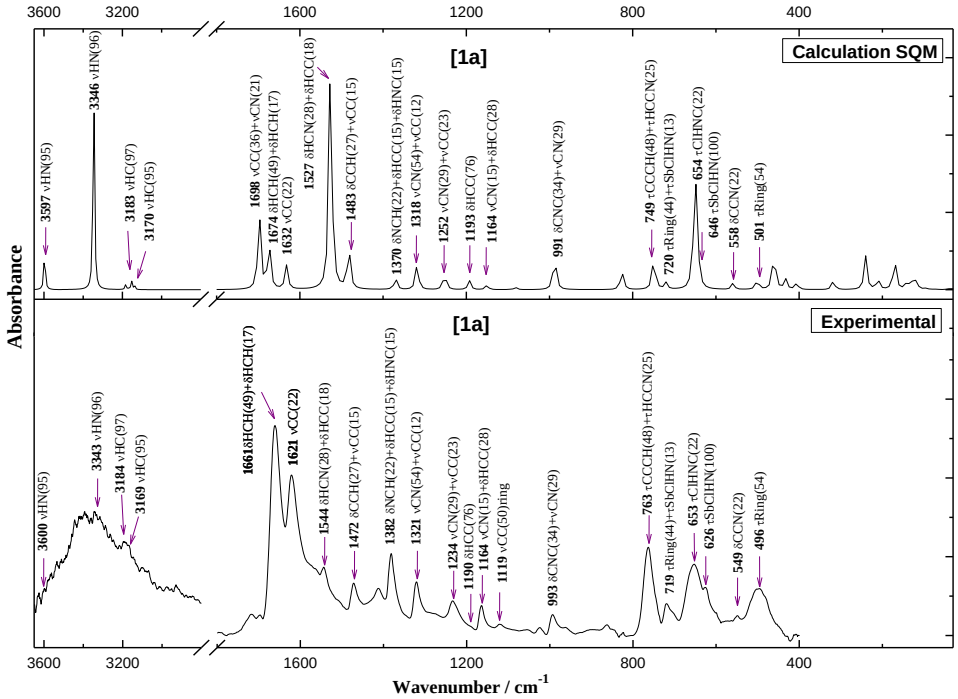

Figure 4. The experimental and simulated infrared spectrum of the complex [1a]

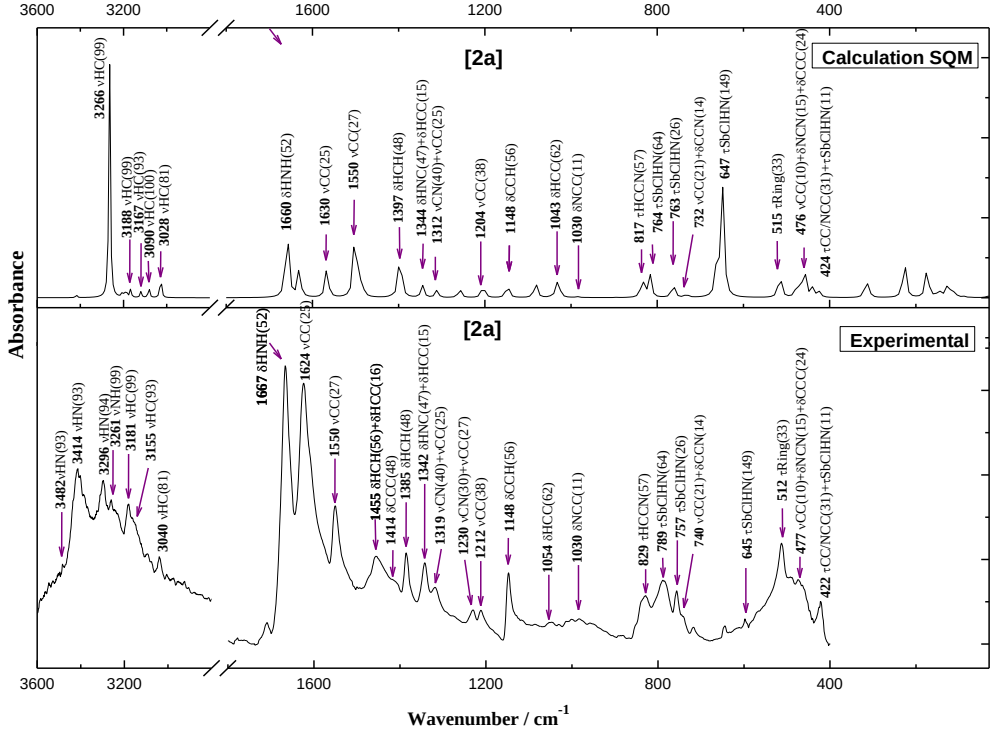

Figure 5. The experimental and simulated infrared spectrum of the complex [2a]

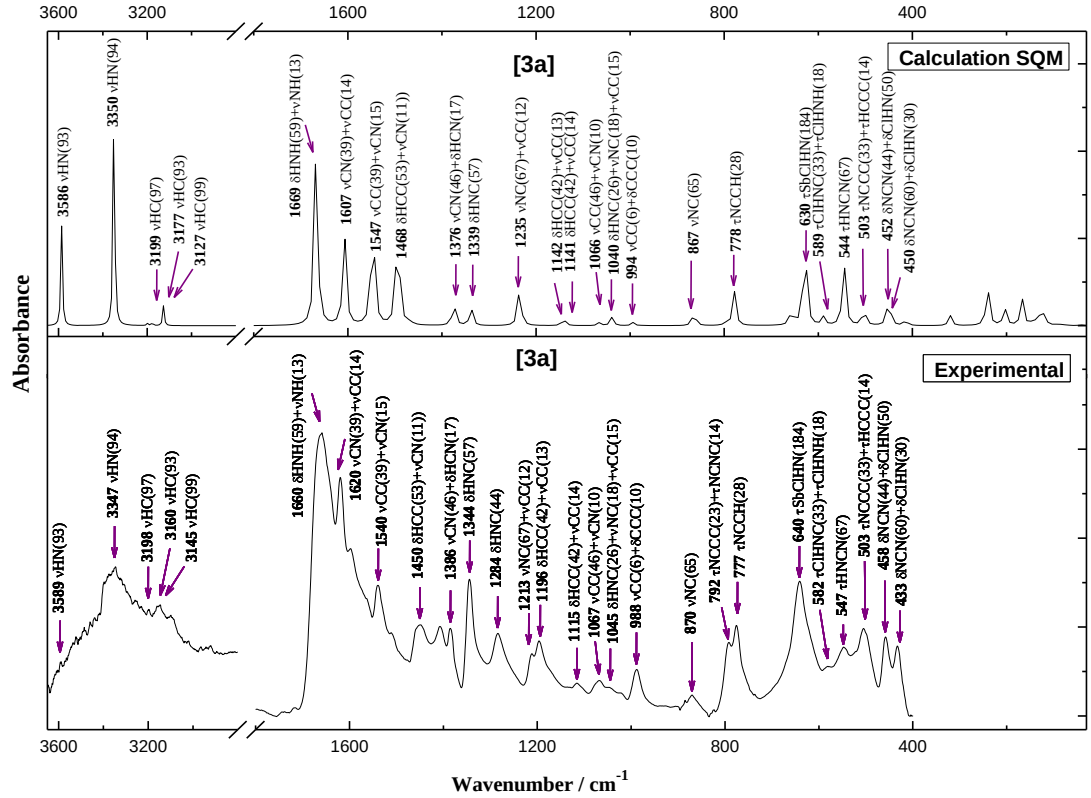

Figure 6. The experimental and simulated infrared spectrum of the complex [3a]

4. CONCLUSIONS

In this study, theoretical electronic and vibrational spectroscopic analyses of antimony (III) complexes were performed with B3LYP method GEN (C, H, N, Cl: 6-31G(d,p) and Sb: LanL2DZ) basis set. Six compounds' partial density of state diagram and the calculated PDOS contribution percentage have been investigated. The HOMO and LUMO orbitals are localized on mostly N-Sb-X (X: Cl, Br). As seen in the molecular electrostatic potential surface map, the negative charge is in the region on the N-Sb-Cl atoms. The calculation of first-order hyperpolarizability reveals that the [3b] complex has the lowest molecular dipole moment as μ = 0.25 Debye, β_{tot} ($\times 10^{-30}$) = 241.85 a.u. and it has a relatively higher average polarizability $\Delta\alpha$ (a.u.) value than the others. The RMS and mean average deviation of fundamental vibrations were found to be the average percentage error RMS was found to be 11.09, 12.64, and 14.26 for the [1a-3a] complexes, respectively. With the use of normal coordinate analysis, which was done by the scaled quantum mechanical force field methodology, the full interpretation of the vibrational spectra was carried out. According to RMS values, there is a fair agreement between experimental and predicted wavenumbers and assignments.

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CONFLICT OF INTEREST

No conflict of interest was declared by the authors.

AUTHORSHIP CONTRIBUTIONS

Berna Çatıkkaş: Writing – review & editing, Supervision, Methodology, Investigation, Conceptualization, Methodology, Calculation. **Özge Şahinler:** Visualition, Editing.

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ESKİŞEHİR TEKNİK ÜNİVERSİTESİ BİLİM VE TEKNOLOJİ DERGİSİ B- TEORİK BİLİMLER

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SOME RESULTS ON THE SMALLEST CARTESIAN GROUP PLANE

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ABSTRACT

Let π be the projective plane of order 25 coordinatised by elements of the smallest cartesian group. In this work, in some cases depending on the choice of the regular quadrangle it is shown that there is no any projective subplane of order 3 of π.

Keywords: Cartesian group, Algebraic structure, Projective plane

1. INTRODUCTION

Projective planes have applications in various branches of mathematics, including combinatorics, geometry, and coding theory. They are also studied for their interesting algebraic and combinatorial structures. it is well known that every projective plane has an algebraic structure obtained by coordinatization. Conversely, certain algebraic structures can be used to construct projective planes. For instance, a general method of generating Cartesian groups has been given by Panella in [6].

The algorithm for the classification of the k – arcs, some examples of the k –arcs, Fano planes, Baer subplanes in the projective planes of order 9 and 25 and embedding of the Projective Planes to the Projective Spaces are given in [2-5] are given.

Definition A projective plane $(P, L, \circ)$ consists of a set P of points, and a set L of subsets of P, called lines, such that every pair of points is contained in exactly one line, every two different lines intersect in exactly one point, and there exist four points, no three of which are collinear.

Definition A subplane of a projective plane $(P, L, \circ)$ is a B of points and lines which is itself a projective plane, relative to the incidence relation given in $(P, L, \circ)$. Let $(P, L, \circ)$ be a projective plane of order n. If $(P', L', \circ')$ is a subplane of order m, then either $n = m^2$ or $n \geq m^2 + m$. $B = (P', L', \circ')$ is called Baer subplane of $(P, L, \circ)$ if it satisfies the following conditions:

1) Every point of $(P, L, \circ)$ is incident with a line of B
2) Every line of $(P, L, \circ)$ is incident with a point of B.

It is clear that for the Baer subplane B of order $n = m^2$.

Cartesian Group: A system $(S, \oplus, \otimes)$ is a Cartesian group if and only if the following conditions are satisfied:

1) $(S, \oplus)$ a group

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2) Each of equations $a \otimes x = b$ and $x \otimes a = b$ has a unique solution for all Where 0 denotes the additive identity.
3) There exists an element $e \in S$ such that $e \otimes x = x \otimes e = x$ for all $x \in S$.
4) $0 \otimes x = x \otimes 0 = x$ for all $x \in S$.
5) Given $a, b, c, d \in S$ such that $a \neq c$, there exists a unique $x \in S$ such that

$$a \otimes x \oplus b = c \otimes x \oplus d$$

6) Given $a, b, c, d \in S$ such that $a \neq c$, there exists a unique pair $(x, y) \in S^2$ such that

$$x \otimes a \oplus y = b$$

and

$$x \otimes c \oplus y = d.$$

The construction of the cartesian group plane of order 25 in [1] is given. We shall be interested in the projective subplanes of order 3 of the smallest Cartesian Group Plane of order 25.

2. THE SMALLEST CARTESIAN GROUP PLANE

The algebraic structure of finite projective planes is a fascinating topic that combines algebraic and geometric concepts. It provides a mathematical framework for studying the properties and relationships of points and lines in a finite projective plane.

We consider the geometrical structure of the projective plane which is constructed on the known the smallest cartesian group.

Definition (See 1) Let $(F_5, +, .)$ be the field of integers modulo 5. Let $S = \{(a,b): a, b \in F_5\}$ and consider the addition and multiplication on S given by

$$(a,b) \oplus (c,d) = (a+b, c+d)$$

and

$$(a,b) \otimes (c,d) = \begin{cases} (a.c, a.d) & ,if\ b = 0 \\ (a.c - (a^2 - 2).d.b^{-1}, b.c - a.d) & ,if\ b \neq 0 \end{cases}.$$

The system $(S, \oplus, \otimes)$ is a proper Cartesian group.

We consider the geometrical structure of the projective plane which is constructed on the known the smallest cartesian group.

A finite projective plane of order n has $n^2 + n + 1$ points and $n^2 + n + 1$ lines. We shall be interested in the projective plane $\boldsymbol{\pi}$ over the smallest Cartesian Group of order 25. The 651 oints of $\boldsymbol{\pi}$ are the elements of the set $\{(x, y): x, y \in S\} \cup \{(m): m \in S\} \cup \{(\infty)\}$.
The points of the form (x, y), are called affine points and the points of the form (m) and the unique point (∞) are called ideal points. The 651 lines of $\boldsymbol{\pi}$ are defined to be set of points satisfying one of the three conditions:

$$[m,k]=\{(x,y)\in S^2 : y=m*x\oplus k\}\cup\{(m)\}$$
$$[\lambda]=\{(x,y)\in S^2 : x=\lambda\}\cup\{(\infty)\}$$
$$[\infty]=\{(m)\in S\ \}\cup\{(\infty)\}.$$

The 625 lines of $\boldsymbol{\pi}$ having form $y=m*x\oplus k$ and 25 lines of $\boldsymbol{\pi}$ having of the form $x=\lambda$ are called the affine lines and the unique line [∞] of $\boldsymbol{\pi}$ is called the ideal line. The system of points, lines and incidence relation given above defines a projective plane of order 25, which is the smallest Cartesian group plane.

3. SUBPLANES OF ORDER 3 OF THE SMALLEST CARTESIAN GROUP PLANE

Let's assume the vertices of the regular quadrangle are O,I,X,P. If the diagonal points E,F,G of this regular quadrangle are not collinear, then this quadrangle does not determine a Fano plane [1].

Let $O=((0,0),(0,0)), I=((1,0),(1,0)), X=((0,0))$ and $P=((0,0),(a,b))$ for $a=b=0$ and $a=1,\ b=0$ be any four points that are known not to form a regular quadrangle.

The following lemmas are taken from [1].

Lemma If $P=((0,0),(a,b))$ with $b\neq 0$, then each a regular quadrangle O,I,X,P determines a Fano subplane of π.

Lemma If $P=((0,0),(a,b))$ with $a\neq 0,1$ and $b=0$, then non of the regular quadrangle O,I,X,P determines a Fano configuration of π.

Lemma If $P=(\infty)$, then the regular quadrangles O,I,X,P doesn't determine a Fano configuration of π.

Theorem Let $O=((0,0),(0,0)),\ I=((1,0),(1,0)),\ X=((0,0))$ and $P=((0,0),(a,b))$ be a regular quadrangle in π. The configurations obtained from completing the some regular quadrangles O,I,X,P of π do not form the respective subplanes of order 3 of π.

Proof To obtain configurations that form a projective plane of order 3 from completing the regular quadrangles O,I,X,P of π, it is necessary for these configurations to satisfy the conditions in Lemma 2. Indeed, the number of such the quadrangles with diagonal points are not collinear is three in Lemma 2. Because in the other conditions, the completions of these quadrangles, known as Fano planes, cannot be subplanes of projective planes of order 3 . Now, let's examine these three cases:

Case 1 If $a=2,b=0$, then P is $((0,0),(2,0))$. The coordinates of the opposite sides and diagonal points of this quadrangle are obtained as follows:

$$OP=[(0,0)],\ IX=[(0,0),(1,0)],\ OI=[(1,0),(0,0)],\ PX=[(0,0),(2,0)],$$
$$OX=[(0,0),(0,0)],\ PI=[(4,0),(2,0)]$$

and

$$E:=OP\wedge IX=((0,0),(1,0)),\ F:=OI\wedge PX=((2,0),(2,0)),\ G:=PI\wedge OX=((2,0),(0,0)).$$

The configuration that completes this the regular quadrangles O, I, X, P should have the property of being a plane of order 3. For this to happen, four lines must pass through each point, and there should be four points on each line.

