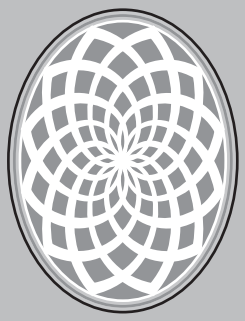

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Polyspherical coordinate systems on orbit spaces with applications to biomolecular conformation

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POLYSPHERICAL COORDINATE SYSTEMS ON ORBIT SPACES WITH APPLICATIONS TO BIOMOLECULAR CONFORMATION

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ABSTRACT. The group G_a of rigid motions, i.e. the semidirect product of $\mathbb{R}^n$ (translations) and $\mathrm{SO}(n)$ (proper rotations), acts on $\mathbb{R}^n$. Let $\mathcal{N}$ be a set with N elements. Let $(\mathbb{R}^n)^{\mathcal{N}}$ denote the set of all mappings $i \mapsto \mathbf{R}_i$ from $\mathcal{N}$ to $\mathbb{R}^n$. G_a also acts on $(\mathbb{R}^n)^{\mathcal{N}}$ by the *diagonal action* $(g \cdot R)_i = g \cdot \mathbf{R}_i$. Let $\mathcal{B}$ consist of those $R \in (\mathbb{R}^n)^{\mathcal{N}}$ whose isotropy subgroup consists only of the identity in G_a. When $N \geq n \geq 2$ we study a particular atlas of polyspherical coordinate charts in the orbit manifold $G_a \backslash \mathcal{B}$ and a related atlas of local trivializations of the principal bundle $\mathcal{B} \to G_a \backslash \mathcal{B}$ with structure group G_a. The coordinate charts are indexed by new combinatorial structures we call *Z-systems* $\Gamma = (\Gamma^1, \ldots, \Gamma^n_*)$, defined as follows. Let $\binom{\mathcal{N}}{k+1}$ denote the set of all abstract k-simplices, i.e. subsets of $\mathcal{N}$ with exactly $k+1$ elements. Define $\Gamma^0 = \binom{\mathcal{N}}{1}$. For each $k = 1, \ldots, n$ we assume that $\Gamma^k \subset \binom{\mathcal{N}}{k+1}$ such that the pair (Γ^{k-1}, Γ^k) is a tree hypergraph, where Γ^{k-1} is the set of vertices and Γ^k is the set of edges, and where a $k-1$ simplex (vertex) v and a k simplex (edge) e are incident if $v \subset e$. Furthermore if $v_1, v_2 \in \Gamma^{k-1}$ such that $v_1 \cup v_2 \in \Gamma^k$ then we require that $v_1 \cap v_2 \in \Gamma^{k-2}$. Γ^n_* is a set of oriented n-simplices, whose set of underlying unoriented n-simplices is Γ^n.

If $e \in \Gamma^k$ and $R \in (\mathbb{R}^n)^{\mathcal{N}}$ then let $R_e = \{\mathbf{R}_i \mid i \in e\}$ be the associated geometrical simplex. Each element $\{i, j\}$ of Γ^1 is associated with the Euclidean distance in $\mathbb{R}^n$ between points $\mathbf{R}_i$ and $\mathbf{R}_j$ of the mapping $R \in (\mathbb{R}^n)^{\mathcal{N}}$. Each element $e \in \Gamma^k$, $k = 2, \ldots, n-1$ is associated with an angle (taking values in $(0, \pi)$) between R_{v_1} and R_{v_2} associated to the two $k-1$ simplices $v_1, v_2 \in \Gamma^{k-1}$ on which e is incident, as measured in a plane perpendicular to the affine subspace of dimension $k-2$ spanned by $R_{v_1 \cap v_2}$ and within the affine subspace of dimension k spanned by R_e. Each element $e^* \in \Gamma^n_*$ is likewise associated with a signed angle (taking values in $(-\pi, \pi]$), where the sign of the angle and the orientation of the underlying abstract simplex $e \in \Gamma^n$ are compatible in a certain natural fashion. Coordinates are assigned to those mappings in $(\mathbb{R}^n)^{\mathcal{N}}$ for which every element $e \in \Gamma^{n-1}$ determines a geometrically independent $n-1$ simplex R_e in $\mathbb{R}^n$; such mappings are said to be in the *coordinate domain* $\mathcal{D}_C(\Gamma)$. We prove that our coordinate system establishes a diffeomorphism between the orbit space $G_a \backslash \mathcal{D}_C(\Gamma)$ and an explicitly given *parameter domain* $\mathcal{D}_P(\Gamma)$ of dimension $Nn - n(n+1)/2$. We also prove that $\mathcal{B}$ is the union of the coordinate domains $\mathcal{D}_C(\Gamma)$, where Γ ranges over all Z-systems on $\mathcal{N}$.

When $n = 3$ our results give an axiomatization of and rigorous mathematical theory for what chemists call valence coordinates, or Z-matrix internal coordinates. Z-systems can be simply manipulated like n-dimensional building blocks; such manipulations are quite complex if one uses Z-matrices. We briefly discuss applications of Z-systems to the study of biomolecular conformation.

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Key words and phrases. molecular conformation, conformational analysis, Z-matrix, Z-system, abstract simplex, spanning tree, line graph, iterated line graph, polyspherical coordinates, internal coordinates, valence coordinates, orbit spaces, diagonal action, principal bundle.

Contents

1. Introduction

Perhaps the reason molecular geometry has not received much attention from mathematicians is that it was perceived that not much *new* mathematics was to be found there. Also, despite the long history of study by chemists and molecular physicists, very little rigorous work has been done formalizing internal coordinate systems, especially those suitable for biological macromolecules. Perhaps this is because it was thought to be either "obvious" how such systems were to be constructed or too complicated or unprofitable to discuss in general. In this work we study a new combinatorial and geometric structure called a Z-system, which is naturally associated with polyspherical coordinate charts in conformation or "shape" spaces, i.e. orbit spaces under the diagonal action of the group of rigid motions on Cartesian products of Euclidean space. In the first five sections we develop from the basic definitions the abstract theory in the n dimensional context. Then in the last section we discuss the applications of our theory to concrete issues in 3 dimensional molecular geometry. In that section other references to previous work will be given. It is through this interplay of theory and application that we hope mathematicians will see the potential for even more new mathematics waiting to be discovered.

2. Z-systems

Suppose $\mathbb{R}^n$ is equipped with the standard Euclidean inner product, and with the usual orientation. The standard basis $I = (\hat{\mathbf{e}}_1, \ldots, \hat{\mathbf{e}}_n)$ is positively oriented and orthonormal. $\mathrm{SO}(n)$ denotes the group of all $n \times n$ real matrices A such that $A^T A = AA^T = I$ and $\det(A) = 1$. (A^T denotes the transpose of the matrix A.) Define $G_a = \mathbb{R}^n \times \mathrm{SO}(n)$ to be the group with the binary operation $(\mathbf{b}_1, A_1)(\mathbf{b}_2, A_2) = (\mathbf{b}_1 + A_1\mathbf{b}_2, A_1A_2)$, identity $(\boldsymbol{\theta}, I)$, and inverse operation $(\mathbf{b}, A)^{-1} = (-A^T\mathbf{b}, A^T)$. The group G_a has a left action on $\mathbb{R}^n$ by the rule $(\mathbf{b}, A) \cdot \mathbf{x} = \mathbf{b} + A\mathbf{x}$. G_a is called the group of n-dimensional *rigid motions*; the subscript a stands for *active*. Define an $n \times (n+1)$ matrix $(\mathbf{e}_0, \mathbf{e}_1, \ldots, \mathbf{e}_n)$ to be a *pose* if $\mathbf{e}_0 \in \mathbb{R}^n$ and $(\mathbf{e}_1, \ldots, \mathbf{e}_n)$ is a positively oriented orthonormal basis of $\mathbb{R}^n$. Every pose defines a Cartesian coordinate system in $\mathbb{R}^n$ with origin $\mathbf{e}_0$ in the usual way. Let $\mathcal{P}$ denote the set of all poses. G_a acts on $\mathcal{P}$ on the left by the rule $(\mathbf{b}, A)(\mathbf{e}_0, \mathbf{e}_1, \ldots, \mathbf{e}_n) = (\mathbf{b} + A\mathbf{e}_0, A\mathbf{e}_1, \ldots, A\mathbf{e}_n)$. This action is transitive and fixed point free. Since $A = (\mathbf{e}_1, \ldots, \mathbf{e}_n) \in \mathrm{SO}(n)$ we see that there is a natural identification of G_a with $\mathcal{P}$; we will mostly ignore it however. Define G_p to be the group of all $(n+1) \times (n+1)$

matrices of the form $\begin{pmatrix} 1 & \boldsymbol{\theta}^T \\ \mathbf{b} & A \end{pmatrix}$, where $\boldsymbol{\theta} \in \mathbb{R}^n$ is the zero (column) vector, and where $(\mathbf{b}, A) \in G_a$. G_p is a group under the operation of ordinary matrix multiplication. In fact the groups G_a and G_p are isomorphic in the obvious manner. G_p acts on $\mathcal{P}$ on the right by ordinary matrix multiplication. This group action is also transitive and fixed point free. We call G_p the *passive* group of coordinate transformations. The left action of G_a on $\mathcal{P}$ commutes with the right action of G_p. If A and B are sets then let A^B denote the set of all mappings from B to A. Let $\mathcal{N}$ be a set of N elements. G_a acts on $(\mathbb{R}^n)^{\mathcal{N}}$ via the *diagonal action*, i.e. if $g \in G_a$, $R \in (\mathbb{R}^n)^{\mathcal{N}}$, and $i \in \mathcal{N}$ then $(g \cdot R)_i = g \cdot \mathbf{R}_i$.

If S is any set define $\binom{S}{k}$ to be the set of all subsets of S with exactly k elements. We call an element of $\binom{\mathcal{N}}{k+1}$ an *abstract k-simplex*. An element of $\binom{\mathbb{R}^n}{k+1}$ is called a *k-simplex*. A k-simplex $\{\mathbf{R}_0, \mathbf{R}_1, \ldots, \mathbf{R}_k\}$ is called *geometrically independent* if the set $\left\{ \begin{pmatrix} 1 \\ \mathbf{R}_0 \end{pmatrix}, \begin{pmatrix} 1 \\ \mathbf{R}_1 \end{pmatrix}, \ldots, \begin{pmatrix} 1 \\ \mathbf{R}_k \end{pmatrix} \right\}$ is linearly independent in $\mathbb{R}^{n+1}$. If $R \in (\mathbb{R}^n)^{\mathcal{N}}$ and $s = \{i_0, i_1, \ldots, i_k\}$ is an abstract k-simplex then define $R_s = \{\mathbf{R}_{i_0}, \mathbf{R}_{i_1}, \ldots, \mathbf{R}_{i_k}\}$ to be the *associated* simplex. If there is no possible confusion we will sometimes call an abstract simplex a simplex. An *oriented* abstract n-simplex S^* is an abstract n-simplex S together with an equivalence class $[\alpha]$ of bijections $\alpha\colon \{0, 1, \ldots, n\} \to S$, where two such bijections α and α' are equivalent if $\alpha' = \alpha \circ p$ for some even permutation $p\colon \{0, 1, \ldots, n\} \to \{0, 1, \ldots, n\}$. If $S^* = (S, [\alpha])$ is an oriented abstract n-simplex, then we also write $S^* = [\alpha(0), \alpha(1), \ldots, \alpha(n)]$ with the understanding that $[\alpha(0), \alpha(1), \ldots, \alpha(n)] = [\alpha(p(0)), \alpha(p(1)), \ldots, \alpha(p(n))]$ for all even permutations p.

A *hypergraph* is a triple $\mathcal{H} = (V, E, \iota)$ where V and E are finite sets and $\iota \subset V \times E$. Elements of V are called *vertices* and elements of E are called *edges*; we write $V = \operatorname{vert} \mathcal{H}$ and $E = \operatorname{edge} \mathcal{H}$. If $(v, e) \in \iota$ then we say the vertex v and the edge e are *incident*. The hypergraph (V, E, ι) is a *graph* if the mapping $e \mapsto \{v \in V \mid (v, e) \in \iota\}$ takes E into $\binom{V}{2}$ and is one-to-one. This means that every edge of E is incident on exactly two vertices, and every unordered pair $\{v_1, v_2\} \in \binom{V}{2}$ corresponds to at most one edge. If (V_1, E_1, ι_1) and (V_2, E_2, ι_2) are hypergraphs then a pair of mappings (f, g) is an isomorphism of hypergraphs if $f\colon V_1 \to V_2$ and $g\colon E_1 \to E_2$ are bijections such that $(f \times g)(\iota_1) = \iota_2$. Consider an ordered list $t = (v_0, e_1, v_1, \ldots, v_{m-1}, e_m, v_m)$ where $v_1, \ldots, v_m$ are distinct vertices of V and $e_1, \ldots, e_m$ are distinct edges from E, such that e_i is incident on both v_{i-1} and v_i for all $i = 1, 2, \ldots, m$. t is called a *path of length m* in (V, E, ι) connecting v_0 to v_m if v_0 is distinct from each of $v_1, \ldots, v_m$. t is called a *cycle* if $v_0 = v_m$ and $m \geq 3$. The hypergraph (V, E, ι) is said to be *connected* if for any two distinct vertices v, v' of V there exists a path connecting v to v'. If a hypergraph contains no cycle it is said to be *acyclic*. A connected acyclic graph is said to be a *tree*. A vertex v is said to be a *leaf* if there is only one edge e incident on v. A graph is said to be *rooted* if a distinguished vertex r of V has been chosen; r is called the root vertex, or simply the root, and the quadruple (V, E, ι, r) is called a rooted graph.