By performing the necessary calculations, the remaining 6 points are found as follows:

$$N := EF \wedge OX = ((3,0),(0,0)),\ N' := EF \wedge PI = ((2,1),(2,3)),\ L := FG \wedge IX = ((2,0),(1,0)),$$
$$L' := FG \wedge OP = (\infty),\ M := EG \wedge OI = ((4,0),(4,0)),\ M' := PX \wedge EG = ((3,0),(2,0)).$$

Since there should be four points on each line, two missing points on the line $PM = [(3,0),(2,0)]$ should be determined.
However, the points *L* and *N* can be on this line *PM*.

$$L \circ PM \Leftrightarrow (1,0) = (3,0) \otimes (2,0) \oplus (2,0)$$

and

$$N \circ PM \Leftrightarrow (0,0) = (3,0) \otimes (3,0) \oplus (2,0)$$

Since the above equations are not satisfied and there are no two points on line *PM* among these 13 points, the resulting configuration cannot be a projective plane of order 3.

Case 2 If $a = 3,\ b = 0$, then *P* is $((0,0),(3,0))$. The coordinates of the opposite sides and diagonal points of this quadrangle are obtained as follows:

$$OP = [(0,0)],\ IX = [(0,0),(1,0)],\ OI = [(1,0),(0,0)],\ PX = [(0,0),(3,0)],$$
$$OX = [(0,0),(0,0)],\ PI = [(3,0),(0,0)]$$

and

$$E := OP \wedge IX = ((0,0),(1,0)),\ F := OI \wedge PX = ((3,0),(3,0)),\ G := PI \wedge OX = ((4,0),(0,0)).$$

By performing the necessary calculations, the remaining 6 points are found as follows:

$$N := ((1,0),(0,0)),\ N' := ((2,0),(4,0)),\ L := ((2,0),(1,0)),$$
$$L' := ((0,0),(2,0)),\ M := (1,0),\ M' := PX \wedge EG = ((2,0),(3,0)),$$

Since there should be four points on each line, two missing points on the line $PM = [(1,0),(3,0)]$ should be determined.

However, the points *L* and *N* can be on this line *PM*.

If calculations are done as in the first case, two points still cannot be found on line *PM*, the resulting configuration cannot be a projective plane of order 3.

Case 3 If $a = 4,\ b = 0,$ then *P* is $((0,0),(4,0))$.

If calculations are done as in the first and second cases, two points still cannot be found on line *PM*. Therefore, a projective plane of order 3 cannot be constructed.

4. CONCLUSION

In this paper, we have presented an approach for finding projective subplanes of order 3 within the cartesian group plane of order 25. By combining principles from algebraic geometry, linear algebra, and computational techniques, we have developed a systematic methodology that enables efficient identification, characterization of some subplanes.

Investigating projective subplanes of order 3 within the cartesian group plane of order 25 by considering different the regular quadrangles is an open problem.

CONFLICT OF INTEREST

The author stated that there are no conflicts of interest regarding the publication of this article.

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ESKİŞEHİR TEKNİK ÜNİVERSİTESİ BİLİM VE TEKNOLOJİ DERGİSİ B- TEORİK BİLİMLER

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RESEARCH ARTICLE

ON SOFT RING AND SOFT TOPOLOGICAL RING

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ABSTRACT

The soft set theory is an affective mathematical tool to solve problems that involves uncertainties. Despite the development in the theoretical structure of soft sets, researchers did not make consensus formulation of soft element. In this study the soft ring is redefined by the help of soft operations which are based on a natural definition of soft element. This new soft ring definition is compared with the soft ring definitions in the literature. Some examples, results and theorems are given to enrich the concept of soft ring. Also soft topological ring structure which is a harmonization of soft ring and soft topology is studied with some results.

Keywords: Soft set, Soft ring, Soft topological ring

1. INTRODUCTION

Frequently solutions of real life problems are not possible with a precise and direct informational point of view. Several models have been developed to date to cope with this complexity. Often these models are not enough to identify the exact solution. The soft set theory is one of these models which was defined by Molodtsov [1]. Soft set theory has excited attention since the year it was defined, due to the freedom it gives to studies on parameters that is increase the application area of soft sets unlike other theories. Some of fundamental soft set operations such as Or, And, Union etc. were introduced by Maji et al in [2]. Soft topological structures were given in [3, 4, 5, 6, 7]. Aktaş and Çağman introduced and investigated the concept of soft group by taking universal set as a group and they also made a comparison with soft sets and other set theories in [8]. After that soft group definition extended soft ring by Acar et al in [9] and some related results about soft ring were derived by them. Another approach to soft group notion was given by Ghosh et al in [10]. Moreover soft modules and fuzzy soft modules were presented by Sun et al in [11] and Gunduz et al in [12].

In the meantime soft element and soft point structures were studied and discussed by some researchers from different perspectives. One of them is Wardowski [13] who defined soft element which provides soft topological structures resembles to pointwise topological structures. After this definition there have been studies on soft topological and soft algebraic structures from an elementary point of view such as [14] and [15] etc.

More combination of algebraic constructions and soft topological structures were studied by many researchers such as [16, 17, 18, 19, 18] and [20]. For example, as an expected extension of the familiar concepts of topological groups were given by Nazmul and Samanta in 2010 [21] and Tanay and Çakmak [16] initiated the idea of soft semi topological groups. Later some improvements were added to the notion of soft topological groups in [20].

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Tahat et al.in [18] introduced the concept of soft topological soft rings by applying soft topological structures on a soft ring and another approach for soft topological rings was given in [17] by applying the topological structures on a soft ring. In [19], the notion soft topological ring which is linked on the soft topological structures over the rings directly, rather than on the topological structures over the subrings were introduced by Tahat et al.

In this paper unlike the studies mentioned above, firstly, definition of a soft ring will be given from the pointwise perspective. Then, definition of a soft topological ring and some theorems will be examined as a result of this study. With this approach soft topological ring structure will depend on a soft topology and a soft ring structure on a single soft set.

We referee for some basic definitions such as soft set, soft subset, intersection and union of soft sets, soft empty set and soft element from [1], [2] and [7]. An application of the these mentioned definitions is given by the following example.

Example 1.1. Mr. X and Mrs. X are deciding to move to a new city, they list the features of the city in which they want to live as follows: Economy, Health, Security, City life, Culture and Art Activities. Features of the cities give the parameter set $E = \{e_1, e_2, e_3, e_4, e_5\}$ where e_1, e_2, e_3, e_4, e_5 stands for economy, health, security, city life and culture and art activities respectively. The universe U of cities that they plan to move to are also listed as London, Paris, New York, Tokyo. Let's define soft sets (F, E) and (G, E) that describe each city with properties determined by Mr. X and Mrs. X respectively.

$(F, E) = \{(e_1, \{\text{London}\}), (e_2, \{\text{Paris}\}), (e_3, \{\text{New York, Tokyo}\})(e_4, \emptyset)\ , (e_5, \emptyset)\}$.

$(G, E) = \{(e_1, \{\text{London, Paris}\}), (e_2, \emptyset)\ (e_3, \{\text{London, New York, Tokyo}\}), (e_4, \emptyset)\ , (e_5, \emptyset)\}$.

The intersection of (F, E) and (G, E) is $(F, E) \,\widetilde{\cap}\, (G, E) =$
$\{(e_1, \{\text{London}\}), (e_2, \emptyset), (e_3, \{\text{New York, Tokyo}\}), (e_4, \emptyset)\ , (e_5, \emptyset)\}$.

The union of (F, E) and (G, E) is, $(F, E)\ \widetilde{\cup}\ (G, E) =$
$\{(e_1, \{\text{London}, B\}), (e_2, \{\text{Paris}\}), (e_3, \{\text{London, New York, Tokyo}\}), (e_4, \emptyset)\ , (e_5, \emptyset)\}$.

The nonempty soft elements of (F, E) are
$\{(e_1, \{\text{London}\}), (e_2, \{\text{Paris}\}), (e_3, \{\text{New York}\}), (e_3, \text{Tokyo})\}$.

Empty soft elements of (F, E) are $\{(e_4, \emptyset), (e_5, \emptyset)\}$.

Soft elements of (G, E) are,

$\{(e_1, \{\text{London}\}), (e_1, \{\text{Paris}\}), (e_2, \emptyset), (e_3, \{\text{London}\}), (e_3, \{\text{New York}\}), (e_3, \{\text{Tokyo}\}), (e_4, \emptyset), (e_5, \emptyset)\}$

$(e_2, \emptyset), (e_4, \emptyset), (e_5, \emptyset)$ are the empty soft elements of (G, E),

$(e_1, \{\text{London}\}), (e_1, \{\text{Paris}\}), (e_3, \{\text{London}\}), (e_3, \{\text{New York}\}), (e_3, \{\text{Tokyo}\})$ are nonempty soft elements of (G, E).

Complement of soft set (F, E) is $(F, E)^{\tilde{C}} =$
$\{(e_1, \{\text{Paris, New York, Tokyo}\}), (e_2, \{\text{London, New York, Tokyo}\}), (e_3, \{\text{London, Paris}\}), (e_4, U), (e_5, U)\}$.

2. SOFT RING AND SOFT TOPOLOGY

2.1.Soft Ring

Definitions such as full soft set, operations on soft sets, properties of operations on soft sets and soft group which are used in this article are taken from the paper [10]. Following the definitions above soft ring definition can be stated as in the below:

Definition 2.1. Let $(E,+_1,\cdot_1)$, $(U,+_2,\cdot_2)$ be two rings, $A \subseteq E$ and $F_A \in S_f(U)$, (F_A is a full soft set on the universe U). Consider the binary operations $\tilde{+},\tilde{\cdot}$ given on the soft set F_A below. For all $(e_1,\{u_1\}),(e_2,\{u_2\}) \tilde{\in} F_A^{\bullet}$.

$$(e_1,\{u_1\})\tilde{+}(e_2,\{u_2\}) = (e_1+_1e_2,\{u_1+_2u_2\})$$
$$(e_1,\{u_1\})\tilde{\cdot}\ (e_2,\{u_2\}) = (e_1\cdot_1 e_2,\{u_1\cdot_2 u_2\})$$

A soft set $(F_A,\tilde{+},\tilde{\cdot})$ over (E,U) is said to be a soft ring if the following conditions are satisfied.

i) $(F_A,\tilde{+})$ is a commutative soft group,

ii) $\alpha\tilde{\cdot}(\beta\tilde{\cdot}\gamma) = (\alpha\tilde{\cdot}\beta)\tilde{\cdot}\gamma$ for all $\alpha,\beta,\gamma \tilde{\in} F_A^{\bullet}$.

iii) $\alpha\tilde{\cdot}(\beta\tilde{+}\gamma)$=($\alpha\tilde{\cdot}\beta)\ \tilde{+}(\alpha\tilde{\cdot}\gamma)$ and $(\alpha\tilde{+}\beta)\tilde{\cdot}\gamma = (\alpha\tilde{\cdot}\gamma)\tilde{+}(\beta\tilde{\cdot}\gamma)$ for all $\alpha,\beta,\gamma \tilde{\in} F_A^{\bullet}$.

Example 2.2. Consider the soft set F_E defined by the set valued function $F: E = \mathbb{Z}_2 \to P\left(\mathbb{Z}(\sqrt{2})\right)$,

$F(\bar{0}) = \{2n + 2n\sqrt{2}: n \in \mathbb{Z}\}$,

$F(\bar{1}) = \{2n + (2n+1)\sqrt{2}: n \in \mathbb{Z}\}$,

$F(\bar{2}) = \{(2n+1) + 2n\sqrt{2}: n \in \mathbb{Z}\}$,

$F(\bar{3}) = \{(2n+1) + (2n+1)\sqrt{2}: n \in \mathbb{Z}\}$ over the rings $(E,+_1,\cdot_1) = (\mathbb{Z}_4,+,\cdot)$, $(U,+_2,\cdot_2) = \left(\mathbb{Z}(\sqrt{2}),+,\cdot\right)$. If we consider the soft elements of F_E $(\bar{1},\{2n + (2n+1)\sqrt{2}: n \in \mathbb{Z}\})$ and $(\bar{3},\{(2n+1) + (2n+1)\sqrt{2}: n \in \mathbb{Z}\})$ then $(\bar{1},\{2n + (2n+1)\sqrt{2}: n \in \mathbb{Z}\})\tilde{+}(\bar{3},\{(2n+1) + (2n+1)\sqrt{2}: n \in \mathbb{Z}\}) = (\bar{0},\{(2n+1) + 2n\sqrt{2}: n \in \mathbb{Z}\})$ which is not belong to soft set F_E. So F_E is not a soft ring over (E,U).

Example 2.3. Consider the soft set F_E defined by the set valued function $F: E = \mathbb{Z}_2 \to P(M_3(\mathbb{R}))$,

$F(\bar{0}) = \{0_{3x3}\}$,

$F(\bar{1}) = \{A: A\ \ upper\ triangular\ matrix\} = U_3$. If one apply the operation $\tilde{+}$ to the soft element $(\bar{1},U_3)$

$(\bar{1},U_3)\tilde{+}(\bar{1},U_3) = (\bar{0},U_3)$ that is not a soft element of the soft set F_E.

F_E is not a soft ring due to $\tilde{+}$ is not closed under the binary operation.

The soft ring definition which was given by [9] in 2010, is not related the definition stated in Definition 2.1. We can deduce this conclusion in view of the fact that a soft set F_E which is given in the above Example 2.3. is a soft ring according to the definition of soft ring stated in [9].

Example 2.4. Consider the soft set F_E defined by the set valued function $F: E = \mathbb{Z}_2 \to P(U = \mathbb{Z}_4)$,

$F(\bar{0}) = \{\bar{0},\bar{2}\}$, $F(\bar{1}) = \{\bar{0},\bar{2}\}$.

One can observe from the tables below that soft operations are closed and F_E is a soft ring over (E, U).

$\tilde{+}$	$(\bar{0},\{\bar{0}\})$	$(\bar{0},\{\bar{2}\})$	$(\bar{1},\{\bar{0}\})$	$(\bar{1},\{\bar{2}\})$
$(\bar{0},\{\bar{0}\})$	$(\bar{0},\{\bar{0}\})$	$(\bar{0},\{\bar{2}\})$	$(\bar{1},\{\bar{0}\})$	$(\bar{1},\{\bar{2}\})$
$(\bar{0},\{\bar{2}\})$	$(\bar{0},\{\bar{2}\})$	$(\bar{0},\{\bar{0}\})$	$(\bar{1},\{\bar{2}\})$	$(\bar{1},\{\bar{0}\})$
$(\bar{1},\{\bar{0}\})$	$(\bar{1},\{\bar{0}\})$	$(\bar{1},\{\bar{2}\})$	$(\bar{0},\{\bar{0}\})$	$(\bar{0},\{\bar{2}\})$
$(\bar{1},\{\bar{2}\})$	$(\bar{1},\{\bar{2}\})$	$(\bar{1},\{\bar{0}\})$	$(\bar{0},\{\bar{2}\})$	$(\bar{0},\{\bar{0}\})$

$\tilde{\cdot}$	$(\bar{0},\{\bar{0}\})$	$(\bar{0},\{\bar{2}\})$	$(\bar{1},\{\bar{0}\})$	$(\bar{1},\{\bar{2}\})$
$(\bar{0},\{\bar{0}\})$	$(\bar{0},\{\bar{0}\})$	$(\bar{0},\{\bar{0}\})$	$(\bar{0},\{\bar{0}\})$	$(\bar{0},\{\bar{0}\})$
$(\bar{0},\{\bar{2}\})$	$(\bar{0},\{\bar{0}\})$	$(\bar{0},\{\bar{0}\})$	$(\bar{0},\{\bar{0}\})$	$(\bar{0},\{\bar{0}\})$
$(\bar{1},\{\bar{0}\})$	$(\bar{0},\{\bar{0}\})$	$(\bar{0},\{\bar{0}\})$	$(\bar{1},\{\bar{0}\})$	$(\bar{1},\{\bar{0}\})$
$(\bar{1},\{\bar{2}\})$	$(\bar{0},\{\bar{0}\})$	$(\bar{0},\{\bar{0}\})$	$(1,\{\bar{0}\})$	$(\bar{1},\{\bar{0}\})$

Definition 2.5. Let $(F_E, \tilde{+}, \tilde{\cdot})$ be a soft ring. If there exist an element $\tilde{1} \tilde{\in} F_E$ such that $\alpha \tilde{\cdot} \tilde{1} = \tilde{1} \tilde{\cdot} \alpha$, for all $\alpha \tilde{\in} F_E$, then F_E is called soft ring with identity.

Theorem 2.6. If E, U are rings with identities e_1 and e_2 and F_E is a soft ring that contains soft element $(e_1,\{e_2\})$, then $(e_1,\{e_2\})$ is the soft identity element.

Proof. Straightforward.

Definition 2.7. Let $(F_E, \tilde{+}, \tilde{\cdot})$ be a soft ring. If $\alpha \tilde{\cdot} \beta = \beta \tilde{\cdot} \alpha$, for all $\alpha, \beta \tilde{\in} F_E$, then F_E is called commutative soft ring .

Example 2.8. The soft ring F_E given in Example 2.4. is a commutative soft ring.

Note 2.9. If E and U are commutative rings so is F_E, that is defined over (E, U).

Theorem 2.10. If $(F_E, \tilde{+}, \tilde{\cdot})$ is a soft ring with additive identity $\tilde{0}$, then for any $\gamma, \beta \tilde{\in} F_E$, we have

i) $\tilde{0} \tilde{\cdot} \gamma = \gamma \tilde{\cdot} \tilde{0} = \tilde{0}$,
ii) $\gamma \tilde{\cdot} (-\beta) = (-\gamma) \tilde{\cdot} \beta = -(\gamma \tilde{\cdot} \beta)$,
iii) $(-\gamma) \tilde{\cdot} (-\beta) = \gamma \tilde{\cdot} \beta$.

Proof: i) $\tilde{0}$ is the soft identity for the operation $\tilde{+}$ and it can be written as $\tilde{0} \tilde{\cdot} \gamma = (\tilde{0} \tilde{+} \tilde{0}) \tilde{\cdot} \gamma$. From the right cancellation law $\tilde{0} \tilde{\cdot} \gamma = \tilde{0}$ is satisfied. The other side of the equality can be done similarly.

ii) Let us prove that $\gamma \tilde{\cdot} (-\beta)$ is the inverse of $\gamma \tilde{\cdot} \beta$ according to the $\tilde{+}$.

$$\gamma \tilde{\cdot} (-\beta) \tilde{+} \gamma \tilde{\cdot} \beta = \gamma \tilde{\cdot} ((-\beta) \tilde{+} \beta) = \gamma \tilde{\cdot} \tilde{0} = \tilde{0}$$

The other side of the equality can be done similarly

The last condition of the theorem can be done similarly.

Definition 2.11. Let $(F_E, \tilde{+}, \tilde{\cdot})$ be a soft ring and $G_B \tilde{\subseteq} F_E$. If G_B is closed under the operations of F_E and satisfies the conditions given in the Definition 2.1. then $(G_B, \tilde{+}, \tilde{\cdot})$ is called a soft subring of $(F_E, \tilde{+}, \tilde{\cdot})$.

Example 2.12. Consider the soft subset $B = \{\bar{0}\} \subseteq \mathbb{Z}_2$. $G_B = \{\bar{0}, \{\bar{0}, \bar{2}\}\}$ of F_E given in Example 2.4. Then $(G_B, \tilde{+}, \tilde{\cdot})$ is a soft sub ring of $(F_E, \tilde{+}, \tilde{\cdot})$.

Theorem 2.13. If $(F_A, \tilde{+}, \tilde{\cdot})$ is a soft ring over (E, U) then

i) A is a subring of E,
ii) $\bigcup_{e_i \in A} F(e_i)$ is a subring of U.

Proof. i) Ghosh et. al. proved that A is a subgroup of E, in [6]. So to show that A is a subring of E, we prove that $e_i \cdot_1 e_j \in A$, for each $e_i, e_j \in A$. Assume that $e_i, e_j \in A$ since $F_A \in S_f(U)$ there exist $u_k, u_l \in U$ such that $(e_i, \{u_k\}), (e_j, \{u_l\}) \tilde{\in} F_A$. Also $(e_i, \{u_k\}) \tilde{\cdot} (e_j, \{u_l\}) = (e_i \cdot_1 e_j, \{u_k \cdot_2 u_l\}) \tilde{\in} F_A$ which proves $e_i \cdot_1 e_j \in A$.

ii) The proof can be done similar with condition i).

Theorem 2.14. Let $(F_A, \tilde{+}, \tilde{\cdot})$ and $(G_B, \tilde{+}, \tilde{\cdot})$ be soft rings over (E, U).

i) If $F_A \tilde{\cap} G_B \in S_f(U)$ and $A \cap B \neq \emptyset$ then $(F_A \tilde{\cap} G_B, \tilde{+}, \tilde{\cdot})$ is a soft ring over (E, U).
ii) If $F_A \tilde{\cup} G_B \in S_f(U)$ and $F_A \tilde{\subseteq} G_B$ or $G_B \tilde{\subseteq} F_A$ then $(F_A \tilde{\cup} G_B, \tilde{+}, \tilde{\cdot})$ is a soft ring over (E, U).

Proof. Straightforward.

Definition 2.16. Let $(F_A, \tilde{+}, \tilde{\cdot})$ be a soft ring and $\tilde{\emptyset} \neq G_B \tilde{\subseteq} F_A$. If G_B satisfies the following conditions

i) for all $\gamma, \beta \tilde{\in} G_B$, $\gamma \tilde{+} \beta \tilde{\in} G_B$,
ii) for all $\beta \tilde{\in} F_A$ and for all $\gamma \tilde{\in} G_B$, $\gamma \tilde{\cdot} \beta \tilde{\in} G_B$ and $\beta \tilde{\cdot} \gamma \tilde{\in} G_B$,

then G_B is called a soft ideal of F_A. In particularly, if for all $\beta \tilde{\in} F_A$ and for all $\gamma \tilde{\in} G_B$,, then $\gamma \tilde{\cdot} \beta \tilde{\in} G_B$ is said to be a soft right ideal of F_A and $\beta \tilde{\cdot} \gamma \tilde{\in} G_B$ then G_B is said to be a soft left ideal of F_A.

Note 2.17. The soft ring $(F_A, \tilde{+}, \tilde{\cdot})$ and $G_B = \{\tilde{0}\}$ where $\tilde{0}$ is the identity of F_A according to the binary operation $\tilde{+}$ are soft ideals of F_A.

It is clear that if $(F_A, \tilde{+}, \tilde{\cdot})$ is a soft ring with an identity $\tilde{1}$ and G_B is the soft ideal of F_A then $G_B = F_A$. Every soft ideal is a soft subring but the converse side is not true in general.

Example 2.17. Consider the Example 2.4. Take the soft subset G_E of F_E where $(\bar{0}) = \{\bar{0}, \bar{2}\}$, $G(\bar{1}) = \emptyset$, is an soft ideal of F_E.

2.2. Soft Topology

Soft topological structures are studied by many authors with their own approaches. In this subsection definitions and some several properties about the soft topological spaces are reminded, which is going to be used in the third section. The essentials of the theory of soft topological structures were introduced by Roy et al. [10].

Example 2.18. [3] Let $U = \{u_1, u_2, u_3\}$, $A = \{p_1, p_2\}$ and $F_A = \{(p_1, \{u_1, u_2\}), (p_2, \{u_2, u_3\})\}$. In that case all soft subsets of F_A are listed below.

$F_{A_1}^1 = \{(p_1, \{u_1\})\}$,

$F_{A_2}^2 = \{(p_1, \{u_2\})\}$,

$F_{A_3}^3 = \{(p_1, \{u_1, u_2\})\}$,

$F_{A_4}^4 = \{(p_2, \{u_2\})\}$,

$F_{A_5}^5 = \{(p_3, \{u_3\})\}$,

$F_{A_6}^6 = \{(p_2, \{u_2, u_3\})\}$,

$F_{A_7}^7 = \{(p_1, \{u_1\}), (p_2, \{u_2\})\}$,

$F_{A_8}^8 = \{(p_1, \{u_1\}), (p_2, \{u_3\})\}$,

$F_{A_9}^9 = \{(p_1, \{u_1\}), (p_2, \{u_2, u_3\})\}$,

$F_{A_{10}}^{10} = \{(p_1, \{u_2\}), (p_2, \{u_2\})\}$,

$F_{A_{11}}^{11} = \{(p_1, \{u_2\}), (p_2, \{u_3\})\}$,

$F_{12}^{12} = \{(p_1, \{u_2\}), (p_2, \{u_2, u_3\})\}$,

$F_{A_{13}}^{13} = \{(p_1, \{u_1, u_2\}), (p_2, \{u_2\})\}$,

$F_{A_{14}}^{14} = \{(p_1, \{u_1, u_2\}), (p_2, \{u_3\})\}$,

$F_{A_{15}}^{15} = F_A$,

$F_{A_{16}}^{16} = \widetilde{\emptyset}$.

Then $\widetilde{\tau_1} = \{\widetilde{\emptyset}, F_A\}$,$\widetilde{\tau_2} = \{F_{A_1}^1, F_{A_2}^2, \dots, F_{A_{16}}^{16}\}$, $\widetilde{\tau_3} = \{\widetilde{\emptyset}, F_A, F_{A_2}^2, F_{A_{11}}^{11}, F_{12}^{12}\}$ are soft topologies on F_A.

Definition 2.19. [14] Let $(F_A, \tilde{\tau})$ be a soft topological space and $(e_j, \{u_l\}) \widetilde{\in} F_A$. Given soft subset G_B of F_A is said to be a soft neighborhood of $(e_j, \{u_l\})$, if there exist an open soft set H_C such that $(e_j, \{u_l\}) \widetilde{\in} H_C \widetilde{\subseteq} G_B$. $N_{(e_j, \{u_l\})}$ is symbolized the all soft neighborhoods of the soft element $(e_j, \{u_l\})$.

Example 2.20. [14] Let F_A be the soft set and $\widetilde{\tau_3}$ be the soft topology on F_A given in Example 2.18. The set of all nonempty soft elements of F_A is

$F_A^{\bullet} = \{(p_1, \{u_1\}), (p_1, \{u_2\}), (p_2, \{u_2\}), (p_2, \{u_3\})\}$. For the soft element $(p_1, \{u_1\}) \widetilde{\in} F_A$, the soft sets containing $(p_1, \{u_1\})$ are $F_A, F_{A_1}^1, F_{A_3}^3, F_{A_7}^7, F_{A_8}^8, F_{A_9}^9, F_{A_{13}}^{13}$ and $F_{A_{14}}^{14}$.

$N_{(p_1, \{u_1\})} = \{F_A, F_{A_{13}}^{13}\}$ is a set of all soft neighborhoods of $(p_1, \{u_1\})$.

$N_{(p_1, \{u_2\})} = \{F_A, F_{A_2}^2, F_{A_{11}}^{11}, F_{A_{13}}^{13}\}$ is a set of soft all neighborhoods of $(p_1, \{u_2\})$.

$N_{(p_2, \{u_2\})} = \{F_A, F_{A_{13}}^{13}\}$ is a set of all soft neighborhoods of $(p_2, \{u_2\})$.

$N_{(p_2, \{u_3\})} = \{F_A, F_{A_{11}}^{11}\}$ is a set of all soft neighborhoods of $(p_2, \{u_3\})$.

Proposition 2.21. [14] Let $(F_A, \tilde{\tau})$ be a soft topological space. A soft set $G_B \widetilde{\subseteq} F_A$ is soft open if and only if for each soft element $\alpha \widetilde{\in} G_B$ there exists a soft set $H_C \in \tilde{\tau}$ such that $\alpha \widetilde{\in} H_C \widetilde{\subseteq} G_B$.

Definition 2.22. [14] Let $(F_A, \tilde{\tau})$ be a soft topological space and $G_B \widetilde{\subseteq} F_A$. The soft topology on G_B induced by the soft topology $\tilde{\tau}$ is the family of $\tilde{\tau}_{G_B}$ of the soft subsets of G_B of the form

$\tilde{\tau}_{G_B} = \{H_C \widetilde{\cap} G_B : H_C \in \tilde{\tau}\}$.

One can prove that the family $\tilde{\tau}_{G_B}$ is a soft topology on G_B. The soft topological space $(G_B, \tilde{\tau}_{G_B})$ is called a soft topological subspace of $(F_A, \tilde{\tau})$.

Definition 2.23. [14] Let $(F_A, \tilde{\tau}_1)$ and $(G_B, \tilde{\tau}_2)$ be soft topological spaces and $\beta = \{F_{A_i} x G_{B_j} : F_{A_i} \in \tilde{\tau}_1, G_{B_j} \in \tilde{\tau}_2\}$. The collection $\tilde{\tau}$ of all arbitrary union of soft elements of β is called the soft product topology over $F_A \times G_B$.

3. SOFT TOPOLOGICAL RING

The structure of the topological ring is more improved in comparison with the concept of a topological group. Also theory of topological rings has several characteristics in common with the theory of topological groups. In the soft set theory, it would be similar. The soft topological group was defined by Polat et. al. in [18] in 2018.

After searching literature on soft rings and soft topological rings reader can deduced that the soft ring structure used the refer to a soft set F_A over a ring U such that $F(x)$ is a subring of universal set U, for every $x \in A$ and the soft topological ring studies based on this soft ring definition defined in [9]. The soft ring definition is redefined in this study. Purpose of this study is to combine soft ring and soft topological space structures on a soft set.

Definition 3.1. Let $(F_A, \tilde{\mp}, \tilde{\cdot})$ be a soft ring and define a soft topology $\tilde{\tau}$ over F_A. If the following three conditions are satisfied then $(F_A, \tilde{\mp}, \tilde{\cdot}, \tilde{\tau})$ is called a soft topological ring.

i) For each soft neighborhood G_B of the soft element $(e_i, \{u_k\}) \tilde{\mp} (e_j, \{u_l\})$ there exist soft neighborhoods H_C of $(e_i, \{u_k\})$ and K_D of $(e_j, \{u_l\})$ satisfies that $H_C \tilde{\mp} K_D \cong G_B$.

ii) For each soft neighborhood G_B of the soft element $(e_i, \{u_k\})^{-1}$ there exist a soft neighborhood H_C of $(e_i, \{u_k\})$ such that ${H_C}^{-1} \cong G_B$.

iii) For each soft neighborhood G_B of the soft element $(e_i, \{u_k\}) \tilde{\cdot} (e_j, \{u_l\})$ there exist soft neighborhoods H_C of $(e_i, \{u_k\})$ and K_D of $(e_j, \{u_l\})$ respectively satisfies that $H_C \tilde{\cdot} K_D \cong G_B$.

Note 3.2. If $(F_A, \tilde{\mp}, \tilde{\cdot}, \tilde{\tau})$ is a soft topological ring then $(F_A, \tilde{\mp}, \tilde{\tau})$ is a soft topological group. Therefore, every property given for soft commutative topological groups is valid for soft topological rings.

Theorem 3.3. Let $(F_A, \tilde{\mp}, \tilde{\cdot})$ be a soft ring and define a soft topology $\tilde{\tau}$ over F_A. If the conditions given in below are satisfied,

i) For each soft neighborhood G_B of the soft element $(e_i, \{u_k\}) \tilde{\mp} (e_j, \{u_l\})^{-1}$ there exist soft neighborhoods H_C of $(e_i, \{u_k\})$ and K_D of $(e_j, \{u_l\})$ respectively satisfy that $H_C \tilde{\mp} {K_D}^{-1} \cong G_B$.

ii) For each soft neighborhood G_B of the soft element $(e_i, \{u_k\}) \tilde{\cdot} (e_j, \{u_l\})$ there exist soft neighborhoods H_C of $(e_i, \{u_k\})$ and K_D of $(e_j, \{u_l\})$ respectively satisfy that $H_C \tilde{\cdot} K_D \cong G_B$

then $(F_A, \tilde{\mp}, \tilde{\cdot}, \tilde{\tau})$ is a soft topological ring.