If (V, E, ι) is a hypergraph then define the *line graph* $L(V, E, \iota)$ to be the graph (E, L, ϵ), where

$$L = \left\{ \{e_1, e_2\} \in \binom{E}{2} \mid \text{there exists } v \in V \text{ such that } (v, e_1) \in \iota \text{ and } (v, e_2) \in \iota \right\},$$

and ϵ represents the incidence relation where a vertex e and an edge l are incident if $e \in l$, i.e. ϵ is represented by the set $\{(e,l) \in E \times L \mid e \in l\}$. Since every edge in L is a two element subset of the vertex set E and the incidence relation is set membership it is clear that this construction always yields a graph. As an example, consider the hypergraph $(\Gamma^{-1}, \Gamma^0, \sigma)$, where $\Gamma^{-1} = \binom{\mathcal{N}}{0} = \{\emptyset\}$, $\Gamma^0 = \binom{\mathcal{N}}{1}$ and σ represents the incidence relation where a vertex v is incident on an edge e if $v \subset e$. There is only one vertex, namely $v = \emptyset$, which is a subset of any set. Hence $L(\Gamma^{-1}, \Gamma^0, \sigma) = (\Gamma^0, \binom{\Gamma^0}{2}, \epsilon)$. This graph is called the *complete graph on the set* Γ^0. It is isomorphic to the graph $(\Gamma^0, \binom{\mathcal{N}}{2}, \sigma)$ via the isomorphism $(1, \beta_1)$, where $1 \colon \Gamma^0 \to \Gamma^0$ is the identity mapping, and where $\beta_1 \colon \binom{\Gamma^0}{2} \to \binom{\mathcal{N}}{2} \colon \{\{i\},\{j\}\} \mapsto \{i,j\}$ is a bijection. Clearly the set membership incidence relation ϵ is carried into the subset incidence relation σ. Suppose (V_1, E_1, ι_1) and (V_2, E_2, ι_2) are graphs. We say (V_1, E_1, ι_1) is a *subgraph* of (V_2, E_2, ι_2) if $V_1 \subset V_2$, $E_1 \subset E_2$, and $\iota_1 \subset \iota_2$. The subgraph (V_1, E_1, ι_1) is said to be *spanning* if $V_1 = V_2$. The subgraph (V_1, E_1, ι_1) is said to be *induced* if $E_1 = \{e \in E_2 \mid \{v \in V_2 \mid (v,e) \in \iota_2\} \in \binom{V_1}{2}\}$ and $\iota_1 = \{(v,e) \in \iota_2 \mid v \in V_1, e \in E_1\}$. If (V, E, ι, r) is a rooted tree then a *leaf-picking order* for this rooted tree is an ordering of the elements of the set $V = \{v_1, v_2, \ldots, v_m\}$ such that $r = v_1$ and for every $2 \leq k \leq m$ the vertex v_k is a leaf of the subgraph of (V, E, ι) induced by the set $\{v_1, \ldots, v_k\}$. Such leaf-picking orders are known to exist for any rooted tree.

Now we are ready to give a definition of *Z-systems*.

Definition. An n-dimensional Z-system on the set $\mathcal{N}$ is an n-tuple $(\Gamma^1, \ldots, \Gamma^{n-1}, \Gamma^n_*)$, where $\Gamma^k \subset \binom{\mathcal{N}}{k+1}$ is a set of abstract k-simplices, $k = 1, \ldots, n$, and Γ^n_* is a set of oriented abstract n-simplices, i.e. a choice of orientation for each of the abstract n-simplices in Γ^n. These sets are required to satisfy the following properties: for each $k = 1, \ldots, n$ the hypergraph $(\Gamma^{k-1}, \Gamma^k, \sigma)$ is a tree, and whenever $v_1, v_2 \in \Gamma^{k-1}$ are such that $v_1 \cup v_2 \in \Gamma^k$ then we have $v_1 \cap v_2 \in \Gamma^{k-2}$.

In the above we are using the notation from the previous paragraph, i.e. $\Gamma^{-1} = \binom{\mathcal{N}}{0} = \{\emptyset\}$, $\Gamma^0 = \binom{\mathcal{N}}{1}$ and σ is the subset incidence relation.

It is not entirely obvious that Z-systems exist in higher dimensions. Thus we will now give an inductive construction proving this existence and showing the degree of flexibility in the concept. In any connected graph it is possible to choose a spanning tree. Furthermore the line graph of any connected graph is always connected. To begin, note that the complete graph $(\Gamma^0, \binom{\Gamma^0}{2}, \epsilon)$ is connected. So choose a spanning tree τ_1 as a subgraph of $(\Gamma^0, \binom{\Gamma^0}{2}, \epsilon)$. Let Γ^1 denote the image under the mapping β_1 of the set edge τ_1 of edges of τ_1. Thus $(\Gamma^0, \Gamma^1, \sigma)$ is a tree isomorphic to the tree τ_1. Notice that if $e \in \Gamma^1$ is incident on the two vertices $v_1, v_2 \in \Gamma^0$ then $v_1 \cap v_2 = \emptyset \in \Gamma^{-1}$. It is always possible to choose one of the two orientations for each of the abstract 1-simplices in Γ^1 to form Γ^1_*. Thus a 1-dimensional Z-system necessarily exists. Now suppose for $n \geq 2$ that an $n-1$-dimensional Z-system $\Gamma^1, \ldots, \Gamma^{n-1}$ has been chosen. Thus, in particular, $(\Gamma^{n-2}, \Gamma^{n-1}, \sigma)$ is a tree. Thus $L(\Gamma^{n-2}, \Gamma^{n-1}, \sigma)$ is a connected graph. The general construction depends on the following result.

Lemma. *Suppose* $(\Gamma^{k-1}, \Gamma^k, \sigma)$ *is a tree for* $k = 1, \ldots, n-1$. *Define the mapping* $\beta_n \colon \text{edge } L(\Gamma^{n-2}, \Gamma^{n-1}, \sigma) \to \binom{\mathcal{N}}{n+1} \colon \{e_1, e_2\} \mapsto e_1 \cup e_2$. *Then* β_n *is an injection.*

Proof. From the definition of the line graph we see that

$$\text{edge } L(\Gamma^{n-2},\Gamma^{n-1},\sigma) = \left\{ \{e_1,e_2\} \in \binom{\Gamma^{n-1}}{2} \mid e_1 \cap e_2 \in \Gamma^{n-2} \right\}.$$

Let $\{e_1,e_2\}$ be an edge in $L(\Gamma^{n-2},\Gamma^{n-1},\sigma)$ and define $S = e_1 \cup e_2 = \beta_n(\{e_1,e_2\})$. Since both e_1 and e_2 are n element sets which intersect in an $n-1$ element set it is clear that S is an $n+1$ element set. Now define for each $k = 0,1,\ldots,n-1$ the sets $\Gamma_S^k = \{s \in \Gamma^k \mid s \subset S\}$. The injectivity of β_n will follow if we show that $\Gamma_S^{n-1} = \{e_1,e_2\}$. Clearly $\{e_1,e_2\} \subset \Gamma_S^{n-1}$, so $|\Gamma_S^{n-1}| \geq 2$. Now for all $k = 1,\ldots,n-1$ we claim that $(\Gamma_S^{k-1},\Gamma_S^k,\sigma)$ is a graph. To see this suppose $e \in \Gamma_S^k \subset \Gamma^k$. Since $(\Gamma^{k-1},\Gamma^k,\sigma)$ is a graph there are exactly two vertices $v_1,v_2 \in \Gamma^{k-1}$ on which e is incident. Since both are subsets of $e \subset S$, both v_1 and v_2 are in Γ_S^{k-1}. Clearly there cannot be in Γ_S^{k-1} any other vertex incident on e. Thus e is incident on exactly two vertices in Γ_S^{k-1}. Also if $v_1,v_2 \in \Gamma_S^{k-1}$ are distinct but otherwise arbitrary then there can be at most one vertex $e \in \Gamma^k$ incident on them. Since any edge in Γ_S^k incident on v_1 and v_2 is necessarily an edge in Γ^k we see that there can be at most one such edge. Therefore our claim is demonstrated. Hence $(\Gamma_S^{n-2},\Gamma_S^{n-1},\sigma)$ is a subgraph of the tree $(\Gamma^{n-2},\Gamma^{n-1},\sigma)$, and hence is acyclic. The connected components of this subgraph are all trees, and hence have one more vertex than the number of edges. Consequently $|\Gamma_S^{n-2}| \geq 3$. By a similar argument we show that $|\Gamma_S^{n-k}| \geq k+1$ for all $k = 1,\ldots,n$. Therefore $n+1 \leq |\Gamma_S^0| \leq |S| = n+1$. Since $(\Gamma_S^0,\Gamma_S^1,\sigma)$ is a subgraph of a tree with $n+1$ vertices, it can have at most n edges. Thus $n \leq |\Gamma_S^1| \leq n$. By a similar argument $|\Gamma_S^k| = n-k+1$ for all $k = 0,1,\ldots,n-1$. Therefore since $|\Gamma_S^{n-1}| = 2$, we must have $\Gamma_S^{n-1} = \{e_1,e_2\}$. □

Now if one chooses a spanning tree τ_n in $L(\Gamma^{n-2},\Gamma^{n-1},\sigma)$ and defines $\Gamma^n = \beta_n(\text{edge } \tau_n)$ then $(\Gamma^{n-1},\Gamma^n,\sigma)$ is a tree isomorphic to τ_n via the isomorphism $(1,\beta_n)$. An n-dimensional Z-system can then be found by choosing one of the two orientations for each of the n-simplices in Γ^n. Thus an n-dimensional Z-system can always be found from an $n-1$-dimensional Z-system by choosing a spanning tree in the line graph of the highest level tree, and choosing orientations for the n-simplices.

It is also true that every Z-sytem can be obtained by means of the inductive procedure just described. This observation is trivial for 1-dimensional Z-systems. Also for $n \geq 2$ suppose $\Gamma^1,\ldots,\Gamma^{n-1}$ of a Z-system of dimension n or higher are obtained by the above inductive construction. By the previous Lemma the map β_n: edge $L(\Gamma^{n-2},\Gamma^{n-1},\sigma) \to \binom{\mathcal{N}}{n+1}$ is an injection. Since $(\Gamma^{n-1},\Gamma^n,\sigma)$ is a graph, each edge $e \in \Gamma^n$ is incident on exactly two edges $v_1,v_2 \in \Gamma^{n-1}$. Because we have a Z-system we know that $v_1 \cap v_2 \in \Gamma^{n-2}$, and hence $\{v_1,v_2\}$ is an edge in $L(\Gamma^{n-2},\Gamma^{n-1},\sigma)$ which β_n maps to e. Thus every edge in Γ^n determines a unique edge in $L(\Gamma^{n-2},\Gamma^{n-1},\sigma)$, and the fact that $(\Gamma^{n-1},\Gamma^n,\sigma)$ is a tree implies that a spanning tree τ_n in $L(\Gamma^{n-2},\Gamma^{n-1},\sigma)$ is thereby determined. Thus in fact, $\Gamma^1,\ldots,\Gamma^n$ are obtained from the inductive construction.

The n-tuple $(\Gamma^1,\ldots,\Gamma^n)$ can be put in one-to-one correspondence with the n-tuple $(\tau_1,\ldots,\tau_n)$, where τ_1 is a spanning tree in the complete graph on $\mathcal{N}$ and τ_{k+1} is a spanning tree in the line graph of τ_k for all $k = 1,\ldots,n-1$. A specification of $(\Gamma^1,\ldots,\Gamma^n)$ is to look at a Z-system in the *poset picture*. A specification of $(\tau_1,\ldots,\tau_n)$ is to look at a Z-system in the *iterated line graph picture*. These pictures

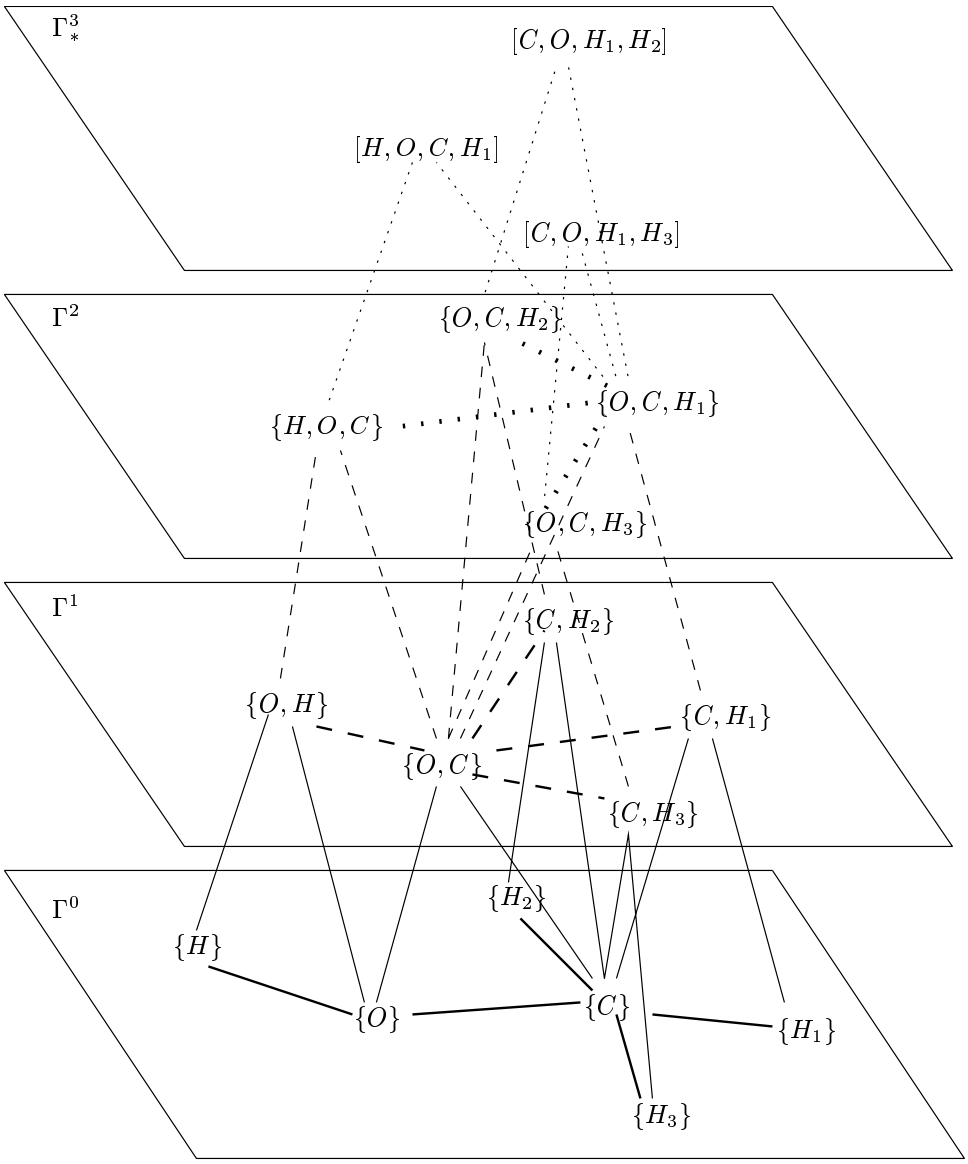

FIGURE 1. A 3-dimensional Z-system Γ for Methanol. The set $\mathcal{N} = \{C, H_1, H_2, H_3, O, H\}$ contains the atom names. The tree for $(\Gamma^{k-1}, \Gamma^k, \subset)$, $k = 1, 2, 3$, is indicated on the part labeled Γ^{k-1}, where the edges are indicated by heavier lines of various styles. Above each such line is the element of Γ^k which is the edge, and it is connected to its two vertices by lighter lines of the same style.