Proof. The proof is obvious from the continuity of composite function.

Example 3.4. [14] Let $E = \{e_1, e_2\}$, $U = \mathbb{Z}_4$ be the classes of residues of integers module 4. E is a ring defined with the operations $+, \cdot$. Tables of the operation $+, \cdot$ on E are given as in the below.

$+$	e_1	e_2
e_1	e_1	e_2
e_2	e_2	e_1

$\cdot$	e_1	e_2
e_1	e_1	e_1
e_2	e_1	e_1

Define a soft set $F: E \to P(U)$ by $F_E = \{(e_1, \{\bar{0}, \bar{2}\}), (e_2, \{\bar{1}, \bar{3}\})\}$. The table of the operations $\tilde{+}$ and $\tilde{\cdot}$ on the soft set F_E given as;

$\tilde{+}$	$(e_1, \{\bar{0}\})$	$(e_1, \{\bar{2}\})$	$(e_2, \{\bar{1}\})$	$(e_2, \{\bar{3}\})$
$(e_1, \{\bar{0}\})$	$(e_1, \{\bar{0}\})$	$(e_1, \{\bar{2}\})$	$(e_2, \{\bar{1}\})$	$(e_2, \{\bar{3}\})$
$(e_1, \{\bar{2}\})$	$(e_1, \{\bar{2}\})$	$(e_1, \{\bar{0}\})$	$(e_2, \{\bar{3}\})$	$(e_2, \{\bar{1}\})$
$(e_2, \{\bar{1}\})$	$(e_2, \{\bar{1}\})$	$(e_2, \{\bar{3}\})$	$(e_1, \{\bar{2}\})$	$(e_1, \{\bar{0}\})$
$(e_2, \{\bar{3}\})$	$(e_2, \{\bar{3}\})$	$(e_2, \{\bar{1}\})$	$(e_1, \{\bar{0}\})$	$(e_1, \{\bar{2}\})$

$\tilde{\cdot}$	$(e_1, \{\bar{0}\})$	$(e_1, \{\bar{2}\})$	$(e_2, \{\bar{1}\})$	$(e_2, \{\bar{3}\})$
$(e_1, \{\bar{0}\})$	$(e_1, \{\bar{0}\})$	$(e_1, \{\bar{0}\})$	$(e_1, \{\bar{0}\})$	$(e_1, \{\bar{0}\})$
$(e_1, \{\bar{2}\})$	$(e_1, \{\bar{0}\})$	$(e_1, \{\bar{0}\})$	$(e_1, \{\bar{2}\})$	$(e_1, \{\bar{2}\})$
$(e_2, \{\bar{1}\})$	$(e_1, \{\bar{0}\})$	$(e_1, \{\bar{2}\})$	$(e_2, \{\bar{1}\})$	$(e_1, \{\bar{3}\})$
$(e_2, \{\bar{3}\})$	$(e_1, \{\bar{0}\})$	$(e_1, \{\bar{2}\})$	$(e_2, \{\bar{3}\})$	$(e_2, \{\bar{1}\})$

In this example one can easily prove that $(F_A, \tilde{+}, \tilde{\cdot})$ is a commutative soft ring with a soft identity element $(e_2, \{\bar{1}\})$. Consider the soft topology $\tilde{\tau} = \{\tilde{\emptyset}, F_A, F_{A_1}^1, F_{A_2}^2\}$ where soft subsets of F_A are given as; $F_{A_1}^1 = \{(e_1, \{\bar{0}, \bar{2}\})\}$ and $F_{A_2}^2 = \{(e_2, \{\bar{1}, \bar{3}\})\}$. Then $(F_A, \tilde{+}, \tilde{\cdot}, \tilde{\tau})$ is a soft topological ring over (E, U).

Theorem 3.5. If $(F_A, \tilde{+}, \tilde{\cdot}, \tilde{\tau})$ is a soft topological ring and G_B is a soft subring of F_A, so is $(G_B, \tilde{+}, \tilde{\cdot}, \tilde{\tau}_{G_B})$.

Proof. Straightforward.

4. CONCLUSION

The soft set theory has wide field of study in different fields especially for the mathematicians in the algebraic and the topological structures. In this paper soft ring and soft topological ring structures are given from the soft element viewpoint which is very naturel approximation. For further studies the other algebraic structures can be studied by the similar viewpoint.

AUTHORSHIP CONTRIBUTIONS

Nazan ÇAKMAK POLAT: Developed the theoretical formalism, wrote the manuscript. played a key role in manuscript preparation and revision.

Gözde YAYLALI: Provided expertise in the specialized mathematical subfield related to the research. Played a crucial role in editing and refining the manuscript for clarity and coherence.

Bekir TANAY: Supervised the project. Contributed mathematical insights during regular group discussions. Contributed the final version of the manuscript.

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ESKİŞEHİR TEKNİK ÜNİVERSİTESİ BİLİM VE TEKNOLOJİ DERGİSİ B- TEORİK BİLİMLER

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RESEARCH ARTICLE

HERMITE INTERPOLATION WITH DICKSON POLYNOMIALS AND BERNSTEIN BASIS POLYNOMIALS

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ABSTRACT

In this manuscript we introduce three new algorithms: (1) An algorithm to recover an unknown polynomial in terms of Dickson polynomials of the first kind, (2) an algorithm to recover an unknown polynomial in terms Dickson polynomials of the second kind, (3) an algorithm to recover an unknown polynomial in terms of Bernstein basis polynomials, from given black boxes for the polynomial itself and its first derivative. In each algorithm, we assume that the unknown polynomial has a sparse representation in the corresponding basis. The methods presented use transformations from Dickson polynomials to Laurent polynomials, a transformation from Bernstein basis polynomials to Laurent polynomials, and a recently developed algorithm as a middle step.

Keywords: Hermite Interpolation, Sparse Polynomials, Dickson Polynomials, Bernstein Basis Polynomials, Algorithms

1. INTRODUCTION

Hermite interpolation is a method of reconstructing an unknown polynomial $f(x)$ by using known evaluations of $f(x)$ and known evaluations of the first few derivatives of $f(x)$. More details about Hermite interpolation can be found at [1] and references therein. In this manuscript, we deal with sparse Hermite interpolation.

A sparse Hermite interpolation algorithm is presented in [2]: Let $f(x) = \sum_{j=1}^{t} c_j x^{e_j} \in K[x, x^{-1}]$ be an unknown sparse univariate Laurent polynomial, i.e. an element in $K[x, x^{-1}]$, in Laurent polynomial basis with $t \ll \deg(f)$ terms, where K is a field and its' characteristic is 0 or a prime p, and where for all $j, c_j \neq 0, e_1 < e_2 < \cdots < e_t$. Let $k \in K - \{0,1\}$. Let black boxes for $f(x)$ and $f'(x)$ be given. [2] introduces a procedure to rebuild the unknown polynomial $f(x)$ from the data sets $\{(k^s, f(k^s))\}_{s=0}^{m}$ and $\{(k^s, f'(k^s))\}_{s=0}^{m}$ where $m = t + \left\lceil \frac{t+1}{2} \right\rceil - 1$. Here the tuples $(*, f(*))$ and $(*, f'(*))$ can be computed with given black boxes. The algorithm presented in [2], which is based on Prony's sparse polynomial interpolation algorithm (a.k.a. Ben-or & Tiwari's Algorithm) [3,4], performs sparse Hermite interpolation using those $2m + 2$, where $t \ll \deg(f)$, data points above. The method in [2] uses "less data points" than the previously known Hermite interpolation algorithms use to reconstruct the unknown polynomial $f(x)$.

Remark 1.1 We note that a black box for an unknown polynomial $f(x)$ is a known mathematical object that takes a value k and evaluates $f(k)$ without revealing any information about the unknown polynomial $f(x)$. Here we assume a black box for a polynomial always computes the correct evaluation with no error. See [5] for more details about computations with black boxes.

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Any polynomial $f(x) \in K[x]$ can be represented in terms of Dickson polynomials (both the first and the second kind). A degree n polynomial with real coefficients can be represented in terms of degree n Bernstein basis polynomials. We want to replace the Laurent polynomial basis with Dickson polynomials and Bernstein basis polynomials and aim to develop new sparse Hermite interpolation algorithms that work directly with those bases.

In this text, we present three new algorithms that solve the following three problems. The algorithms in the present manuscript perform sparse Hermite interpolation with Dickson polynomials (both the first and the second kind) and Bernstein basis polynomials. The algorithms use transformations from Dickson polynomials to Laurent polynomials, a transformation from Bernstein basis polynomials to Laurent polynomials, and the algorithm given in [2] as a middle step.

Problem 1.1

i. Let

$$f(x) = \sum_{j=0}^{t} c_j D_{e_j}(x, a) \in K[x]$$

where for all $j, c_j \neq 0, e_1 < e_2 < \cdots < e_t$, be an unknown polynomial. Here $D_{e_j}(x, a)$ is the Dickson polynomial of the first kind of degree e_j. Here we assume that $t \ll \deg(f)$, i.e., $f(x)$ has sparse representation in terms of Dickson polynomials of the first kind.

Construct $f(x)$ from given black boxes for $f(x)$ and $f'(x)$, $a \in K$, the integer t, from the sets of tuples $\{(k^s, f(k^s))\}_{s=0}^{m}$ and $\{(k^s, f'(k^s))\}_{s=0}^{m}$ where $k \in K$ and $m = t + \left\lceil \frac{t+1}{2} \right\rceil - 1$. Here the data points are computed by the given black boxes.

ii. Let

$$f(x) = \sum_{j=0}^{t} c_j E_{e_j}(x, a) \in K[x]$$

where for all $j, c_j \neq 0, e_1 < e_2 < \cdots < e_t$, be an unknown polynomial. Here $E_{e_j}(x, a)$ is the Dickson polynomial of the second kind of degree e_j. Here we assume that $t \ll \deg(f)$, i.e., $f(x)$ has sparse representation in terms of Dickson polynomials of the second kind.

Construct $f(x)$ from given a black boxes for $f(x)$ and $f'(x)$, $a \in K$, the integer t, from the sets of tuples $\{(k^s, f(k^s))\}_{s=0}^{m}$ and $\{(k^s, f'(k^s))\}_{s=0}^{m}$ where $k \in K$ and $m = t + \left\lceil \frac{t+1}{2} \right\rceil - 1$. Here the data points are computed by the given black boxes.

iii. Let

$$f(x) = \sum_{j=0}^{t} c_j B_{e_j,n}(x) \in K[x]$$

where for all $j, c_j \neq 0, e_1 < e_2 < \cdots < e_t$, be an unknown polynomial. Here $B_{e_j,n}(x)$ is the e_j-th Bernstein basis polynomial of degree n. Here we assume $n = \deg(f(x))$ is known, $K = \mathbb{R}$, and $t \ll \deg(f)$, i.e., $f(x)$ has sparse representation in terms of Bernstein basis polynomials.

Construct $f(x)$ from given black boxes for $f(x)$ and $f'(x)$, $a \in K$, the integer t, $n = \deg(f(x))$ from the sets of tuples $\{(k^s, f(k^s))\}_{s=0}^{m}$ and $\{(k^s, f'(k^s))\}_{s=0}^{m}$ where $k \in K$ and $m = t + \left\lceil \frac{t+1}{2} \right\rceil - 1$. Here the data points are computed by the given black boxes.

Before we state our procedures, we briefly mention about Dickson polynomials and Bernstein basis polynomials.

1.1. Dickson Polynomials

Dickson polynomials are introduced in [6]. Let K be a finite field with characteristic p and $a \in K$. Degree n Dickson polynomial of the first kind, $D_n(x, a)$, can be defined by the following recursion:

$$D_0(x, a) \coloneqq 2$$
$$D_1(x, a) \coloneqq x$$
$$D_n(x, a) \coloneqq xD_{n-1}(x, a) - aD_{n-2}(x, a), \forall n \geq 2.$$

Similarly, degree n Dickson polynomial of the second kind, $E_n(x, a)$, can be defined by the same recursion as above, but with a different zero-degree polynomial:

$$E_0(x, a) \coloneqq 1$$
$$E_1(x, a) \coloneqq x$$
$$E_n(x, a) \coloneqq xE_{n-1}(x, a) - aE_{n-2}(x, a), \forall n \geq 2.$$

Dickson polynomials form a K vector space bases for $K[x]$: Any $f(x) \in K[x]$ can be represented in terms of Dickson polynomials (both the first and the second kind).

Dickson polynomials are one of the examples of many orthogonal polynomials and they occur in various areas of mathematical research, such as cryptography and number theory [8,9]. The polynomials possess many useful properties. Details of Dickson polynomials and their further properties can be found at [6-9] and references in [6-9].

1.2 Bernstein Basis Polynomials

The i-th degree n Bernstein basis polynomial, which is denoted by $B_{i,n}(x)$, is defined as

$$B_{i,n}(x) = \binom{n}{i} x^i (1-x)^{n-i}.$$

Here $\binom{n}{i}$ denotes the binomial coefficient. The set $\{B_{s,n}(x)\}_{s=0}^{n}$ form a vector space basis (a.k.a. Bernstein-Bezier basis) for the polynomials in Π_n, where Π_n is the vector space of polynomials of degree $\leq n$ with real coefficients. Bernstein-Bezier basis is the standard way of representing a polynomial curve. We refer to [10,11] for further properties of Bernstein basis polynomials.

2. DISCUSSION AND ALGORITHMS

2.1. Sparse Hermite Interpolation with Dickson Polynomials of the First Kind

In [9], it is stated that Dickson polynomials satisfy the transformation formulas below: If $x \neq 0$ and $x^2 \neq a$,

$$D_n\left(x+\frac{a}{x},a\right)=x^n+\left(\frac{a}{x}\right)^n$$

$$E_n\left(x+\frac{a}{x},a\right)=\frac{x^{n+1}-\left(\frac{a}{x}\right)^{n+1}}{x-\left(\frac{a}{x}\right)}.$$

If we let $b^2=a$, then:

$$D_n\left(bx+\frac{a}{bx},a\right)=b^nx^n+\left(\frac{a}{bx}\right)^n=b^n\left(x^n+\frac{1}{x^n}\right) \tag{1}$$

$$\left(bx-\frac{a}{bx}\right)E_n\left(bx+\frac{a}{bx},a\right)=\left(bx-\frac{a}{bx}\right)\left(\frac{b^{n+1}x^{n+1}-\left(\frac{a}{bx}\right)^{n+1}}{bx-\left(\frac{a}{bx}\right)}\right)=b^{n+1}\left(x^{n+1}-\frac{1}{x^{n+1}}\right). \tag{2}$$

Equations (1) and (2) are also used in [12] to perform sparse polynomial interpolation in Dickson polynomial bases.

Assume that $f(x)=\sum_{j=0}^{t}c_jD_{e_j}(x,a)$. Then, with the help of Equation (1), we can define $g(x)$ from $f(x)$:

$$\begin{aligned} g(x) &\coloneqq f\left(b\left(x+\frac{1}{x}\right)\right)\\ &=f\left(bx+\frac{a}{bx}\right)\\ &=\sum_{j=0}^{t}c_jD_{e_j}\left(bx+\frac{a}{bx},a\right)\\ &=\sum_{j=1}^{t}G_j\left(x^{e_j}+\frac{1}{x^{e_j}}\right)\in K[x,x^{-1}] \end{aligned} \tag{3}$$

where $G_j=b^{e_j}c_j$.

Here, $g(x)$ has $T=2t$ terms in Laurent polynomial bases and $g\left(k^i\right)=g\left(k^{-i}\right)$ for $k\in K$. To compute the two evaluations $g\left(k^i\right)$ and $g\left(k^{-i}\right)$, we need to evaluate $f(x)$ only once at $x=b\left(k^i+\frac{1}{k^i}\right)$.

Here, we have

$$g'(x)=f'\left(b\left(x+\frac{1}{x}\right)\right)\left(b\left(1-\frac{1}{x^2}\right)\right)$$

and

$$g'(x)=\sum_{j=1}^{t}\frac{G_je_j}{x}\left(x^{e_j}-\frac{1}{x^{e_j}}\right).$$

Note that, $k^i g'(k^i) = -(k^{-i} g'(k^{-i}))$. To compute the two evaluations $g'(k^i)$ and $g'(k^{-i})$), we need to evaluate $f'(x)$ only once at $x = b\left(k^i + \frac{1}{k^i}\right)$.