can be used to visualize a Z-system. For example in Figure 1 we give a 3-dimensional Z-system for the molecule methanol in the poset picture. Figure 2 is the same Z-system, but given in the iterated line graph picture. (See section 6 for a discussion of dihedrals and impropers in the 3-dimensional case.) Although the diagrams are

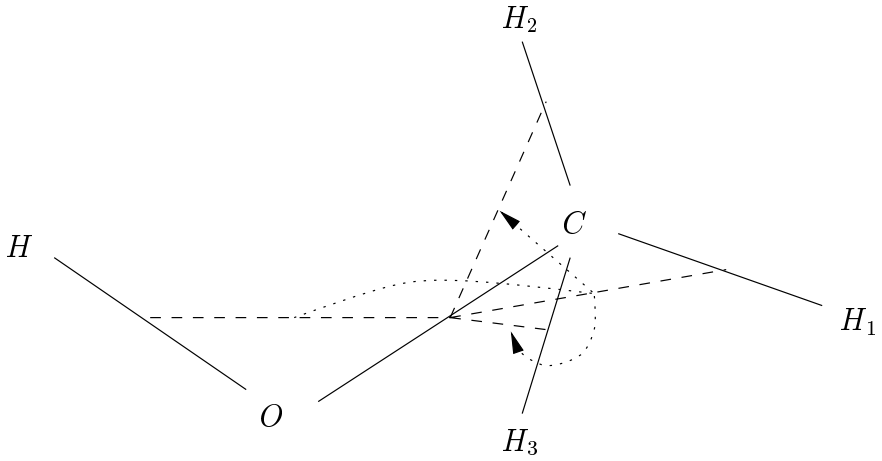

FIGURE 2. The iterated line graph form (used by IMIMOL) of the same Z-system Γ for Methanol as in Figure 1. Bonds (1-simplices, or edges of τ_1) are indicated by solid lines. Triangles (2-simplices) are in one-to-one correspondence with angles (edges of τ_2), and are indicated by dashed lines from one vertex bond to the other. Tetrahedra (3-simplices) are in one-to-one correspondence with unordered pairs of angles (edges of τ_3), and are indicated by curved or straight dotted lines from one vertex angle to the other. Impropers must be given a direction; dihedrals assume their canonical orientation (see section 6).

easier to draw in the (3-dimensional) iterated line graph picture, the set theoretical nature of the vertices and edges involved become quite complex for the higher level trees. Furthermore, the "orientations" of the edges of τ_n are more correctly described as orientations of the corresponding n-simplices. So we commonly use the iterated line graph picture to display Z-systems, but use the poset picture for theoretical discussions.

A "top down" construction of a Z-system satisfying certain geometrical constraints will be given in the proof of the second theorem of section 4.

As a mathematical concept Z-systems are related to abstract simplicial complexes [57], and in fact are special types of skeleton complexes [4]. However the concept is not mentioned in [30].

3. Polyspherical Coordinates

As natural combinatorial objects as Z-systems might be, their true nature is revealed when they are considered as defining polyspherical coordinate systems. Let $(\Gamma^1, \ldots, \Gamma^n_*)$ be an n-dimensional Z-system on the set $\mathcal{N} = \{1, \ldots, N\}$. Define

$$\mathcal{D}_C(\Gamma) = \{R \in (\mathbb{R}^n)^{\mathcal{N}} \mid \text{for all } s \in \Gamma^{n-1} \text{ the associated simplex } R_s \text{ is geometrically independent}\}.$$

This is called the *coordinate domain* corresponding to the given Z-system. If the Z-system Γ is understood we will write $\mathcal{D}_C(\Gamma) = \mathcal{D}_C$. Notice that if $R \in \mathcal{D}_C$

and $(\mathbf{b}, A) \in G_a$ then $(\mathbf{b}, A) \cdot R \in \mathcal{D}_C$. Let $R \in \mathcal{D}_C$ be given. Then for every $e = \{i, j\} \in \Gamma^1$ we define

$$L_e(R) = \|\mathbf{R}_i - \mathbf{R}_j\|.$$

Note that the associated simplex R_e must be geometrically independent, and hence $L_e(R) > 0$.

For any $k = 2, \ldots, n$ suppose $e = v_1 \cup v_2 \in \Gamma^k$ where $v_1, v_2 \in \Gamma^{k-1}$ and $s = v_1 \cap v_2 \in \Gamma^{k-2}$. Define Π_s to be the orthogonal projection onto the subspace of $\mathbb{R}^n$ spanned by the set of vectors $\{\mathbf{R}_j - \mathbf{R}_i \mid j \in s \setminus \{i\}\}$, where $i \in s$. When $k = 2$ so that $s = \{i\}$ we have that Π_s maps every vector to the zero vector. For larger values of k we have that Π_s does not depend on $i \in s$, as is easy to see. Now suppose $i \in s$, $\{j_1\} = v_1 \setminus s$, and $\{j_2\} = v_2 \setminus s$. Then define

$$C_e(R) = \frac{(1 - \Pi_s)(\mathbf{R}_{j_1} - \mathbf{R}_i)}{\|(1 - \Pi_s)(\mathbf{R}_{j_1} - \mathbf{R}_i)\|} \cdot \frac{(1 - \Pi_s)(\mathbf{R}_{j_2} - \mathbf{R}_i)}{\|(1 - \Pi_s)(\mathbf{R}_{j_2} - \mathbf{R}_i)\|}.$$

Since the associated $k-1$-simplices R_{v_1} and R_{v_2} must each be contained in a geometrically independent $n-1$-simplex, we see that each of the denominators must be positive. However, we must show that each of the unit vectors in the above expression is independent of $i \in s$. To see this suppose $i' \neq i$, $i' \in s$. Then $\mathbf{R}_j - \mathbf{R}_i = \mathbf{R}_j - \mathbf{R}_{i'} + (\mathbf{R}_{i'} - \mathbf{R}_i)$. Since $\Pi_s(\mathbf{R}_{i'} - \mathbf{R}_i) = (\mathbf{R}_{i'} - \mathbf{R}_i)$ we have that $(1 - \Pi_s)(\mathbf{R}_j - \mathbf{R}_i) = (1 - \Pi_s)(\mathbf{R}_j - \mathbf{R}_{i'})$, as desired. If $2 \leq k \leq n-1$ then the asociated simplex R_e must be geometrically independent, and hence $C_e(R) \in (-1, 1)$. We will use the coordinate $C_e(R)$ rather than the angle $\theta = \cos^{-1} C_e(R)$.

Now suppose $e^* = [i_0, i_1, \ldots, i_n] \in \Gamma^n_*$, where $e = \{i_0, i_1, \ldots, i_n\}$, $s = \{i_0, i_1, \ldots, i_{n-2}\}$, $v_1 = s \cup \{i_{n-1}\} \in \Gamma^{n-1}$, and $v_2 = s \cup \{i_n\} \in \Gamma^{n-1}$. It is always possible to arrange this. $C_e(R)$ is defined as above except now we do not know R_e is geometrically independent, so we only have that $C_e(R) \in [-1, 1]$. Since R_{v_1} is geometrically independent there is a unique unit vector $\mathbf{e}_n$ which is orthogonal to the span of $\{\mathbf{R}_{i_1} - \mathbf{R}_{i_0}, \ldots, \mathbf{R}_{i_{n-1}} - \mathbf{R}_{i_0}\}$ and such that $(\mathbf{R}_{i_1} - \mathbf{R}_{i_0}, \ldots, \mathbf{R}_{i_{n-1}} - \mathbf{R}_{i_0}, \mathbf{e}_n)$ is positively oriented. We define

$$S_{e^*}(R) = \mathbf{e}_n \cdot \frac{(1 - \Pi_s)(\mathbf{R}_{i_n} - \mathbf{R}_{i_0})}{\|(1 - \Pi_s)(\mathbf{R}_{i_n} - \mathbf{R}_{i_0})\|}.$$

Since R_{v_2} must be geometrically independent, the denominator in the above expression is positive. Since R_s is geometrically independent there exists a unique orthonormal set $(\mathbf{e}_1, \ldots, \mathbf{e}_{n-2})$ of vectors from $\mathbb{R}^n$ and a unique upper triangular $(n-2) \times (n-2)$ matrix U with positive diagonal entries such that $(\mathbf{R}_{i_1} - \mathbf{R}_{i_0}, \ldots, \mathbf{R}_{i_{n-2}} - \mathbf{R}_{i_0}) = (\mathbf{e}_1, \ldots, \mathbf{e}_{n-2})U$. This is simply Gram-Schmidt orthogonalization, or QR factorization [29]. The entries of the vectors $\mathbf{e}_k$ and of the matrix U are smooth functions of R. It follows that $\Pi_s = \sum_{k=1}^{n-2} \mathbf{e}_k \mathbf{e}_k^T$. Define

$$\mathbf{e}_{n-1} = \frac{(1 - \Pi_s)(\mathbf{R}_{i_{n-1}} - \mathbf{R}_{i_0})}{\|(1 - \Pi_s)(\mathbf{R}_{i_{n-1}} - \mathbf{R}_{i_0})\|}, \quad \text{and} \quad \mathbf{v} = \frac{(1 - \Pi_s)(\mathbf{R}_{i_n} - \mathbf{R}_{i_0})}{\|(1 - \Pi_s)(\mathbf{R}_{i_n} - \mathbf{R}_{i_0})\|}.$$

It follows that $(\mathbf{e}_1, \ldots, \mathbf{e}_n)$ is a positively oriented orthonormal basis of $\mathbb{R}^n$. From the definitions above we see that $C_e(R) = \mathbf{e}_{n-1} \cdot \mathbf{v}$, $S_{e^*}(R) = \mathbf{e}_n \cdot \mathbf{v}$, and hence $\mathbf{v} = C_s(R)\mathbf{e}_{n-1} + S_{e^*}(R)\mathbf{e}_n$. Thus

$$\det(\mathbf{e}_1, \ldots, \mathbf{e}_{n-1}, \mathbf{v}) = S_{e^*}(R).$$

This proves that $S_{e^*}(R)$ is a smooth function of R. See figure 3 for the 3-dimensional case.

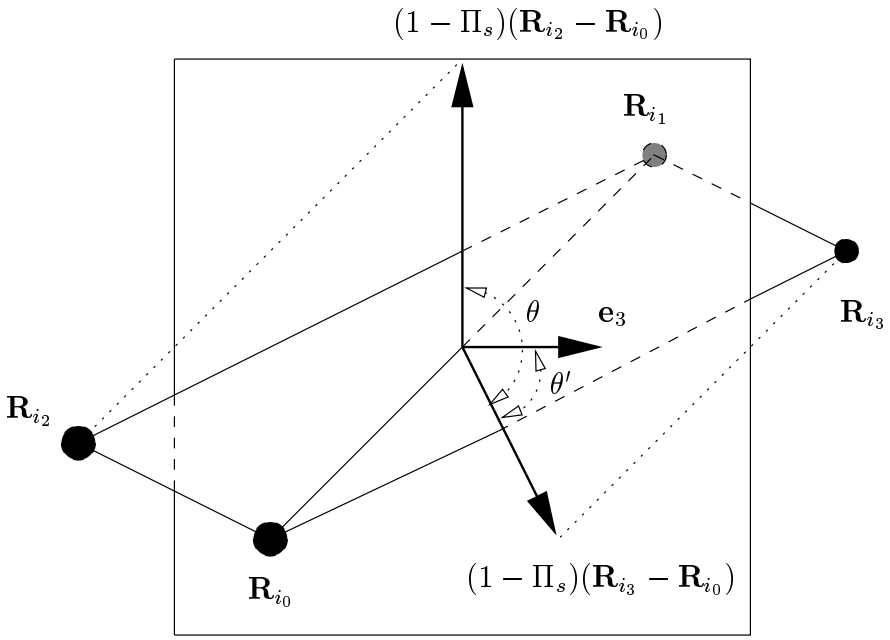

FIGURE 3. The geometry of wedge angles in dimension $n = 3$. In this case $e^* = [i_0, i_1, i_2, i_3]$, $s = \{i_0, i_1\}$, $v_1 = \{i_0, i_1, i_2\}$, and $v_2 = \{i_0, i_1, i_3\}$. The square lies in a plane perpendicular to the line through $\mathbf{R}_{i_0}$ and $\mathbf{R}_{i_1}$. Both of the vectors $(1-\Pi_s)(\mathbf{R}_{i_2}-\mathbf{R}_{i_0})$ and $(1-\Pi_s)(\mathbf{R}_{i_3}-\mathbf{R}_{i_0})$ lie in this plane since $1-\Pi_s$ is an orthogonal projection into this plane. $C_e(R) = \cos(\theta)$ and $S_{e^*}(R) = \cos(\theta') = \sin(\theta) > 0$ in this picture.

Lemma. *The number $S_{e^*}(R)$ does not depend on the representative $(i_0, i_1, \ldots, i_n)$ of the chosen orientational equivalence class e^*, provided $s = \{i_0, i_1, \ldots, i_{n-2}\}$.*

Proof. So suppose $[i_0, i_1, \ldots, i_n] = [j_0, j_1, \ldots, j_n]$, where $s = \{j_0, j_1, \ldots, j_{n-2}\}$. Then $\{i_{n-1}, i_n\} = \{j_{n-1}, j_n\}$, and there are therefore two cases: $(i_{n-1}, i_n) = (j_{n-1}, j_n)$ and $(i_{n-1}, i_n) = (j_n, j_{n-1})$. In the first case, $(i_{n-1}, i_n) = (j_{n-1}, j_n)$, which cannot happen in a nontrivial way in dimensions 2 and 3, we see that $(j_0, j_1, \ldots, j_{n-2})$ is an even permutation of $(i_0, i_1, \ldots, i_{n-2})$. Hence $(j_0, j_1, \ldots, j_{n-1})$ is an even permutation of $(i_0, i_1, \ldots, i_{n-1})$. Let P be the $n \times n$ permutation matrix such that $(j_0, \ldots, j_{n-1}) = (i_0, \ldots, i_{n-1})P$. Let $\mathbf{u}^T = (0, 1, \ldots, 1) \in (\mathbb{R}^n)^*$, and $G = I - \hat{\mathbf{e}}_1 \mathbf{u}^T$ an $n \times n$ Gauss transformation; note that $G^{-1} = I + \hat{\mathbf{e}}_1 \mathbf{u}^T$. Then we have that

$$\begin{aligned}
&\begin{pmatrix} 1 & 0 & \ldots & 0 & 0 \\ \mathbf{R}_{j_0} & \mathbf{R}_{j_1} - \mathbf{R}_{j_0} & \ldots & \mathbf{R}_{j_{n-1}} - \mathbf{R}_{j_0} & \mathbf{e}_n \end{pmatrix} \\
&\quad = \begin{pmatrix} 1 & 1 & \ldots & 1 & 0 \\ \mathbf{R}_{j_0} & \mathbf{R}_{j_1} & \ldots & \mathbf{R}_{j_{n-1}} & \mathbf{e}_n \end{pmatrix} \begin{pmatrix} G & \boldsymbol{\theta} \\ \boldsymbol{\theta}^T & 1 \end{pmatrix} \\
&\quad = \begin{pmatrix} 1 & 1 & \ldots & 1 & 0 \\ \mathbf{R}_{i_0} & \mathbf{R}_{i_1} & \ldots & \mathbf{R}_{i_{n-1}} & \mathbf{e}_n \end{pmatrix} \begin{pmatrix} P & \boldsymbol{\theta} \\ \boldsymbol{\theta}^T & 1 \end{pmatrix} \begin{pmatrix} G & \boldsymbol{\theta} \\ \boldsymbol{\theta}^T & 1 \end{pmatrix}
\end{aligned}$$

$$= \begin{pmatrix} 1 & 0 & \dots & 0 & 0 \\ \mathbf{R}_{i_0} & \mathbf{R}_{i_1} - \mathbf{R}_{i_0} & \dots & \mathbf{R}_{i_{n-1}} - \mathbf{R}_{i_0} & \mathbf{e}_n \end{pmatrix} \begin{pmatrix} G^{-1} & \boldsymbol{\theta} \\ \boldsymbol{\theta}^T & 1 \end{pmatrix} \begin{pmatrix} PG & \boldsymbol{\theta} \\ \boldsymbol{\theta}^T & 1 \end{pmatrix}$$

Since $\det(G^{-1}PG) = \det(P) = 1$ we see that

$$\det(\mathbf{R}_{j_1} - \mathbf{R}_{j_0}, \dots, \mathbf{R}_{j_{n-1}} - \mathbf{R}_{j_0}, \mathbf{e}_n) = \det(\mathbf{R}_{i_1} - \mathbf{R}_{i_0}, \dots, \mathbf{R}_{i_{n-1}} - \mathbf{R}_{i_0}, \mathbf{e}_n) > 0.$$

Also $\hat{\mathbf{e}}_1^T(I + \hat{\mathbf{e}}_1\mathbf{u}^T)P(I - \hat{\mathbf{e}}_1\mathbf{u}^T) = (\hat{\mathbf{e}}_1^T + \mathbf{u}^T)P(I - \hat{\mathbf{e}}_1\mathbf{u}^T) = (\hat{\mathbf{e}}_1^T + \mathbf{u}^T)(I - \hat{\mathbf{e}}_1\mathbf{u}^T) = \hat{\mathbf{e}}_1^T + \mathbf{u}^T - (\hat{\mathbf{e}}_1^T\hat{\mathbf{e}}_1)\mathbf{u}^T - (\mathbf{u}^T\hat{\mathbf{e}}_1)\mathbf{u}^T = \hat{\mathbf{e}}_1^T$. Therefore $G^{-1}PG = \begin{pmatrix} 1 & \boldsymbol{\theta}^T \\ \mathbf{v} & H \end{pmatrix}$, where H is an $(n-1) \times (n-1)$ matrix with unit determinant. Since

$$(\mathbf{R}_{j_0}, \mathbf{R}_{j_1} - \mathbf{R}_{j_0}, \dots, \mathbf{R}_{j_{n-1}} - \mathbf{R}_{j_0}) = (\mathbf{R}_{i_0}, \mathbf{R}_{i_1} - \mathbf{R}_{i_0}, \dots, \mathbf{R}_{i_{n-1}} - \mathbf{R}_{i_0}) \begin{pmatrix} 1 & \boldsymbol{\theta}^T \\ \mathbf{v} & H \end{pmatrix}$$

we see that

$$(\mathbf{R}_{j_1} - \mathbf{R}_{j_0}, \dots, \mathbf{R}_{j_{n-1}} - \mathbf{R}_{j_0}) = (\mathbf{R}_{i_1} - \mathbf{R}_{i_0}, \dots, \mathbf{R}_{i_{n-1}} - \mathbf{R}_{i_0})H,$$

and hence the same vector $\mathbf{e}_n$ works for both representatives of the orientational equivalence class. Since we have already seen that $(1 - \Pi_s)(\mathbf{R}_{j_n} - \mathbf{R}_{j_0}) = (1 - \Pi_s)(\mathbf{R}_{i_n} - \mathbf{R}_{i_0})$, we have that $S_{e^*}(R)$ is independent of the representative of the orientational equivalence class in this case.

Now consider the case where $(i_{n-1}, i_n) = (j_n, j_{n-1})$. Therefore $(j_0, j_1, \dots, j_{n-2})$ is an odd permutation of $(i_0, i_1, \dots, i_{n-2})$. Let $B = (\mathbf{R}_{i_1} - \mathbf{R}_{i_0}, \dots, \mathbf{R}_{i_{n-2}} - \mathbf{R}_{i_0})$. Using an argument similar to that given in the first case we have that there is an $(n-2)\times(n-2)$ matrix K such that $\det K = -1$ and $(\mathbf{R}_{j_1} - \mathbf{R}_{j_0}, \dots, \mathbf{R}_{j_{n-2}} - \mathbf{R}_{j_0}) = BH$. There exists a vector $\mathbf{z} \in \mathbb{R}^{n-1}$ such that $\mathbf{R}_{i_0} - \mathbf{R}_{j_0} = B\mathbf{z}$. Therefore $\mathbf{R}_{j_{n-1}} - \mathbf{R}_{j_0} = \mathbf{R}_{i_n} - \mathbf{R}_{i_0} + B\mathbf{z}$ and $\mathbf{R}_{j_n} - \mathbf{R}_{j_0} = \mathbf{R}_{i_{n-1}} - \mathbf{R}_{i_0} + B\mathbf{z}$. Consequently $(1 - \Pi_s)(\mathbf{R}_{j_{n-1}} - \mathbf{R}_{j_0}) = (1 - \Pi_s)(\mathbf{R}_{i_n} - \mathbf{R}_{i_0})$ and $(1 - \Pi_s)(\mathbf{R}_{j_n} - \mathbf{R}_{j_0}) = (1 - \Pi_s)(\mathbf{R}_{i_{n-1}} - \mathbf{R}_{i_0})$, and hence $\tilde{\mathbf{e}}_{n-1} = \mathbf{v}$, and $\tilde{\mathbf{v}} = \mathbf{e}_{n-1}$. Since $\tilde{\mathbf{e}}_{n-1} = \mathbf{v} = C_s(R)\mathbf{e}_{n-1} + S_{e^*}(R)\mathbf{e}_n$ it is reasonable to define $\tilde{\mathbf{e}}_n = S_{e^*}(R)\mathbf{e}_{n-1} - C_e(R)\mathbf{e}_n$, since then we would have $\tilde{\mathbf{e}}_{n-1} \cdot \tilde{\mathbf{e}}_n = 0$ and $\tilde{\mathbf{e}}_n \cdot \tilde{\mathbf{v}} = [S_{e^*}(R)\mathbf{e}_{n-1} - C_e(R)\mathbf{e}_n] \cdot \mathbf{e}_{n-1} = S_{e^*}(R)$ as desired. Since $\tilde{\mathbf{e}}_n \cdot \tilde{\mathbf{e}}_n = S_{e^*}(R)^2 + C_e(R)^2 = \mathbf{v} \cdot \mathbf{v} = 1$ we see that $\tilde{\mathbf{e}}_n$ is a unit vector. To finish showing that this choice for $\tilde{\mathbf{e}}_n$ has all the properties specified for it in the definition, we compute

$$\begin{aligned}
&(\mathbf{R}_{j_1} - \mathbf{R}_{j_0}, \dots, \mathbf{R}_{j_{n-1}} - \mathbf{R}_{j_0}, \tilde{\mathbf{e}}_n) \\
&\quad = (\mathbf{R}_{i_1} - \mathbf{R}_{i_0}, \dots, \mathbf{R}_{i_{n-2}} - \mathbf{R}_{i_0}, \mathbf{R}_{j_{n-1}} - \mathbf{R}_{j_0}, \tilde{\mathbf{e}}_n) \begin{pmatrix} K & \boldsymbol{\theta} & \boldsymbol{\theta} \\ \boldsymbol{\theta}^T & 1 & 0 \\ \boldsymbol{\theta}^T & 0 & 1 \end{pmatrix} \\
&\quad = (\mathbf{e}_1, \dots, \mathbf{e}_{n-2}, \mathbf{R}_{j_{n-1}} - \mathbf{R}_{j_0}, \tilde{\mathbf{e}}_n) \begin{pmatrix} U & \boldsymbol{\theta} & \boldsymbol{\theta} \\ \boldsymbol{\theta}^T & 1 & 0 \\ \boldsymbol{\theta}^T & 0 & 1 \end{pmatrix} \begin{pmatrix} K & \boldsymbol{\theta} & \boldsymbol{\theta} \\ \boldsymbol{\theta}^T & 1 & 0 \\ \boldsymbol{\theta}^T & 0 & 1 \end{pmatrix} \\
&\quad = (\mathbf{e}_1, \dots, \mathbf{e}_{n-2}, \tilde{\mathbf{e}}_{n-1}, \tilde{\mathbf{e}}_n) \begin{pmatrix} I & \mathbf{y} & \boldsymbol{\theta} \\ \boldsymbol{\theta}^T & l & 0 \\ \boldsymbol{\theta}^T & 0 & 1 \end{pmatrix} \begin{pmatrix} UK & \boldsymbol{\theta} & \boldsymbol{\theta} \\ \boldsymbol{\theta}^T & 1 & 0 \\ \boldsymbol{\theta}^T & 0 & 1 \end{pmatrix} \\
&\quad = (\mathbf{e}_1, \dots, \mathbf{e}_{n-2}, \mathbf{e}_{n-1}, \mathbf{e}_n) \begin{pmatrix} I & \boldsymbol{\theta} & \boldsymbol{\theta} \\ \boldsymbol{\theta}^T & C_e(R) & S_{e^*}(R) \\ \boldsymbol{\theta}^T & S_{e^*}(R) & -C_e(R) \end{pmatrix} \begin{pmatrix} UK & \mathbf{y} & \boldsymbol{\theta} \\ \boldsymbol{\theta}^T & l & 0 \\ \boldsymbol{\theta}^T & 0 & 1 \end{pmatrix},
\end{aligned}$$

where $\mathbf{x} = \mathbf{R}_{j_{n-1}} - \mathbf{R}_{j_0}$, $\mathbf{y} = (\mathbf{e}_1, \ldots, \mathbf{e}_{n-2})^T \mathbf{x}$, and $l = \|(1 - \Pi_s)\mathbf{x}\|$. Thus $(\mathbf{R}_{j_1} - \mathbf{R}_{j_0}, \ldots, \mathbf{R}_{j_{n-1}} - \mathbf{R}_{j_0}, \tilde{\mathbf{e}}_n)$ is positively oriented. □

Thus we define $Z_{e^*}(R) = C_e(R) + iS_{e^*}(R) \in S^1 = \{z \in \mathbb{C} \mid |z| = 1\}$. Clearly if e^* is replaced by the opposite orientational equivalence class $-e^*$ with the same underlying n-simplex e then $S_{-e^*}(R) = -S_{e^*}(R)$. We will use the coordinate $Z_{e^*}(R)$ rather than choosing a branch for the angle φ, where $Z_{e^*}(R) = e^{i\varphi}$. We consider S^1 to be a one dimensional real manifold.