We make use of Equation (3) to present Algorithm 2.1.1 below that solves Problem 1.1.i. Algorithm 2.1.1 first uses Equation (3) to convert Problem 1.1.i to another problem that the Algorithm in [2] can solve, then uses Algorithm [2], and then recovers the coefficient-degree tuples (c_j, e_j) such that $f(x) = \sum_{j=0}^{t} c_j D_{e_j}(x, a)$.

Algorithm 2.1.1

Input:

- Black boxes for $f(x)$ and $f'(x)$.
- The integer t.
- $k \in K - \{0,1\}$.
- $a \in K - \{0\}$ such that $b^2 = a$.

Output:

- The c_j and the e_j such that $f(x) = \sum_{j=0}^{t} c_j D_{e_j}(x, a)$.
- The δ_j and the ε_j such that for $f_\varepsilon(x) = \sum_{j=0}^{t} \delta_j D_{\varepsilon_j}(x, a)$; $f\left(k^{i_0+i}\right) = f_\varepsilon\left(k^{i_0+i}\right)$ and $f'\left(k^{i_0+i}\right) = f'_\varepsilon\left(k^{i_0+i}\right)$.

1.

i. Use Equation (3) and form $g(x)$.

ii. Let $\ell = -\left\lceil \frac{3t-1}{2} \right\rceil$.

a. By using the black box for $f(x)$, for $i = 0,1, \ldots, |\ell|, \ldots 3t-1$, compute the $a_i = g\left(k^{\ell+i}\right)$ by using $g(x) = f\left(b\left(x + \frac{1}{x}\right)\right)$.

Use the equality $g\left(k^{\ell+i}\right) = g\left(k^{-\ell-i}\right)$ to generate the a_i with less computation.

b. By using the black box for $f'(x)$, for $i = 0,1, \ldots, |\ell|, \ldots, 3t-1$, compute the $a'_i = g'\left(k^{\ell+i}\right)$ by using $g'(x) = f'\left(b\left(x + \frac{1}{x}\right)\right)\left(b\left(1 - \frac{1}{x^2}\right)\right)$.

Use the equality $k^{\ell+i} g'\left(k^{\ell+i}\right) = -\left(k^{-\ell-i} g'\left(k^{-\ell-i}\right)\right)$ to generate the a'_i with less computation.

We encounter the same scenario as in Section 5.2 of [1]: Similarly, here we have $i_0 = \ell = -\left\lceil \frac{3t-1}{2} \right\rceil$, $g\left(k^{\ell+i}\right) = g\left(k^{-\ell-i}\right)$, $k^{\ell+i} g'\left(k^{\ell+i}\right) = -\left(k^{-\ell-i} g'\left(k^{-\ell-i}\right)\right)$. As stated in Section 5.2 of [1], we can compute the a_i and the a'_i above from $2(|\ell| + 1) \leq 3t + 2$ values of $f(x)$ and $f'(x)$. To generate those values of $f(x)$ and $f'(x)$, we need to use given black boxes for $f(x)$ and $f'(x)$ only $\leq t + \left\lfloor \frac{t}{2} \right\rfloor + 1$ times.

2. Use the Algorithm 2.1 in [1] with inputs $T = 2t, k, i_0 = \ell, r = \left\lfloor \frac{t}{2} \right\rfloor$, and $a_i = g\left(k^{\ell+i}\right)$ and $a_i'' = k^{\ell+i}a_i' = k^{\ell+i}g'\left(k^{\ell+i}\right)$. Note that here we have $3T = 6t$ values of $g(x)$ and $g'(x)$.

3.

i. If Step 2 decides there is no T sparse polynomial $g(x)$ in Laurent basis that interpolates a_i and a_i'', then print that information and stop.

ii. If $char(K) = 0$, or, $char(K) > 0$ and $k^s \neq 1$ for all $s \geq 1$, then the algorithm in Step 2 returns the G_j and the e_j such that $g(x) = \sum_{j=1}^{t} G_j \left(x^{e_j} + \frac{1}{x^{e_j}}\right)$.

In this case, compute the c_j from $G_j = b^{e_j}c_j$ and return the c_j and the e_j such that $f(x) = \sum_{j=0}^{t} c_j D_{e_j}(x, a)$.

iii. If $char(K) > 0$ and there exists $s \geq 2$ such that $k^s = 1$, then the algorithm in Step 2 returns Γ_j and ε_j such that $g_\varepsilon(x) = \sum_{j=1}^{t} \Gamma_j \left(x^{\varepsilon_j} + \frac{1}{x^{\varepsilon_j}}\right)$ such that $g\left(k^{\ell+i}\right) = g_\varepsilon\left(k^{\ell+i}\right)$ and $g'\left(k^{\ell+i}\right) = g_\varepsilon'\left(k^{\ell+i}\right)$.

In this case, compute the δ_j from $\Gamma_j = b^{\varepsilon_j}c_j$ and return the c_j and the ε_j such that $f_\varepsilon(x) = \sum_{j=0}^{t} \delta_j D_{\varepsilon_j}(x, a)$, such that $f\left(k^{\ell+i}\right) = f_\varepsilon\left(k^{\ell+i}\right)$ and $f'\left(k^{\ell+i}\right) = f_\varepsilon'\left(k^{\ell+i}\right)$.

2.2 Sparse Hermite Interpolation with Dickson Polynomials of the Second Kind

Assume that $f(x) = \sum_{j=0}^{t} c_j E_{e_j}(x, a)$. Then, with the help of Equation (2), we can define $h(x)$ from $f(x)$:

$$\begin{aligned} h(x) &:= \left(b\left(x - \frac{1}{x}\right)\right) f\left(b\left(x + \frac{1}{x}\right)\right) \\ &= \left(bx - \frac{a}{bx}\right) f\left(bx + \frac{a}{bx}\right) \\ &= \left(bx - \frac{a}{bx}\right) \sum_{j=0}^{t} c_j E_{e_j}\left(bx + \frac{a}{bx}, a\right) \\ &= \sum_{j=1}^{t} H_j \left(x^{e_j+1} - \frac{1}{x^{e_j+1}}\right) \in K[x, x^{-1}] \end{aligned} \tag{4}$$

where $H_j = b^{e_j+1}c_j$.

Here, $h(x)$ has $T = 2t$ terms in Laurent polynomial bases and $h\left(k^i\right) = -h\left(k^{-i}\right)$ for $k \in K$. To compute two evaluations $h\left(k^i\right)$ and $h\left(k^{-i}\right)$, we need to evaluate $f(x)$ only once at $x = b\left(k^i + \frac{1}{k^i}\right)$.

Here, we have

$$h'(x) = b\left(1 + \frac{1}{x^2}\right) f\left(b\left(x + \frac{1}{x}\right)\right) + a\left(x - \frac{1}{x}\right)\left(1 - \frac{1}{x^2}\right) f'\left(b\left(x + \frac{1}{x}\right)\right)$$

and

$$h'(x) = \sum_{j=1}^{t} \frac{H_j(e_j+1)}{x}\left(x^{e_j+1} + \frac{1}{x^{e_j+1}}\right).$$

Note that, $k^i h'(k^i) = k^{-i}h'(k^{-i})$. To compute the two evaluations $h'(k^i)$ and $h'(k^{-i})$, we need to evaluate $f(x)$ and $f'(x)$ only once at $x = b\left(k^i + \frac{1}{k^i}\right)$.

One can make use of Equation (4) and can design an algorithm (which is similar to Algorithm 2.1.1) that solves Problem 1.1.ii.

2.3 Sparse Hermite Interpolation with Bernstein Basis Polynomials

In [13], it is introduced that

$$(1+x)^n B_{i,n}\left(\frac{x}{1+x}\right) = \binom{n}{i} x^i. \tag{5}$$

Assume $f(x) = \sum_{j=0}^{t} c_j B_{e_j,n}(x)$. Then, with the help of Equation (5), we can define $z(x)$ from $f(x)$:

$$\begin{aligned} z(x) &\coloneqq (1+x)^n f\left(\frac{x}{1+x}\right) \\ &= (1+x)^n \sum_{j=0}^{t} c_j B_{e_j,n}\left(\frac{x}{1+x}\right) \\ &= \sum_{j=0}^{t} Z_j\, x^{e_j} \end{aligned} \tag{6}$$

where $Z_j = \binom{n}{j} c_j$. Here $z(x)$ and $f(x)$ have the same number of terms and $z(k^i), z'(k^i)$ can be computed from $f\left(\frac{k^i}{1+k^i}\right), f'\left(\frac{k^i}{1+k^i}\right)$.

We can make use of Equation (6) and can design an algorithm that solves Problem 1.1.iii. Algorithm 2.3.1 first uses Equation (6) to convert Problem 1.1.iii to another problem that the Algorithm in [2] can solve, then uses Algorithm [2], and then recovers the coefficient-degree tuples (c_j, e_j) such that $f(x) = \sum_{j=0}^{t} c_j B_{e_j,n}(x)$.

Algorithm 2.3.1

Input:

- Black boxes for $f(x)$ and $f'(x)$.
- The integer t.
- An integer r such that $1 \le r \le t-1$.
- An integer ℓ.
- $k \in \mathbb{R} - \{0,1\}$.
- $n = \deg(f(x))$.

Output:

- The c_j and the e_j such that $f(x) = \sum_{j=0}^{t} c_j B_{e_j,n}(x)$.

1.
   i. Use Equation (6) and form $z(x)$.

   ii. By using black the boxes for $f(x)$ and $f'(x)$, for $i = 0, \ldots, 2t - r - 1$, compute $a_i = z(k^{\ell+i})$ and $a_i'' = k^{\ell+i} z'(k^{\ell+i})$ by using $z(x) = (1+x)^n f\left(\frac{x}{1+x}\right)$.

2. Use the algorithm 2.1 in [1] with inputs $t, k, i_0 = \ell, r$, and $a_i = z(k^{\ell+i})$ and $a_i'' = k^{\ell+i} z'(k^{\ell+i})$.

3.
   i. If Step 2 decides there is no t sparse polynomial $z(x)$ in Laurent basis that interpolates a_i and a_i'', then print that information and stop.

   ii. If Step 2 returns the Z_j and the e_j such that $z(x) = \sum_{j=0}^{t} Z_j\, x^{e_j}$, then compute the c_j from $Z_j = \binom{n}{j} c_j$, and then return the c_j and the e_j.

3. CONCLUSION

In this manuscript, we present three sparse Hermite interpolation algorithms: An algorithm that computes an unknown polynomial directly as a linear combination of Dickson polynomials of the first kind, an algorithm that recovers an unknown polynomial directly in terms of Dickson polynomials of the second kind, and an algorithm that rebuilds an unknown polynomial as a combination of Bernstein basis polynomials. Future work may include developing sparse Hermite interpolation algorithms that perform similar compuations with orthogonal polynomial bases, such as Legendre polynomials and Jacobi polynomials.

CONFLICT OF INTEREST

The author stated that there are no conflicts of interest regarding the publication of this article.

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RESEARCH ARTICLE

FIVE POINT METRIC SPACES: GROMOV PRODUCT STRUCTURES, QUADRANGLE STRUCTURES AND EXPLICIT PARAMETERIZATIONS

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ABSTRACT

Let (X,d) be a finite metric space with elements $P_i, i=1,\dots,n$ and with distances $d_{ij}:=d(P_i,P_j)$ for $i,j=1,\dots,n$. The "Gromov product" Δ_{ijk}, is defined as $\Delta_{ijk}=\frac{1}{2}(d_{ij}+d_{ik}-d_{jk})$. (X,d) is called Δ-generic, if for each fixed i, the set of Gromov products has a unique least element, $\Delta_{ij_ik_i}$. The Gromov product structure on a Δ-generic finite metric space (X,d) is the map that assigns the edge $E_{j_ik_i}$ to P_i. A finite metric space is called "quadrangle generic", if for all 4-point subsets $\{P_i,P_j,P_k,P_l\}$, the set $\{d_{ij}+d_{kl},d_{ik}+d_{jl},d_{il}+d_{jk}\}$ has a unique maximal element. We define the "quadrangle structure" on a quadrangle generic finite metric space (X,d) as the map that assigns to each 4-point subset of X, the pair of edges corresponding to the maximal element of the sums of the distances. Two metric spaces (X,d) and (X,d') are said to be Δ-equivalent (Q-equivalent), if the corresponding Gromov product (quadrangle) structures are the same up to a permutation of X.

In this paper, Gromov product structures, quadrangle structures, optimal reductions and explicit parameterizations for 5-point spaces are obtained and compared with previous results in the literature. In the final part of this paper, we have used the Monte Carlo method to obtain the relative volume of each of the 5-point metric types inside the corresponding metric cone for 5-point spaces, meanwhile 102 different partitions of metric cone for 5-point spaces are derived, considering Gromov product structures. These 102 partitions, come in three symmetric classes forming three types of metrics for 5-point spaces. Thus, one can say that all the methods of classification given here or given before in the literature of finite metric spaces, give 3 types of metrics for 5-point spaces.

Keywords: Finite metric spaces, Split metric decompositions, Gromov products, Quadrangle structures

1. INTRODUCTION

The notions of Gromov product structures, Δ-equivalence, quadrangle structures and Q-equivalence have been defined in previous work [1]. Here, we present the applications of these notions to 5-point spaces. Basic definitions are quoted from [1].

Notation: Let (X,d) be a finite metric space with n elements P_i, $i=1,\dots,n$ $(n\geq 3)$ and let d_{ij} be the distance between P_i and P_j. The elements of X are also referred to as "vertices" or "nodes". E_{ij} and T_{ijk} denote respectively an edge and a triangle with corresponding vertices.

Gromov products: The quantity Δ_{ijk}, defined as

$$\Delta_{ijk}=\Delta_{ikj}=\frac{1}{2}(d_{ij}+d_{ik}-d_{jk})$$

is called the Gromov product of the triangle T_{ijk} at the vertex P_i [2].

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Δ-generic metrics: A metric space is called Δ-generic, if for each P_i the set of Gromov products Δ_{ijk} has a unique smallest element.

Gromov product structures: Let (X, d) be a Δ-generic finite metric space. Let $P_i \in X$, and let Δ_{ijk} be the minimal Gromov product at P_i, $(i = 1, \dots, n)$. The function that assigns the edge E_{jk} to the vertex P_i is called the Gromov product structure on X. Two Δ-generic metric spaces (X, d) and (X, d') are Δ-equivalent, if the corresponding Gromov product structures are the same up to a permutation of X.

The metric cone: The set C_n of all pseudo-metrics $d = (d_{ij}) \in \mathbb{R}^{\binom{n}{2}}$ on a given n-point set X, is called the metric cone.

The metric fan: A decomposition of metric cone C_n into some sub-cones defined as below is called the metric fan [3]. Consider the $\binom{n}{2} \times$ n matrix $\mathcal{A}$ where the rows are numbered by the edges as

$$(1,2), (1,3), \dots, (1,n), (2,3), (2,4), \dots, (2,n), \dots, (n-1,n)$$

and the (i,j)-row $(i < j)$ is given by $e_i + e_j = (0, \dots, 1, \dots, 1, \dots, 0) \in \mathbb{R}^n$. Let $\mathcal{B}$ be an invertible $n \times n$ submatrix of $\mathcal{A}$ and denote the $\left[\binom{n}{2} - n\right] \times n$ matrix obtained by deleting $\mathcal{B}$ from $\mathcal{A}$ by $\mathcal{B}'$. Likewise, define $d_{\mathcal{B}} \in \mathbb{R}^n$ by choosing the components of $d \in \mathbb{R}^{\binom{n}{2}}$ corresponding to $\mathcal{B}$ and $d_{\mathcal{B}'} \in \mathbb{R}^{\binom{n}{2}-n}$ corresponding to $\mathcal{B}'$. Now consider the following system of equations and inequalities for $x \in \mathbb{R}^n$:

$$\mathcal{B}x = d_{\mathcal{B}} \text{ and } \mathcal{B}'x > d_{\mathcal{B}'}.$$

If this system has a solution we say that the matrix $\mathcal{B}$ is a "cell" or a "thrackle" for the metric d. The collection of cells of a metric d is denoted by $Cell(d)$. Two metrics d and d' on an n-point metric space X are said to be equivalent in the metric-fan sense, if they have the same collection of cells or what amounts to the same collection of sub-graphs, i.e. $Cell(d) = Cell(d')$. The equivalence class of a metric d is a sub-cone of the metric cone and these sub-cones constitute altogether the metric fan.