We define the *parameter domain* $\mathcal{D}_P(\Gamma)$ to be

$$\mathcal{D}_P(\Gamma) = (0, \infty)^{\Gamma^1} \times \left[\prod_{k=2}^{n-1} (-1, 1)^{\Gamma^k}\right] \times (S^1)^{\Gamma^n_*}.$$

When the Z-system Γ is understood we write $\mathcal{D}_P(\Gamma) = \mathcal{D}_P$. When $R \in \mathcal{D}_C$ is given, then taken together all the coordinate functions we have defined determine an element

$$((L_e(R) \mid e \in \Gamma^1), (C_e(R) \mid e \in \Gamma^2), \ldots, (C_e(R) \mid e \in \Gamma^{n-1}), (Z_{e^*}(R) \mid e^* \in \Gamma^n_*))$$

in $\mathcal{D}_P$. Thus we can think of elements of $\mathcal{D}_P$ as being a labelling of each of the edges of each of the trees of the given Z-system $(\Gamma^1, \ldots, \Gamma^n_*)$ with appropriate numerical coordinate values. Thus an element of $\mathcal{D}_P$ will be called a *labelled Z-system.*

Suppose $r = (i_0, \ldots, i_{n-1}) \in \mathcal{N}^n$ is such that $s_k(r) = \{i_0, \ldots, i_k\} \in \Gamma^k$ for $k = 0, \ldots, n-1$. We call r a *site* of the Z-system. The simplices $s_0(r), \ldots, s_{n-1}(r)$ are said to be *associated* to the site r. Given a site r and $R \in \mathcal{D}_C$ we can define the *pose at the site* r as follows:

$$\mathbf{e}_0 = \mathbf{R}_{i_0}, \qquad \mathbf{e}_1 = \frac{\mathbf{R}_{i_1} - \mathbf{R}_{i_0}}{\|\mathbf{R}_{i_1} - \mathbf{R}_{i_0}\|}, \qquad \mathbf{e}_2 = \frac{(1 - \mathbf{e}_1\mathbf{e}_1^T)(\mathbf{R}_{i_2} - \mathbf{R}_{i_0})}{\|(1 - \mathbf{e}_1\mathbf{e}_1^T)(\mathbf{R}_{i_2} - \mathbf{R}_{i_0})\|}, \ldots,$$

$$\mathbf{e}_{n-1} = \frac{(1 - \sum_{k=1}^{n-2} \mathbf{e}_k\mathbf{e}_k^T)(\mathbf{R}_{i_{n-1}} - \mathbf{R}_{i_0})}{\|(1 - \sum_{k=1}^{n-2} \mathbf{e}_k\mathbf{e}_k^T)(\mathbf{R}_{i_{n-1}} - \mathbf{R}_{i_0})\|},$$

$\mathbf{e}_n =$ the unique unit vector in $\mathbb{R}^n$ perpendicular to $\mathbf{e}_1, \ldots, \mathbf{e}_{n-1}$ such that $(\mathbf{e}_1, \ldots, \mathbf{e}_n)$ is positively oriented.

Each of these vectors is well-defined since the simplex $R_{s_{n-1}(r)}$ is geometrically independent for $R \in \mathcal{D}_C$. Let $E_r(R) = (\mathbf{e}_0, \mathbf{e}_1, \ldots, \mathbf{e}_n) \in \mathcal{P}$ denote this pose. Notice that $\Pi_{s_j(r)} = \sum_{k=1}^{j-1} \mathbf{e}_k\mathbf{e}_k^T$, for $j = 1, \ldots, n-1$. If $(\mathbf{b}, A) \in G_a$ then it is clear that $E_r((\mathbf{b}, A) \cdot R) = (\mathbf{b}, A)E_r(R)$.

Let vert $\mathcal{S}(\Gamma)$ denote the set of all sites for the Z-system $\Gamma = (\Gamma^1, \ldots, \Gamma^n_*)$. Let edge $\mathcal{S}(\Gamma)$ denote the set of all two element subsets $\{(i_0, \ldots, i_{n-1}), (j_0, \ldots, j_{n-1})\}$ of vert $\mathcal{S}(\Gamma)$ such that $(j_0, \ldots, j_{n-1})$ can be obtained from $(i_0, \ldots, i_{n-1})$ by a single transposition of adjacent entries. Taken together the data (vert $\mathcal{S}(\Gamma)$, edge $\mathcal{S}(\Gamma)$, ϵ) forms a graph, called the *site graph* $\mathcal{S}(\Gamma)$. Let $\mathcal{G}(\Gamma)$ be the set of all ordered pairs $((i_0, \ldots, i_{n-1}), (j_0, \ldots, j_{n-1}))$ of sites in vert $\mathcal{S}(\Gamma)$ such that $(i_0, \ldots, i_{n-2}) = (j_0, \ldots, j_{n-2})$. Let this set $\mathcal{G}(\Gamma)$ be equipped with the following partially defined binary operation: $(r_1, r_2)(r_2, r_3) = (r_1, r_3)$. Thus the operation $(r_1, r_2)(r_3, r_4)$ is undefined unless $r_2 = r_3$. With this definition, $\mathcal{G}(\Gamma)$ becomes what is called a *pair groupoid.* The pair $(\mathcal{S}(\Gamma), \mathcal{G}(\Gamma))$ is called the *site network* of Γ (see Figure 4).

The site network associated to a Z-system may seem to be an unnecessary construct, but it greatly illuminates the features of the coordinates we have defined.

To see this, define the following $(n+1)\times(n+1)$ matrix-valued functions:

$$T_1(L) = \begin{pmatrix} 1 & 0 & \boldsymbol{\theta}^T & 0 \\ L & -1 & \boldsymbol{\theta}^T & 0 \\ \boldsymbol{\theta} & \boldsymbol{\theta} & I & \boldsymbol{\theta} \\ 0 & 0 & \boldsymbol{\theta}^T & -1 \end{pmatrix}, \qquad L > 0;$$

$$T_k(C) = \begin{pmatrix} I_1 & \boldsymbol{\theta}_1 & \boldsymbol{\theta}_1 & \Theta & \boldsymbol{\theta}_1 \\ \boldsymbol{\theta}_1^T & C & S & \boldsymbol{\theta}_2^T & 0 \\ \boldsymbol{\theta}_1^T & S & -C & \boldsymbol{\theta}_2^T & 0 \\ \Theta^T & \boldsymbol{\theta}_2 & \boldsymbol{\theta}_2 & I_2 & \boldsymbol{\theta}_2 \\ \boldsymbol{\theta}_1^T & 0 & 0 & \boldsymbol{\theta}_2^T & -1 \end{pmatrix},$$

where I_1 is a $(k-1)\times(k-1)$ identity matrix,

for $C \in (-1,1), S = \sqrt{1-C^2}, 2 \leq k \leq n-1$;

$$T_n(Z) = \begin{pmatrix} I & \boldsymbol{\theta} & \boldsymbol{\theta} \\ \boldsymbol{\theta}^T & C & -S \\ \boldsymbol{\theta}^T & S & C \end{pmatrix}, \qquad Z = C + iS \in S^1.$$

Note that each of the mappings T_k takes values in G_p and is injective for all $1 \leq k \leq n$, and $T_k^{-1} = T_k$ whenever $1 \leq k < n$. The mapping $T_n \colon S^1 \to G_p$ is a group homomorphism.

Now suppose $R \in \mathcal{D}_C$ is given. To each site $r \in \operatorname{vert} \mathcal{S}(\Gamma)$ we assign the pose $E_r(R)$ at that site. Thus the vertices of the site graph become labelled with poses. Now for every edge $e = \{r, r'\}$ of the site graph, or for every pair $e = (r, r')$ of the pair groupoid, there is a unique matrix $\mathcal{A}_e(R) \in G_p$ such that $E_r(R)\mathcal{A}_e(R) = E_{r'}(R)$. Because of the special structure of the poses this matrix always turns out to be one of the above three types.

Theorem. *Suppose Γ is a Z-system and $R \in \mathcal{D}_C(\Gamma)$. Suppose r, r' are sites of Γ.*

1. *If $r = (i_0, i_1, i_2, \ldots, i_{n-1})$ and $r' = (i_1, i_0, i_2, \ldots, i_{n-1})$, and if $e = \{i_0, i_1\}$, then $E_{r'}(R) = E_r(R)T_1(L_e(R))$.*
2. *If for $2 \leq k \leq n-1$ we have that r' is obtained from r by interchanging the $k-1$st and kth elements, and $e = s_k(r) = s_k(r')$, then $E_{r'}(R) = E_r(R)T_k(C_e(R))$.*
3. *If $r = (i_0, \ldots, i_{n-2}, i_{n-1})$ and $r' = (i_0, \ldots, i_{n-2}, i_n)$ and $e^* = [i_0, \ldots, i_{n-2}, i_{n-1}, i_n] \in \Gamma^n_*$, then $E_{r'}(R) = E_r(R)T_n(Z_{e^*}(R))$.*

Proof. (1) We begin by considering an edge such as $e = \{r = (i_0, i_1, i_2, \ldots, i_{n-1}), r' = (i_1, i_0, i_2, \ldots, i_{n-1})\}$, where $r, r' \in \operatorname{vert} \mathcal{S}(\Gamma)$. Define $s = \{i_0, i_1\}$, which determines an edge in the tree $(\Gamma^0, \Gamma^1, \sigma)$ between the 0-simplices $\{i_0\}$ and $\{i_1\}$. If $E_r(R) = (\mathbf{e}_0, \mathbf{e}_1, \ldots, \mathbf{e}_n)$, then

$$E_r(R)T_1(L_s(R)) = (\mathbf{e}_0 + L_s(R)\mathbf{e}_1, -\mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_{n-1}, -\mathbf{e}_n).$$

Our definitions immediate imply that this is the pose $E_{r'}(R)$.

(2) Now suppose $e = \{r = (i_0, \ldots, i_{n-1}), r' = (j_0, \ldots, j_{n-1})\} \in \operatorname{edge} \mathcal{S}(\Gamma)$ where for some $2 \leq k \leq n-1$ we have

$$(i_0, \ldots, i_{k-2}) = (j_0, \ldots, j_{k-2}),$$
$$(i_{k+1}, \ldots, i_{n-1}) = (j_{k+1}, \ldots, j_{n-1}), \text{and}$$

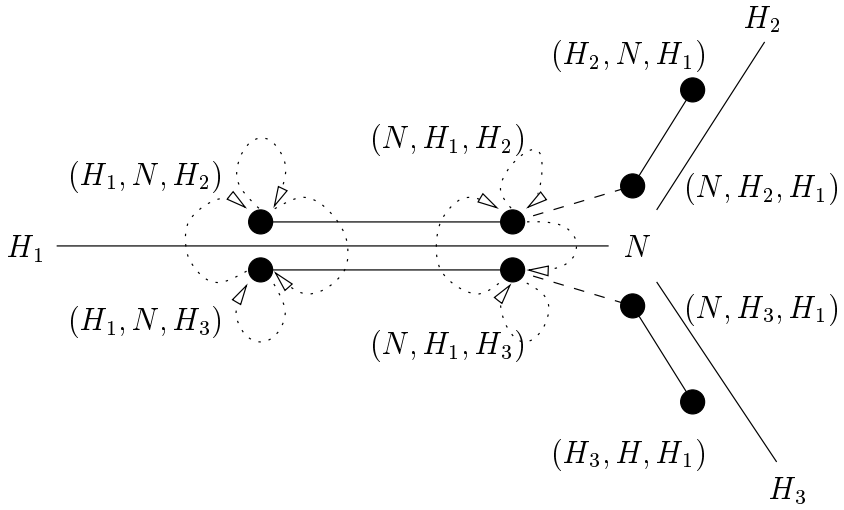

FIGURE 4. The site network for ammonia, superimposed on the molecular graph for the molecule. The Z-system has $\mathcal{N} = \{N, H_1, H_2, H_3\}$, $\Gamma^1 = \{\{N, H_1\}, \{N, H_2\}, \{N, H_3\}\}$, $\Gamma^2 = \{\{H_1, N, H_2\}, \{H_1, N, H_3\}\}$, and $\Gamma^3_* = \{[N, H_1, H_2, H_3]\}$. Sites are indicated by dark circles, and labeled with the corresponding ordered triples of atom names. Edges in the site graph are indicated by solid and dashed lines. Elements of the pair groupoid are indicated by dotted curving arrows.

$$(i_{k-1}, i_k) = (j_k, j_{k-1}).$$

$s_k(r) = \{i_0, \ldots, i_k\}$ is equal to $s_k(r') = \{j_0, \ldots, j_k\}$, and corresponds to an edge s in the tree $(\Gamma^{k-1}, \Gamma^k, \sigma)$ with vertices $v_1 = s_{k-1}(r)$ and $v_2 = s_{k-1}(r')$ in Γ^{k-1}. Let $u = v_1 \cap v_2 = s_{k-2}(r) = s_{k-2}(r') \in \Gamma^{k-2}$. Let $E_r(R) = (\mathbf{e}_0, \mathbf{e}_1, \ldots, \mathbf{e}_n)$ and $E_{r'}(R) = (\mathbf{e}'_0, \mathbf{e}'_1, \ldots, \mathbf{e}'_n)$. Then for $C = C_s(R)$ note that

$$E_r(R)T_k(C) = (\mathbf{e}_0, \ldots, \mathbf{e}_{k-2}, \mathbf{e}_{k-1}C + \mathbf{e}_k S, \mathbf{e}_{k-1}S - \mathbf{e}_k C, \mathbf{e}_{k+1}, \ldots, \mathbf{e}_{n-1}, -\mathbf{e}_n).$$