The classification of 6-point spaces with respect to Gromov product structures (Δ-equivalence) is obtained in [4]. In that work it is shown that there are 26 Δ-equivalence classes and also presented their correspondences to the classification by the decomposition of the metric fan. The list of Gromov product structures and the corresponding metric fan types for the 26 Δ-generic metrics are given in [4].

In [5], the Gromov classification of 7-point spaces has been obtained and shown that there are 431 equivalence classes. For 8-point metric spaces, we have obtained the Δ-equivalence classifications and found 11470 equivalence classes in the work on our website:
http://finitemetricspaces.khas.edu.tr/118F412_webpage_8pointspaces.pdf

The metric fan classification of n-point spaces for $n > 6$ is not known. It looks like the number of classes will be increasingly large and such a classification would not be practical. Even the Gromov product classification is becoming impractical for $n > 8$. Thus, we are looking for coarser equivalences that would reflect essential properties of a finite metric space.

Quadrangle generic metric spaces: An n-point finite metric space X is called "quadrangle generic", or Q-generic, if for every 4-point subset $\{P_a, P_b, P_c, P_d\} \subseteq X$, the set of distances

$$\{d_{ab} + d_{cd}, d_{ac} + d_{bd}, d_{ad} + d_{bc}\}$$

has a unique maximal element.

Quadrangle Structures: A quadrangle structure on a Q-generic finite metric space (X, d) is a map which assigns to any 4-point subset $\{P_a, P_b, P_c, P_d\}$ of X, the pair of edges corresponding to the maximal element of the set $\{d_{ab} + d_{cd}, d_{ac} + d_{bd}, d_{ad} + d_{bc}\}$. We denote the 4-point subset $\{P_a, P_b, P_c, P_d\}$ without any restriction on the sides by $Q(a, b, c, d)$ in which the ordering of the indices is irrelevant. If $d_{ac} + d_{bd}$ is maximal, the vertices are ordered as (P_a, P_b, P_c, P_d) and we denote this structured quadrangle by $Q(abcd)$ in which the cyclic permutations and reversal of the order of the indices give equivalent quadrangles.

***Q*-equivalence:** Two Q-generic metric spaces (X, d) and (X, d') are called Q-equivalent, if the corresponding quadrangle structures are the same up to a permutation of X.

Parameterization of 4-point spaces: Let the set of minimal Gromov products of the quadrangle $Q(abcd)$ be $\{\Delta_{abd}, \Delta_{bac}, \Delta_{cbd}, \Delta_{dac}\}$ and let α and β be defined as

$$\alpha = \Delta_{\mathrm{abc}} - \Delta_{\mathrm{abd}}, \qquad \beta = \Delta_{\mathrm{adc}} - \Delta_{\mathrm{adb}},$$

then, one has the following equalities between Gromov products

$$\alpha = \Delta_{abc} - \Delta_{abd} = \Delta_{bad} - \Delta_{bac} = \Delta_{cda} - \Delta_{cdb} = \Delta_{dcb} - \Delta_{dca},$$
$$\beta = \Delta_{adc} - \Delta_{adb} = \Delta_{bcd} - \Delta_{bca} = \Delta_{cba} - \Delta_{cbd} = \Delta_{dab} - \Delta_{dac},$$

and the distances are expressed as

$$d_{ab} = \Delta_{abd} + \Delta_{bac} + \alpha, \qquad d_{cd} = \Delta_{cbd} + \Delta_{dac} + \alpha,$$
$$d_{bc} = \Delta_{bac} + \Delta_{cbd} + \beta, \qquad d_{ad} = \Delta_{abd} + \Delta_{dac} + \beta,$$
$$d_{ac} = \Delta_{abd} + \Delta_{cbd} + \alpha + \beta, \quad d_{bd} = \Delta_{bac} + \Delta_{dac} + \alpha + \beta.$$

This is shown in Figure 1 below.

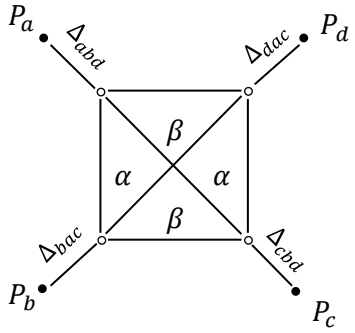

Figure 1. A quadrangle with the set of minimal Gromov products $\{\Delta_{abd}, \Delta_{bac}, \Delta_{cbd}, \Delta_{dac}\}$.

Matrix representation of Gromov product structures: Gromov product structures on an n-point space are represented by the $n \times n$ matrix M_Δ defined by $M_\Delta(i, j) = 1$ and $M_\Delta(i, k) = 1$ if Δ_{ijk} is the minimal Gromov product at P_i and 0 otherwise [6].

Matrix representation of quadrangle structures: The matrix of a quadrangle structure Q, M_Q on an n-point space is an $n_d \times n_d$ matrix ($n_d = \frac{n(n-1)}{2}$) such that $M_Q(ab, cd) = 1$ if the edges E_{ab} and E_{cd} are diagonals in $\{P_a, P_b, P_c, P_d\}$ and $M_Q(ab, cd) = 0$ otherwise.

These matrix representations proved to be useful in determining equivalences/inequivalences of Δ- and Q-equivalence classes. We recall that two structures are equivalent if their matrices can be mapped to each other by a permutation of indices. Similarity and isospectrality of matrices leads to coarser classifications [6].

Split pseudo-metrics: A "split" $S = \{A, B\}$ of a finite set X is a partition of X into two non-empty subsets A and B. For simplicity we often identify the set of points of A with its index set. For each

$P_a \in X$, we denote by $S(a)$ the subset A or B that contains P_a. Corresponding to each split S we define the pseudo-metric δ_S by

$$\delta_S(a,a') = \begin{cases} 1, & if\ \ S(a) \neq S(a'), \\ 0, & if\ \ S(a) = S(a'). \end{cases}$$

If the number of elements of A or B is equal to k, the split is referred to as a k-split.

Totally split decomposable metrics: A metric on X is called totally split decomposable if it can be expressed as a linear combination (with non-negative coefficients) of the split metrics [7].

The isolation index of a split: The isolation index of a split $S = \{A, B\}$ is defined as

$$\alpha_{\{A,B\}} = \frac{1}{2} \min_{\{a,a' \in A, b,b' \in B\}} \{ \max \{ d_{ab} + d_{a'b'}\ , d_{ab'}\ + d_{a'b}\ , d_{aa'} + d_{bb'} \}\ - (d_{aa'} + d_{bb'}) \}.$$

Split prime: A pseudo-metric is called a split prime if all of its isolation indices are equal to zero [7].

Lemma 1: Let (X, d) be a finite metric space with n elements $P_i\ (i\ =\ 1, \dots, n)$ and let $S\ = \{A, B\}$ be a split for X. Then,

i. The isolation index for the 1-split with $A = \{P_a\}$ is the minimal Gromov product at P_a,
ii. If (X, d) is Q-generic, then the isolation index for the k-split with $A = \{P_{i_1}, \dots, P_{i_k}\}$ is non-zero if and only if for no pair of indices $a, a' \in A$, $E_{aa'}$ is a diagonal of the quadrangles $Q(a, a', b, b')$ where $b, b' \in B$.

Proof: See [1].

In [1], we have shown that the number of 2-splits in an n-point space is at most n. We have discussed the case $n = 6$ in terms of 3-splits, relating to the results of [7].

2. PARAMETERIZATION OF 5-POINT METRIC SPACES

In this section we will give an explicit parameterization of 5-point spaces using Gromov product structures, quadrangle structures and partial orders on Gromov products at each P_a. This parameterization coincides with the parameterization given in [8].

It is known that the Gromov product equivalence gives the known classification of 5-point Δ-generic metric spaces [4].

A: $\{\Delta_{125}, \Delta_{213}, \Delta_{324}, \Delta_{435}, \Delta_{514}\}$
B: $\{\Delta_{125}, \Delta_{213}, \Delta_{325}, \Delta_{425}, \Delta_{514}\}$,
C: $\{\Delta_{125}, \Delta_{213}, \Delta_{325}, \Delta_{425}, \Delta_{513}\}$.

Note that, if say Δ_{ijk} is minimal in the metric space X, then it is also minimal in every quadrangle $Q = \{P_i, P_j, P_k, P_l\}$. In a graphical presentation we indicate this by marking the corresponding angle by a filled arc as shown in Figure 2. For a 5-point metric space X, at least one of the Gromov products in any quadrangle belongs to the list of minimal Gromov products. It follows that for a 5-point space, the Gromov product structure determines the quadrangle structure. The determination of the parameters displayed in the quadrangles will be explained below.

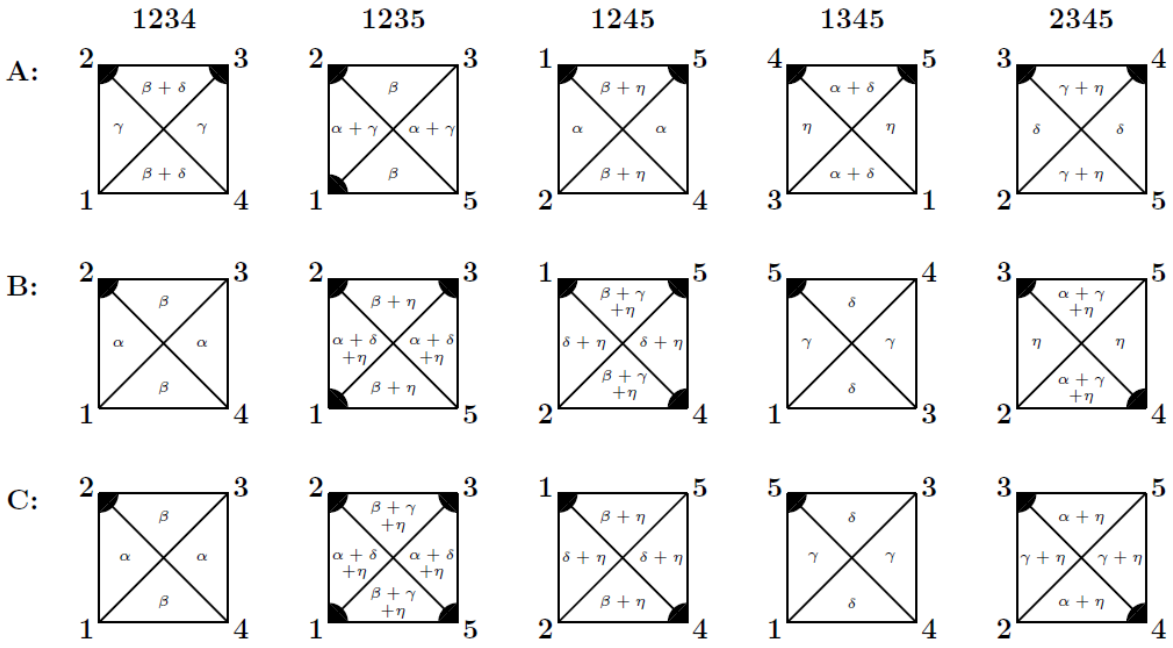

Figure 2. The structure of the 4-point subsets for the three types of 5-point metric spaces.

From Figure 2, we can see that, in Type A, the edges $E_{12}, E_{23}, E_{34}, E_{45}$ and E_{15} are "sides" in all quadrangles, hence Type A metrics are totally split-decomposable by Lemma 1. For Type B, there are 4 edges E_{45}, E_{15}, E_{12} and E_{23} that occur as sides in all quadrangles. Therefore it is not totally split-decomposable. Similarly for Type C, the edges that occur as "sides" in all quadrangles are E_{12}, E_{23}, E_{34} and E_{45}, hence it is not totally split-decomposable.

In order to obtain an explicit parameterization of these metrics, we will use the quadrangle structure to obtain partial order relations among the Gromov products, then use the relations $d_{ij} = \Delta_{ijk} + \Delta_{jik}$. The structure of the quadrangles in Figure 2 lead to the following order relations for each of the types A, B, C in the following way: Take quadrangle $Q(1234)$ of Type A for instance. Since $d_{12} + d_{34} < d_{13} + d_{24}$, equivalently $\frac{1}{2}(d_{12} + d_{14} - d_{24}) < \frac{1}{2}(d_{13} + d_{14} - d_{34})$ which is to say $\Delta_{124} < \Delta_{134}$; we can also say that since $d_{14} + d_{23} < d_{13} + d_{24}$ is equivalent to $\frac{1}{2}(d_{12} + d_{14} - d_{24}) < \frac{1}{2}(d_{12} + d_{13} - d_{23})$ which means $\Delta_{124} < \Delta_{123}$. Thus for each vertex of a quadrangle, two inequalities among three Gromov products could be derived by similar algebraic manipulations. The list of these inequalities for each type is given below. These order relations are used to determine isolation indices for 2-splits and the split primes.

From quadrangles of Type A, we have the following relations among Gromov products:

$$
\begin{array}{llll}
Q(1234): \Delta_{124} < \Delta_{123}, \Delta_{134}, & \Delta_{213} < \Delta_{214}, \Delta_{234}, & \Delta_{324} < \Delta_{312}, \Delta_{314}, & \Delta_{413} < \Delta_{412}, \Delta_{423}, \\
Q(1235): \Delta_{125} < \Delta_{123}, \Delta_{135}, & \Delta_{213} < \Delta_{215}, \Delta_{235}, & \Delta_{325} < \Delta_{312}, \Delta_{315}, & \Delta_{513} < \Delta_{512}, \Delta_{523}, \\
Q(1245): \Delta_{125} < \Delta_{124}, \Delta_{145}, & \Delta_{214} < \Delta_{215}, \Delta_{245}, & \Delta_{425} < \Delta_{412}, \Delta_{415}, & \Delta_{514} < \Delta_{512}, \Delta_{524}, \\
Q(1345): \Delta_{135} < \Delta_{134}, \Delta_{145}, & \Delta_{314} < \Delta_{315}, \Delta_{345}, & \Delta_{435} < \Delta_{413}, \Delta_{415}, & \Delta_{514} < \Delta_{513}, \Delta_{534}, \\
Q(2345): \Delta_{235} < \Delta_{234}, \Delta_{245}, & \Delta_{324} < \Delta_{325}, \Delta_{345}, & \Delta_{435} < \Delta_{423}, \Delta_{425}, & \Delta_{524} < \Delta_{523}, \Delta_{534}.
\end{array}
$$

which lead to the following Hasse diagrams given in Figure 3.

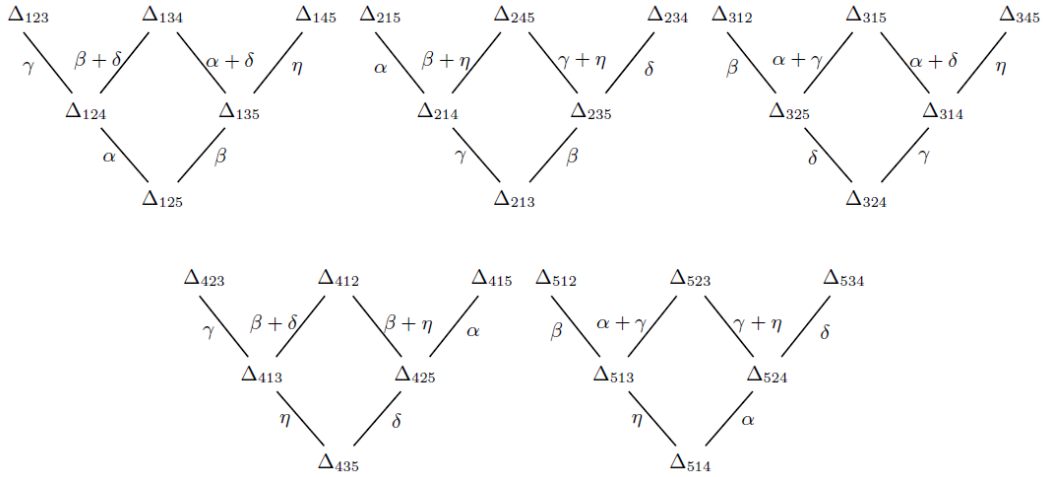

Figure 3. The partial order diagrams for the Type A.

For Type B, we have:

$$Q(1234):\ \Delta_{124}<\Delta_{123},\Delta_{134},\quad \Delta_{213}<\Delta_{214},\Delta_{234},\quad \Delta_{324}<\Delta_{312},\Delta_{314},\quad \Delta_{413}<\Delta_{412},\Delta_{423},$$
$$Q(1235):\ \Delta_{125}<\Delta_{123},\Delta_{135},\quad \Delta_{213}<\Delta_{215},\Delta_{235},\quad \Delta_{325}<\Delta_{312},\Delta_{315},\quad \Delta_{513}<\Delta_{512},\Delta_{523},$$
$$Q(1245):\ \Delta_{125}<\Delta_{124},\Delta_{145},\quad \Delta_{214}<\Delta_{215},\Delta_{245},\quad \Delta_{425}<\Delta_{412},\Delta_{415},\quad \Delta_{514}<\Delta_{512},\Delta_{524},$$
$$Q(1345):\ \Delta_{135}<\Delta_{134},\Delta_{145},\quad \Delta_{314}<\Delta_{315},\Delta_{345},\quad \Delta_{435}<\Delta_{413},\Delta_{415},\quad \Delta_{514}<\Delta_{513},\Delta_{534},$$
$$Q(2354):\ \Delta_{234}<\Delta_{235},\Delta_{245},\quad \Delta_{325}<\Delta_{324},\Delta_{345},\quad \Delta_{425}<\Delta_{423},\Delta_{435},\quad \Delta_{534}<\Delta_{523},\Delta_{524}.$$

which give the following Hasse diagrams given in Figure 4.

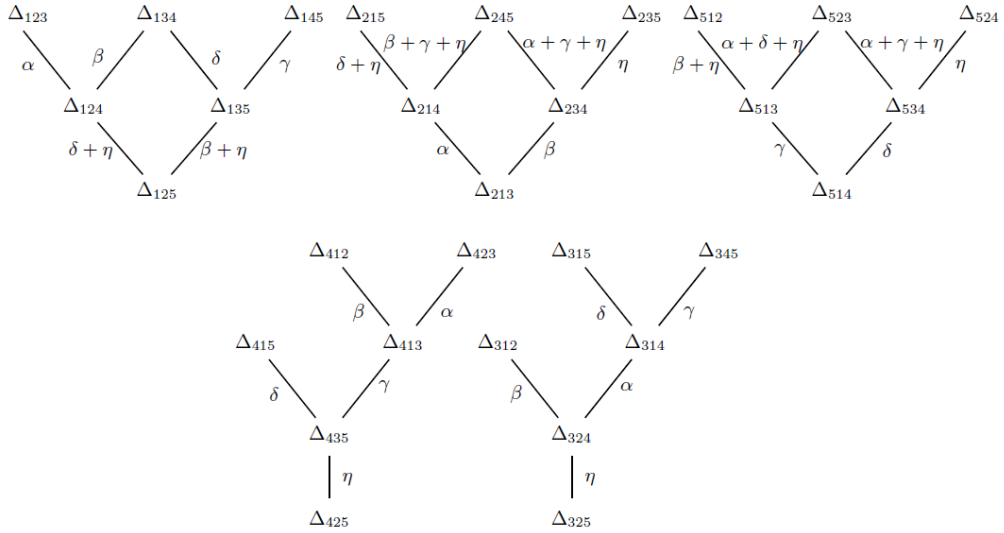

Figure 4. The partial order diagrams for the Type B.

For Type C, the quadrangles give the following relations:

$$Q(1234):\Delta_{124}<\Delta_{123},\Delta_{134},\quad \Delta_{213}<\Delta_{214},\Delta_{234},\quad \Delta_{324}<\Delta_{312},\Delta_{314},\quad \Delta_{413}<\Delta_{412},\Delta_{423},$$
$$Q(1235):\Delta_{125}<\Delta_{123},\Delta_{135},\quad \Delta_{213}<\Delta_{215},\Delta_{235},\quad \Delta_{325}<\Delta_{312},\Delta_{315},\quad \Delta_{513}<\Delta_{512},\Delta_{523},$$
$$Q(1245):\Delta_{125}<\Delta_{124},\Delta_{145},\quad \Delta_{214}<\Delta_{215},\Delta_{245},\quad \Delta_{425}<\Delta_{412},\Delta_{415},\quad \Delta_{514}<\Delta_{512},\Delta_{524},$$
$$Q(1435):\Delta_{145}<\Delta_{134},\Delta_{135},\quad \Delta_{345}<\Delta_{314},\Delta_{315},\quad \Delta_{413}<\Delta_{415},\Delta_{435},\quad \Delta_{513}<\Delta_{514},\Delta_{534},$$
$$Q(2354):\Delta_{234}<\Delta_{235},\Delta_{245},\quad \Delta_{325}<\Delta_{324},\Delta_{345},\quad \Delta_{425}<\Delta_{423},\Delta_{435},\quad \Delta_{534}<\Delta_{523},\Delta_{524}.$$

which lead to the Hasse diagrams given in Figure 5.

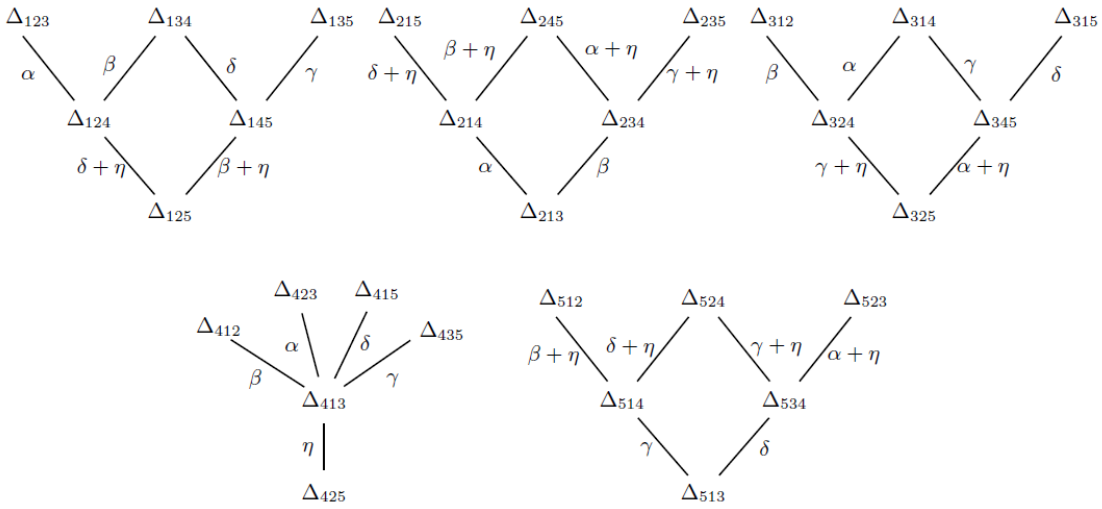

Figure 5. The partial order diagrams for the Type C.

Remark 1 For Types A and B, the quadrangle structure determines the Gromov product structure, in the sense that the partial order relations deduced from the quadrangle structure determine the smallest Gromov product at each P_i. On the other hand, for Type C, the partial order relations imply that both Δ_{413} and Δ_{425} are smaller than $\Delta_{412}, \Delta_{415}, \Delta_{423}$ and Δ_{435}, but the order relation between Δ_{413} and Δ_{425} is not determined by the quadrangle structure. This is an example for the case where the quadrangle structure does not determine the Gromov product structure.

Recall that the minimal Gromov products at each P_a are the isolation indices of 1-splits. In what follows, we assume that minimal Gromov products are zero.
The isolation indices for 2-splits will serve as free variables for the parameterization of the distances. For example, for Type A,

$$\begin{aligned}\alpha_{12} = \frac{1}{2}\min\{\ &\max\{d_{13}+d_{24}, d_{14}+d_{23}, d_{12}+d_{34}\} - (d_{12}+d_{34}),\\ &\max\{d_{13}+d_{25}, d_{15}+d_{23}, d_{12}+d_{35}\} - (d_{12}+d_{35}),\\ &\max\{d_{14}+d_{25}, d_{15}+d_{24}, d_{12}+d_{45}\} - (d_{12}+d_{45})\}\\ = \min\{\ &d_{13}+d_{24}-d_{12}-d_{34},\ d_{13}+d_{25}-d_{12}-d_{35},\ d_{14}+d_{25}-d_{12}-d_{45}\}.\end{aligned}$$

Which reformulating by using Gromov products gives:

$$\alpha_{12} = \min\{\Delta_{134} - \Delta_{124} = \Delta_{234} - \Delta_{213}, \Delta_{135} - \Delta_{125} = \Delta_{235} - \Delta_{213}, \Delta_{145} - \Delta_{125} = \Delta_{245} - \Delta_{214}\}.$$

Finally since $\Delta_{125} = \Delta_{213} = 0$ we may write it as:

$$\alpha_{12} = \min\{\Delta_{234}, \Delta_{135} = \Delta_{235}, \Delta_{145}\}.$$

From the partial order relations it is clear that α_{12} cannot be equal to Δ_{145}. Similarly, as $\Delta_{234} > \Delta_{235}$, we choose Δ_{135} as a free variable for the parameterization. By similar arguments and what is given when discussing "Parameterization of 4-point spaces" and Figure 1 in the introduction, the parameterization of the Gromov products and of the distance functions can be obtained as given below.

Type A: $\Delta_{125} = \Delta_{213} = \Delta_{324} = \Delta_{435} = \Delta_{514} = 0$.

$$\begin{aligned}&\Delta_{124} = \alpha, \quad \Delta_{135} = \beta, \quad \Delta_{123} = \alpha+\gamma, \quad \Delta_{145} = \beta+\eta, \quad \Delta_{134} = \alpha+\beta+\delta,\\ &\Delta_{214} = \gamma, \quad \Delta_{235} = \beta, \quad \Delta_{215} = \alpha+\gamma, \quad \Delta_{234} = \beta+\delta, \quad \Delta_{245} = \beta+\gamma+\eta,\\ &\Delta_{314} = \gamma, \quad \Delta_{325} = \delta, \quad \Delta_{312} = \beta+\delta, \quad \Delta_{345} = \gamma+\eta, \quad \Delta_{315} = \alpha+\delta+\gamma,\end{aligned}$$

$$\Delta_{413} = \eta, \quad \Delta_{425} = \delta, \quad \Delta_{415} = \alpha + \delta, \quad \Delta_{423} = \gamma + \eta, \quad \Delta_{412} = \beta + \delta + \eta,$$
$$\Delta_{513} = \eta, \quad \Delta_{524} = \alpha, \quad \Delta_{512} = \beta + \eta, \quad \Delta_{534} = \alpha + \delta, \quad \Delta_{523} = \alpha + \gamma + \eta.$$

$$d_{12} = \alpha + \gamma, \quad d_{13} = \alpha + \beta + \delta + \gamma, \quad d_{14} = \alpha + \beta + \delta + \eta, \quad d_{15} = \beta + \eta, \quad d_{23} = \beta + \delta,$$
$$d_{24} = \beta + \delta + \gamma + \eta, \; d_{25} = \alpha + \beta + \gamma + \eta, \; d_{34} = \gamma + \eta, \; d_{35} = \alpha + \delta + \gamma + \eta, \; d_{45} = \alpha + \delta.$$

Type B: $\Delta_{125} = \Delta_{213} = \Delta_{325} = \Delta_{425} = \Delta_{514} = 0.$

$$\Delta_{124} = \delta + \eta, \quad \Delta_{135} = \beta + \eta, \quad \Delta_{134} = \beta + \delta + \eta, \quad \Delta_{123} = \alpha + \delta + \eta, \quad \Delta_{145} = \beta + \gamma + \eta,$$
$$\Delta_{214} = \alpha, \quad \Delta_{234} = \beta, \quad \Delta_{235} = \beta + \eta, \quad \Delta_{215} = \alpha + \delta + \eta, \quad \Delta_{245} = \alpha + \beta + \gamma + \eta,$$
$$\Delta_{324} = \eta, \quad \Delta_{312} = \beta + \eta, \quad \Delta_{314} = \alpha + \eta, \quad \Delta_{315} = \alpha + \delta + \eta, \quad \Delta_{345} = \alpha + \gamma + \eta,$$
$$\Delta_{435} = \eta, \quad \Delta_{413} = \gamma + \eta, \quad \Delta_{415} = \delta + \eta, \quad \Delta_{423} = \alpha + \gamma + \eta, \quad \Delta_{412} = \beta + \gamma + \eta,$$
$$\Delta_{534} = \delta, \quad \Delta_{513} = \gamma, \quad \Delta_{524} = \delta + \eta, \quad \Delta_{512} = \beta + \gamma + \eta, \quad \Delta_{523} = \alpha + \delta + \gamma + \eta.$$

$$d_{12} = \alpha + \delta + \eta, \; d_{13} = \alpha + \beta + \delta + 2\eta, \; d_{14} = \beta + \delta + \gamma + 2\eta, \; d_{15} = \beta + \gamma + \eta, \; d_{23} = \beta + \eta,$$
$$d_{24} = \alpha + \beta + \gamma + \eta, \; d_{25} = \alpha + \beta + \delta + \gamma + 2\eta, \; d_{35} = \alpha + \delta + \gamma + \eta, \; d_{45} = \delta + \eta.$$

Type C : $\Delta_{125} = \Delta_{213} = \Delta_{325} = \Delta_{425} = \Delta_{513} = 0.$

$$\Delta_{123} = \alpha + \delta + \eta, \quad \Delta_{124} = \delta + \eta, \quad \Delta_{134} = \beta + \delta + \eta, \quad \Delta_{135} = \beta + \gamma + \eta, \quad \Delta_{145} = \beta + \eta,$$
$$\Delta_{214} = \alpha, \quad \Delta_{215} = \alpha + \delta + \eta, \quad \Delta_{234} = \beta, \quad \Delta_{235} = \beta + \gamma + \eta, \quad \Delta_{245} = \alpha + \beta + \eta,$$
$$\Delta_{312} = \beta + \gamma + \eta, \quad \Delta_{314} = \alpha + \gamma + \eta, \quad \Delta_{315} = \alpha + \delta + \eta, \quad \Delta_{324} = \gamma + \eta, \quad \Delta_{345} = \alpha + \eta,$$
$$\Delta_{412} = \beta + \eta, \quad \Delta_{413} = \eta, \quad \Delta_{415} = \delta + \eta, \quad \Delta_{423} = \alpha + \eta, \quad \Delta_{435} = \gamma + \eta,$$
$$\Delta_{512} = \beta + \gamma + \eta, \quad \Delta_{514} = \gamma, \quad \Delta_{523} = \alpha + \delta + \eta, \quad \Delta_{524} = \delta + \gamma + \eta, \quad \Delta_{534} = \delta.$$

$$d_{12} = \alpha + \delta + \eta, \; d_{13} = \alpha + \beta + \delta + \gamma + 2\eta, \; d_{14} = \beta + \delta + 2\eta, \; d_{15} = \beta + \gamma + \eta, \; d_{23} = \beta + \gamma + \eta,$$
$$d_{24} = \alpha + \beta + \eta, \; d_{25} = \alpha + \beta + \delta + \gamma + 2\eta, \; d_{34} = \alpha + \gamma + 2\eta, \; d_{35} = \alpha + \delta + \eta, \; d_{45} = \delta + \gamma + \eta.$$

These parameterizations are exactly the ones given by Koolen, Lesser and Moulton [8]. In the paper [8], the classes obtained via the decomposition of the metric cone are denoted as Type I, Type II and Type III. These correspond respectively to our equivalence classes denoted by Type A, Type C and Type B. The metrics of Type I, II and III are defined by their split decompositions, given as below. For simplicity we consider the pendant free case, i.e, we take the coefficients of the 1-splits as zero, equivalently the minimal Gromov products at each node are zero.

We use the labeling of the nodes by $\{x, y, u, v, w\}$.
(Type I): $d = \alpha_{xy}\delta_{xy} + \alpha_{yu}\delta\_yu + \alpha_{uv}\delta_{uv} + \alpha_{vw}\delta_{vw} + \alpha_{wx}\delta_{wx}$,
(Type II): $d = \alpha_{xu}\delta_{xu} + \alpha_{xv}\delta_{xv} + \alpha_{uy}\delta_{uy} + \alpha_{vy}\delta_{vy} + c\ d'$,
(Type III): $d = \alpha_{xu}\delta_{xu} + \alpha_{xv}\delta_{xv} + \alpha_{wy}\delta_{wy} + \alpha_{vy}\delta_{vy} + c\ \ d'$,
where $d'(a, b) = 0\ if\ a = b,\ d'(x, y) = d'(u, v) = d'(u, w) = d'(v, w) = 2$ and $d'(a, b) = 1$ for all other cases.