Since $(i_0, \ldots, i_{k-2}) = (j_0, \ldots, j_{k-2})$ it is clear that $\mathbf{e}'_0 = \mathbf{e}_0, \ldots, \mathbf{e}'_{k-2} = \mathbf{e}_{k-2}$. We claim that $\mathbf{e}'_{k-1} = \mathbf{e}_{k-1}C + \mathbf{e}_k S$. To see this, note that $1 - \Pi_{v_1} = (1 - \mathbf{e}_{k-1}\mathbf{e}^T_{k-1})(1 - \Pi_u)$. Therefore $\mathbf{e}_k$ is the unit vector in the direction of $(1 - \Pi_{v_1})(\mathbf{R}_{i_k} - \mathbf{R}_{i_0}) = (1 - \mathbf{e}_{k-1}\mathbf{e}^T_{k-1})(1 - \Pi_u)(\mathbf{R}_{i_k} - \mathbf{R}_{i_0})$. Since $j_{k-1} = i_k$ it follows that $\mathbf{e}'_{k-1}$ is the unit vector in the direction of $(1 - \Pi_u)(\mathbf{R}_{i_k} - \mathbf{R}_{i_0})$, and thus that $\mathbf{e}_k$ is the unit vector in the direction of $(1 - \mathbf{e}_{k-1}\mathbf{e}^T_{k-1})\mathbf{e}'_{k-1}$. Thus there is a positive constant α such that $\mathbf{e}_k\alpha = \mathbf{e}'_{k-1} - \mathbf{e}_{k-1}(\mathbf{e}_{k-1} \cdot \mathbf{e}'_{k-1})$. But $\mathbf{e}_{k-1} \cdot \mathbf{e}'_{k-1} = C_s(R) = C$. Thus $\mathbf{e}'_{k-1} = \mathbf{e}_{k-1}C + \mathbf{e}_k\alpha$. Since $\mathbf{e}'_{k-1}$ is a unit vector and $\{\mathbf{e}_{k-1}, \mathbf{e}_k\}$ is an orthonormal set we have that $C^2 + \alpha^2 = 1$. Since $\alpha > 0$ we have $\alpha = \sqrt{1 - C^2} = S$. Thus $\mathbf{e}'_{k-1} = \mathbf{e}_{k-1}C + \mathbf{e}_k S$, as claimed. In the same vein we claim that $\mathbf{e}'_k = \mathbf{e}_{k-1}S - \mathbf{e}_k C$. To see this, note that $1 - \Pi_{v_2} = (1 - \mathbf{e}'_{k-1}(\mathbf{e}'_{k-1})^T)(1 - \Pi_u)$. $\mathbf{e}'_k$ is the unit vector in the direction of $(1 - \Pi_{v_2})(\mathbf{R}_{j_k} - \mathbf{R}_{j_0}) = (1 - \mathbf{e}'_{k-1}(\mathbf{e}'_{k-1})^T)(1 - \Pi_u)(\mathbf{R}_{i_{k-1}} - \mathbf{R}_{i_0})$, or of $(1 - \mathbf{e}'_{k-1}(\mathbf{e}'_{k-1})^T)\mathbf{e}_{k-1}$. Hence there is a positive constant β such that $\mathbf{e}'_k\beta = \mathbf{e}_{k-1} - \mathbf{e}'_{k-1}(\mathbf{e}'_{k-1} \cdot \mathbf{e}_{k-1}) = \mathbf{e}_{k-1} - \mathbf{e}'_{k-1}C_s(R)$. Using our known expression for $\mathbf{e}'_{k-1}$, we can easily derive the claim from this. Since $(i_{k+1}, \ldots, i_{n-1}) = (j_{k+1}, \ldots, j_{n-1})$

and $s_j(r) = s_j(r')$ for $j = k, \ldots, n-2$, we see that $\mathbf{e}'_{k+1} = \mathbf{e}_{k+1}, \ldots, \mathbf{e}'_{n-1} = \mathbf{e}_{n-1}$. Finally, $\mathbf{e}'_n$ is either $\mathbf{e}_n$ or $-\mathbf{e}_n$, and it must be the latter since $\det \begin{pmatrix} C & S \\ S & -C \end{pmatrix} = -1$. Thus we have shown that $E_r(R)T_k(C) = E_{r'}(R)$.

(3) Now consider a pair $(r, r') \in \mathcal{G}(\Gamma)$ of the form $r = (i_0, \ldots, i_{n-2}, i_{n-1})$, $r' = (i_0, \ldots, i_{n-2}, i_n)$, where $e^* = [i_0, \ldots, i_{n-1}, i_n] \in \Gamma^n_*$, $v = \{i_0, \ldots, i_{n-2}, i_{n-1}\} \in \Gamma^{n-1}$, $v' = \{i_0, \ldots, i_{n-2}, i_n\} \in \Gamma^{n-1}$, $e = v \cup v' \in \Gamma^n$, and $s = v \cap v' \in \Gamma^{n-2}$. Let $E_r(R) = (\mathbf{e}_0, \mathbf{e}_1, \ldots, \mathbf{e}_n)$ and $E_{r'}(R) = (\mathbf{e}'_0, \mathbf{e}'_1, \ldots, \mathbf{e}'_n)$. Clearly we have $\mathbf{e}'_k = \mathbf{e}_k$ for $k = 0, 1, \ldots, n-2$. Then our definitions show that $C_e(R) = \mathbf{e}_{n-1} \cdot \mathbf{e}'_{n-1}$ and $S_{e^*}(R) = \mathbf{e}_n \cdot \mathbf{e}'_{n-1}$. Since $\mathbf{e}'_{n-1}$ is in the two-dimensional space perpendicular to the span of $\{\mathbf{e}_1, \ldots, \mathbf{e}_{n-2}\}$, and $\{\mathbf{e}_{n-1}, \mathbf{e}_n\}$ is an orthonormal basis of this subspace, then we have that $\mathbf{e}'_{n-1} = \mathbf{e}_{n-1}C_e(R) + \mathbf{e}_n S_{e^*}(R)$. Also the vector $-\mathbf{e}_{n-1}S_{e^*}(R) + \mathbf{e}_n C_e(R)$ is a unit vector perpendicular to the span of $\{\mathbf{e}'_1, \ldots, \mathbf{e}'_{n-2}, \mathbf{e}'_{n-1}\}$ and

$$\begin{aligned} \det(\mathbf{e}'_1, \ldots, &\mathbf{e}'_{n-2}, \mathbf{e}'_{n-1}, -\mathbf{e}_{n-1}S_{e^*}(R) + \mathbf{e}_n C_e(R)) \\ &= \det(\mathbf{e}_1, \ldots, \mathbf{e}_{n-2}, \mathbf{e}_{n-1}C_e(R) + \mathbf{e}_n S_{e^*}(R), -\mathbf{e}_{n-1}S_{e^*}(R) + \mathbf{e}_n C_e(R)) \\ &= \det(\mathbf{e}_1, \ldots, \mathbf{e}_n) \det \begin{pmatrix} C_e(R) & -S_{e^*}(R) \\ S_{e^*}(R) & C_e(R) \end{pmatrix} = 1 \end{aligned}$$

Hence $\mathbf{e}'_n = -\mathbf{e}_{n-1}S_{e^*}(R) + \mathbf{e}_n C_e(R)$. We have shown that $E_r(R)T_n(C_e(R) + iS_{e^*}(R)) = E_{r'}(R)$. □

Since the numbers L, C, and Z can be uniquely recovered from the matrices $T_1(L), T_k(C)$, and $T_n(Z)$, and every element of Γ^k, $1 \leq k \leq n$, can be associated with at least one pair of sites, this theorem gives an alternate way to define the coordinate functions $L_e(R), C_e(R)$, and $Z_{e^*}(R)$.

Thus given $R \in \mathcal{D}_C(\Gamma)$ we can label each edge $e \in \text{edge}\,\mathcal{S}(\Gamma)$ with an element $\mathcal{A}_e(R) \in G_p$ such that $E_{r_1}(R)\mathcal{A}_e(R) = E_{r_2}(R)$ as follows. The edge $e = \{r, r'\}$, where r' is obtained from r by interchanging the first two entries, should be labelled with $\mathcal{A}_e(R) = T_1(L_s(R))$, where $s = s_1(r) = s_1(r')$. When r' is obtained from r by interchanging the $k-1$st and the kth entries, where $2 \leq k \leq n-1$, then we label the edge $e = \{r, r'\}$ in the site graph with $\mathcal{A}_e(R) = T_k(C_s(R))$, where $s = s_k(r) = s_k(r')$. Since $\mathcal{A}_e(R) = \mathcal{A}_e(R)^{-1}$ this means it will also be true that $E_r(R)\mathcal{A}_e(R) = E_{r'}(R)$.

Part (3) of the above theorem also tells us how to label certain pairs (r, r') of the pair groupoid $\mathcal{G}(\Gamma)$ with an element $a_{rr'}(R) = Z_{e^*}(R)$ of the group S^1, so that $E_r(R)T_n(a_{rr'}(R)) = E_{r'}(R)$. The pair (r, r') and the oriented n-simplex $e^* \in \Gamma^n_*$ must be related as specified in part (3) of the theorem. However, this turns out to be exactly the information we need to uniquely extend this labelling to a mapping $a_\cdot(R)\colon \mathcal{G}(\Gamma) \to S^1 \colon (r, r') \mapsto a_{rr'}(R)$ such that $E_r(R)T_n(a_{rr'}(R)) = E_{r'}(R)$ holds for all $(r, r') \in \mathcal{G}(\Gamma)$, or equivalently, $a_{r_1 r_3}(R) = a_{r_1 r_2}(R)a_{r_2 r_3}(R)$ for all $(r_1, r_2), (r_2, r_3) \in \mathcal{G}(\Gamma)$. Mappings $a_\cdot(R)$ with this property are said to be S^1-valued *cocycles*, or *groupoid homomorphisms*.

To see how this extended labelling should be done we proceed as follows. We should label all pairs (r, r) with the number 1, i.e. $a_{r\,r}(R) = 1$. Furthermore, if $(r, r') \in \mathcal{G}(\Gamma)$ is one of the special pairs related to an oriented n-simplex $e^* \in \Gamma^n_*$ as above, then we should define $a_{r'r}(R) = a_{r\,r'}(R)^{-1}$. But these instructions might not label all the pairs in $\mathcal{G}(\Gamma)$, although they do suffice for the pair groupoid of ammonia (see Figure 4). So suppose $(r, r') \in \mathcal{G}(\Gamma)$ is one of the pairs not yet

labelled. Let $r = (i_0, \ldots, i_{n-2}, i)$, $r' = (i_0, \ldots, i_{n-2}, i')$; since r and r' are sites we have $v = \{i_0, \ldots, i_{n-2}, i\} \in \Gamma^{n-1}$, $v' = \{i_0, \ldots, i_{n-2}, i'\} \in \Gamma^{n-1}$, and $s = \{i_0, \ldots, i_{n-2}\} \in \Gamma^{n-2}$. We are assuming that $v \cup v' \notin \Gamma^n$ and $i \neq i'$, so that $s = v \cap v'$. We need the following result when $k = n$.

Lemma. *Suppose Γ is a Z-system, $1 \leq k \leq n$, and v and v' are distinct vertices in the tree $(\Gamma^{k-1}, \Gamma^k, \sigma)$, where $v \cup v' \notin \Gamma^k$ and $s = v \cap v' \in \Gamma^{k-2}$. Let $(v = v_0, e_1, v_1, \ldots, v_{m-1}, e_m, v_m = v')$ be the unique path $(m \geq 2)$ connecting them. (The distinct vertices $v_j \in \Gamma^{k-1}$ and the distinct edges $e_j \in \Gamma^k$ are such that e_j is incident on v_{j-1} and v_j.) Then $v_{j-1} \cap v_j = s$ for all $j = 1, \ldots, m$.*

Proof. If $k = 1$ then $\Gamma^{-1} = \{\emptyset\}$, and so the assertion of the lemma is trivial. So suppose $k \geq 2$. Consider the list $(v_0 \cap v_1, v_1 \cap v_2, \ldots, v_{m-1} \cap v_m, s)$ of simplices in Γ^{k-2}. Suppose by way of contradiction that this list contains a simplex other than s. Define $h_1 = \min\{1 \leq h \leq m \mid v_{h-1} \cap v_h \neq s\}$, and recursively $h_{j+1} = \min\{h_j < h \leq m \mid v_{h-1} \cap v_h \neq v_{h_j - 1} \cap v_{h_j}\}$ for all $j \geq 1$ for which the set over which the minimum is taken is nonempty. Let h_p be the last one defined; clearly $p \leq m$. Define $s_j = v_{h_j - 1} \cap v_{h_j}$. $v_{h_1 - 1}$ is incident on s (since either $h_1 = 1$ or $s = v_0 \cap v_1 = \cdots = v_{h_1 - 2} \cap v_{h_1 - 1}$) and on $s_1 \neq s$. Also v_m is incident on s_p, since $\{h_p < h \leq m \mid v_{h-1} \cap v_h \neq v_{h_p - 1} \cap v_{h_p}\} = \emptyset$ can only happen if $h_p = m$ (in which case $s_p = v_{h_p - 1} \cap v_{h_p} = v_{m-1} \cap v_m$) or if $h_p < m$ and (taking $h = m$) $s_p = v_{h_p - 1} \cap v_{h_p} = v_{m-1} \cap v_m$. Also $v_m = v'$ is incident on s. Thus if $p = 1$ then $v_{h_1 - 1}$ would equal v_m because both would be incident on s and s_1, which contradicts the fact that the vertices $(v_0, v_1, \ldots, v_m)$ are distinct. Therefore $p \geq 2$. $v_{h_2 - 1}$ is incident on s_1 and on s_2. $s_2 \neq s$ because otherwise $v_{h_2 - 1} = v_{h_1 - 1}$ (both being incident on s and s_1), again contradicting distinctness. In general $v_{h_j - 1}$ is incident on both s_{j-1} and s_j $(\neq s_{j-1})$. $s_j \neq s_{j-2}$ by distinctness of the vertices $(v_0, v_1, \ldots, v_m)$. Furthermore s_j for $j \geq 3$ cannot cannot equal any of $s_{j-3}, s_{j-4}, \ldots, s$ because otherwise there would be a cycle in the tree $(\Gamma^{k-2}, \Gamma^{k-1}, \sigma)$. In particular $s_p \neq s$. Hence $(s, v_{h_1 - 1}, s_1, v_{h_2 - 1}, \ldots, v_{h_p - 1}, s_p, v_m, s)$ constitutes a cycle in the tree $(\Gamma^{k-2}, \Gamma^{k-1}, \sigma)$. This contradiction shows that the list $(v_0 \cap v_1, v_1 \cap v_2, \ldots, v_{m-1} \cap v_m, s)$ cannot contain a simplex other than s, which finishes the proof. □

Each vertex v_j in the list $v_0, v_1, \ldots, v_m$ determines a site $r_j = (i_0, \ldots, i_{n-2}, i(j))$ where $\{i(j)\} = v_j \setminus s$. Furthermore, for each $j = 1, \ldots, m$, the label $a_{r_{j-1} r_j}(R)$ has been previously assigned, since $e_j = v_{j-1} \cup v_j = \{i_0, \ldots, i_{n-2}, i(j-1), i(j)\} \in \Gamma^n$. Therefore we define

$$a_{r\,r'}(R) = a_{r_0 r_1}(R) a_{r_1 r_2}(R) \ldots a_{r_{m-1} r_m}(R).$$

This is a complete and unique way to define the labels so that the result is a groupoid homomorphism.

Thus a labelled Z-system induces a labelling of the edges of the site graph and of the pairs of the pair groupoid with appropriate elements of G_p. This pattern of labelling is consistent with a labelling of the sites with poses arising from a choice of $R \in \mathcal{D}_C$. But if R is replaced by $(\mathbf{b}, A) \cdot R$, the poses which are assigned to the sites change accordingly but the elements of G_p assigned to the edges of the site network are unchanged, since G_a acts on poses on the left whereas G_p acts on poses on the right. The labelled site network is a natural—albeit elaborate—structure which has other properties which we will not discuss here. It provides a convenient formalism

for the detailed mathematical study of molecular conformations. It is compactly coded by and most easily manipulated in terms of its underlying Z-system.

If a distinguished site r is chosen for a Z-system Γ it will be called a *root* of Γ, because $s_k(r)$ is thought of as a choice of root vertex for the tree $(\Gamma^k, \Gamma^{k+1}, \sigma)$ for all $k = 0, \ldots, n-1$.

Definition. Suppose $\Gamma = (\Gamma^1, \ldots, \Gamma^n_*)$ is a Z-system and r is a root for Γ. Then define the mapping $\eta\colon \mathcal{D}_C \to \mathcal{P} \times \mathcal{D}_P$ by the rule:

$$R \mapsto (E_r(R), (L_e(R) \mid e \in \Gamma^1), (C_e(R) \mid e \in \Gamma^k, 2 \leq k \leq n-1), (Z_{e^*}(R) \mid e^* \in \Gamma^n_*)).$$

We will call this the *polyspherical coordinate mapping* associated to (Γ, r).

η is clearly a smooth mapping. In fact it is algebraic. Now suppose $(\mathbf{b}, A) \in G_a$ and $(E, \gamma) \in \mathcal{P} \times \mathcal{D}_P$. Define $(\mathbf{b}, A)(E, \gamma) = ((\mathbf{b}, A)E, \gamma)$. With this convention in place we claim that the mapping η satisfies $\eta((\mathbf{b}, A) \cdot R) = (\mathbf{b}, A)\eta(R)$ for all $R \in \mathcal{D}_C$. We will refer to this property of η by saying η is *left G_a-equivariant*. This property reduces to the already established fact that each of the mappings L_e, C_e, and Z_{e^*} are invariant with respect to the action of G_a.

It is not yet clear why we use the term "polyspherical coordinates" to describe this mapping. This will become clear in the next section where we learn how to invert the mapping η.

4. The Main Theorems

A comparison of the dimensions of $\mathcal{D}_C$ and $\mathcal{P} \times \mathcal{D}_P$ suggests that the mapping η defined in the previous section might be invertible. $\mathcal{D}_C$ is a dense open subset of $(\mathbb{R}^n)^{\mathcal{N}}$ and so has dimension nN. $\mathcal{P}$ is diffeomorphic to $\mathbb{R}^n \times \mathrm{SO}(n)$, and so has dimension $n + n(n-1)/2 = n(n+1)/2$. ($\mathrm{SO}(n)$ has the same dimension as its Lie algebra, namely the set of all $n \times n$ real antisymmetric matrices.) Since $|\Gamma^0| = N$ and $(\Gamma^0, \Gamma^1, \sigma)$ is a tree we have that $|\Gamma^1| = N - 1$. Similarly $|\Gamma^k| = N - k$, for $k = 1, \ldots, n$. Thus $\mathcal{D}_P$ has dimension $\sum_{k=1}^n (N-k) = nN - n(n+1)/2$. Therefore $\mathcal{P} \times \mathcal{D}_P$ also has dimension nN, as claimed.

Main Theorem. *Suppose $N \geq n \geq 2$, $\Gamma = (\Gamma^1, \ldots, \Gamma^n_*)$ is an n-dimensional Z-system on the set $\mathcal{N}$, $r = (i_0, \ldots, i_{n-1})$ is a root for Γ, and $\eta\colon \mathcal{D}_C \to \mathcal{P} \times \mathcal{D}_P$ is the polyspherical coordinate mapping defined in the previous section. Then η is a diffeomorphism. Furthermore η induces a diffeomorphism $\hat{\eta}\colon G_a \backslash \mathcal{D}_C \to \mathcal{D}_P$, which is independent of the root r.*

Proof. We will proceed by constructing the inverse $\zeta\colon \mathcal{P} \times \mathcal{D}_P \to \mathcal{D}_C$ to η via induction on N. We start with the case $N = n$. So let $(E, \gamma) \in \mathcal{P} \times \mathcal{D}_P$ be given, where $E = (\mathbf{e}_0, \mathbf{e}_1, \ldots, \mathbf{e}_n) \in \mathcal{P}$ and

$$\gamma = ((L_e \mid e \in \Gamma^1), (C_e \mid e \in \Gamma^k, 2 \leq k \leq n-1)) \in \mathcal{D}_P.$$

When $N = n$ we have $\Gamma^n = \emptyset$, so we have not included any coordinates of type Z_{e^*} in the definition of γ. Let $r = (i_0, i_1, \ldots, i_{n-1})$ be the root site. Define $\mathbf{R}_{i_0} = \mathbf{e}_0$, and $\mathbf{R}_{i_1} = \mathbf{R}_{i_0} + \mathbf{e}_1 L_{\{i_0, i_1\}}$. Because $\gamma \in \mathcal{D}_P$ we have $L_{\{i_0,i_1\}} > 0$, and hence the 1 simplex $\{\mathbf{R}_{i_0}, \mathbf{R}_{i_1}\}$ is geometrically independent. Now suppose $\mathbf{R}_{i_j}$ has been defined for all $0 \leq j \leq k-1$, where $2 \leq k \leq n-1$. Assume that the $k-1$ simplex $\{\mathbf{R}_{i_0}, \ldots, \mathbf{R}_{i_{k-1}}\}$ is geometrically independent. $s^1_k = s_k(r) = \{i_0, i_1, \ldots, i_k\} \in \Gamma^k$ is incident on two $k-1$ simplices in Γ^{k-1}, one of which is $s^0_{k-1} = s_{k-1}(r) = \{i_0, \ldots, i_{k-1}\}$ and the other we will denote by s^1_{k-1}; the intersection of these two

being denoted by $s^0_{k-2} \in \Gamma^{k-2}$. Define j_{k-1} by the relation $s^0_{k-1} \setminus s^0_{k-2} = \{j_{k-1}\}$. Notice that $s^1_{k-1} \setminus s^0_{k-2} = \{i_k\}$.

$$\begin{array}{ccccccccccccc} s^1_k & \hookleftarrow & s^1_{k-1} & \hookleftarrow & s^1_{k-2} & \hookleftarrow & \dots & \hookleftarrow & s^1_2 & \hookleftarrow & s^1_1 & \hookleftarrow & s^1_0 \\ \uparrow & & \uparrow & & \uparrow & & & & \uparrow & & \uparrow & & \\ s^0_{k-1} & \hookleftarrow & s^0_{k-2} & \hookleftarrow & s^0_{k-3} & \hookleftarrow & \dots & \hookleftarrow & s^0_1 & \hookleftarrow & s^0_0 & & \end{array}$$

If the smallest simplex in this array is a 0-simplex then we stop, otherwise we continue as follows: s^1_{k-1} is incident on s^0_{k-2} and one other $k-2$ simplex, call it $s^1_{k-2} \in \Gamma^{k-2}$. The intersection of s^0_{k-2} and s^1_{k-2} is a $k-3$ simplex called $s^0_{k-3} \in \Gamma^{k-3}$. Define j_{k-2} such that $s^0_{k-2} \setminus s^0_{k-3} = \{j_{k-2}\}$. Notice that $s^1_{k-2} \setminus s^0_{k-3} = \{i_k\}$. When this process stops we will have that s^0_0 and $s^1_0 = \{i_k\}$ are 0-simplices. Let $s^0_0 = \{j_0\}$. Then $s^0_h = \{j_0, \dots, j_h\}$ and $s^1_h = \{j_0, \dots, j_{h-1}, i_k\}$, for $h = 0, \dots, k$. Thus $\{j_0, \dots, j_{k-1}\} = s^0_{k-1} = \{i_0, \dots, i_{k-1}\}$, and hence $\mathbf{R}_{j_0}, \dots, \mathbf{R}_{j_{k-1}}$ are already defined. Thus the following are sites of our Z-system:

$$\begin{aligned} r_k &= (j_0, \dots, j_{k-2}, j_{k-1}, i_k, i_{k+1}, \dots, i_{n-1}) \\ r_{k-1} &= (j_0, \dots, j_{k-2}, i_k, j_{k-1}, i_{k+1}, \dots, i_{n-1}) \\ &\vdots \\ r_2 &= (j_0, j_1, i_k, j_2, \dots, j_{k-1}, i_{k+1}, \dots, i_{n-1}) \\ r_1 &= (j_0, i_k, j_1, \dots, j_{k-1}, i_{k+1}, \dots, i_{n-1}) \\ r_0 &= (i_k, j_0, j_1, \dots, j_{k-1}, i_{k+1}, \dots, i_{n-1}) \end{aligned}$$

Each one is obtained from its predecessor by a single interchange of adjacent entries. Define $E_{r_k} = (\mathbf{e}'_0, \mathbf{e}'_1, \dots, \mathbf{e}'_{k-1}, \mathbf{e}_k, \dots, \mathbf{e}_{n-1}, \pm\mathbf{e}_n)$, where

$$\mathbf{e}'_0 = \mathbf{R}_{j_0}, \qquad \mathbf{e}'_h = \frac{(1 - \Pi_{s_{h-1}(r^k)})(\mathbf{R}_{j_h} - \mathbf{R}_{j_0})}{\|(1 - \Pi_{s_{h-1}(r^k)})(\mathbf{R}_{j_h} - \mathbf{R}_{j_0})\|}, \qquad h = 1, \dots, k-1,$$

and where the sign is chosen to assure that this is indeed a pose. Note that

$$\begin{aligned} \text{span } \{\mathbf{e}'_1, \dots, \mathbf{e}'_{k-1}\} &= \text{span } \{\mathbf{R}_{j_1} - \mathbf{R}_{j_0}, \dots, \mathbf{R}_{j_{k-1}} - \mathbf{R}_{j_0}\} \\ &= \text{span } \{\mathbf{R}_{i_1} - \mathbf{R}_{i_0}, \dots, \mathbf{R}_{i_{k-1}} - \mathbf{R}_{i_0}\} \\ &= \text{span } \{\mathbf{e}_1, \dots, \mathbf{e}_{k-1}\}, \end{aligned}$$

and hence $\mathbf{e}_k, \dots, \mathbf{e}_n$ are perpendicular to this span. Consider the product

$$E_{r_0} = E_{r^k} \mathcal{A}_{r_k r_{k-1}} \dots \mathcal{A}_{r_2 r_1} \mathcal{A}_{r_1 r_0},$$

where $\mathcal{A}_{r_1 r_0} = T_1(L_{s^1_1})$ and $\mathcal{A}_{r_h r_{h-1}} = T_h(C_{s^1_h})$, $h = 2, \dots, k$. This should be a pose whose origin is located at $\mathbf{R}_{i_k}$, the quantity we are trying to define. Thus $\mathbf{R}_{i_k} = E_{r_0}(1, 0, \dots, 0)^T$ or

$$\mathbf{R}_{i_k} = E_{r^k} T_k(C_{s^1_k}) T_{k-1}(C_{s^1_{k-1}}) \dots T_2(C_{s^1_2}) T_1(L_{s^1_1}) \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

$$= (\mathbf{e}'_0, \mathbf{e}'_1, \ldots, \mathbf{e}'_{k-1}, \mathbf{e}_k, \ldots, \mathbf{e}_{n-1}, \pm\mathbf{e}_n) \begin{pmatrix} 1 \\ C_{s^1_2} L_{s^1_1} \\ C_{s^1_3} S_{s^1_2} L_{s^1_1} \\ \vdots \\ C_{s^1_k} S_{s^1_{k-1}} \ldots S_{s^1_2} L_{s^1_1} \\ S_{s^1_k} S_{s^1_{k-1}} \ldots S_{s^1_2} L_{s^1_1} \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

In the above, we are using the notation $S_s = \sqrt{1 - C_s^2}$. Because $\gamma \in \mathcal{D}_P$ it follows that the component of $\mathbf{e}_k$ is nonzero, which implies that the simplex $\{\mathbf{R}_{i_0}, \ldots, \mathbf{R}_{i_k}\}$ is geometrically independent. Clearly $\mathbf{R}_{i_k}$ does not depend on the vectors $\mathbf{e}_{k+1}, \ldots, \mathbf{e}_n$ at all. This formula also explains why we describe our coordinates as polyspherical coordinates, for this is exactly how R_{i_k} is located relative to the pose E_{r_k}. Thus by induction all n points $(\mathbf{R}_{i_0}, \ldots, \mathbf{R}_{i_{n-1}})$ have now been defined and the resulting $n-1$ simplex is geometrically independent. This list of n points defines the value of the mapping ζ on the argument (E, γ). Clearly ζ is a smooth function. We have defined ζ by inverting the formulae for η at every point, so $\eta \circ \zeta$ and $\zeta \circ \eta$ are identity mappings.