We identify the indices x, y, u, v, w with our notation. For example, for Type I, i.e, our Type A, x, y, u, v, w correspond to $1, 2, 3, 4, 5$ respectively and the correspondence of the parameters are

$$\alpha_{xy} = \beta, \qquad \alpha_{yu} = \gamma, \qquad \alpha_{uv} = \delta, \qquad \alpha_{vw} = \eta, \qquad \alpha_{wx} = \alpha.$$

For Type II, i.e, our Type C, x, y, u, v, w correspond to $5, 2, 1, 3, 4$ respectively and the correspondence of the parameters are

$$\alpha_{xu} = \delta, \qquad \alpha_{xv} = \gamma, \qquad \alpha_{uy} = \beta, \qquad \alpha_{vy} = \alpha, \qquad c = \eta.$$

For Type III, i.e, our Type B, x, y, u, v, w correspond to $2, 5, 3, 1, 4$ respectively and the correspondence of the parameters are

$$\alpha_{xu} = \alpha, \qquad \alpha_{xv} = \beta, \qquad \alpha_{wy} = \gamma, \qquad \alpha_{vy} = \delta, \qquad c = \eta.$$

Explicit parametrizations for certain 6-point spaces have been also obtained via partial order relations and quadrangle classifications. It is available on http://finitemetricspaces.khas.edu.tr/Optimal%20Realizations,%20h-optimal%20Realizations%20and%20Tight%20Spans%20of%20Metric%20Spaces.pdf}.

3. OPTIMAL REDUCTIONS OF 5-POINT METRIC SPACES

Optimal realizations of 5-point metric spaces for three types are given in [8], in what follows we will give underlying graphs for each metric type and will drive their optimal reductions.

The weighted graph $G = (V, E, w)$ is called a realization of the finite metric space (X, d) if there is a labeling function $\phi : X \to V$ such that for all $x, y \in X$ the weight of any path between $\phi(x)$ and $\phi(y)$ is equal to $d(x, y)$. Any such realization is called optimal if $||G||$, the total edge weight of the graph G, is minimal among all realizations of the metric space (X, d) [8].

As it is clear from the definition above that a finite metric space can have many realizations. In the following, we will start with the pendant free reductions and use certain "moves" as defined in [9] to reduce the total weight and reach the optimal representation. This kind of operations are generally done by adjoining new vertices to the original graph, which in this case the added vertices are called secondary vertices and the original vertices as primary, discarding some edges or adding new edges between the enlarged set of vertices and assigning weights to the new edges in a way that the distance between primary nodes are unchanged but the weight of the graph, namely $||G||$, is reduced.

The first move, which is called *joining edges*, is done in the following way: Consider a vertex u and all (or some) of the other nodes $v_1, v_2, \dots, v_k$ of G, which are neighbors of u. Calculate the Gromov products of all triangles $T_{uv_iv_j}$ with $1 \leq i, j \leq k$ at vertex u and call the minimum m_u. Now delete all the edges between u and v_i's, introduce a new vertex v and connect v_i's to v by edges of weight $w_{uv_i} - m_u$ for $1 \leq i \leq k$ and also u to v by an edge of weight m_u; hence the nodes v_i become connected to u by two edges through v and the total weight of the graph is reduced by an amount of $(k-1)m_u$.

The second move, which is called *edge removing*, is done by deleting the edge between two nodes u and v if it can be avoided by a shortest path. This move reduces $||G||$ by an amount of the weight of the deleted edge.

The "$\Delta - Y$" transform is a consequence of the above moves and can be applied to any triangle with 1-connected vertices in G. It is called a $\Delta - Y$ transform, because a triangle shape (Δ) turns to a Y shape after the operation.

We should also note that what we mean by *underlying graph of a metric*, is the complete graph with the same set of vertices as the metric space and all the edges with weight d_{ij} removed for which there is a point in space p_k such that $d_{ij} = d_{ik} + d_{kj}$.

For Type A with the Gromov product structure as $\{\Delta_{125}, \Delta_{213}, \Delta_{324}, \Delta_{435}, \Delta_{514}\}$, when edge removing operations are applied and passed to pendant-free reduction, a 5-cycle given in Figure 6 is obtained. The optimal realization given in [8] is a 5-cycle with edges connected to each of its nodes (Type (a) of [8]).

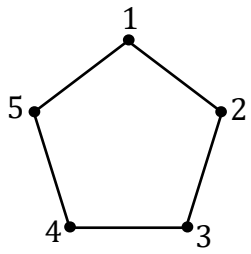

Figure 6. Optimal reduction of metric Type A.

For Type B with the Gromov product structure as $\{\Delta_{125}, \Delta_{213}, \Delta_{325}, \Delta_{425}, \Delta_{514}\}$, the underlying graph is given in Figure 7:

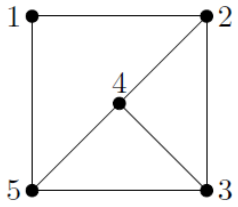

Figure 7. Underlying graph of metric Type B.

By applying a $\Delta - Y$ transform to T_{345} we have Figure 8

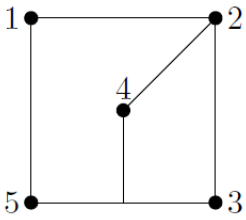

Figure 8. Graph with $\Delta - Y$ transformed.

In this step, one can follow two different approaches which reduce the metric to Type (b) or (c) of [8]. To observe the process closely we need to point out that the parameterization of Type B is given in Figure 9:

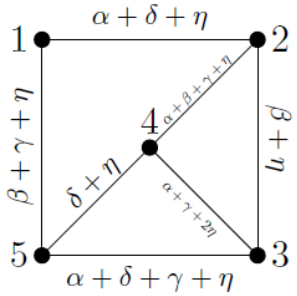

Figure 9. Underlying graph of metric Type B with distances parameterized.

Here we have $\Delta_{345} = \alpha + \gamma + \eta$, $\Delta_{435} = \eta$ and $\Delta_{534} = \delta$, and applying a $\Delta - Y$ transform to T_{345} will be as in Figure 10:

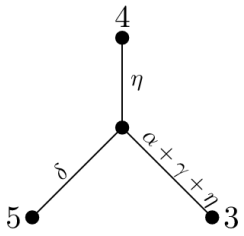

Figure 10. T_{345} of Type B after $\Delta - Y$ transform.

So the Type B with parameters are as following:

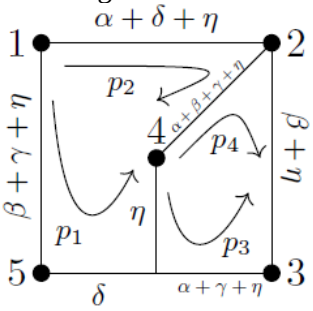

Figure 11. Metric Type B with the parameters.

Now according to the graph above, we have d_{14} equal to $\beta + \delta + \gamma + 2\eta$ (path p_1) or equal to $2\alpha + \beta + \gamma + \delta + 2\eta$ (path p_2). Path p_2 is longer than path p_1 by an amount of 2α. Likewise d_{34} is equal to $\alpha + \gamma + 2\eta$ (path p_3) or equal to $\alpha + 2\beta + \gamma + 2\eta$ (path p_4). Here path p_4 is longer than path p_3 by a difference of 2β. It should be noted that $\alpha = \Delta_{214}$ and $\beta = \Delta_{234}$ and two scenarios are possible: either $\alpha > \beta$ or $\beta > \alpha$. If $\alpha > \beta$, in order to decrease the total weight of the graph, we will introduce a new node called v on the edge joining 1 to 2 as shown below:

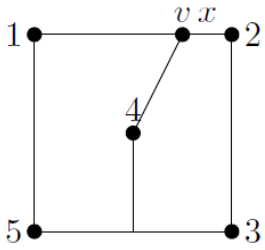

Figure 12. Reduction of Type B to (b).

This will reduce the total weight as $x = \Delta_{214}$ and that results the Type B to reduced into (b) of [8] and the metric will be as following:

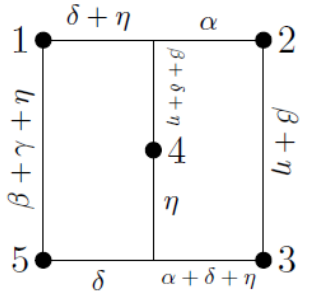

Figure 13. Reduction of Type B to (b) when $\alpha > \beta$ (parameters given).

In the other case, when $\beta > \alpha$, if we do the same operation as before, but this time for the edge joining 2 to 3 we will have the following reduction:

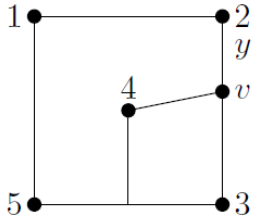

Figure 14. Reduction of Type B to (c).

This reduces the weight of graph as $y = \Delta_{234}$ and turns it into Type (c) given as below:

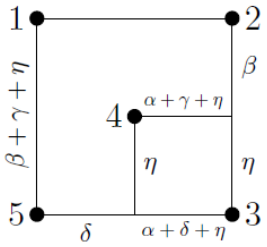

Figure 15. Reduction of Type B to (c) when $\beta > \alpha$ (parameters given).

For Type C which the underlying graph with the parameters given is depicted below, the following can be done:

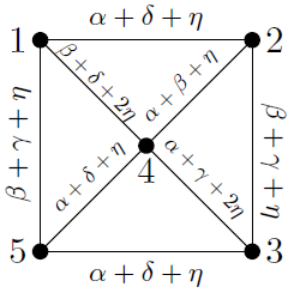

Figure 16. Underlying graph of metric Type C with the metric parameterized.

Since $\Delta_{124} = \delta + \eta$, $\Delta_{214} = \alpha$ and $\Delta_{412} = \beta + \eta$, applying a $\Delta - Y$ transform to T_{124} will result in the following:

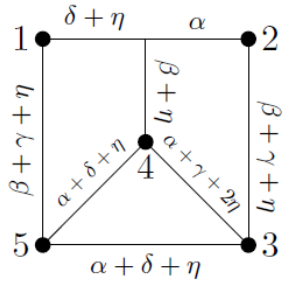

Figure 17. Type C with a $\Delta - Y$ transform applied to T_{124}.

Finally considering that $\Delta_{345} = \alpha + \eta$, $\Delta_{435} = \gamma + \eta$ and $\Delta_{534} = \delta$, applying another $\Delta - Y$ transform to T_{345} will result in the following:

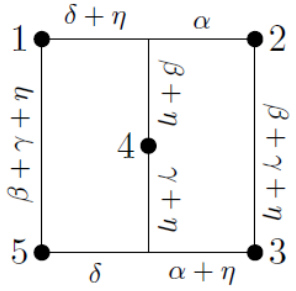

Figure 18. Type C with a second $\Delta - Y$ transform applied to T_{345} and reduced to (b).

4. VOLUMES OF GROMOV METRIC TYPES

One of the ways to study the stability of Δ-equivalence classes under small numerical perturbations on components of metric represented as the vector $d = (d_{ij})$, is to consider the relative volume of each class inside the metric cone. To estimate these relative sizes of Δ-equivalence classes in an n-point space, we generate random points that lie in the intersection of the metric cone with unit ball in $\mathbb{R}^{\frac{n(n-1)}{2}}$ and then count the occurrence of points in each class.

We note that the volume of unit ball in $\mathbb{R}^N$ is equal to $V_N = \frac{\pi^{\frac{N}{2}}}{\Gamma\left(\frac{N}{2}+1\right)}$, where Γ is the Gamma function. It should also be noted that since the rate of growth of Gamma function is greater than the exponentials, as the dimension of space increases this volume decreases. It is known that the maximum volume is obtained for $N = 6$ and for the values of N greater than 6, V_N starts to decrease. On the other hand by keeping in mind that a metric d on an n-point space can be shown by a vector of positive coordinates in $\mathbb{R}^N$ where $N = \frac{n(n-1)}{2}$, we need to work with the intersection of unit ball with the orthant in which all the coordinates are positive (the first orthant in higher dimensions). Both of these issues leave us with only a few samples to work with.

To deal with the problem of generating a statistically significant number of points in the metric cone in $\mathbb{R}^{10}$ (since every metric on a 5-point space can be shown by a vector in $\mathbb{R}^{10}$) on a standard computer, we generate 10^7 random points $P = (x_1, x_2, \dots, x_{10}), 0 < x_i < 1$ and accumulate these points from 10 such runs to get 10^8 points. Each of these points has 10 positive coordinates that are uniformly distributed random numbers in the range (0,1). Then the points that fall inside the unit ball are chosen and in the next step by checking which points satisfy the triangle inequalities, we select the points inside the metric cone. Finally, for each of these points (metrics) we calculate the Gromov product structure in order to determine the metric type. This process is repeated 30 times and some of the results are given in Table \ref{table:random} below. The Matlab code for this program is available at http://finitemetricspaces.khas.edu.tr/Volume_of_Metric_Cone_n=5.m.

Table 1. Sample results of accumulating 10^8 points in $\mathbb{R}^{10}$. Each row is a single run of the program and shows how many points fall inside the unit ball, metric cone, and each type.

points in unit ball	points in metric cone	Type A	Type B	Type C
274578	705	142	360	203
273136	735	186	351	198
273891	716	161	362	193
273426	733	170	376	187
272959	721	167	363	191

As shown in Table 1, from 10^8 points in the cube, around 2.7×10^5 points (0.275%) fall inside the unit ball and around 0.25% of these points fall inside the metric cone. To understand why these small amounts of points in unit cube of $\mathbb{R}^{10}$ fall inside the unit ball, it should be noted that the volume of unit ball V_{10} in $\mathbb{R}^{10}$ is equal to $\frac{\pi^5}{120}$ and we work only with the portion of unit ball intersecting the first orthant. This volume is approximately 0.00249 which is 0.24% of the volume of the unit cube.

In order to interpret the data given in Table 1, some clarifications must be made. 5-point metrics inside the metric cone in $\mathbb{R}^{10}$, when the Gromov product structure is considered, fall into 102 classes. Under permutation of the points of underlying metric space, these 102 classes form 3 families. In a family which is the orbit of the Gromov product structure $\{\Delta_{125}, \Delta_{213}, \Delta_{324}, \Delta_{435}, \Delta_{514}\}$ under the action of the permutation group S_5, there are 12 elements. The metrics that have a Gromov product structure in this family are called Type A metrics. Furthermore, the orbit of the Gromov product structure $\{\Delta_{125}, \Delta_{213}, \Delta_{325}, \Delta_{425}, \Delta_{514}\}$ and $\{\Delta_{125}, \Delta_{213}, \Delta_{325}, \Delta_{425}, \Delta_{513}\}$ have 60 and 30 elements respectively and the metrics of these families are called Type B and Type C in this order.

For calculating the type of a metric inside the metric cone to obtain the results given in Table 1, these 102 classes are taken into consideration. With this view in hand, the volume of Type A, Type B and Type C metrics on average are $22.07\%, 51.02\%$ and $26.26\ \%$ of the metric cone (within a standard deviation of 21.1 for points inside the metric cone, 10.83 for Type A metrics, 17.03 for Type B metrics and 12.43 for Type C metrics in our runs to obtain the data given in Table 1). If we take the other view, without considering the permutations, results of Type A, B and C should be divided by 12, 60 and 30 respectively to obtain the volume of a single representative of each class. This means that within error bounds, the volumes of a single representative of Type A, B and C are respectively $1.84\ \%, 0.85\ \%$ and $0.87\ \%$ of the metric cone.

The results above, give us the following intuitive conclusions: first that the volume of a single representative of Type B and Type C metrics are almost equal and Type A is "thicker"' than these two types. Second, although a single representative of metric Type A is thicker than other types, these representatives are small in number (12 among 102 classes) with respect to Type B (60 among 102) and Type C (30 among 102) inside the metric cone.

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CONFLICT OF INTEREST

The authors stated that there are no conflicts of interest regarding the publication of this article.

AUTHORSHIP CONTRIBUTIONS

All authors contributed to the theoretical part of this article. Computer aided results were carried out by Arash M. Rezaeinazhad.

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