Now suppose for $N \geq n+1$ that a smooth inverse ζ exists for the polyspherical coordinate mapping η for all n-dimensional Z-systems on any set of $N-1$ elements. Suppose $\mathcal{N} = \{1, \ldots, N\}$ and $\Gamma = (\Gamma^1, \ldots, \Gamma^n_*)$ is an n-dimensional Z-system on $\mathcal{N}$, with its coordinate domain $\mathcal{D}_C = \mathcal{D}_C(\Gamma)$, parameter domain $\mathcal{D}_P = \mathcal{D}_P(\Gamma)$, root site $r = (i_0, \ldots, i_{n-1})$, and smooth left G_a-equivariant polyspherical coordinate mapping $\eta \colon \mathcal{D}_C \to \mathcal{P} \times \mathcal{D}_P$. The tree $(\Gamma^{n-1}, \Gamma^n, \sigma)$ has leaves, which are vertices with degree one (having only one edge incident on them). Since $N \geq n+1$ we have $|\Gamma^{n-1}| = N - (n-1) \geq 2$. Thus, since every tree with at least two vertices has at least two leaves, we can choose a leaf vertex $s^1_{n-1} \in \Gamma^{n-1}$ which is not the root vertex $s_{n-1}(r) = \{i_0, \ldots, i_{n-1}\} \in \Gamma^{n-1}$. Let $s^1_n \in \Gamma^n$ denote the single edge incident on this leaf, and let $s^0_{n-1} \in \Gamma^{n-1}$ denote the other vertex on which this edge is incident. Define $s^0_{n-2} = s^0_{n-1} \cap s^1_{n-1} \in \Gamma^{n-2}$. Note that s^1_{n-1} is an edge in the tree $(\Gamma^{n-2}, \Gamma^{n-1}, \sigma)$ incident on the vertex s^0_{n-2}; hence there is exactly one other vertex $s^1_{n-2} \in \Gamma^{n-2}$ on which it is also incident. If the smallest of these simplices is a 0 simplex then we stop the process, but otherwise we continue the process by defining $s^0_{n-3} = s^0_{n-2} \cap s^1_{n-2} \in \Gamma^{n-3}$ and noting that s^1_{n-2} is an edge in the tree $(\Gamma^{n-3}, \Gamma^{n-2}, \sigma)$ incident on the vertex s^0_{n-3}, and therefore also on exactly on other vertex $s^1_{n-3} \in \Gamma^{n-3}$. Continuing this process until the smallest simplices are 0 simplices we obtain the following scheme:

$$\begin{array}{ccccccccccccc}
s^1_n & \hookleftarrow & s^1_{n-1} & \hookleftarrow & s^1_{n-2} & \hookleftarrow & \ldots & \hookleftarrow & s^1_2 & \hookleftarrow & s^1_1 & \hookleftarrow & s^1_0 \\
\uparrow & & \uparrow & & \uparrow & & & & \uparrow & & \uparrow & & \\
s^0_{n-1} & \hookleftarrow & s^0_{n-2} & \hookleftarrow & s^0_{n-3} & \hookleftarrow & \ldots & \hookleftarrow & s^0_1 & \hookleftarrow & s^0_0 & &
\end{array}$$

Suppose s^1_{k-1} is a leaf vertex in the tree $(\Gamma^{k-1}, \Gamma^k, \sigma)$ for some $2 \leq k \leq n$. We claim that s^1_{k-2} is a leaf vertex in the tree $(\Gamma^{k-2}, \Gamma^{k-1}, \sigma)$. Suppose by way of contradiction that s^1_{k-2} is a vertex of degree at least two in the tree $(\Gamma^{k-2}, \Gamma^{k-1}, \sigma)$,

i.e. there is an edge $s \in \Gamma^{k-1}$ which is incident on s^1_{k-2} and is distinct from s^1_{k-1}. Suppose $s = s^0_{k-1}$. Then $s^0_{k-2} = s^0_{k-1} \cap s^1_{k-1} = s \cap s^1_{k-1} = s^1_{k-2}$, which is a contradiction. So $s \neq s^0_{k-1}$. If $s \cup s^1_{k-1} \in \Gamma^k$ then s^1_{k-1} would have two distinct edges incident on it, namely s^1_k and $s \cup s^1_{k-1}$, contradicting the assumption that s^1_{k-1} is a leaf. Therefore $s \cup s^1_{k-1} \notin \Gamma^k$. Consider the unique path in the tree $(\Gamma^{k-1}, \Gamma^k, \sigma)$ connecting s to s^1_{k-1}. This path must have length at least two, and must contain the edge s^1_k. By the second lemma from section 3 the intersection of the pair of vertices for each edge of this path must be the same element of Γ^{k-2}. This element can be computed as the intersection of the two vertices of the edge s^1_k, namely $s^0_{k-1} \cap s^1_{k-1} = s^0_{k-2}$. But this would require that $s^0_{k-2} \subset s$, i.e. s is incident on s^0_{k-2}, which is impossible, since s would coincide with s^1_{k-1}, both being incident on s^0_{k-2} and s^1_{k-2}. This contradiction shows that s^1_{k-2} has degree one as a vertex in $(\Gamma^{k-2}, \Gamma^{k-1}, \sigma)$, as claimed.

Thus each of $s^1_{n-1}, \ldots, s^1_1, s^1_0$ are leaf vertices in their respective trees. Define $\tilde{\Gamma}^j = \Gamma^j \setminus \{s^1_j\}$ for all $j = 0, 1, \ldots, n$. In each case we have deleted a leaf vertex and the single edge which was incident on it, so $(\tilde{\Gamma}^{j-1}, \tilde{\Gamma}^j, \sigma)$ is a tree for all $j = 1, \ldots, n$. If $v_1, v_2 \in \tilde{\Gamma}^{j-1}$ satisfy $v_1 \cup v_2 \in \tilde{\Gamma}^j$ then $v_1 \cap v_2 \in \Gamma^{j-2}$. Since $v_1 \neq s^1_{j-1}$ and $v_2 \neq s^1_{j-1}$ and s^1_{j-1} is the only simplex in Γ^{j-1} which is incident on s^1_{j-2}, we have that $v_1 \cap v_2 \neq s^1_{j-2}$ and hence $v_1 \cap v_2 \in \tilde{\Gamma}^{j-2}$. Thus $\tilde{\Gamma} = (\tilde{\Gamma}^1, \ldots, \tilde{\Gamma}^n_*)$ is an n-dimensional Z-system on the set $\tilde{\mathcal{N}} = \mathcal{N} \setminus s^1_0$. If $s^1_0 \subset s_{n-1}(r)$ then one, say $\tilde{s}_{n-2}$, of the two $n-2$ simplices in Γ^{n-2} on which $s_{n-1}(r)$ is incident must satisfy $s^1_0 \subset \tilde{s}_{n-2}$. Continuing this sort of argument, we show that $s^1_0 \subset \tilde{s}_1 \subset \cdots \subset \tilde{s}_{n-2} \subset s_{n-1}(r)$. Since the only 1 simplex in Γ^1 incident on s^1_0 is s^1_1 we must have $\tilde{s}_1 = s^1_1$. Since the only 2 simplex in Γ^2 incident on s^1_1 is s^1_2 we must have $\tilde{s}_2 = s^1_2$. Continuing this argument we find that $s_{n-1}(r) = s^1_{n-1}$. This contradicts our original choice of the leaf $s^1_{n-1} \neq s_{n-1}(r)$. Therefore $s^1_0 \not\subset s_{n-1}(r)$. Thus for all $0 \leq j \leq n-1$ we have $s_j(r) \neq s^1_j$, since $s^1_0 \subset s^1_j$ but $s^1_0 \not\subset s_j(r)$. Therefore r is a root for the Z-system $\tilde{\Gamma}$.

Define $\mathcal{D}_C(\tilde{\Gamma}) = \{\tilde{R}\colon \tilde{\mathcal{N}} \to \mathbb{R}^n \mid \text{for all } s \in \tilde{\Gamma}^{n-1} \text{ the simplex } R_s \text{ is geometrically independent}\}$. The restriction mapping maps $(\mathbb{R}^n)^{\mathcal{N}} \to (\mathbb{R}^n)^{\tilde{\mathcal{N}}}\colon R \mapsto \tilde{R}$. If $R \in \mathcal{D}_C$ then clearly its restriction $\tilde{R}$ is in $\tilde{\mathcal{D}}_C$. Define $\mathcal{D}_P(\tilde{\Gamma}) = (0,\infty)^{\tilde{\Gamma}^1} \times \left[\prod_{k=2}^{n-1}(-1,1)^{\tilde{\Gamma}^k}\right] \times (S^1)^{\tilde{\Gamma}^n_*}$. Clearly the restriction mapping $\gamma \mapsto \tilde{\gamma}$ maps $\mathcal{D}_P$ onto $\mathcal{D}_P(\tilde{\Gamma})$. If $\tilde{\eta}\colon \mathcal{D}_C(\tilde{\Gamma}) \to \mathcal{P} \times \mathcal{D}_P(\tilde{\Gamma})$ is the polyspherical coordinate mapping for the rooted Z-system $(\tilde{\Gamma}, r)$ then we claim the following diagram commutes:

$$\begin{array}{ccc} \mathcal{D}_C & \xrightarrow{\eta} & \mathcal{P} \times \mathcal{D}_P \\ {\scriptstyle\text{restriction}}\downarrow & & \downarrow{\scriptstyle\text{restriction}} \\ \mathcal{D}_C(\tilde{\Gamma}) & \xrightarrow{\tilde{\eta}} & \mathcal{P} \times \mathcal{D}_P(\tilde{\Gamma}) \end{array}$$

This is because the only simplices which contain $s^1_0 = \{i\}$ as a subset are the ones which are excluded from $\tilde{\Gamma}^j$. Hence the labels of all the simplices in $\tilde{\Gamma}^j$ can be computed without knowing $\mathbf{R}_i$, and these computations are performed in exactly the same manner, whether by η or by $\tilde{\eta}$. By the induction hypothesis there is a smooth inverse $\tilde{\zeta}\colon \mathcal{P} \times \mathcal{D}_P(\tilde{\Gamma}) \to \mathcal{D}_C(\tilde{\Gamma})$ to the mapping $\tilde{\eta}$.

Let $(E, \gamma) \in \mathcal{P} \times \mathcal{D}_P$ be given, where

$$\gamma = ((L_e \mid e \in \Gamma^1), (C_e \mid e \in \Gamma^k, 2 \leq k \leq n-1), (Z_{e^*} \mid e^* \in \Gamma^n_*)) \in \mathcal{D}_P.$$

We wish to define $\zeta(E,\gamma) \in \mathcal{D}_C$ such that the mapping ζ is a smooth inverse to the polyspherical coordinate mapping η. Define the site $r_n = (j_0, j_1, \ldots, j_{n-1})$ such that $\{j_0, \ldots, j_k\} = s^0_k \in \tilde{\Gamma}^k$ for all $k = 0, 1, \ldots, n-1$. r_n is a site of the Z-system $\tilde{\Gamma}$. If $\tilde{R} = \tilde{\zeta}(E, \tilde{\gamma})$, then the pose $E_{r_n}(\tilde{R}) = (\tilde{\mathbf{e}}_0, \tilde{\mathbf{e}}_1, \ldots, \tilde{\mathbf{e}}_n)$ is well-defined, and a smooth function of (E,γ). To define $R = \zeta(E,\gamma)$ we augment $\tilde{R}$ by defining $\mathbf{R}_i$. Note that $s^1_k = \{j_0, \ldots, j_{k-1}, i\}$ for all $k = 0, 1, \ldots, n$. Thus we have the sequence of sites:

$$\begin{aligned} r_n &= (j_0, j_1, j_2, j_3, \ldots, j_{n-2}, j_{n-1}) \\ r_{n-1} &= (j_0, j_1, j_2, j_3, \ldots, j_{n-2}, i) \\ &\vdots \\ r_2 &= (j_0, j_1, i, j_2, \ldots, j_{n-3}, j_{n-2}) \\ r_1 &= (j_0, i, j_1, j_2, \ldots, j_{n-3}, j_{n-2}) \\ r_0 &= (i, j_0, j_1, j_2, \ldots, j_{n-3}, j_{n-2}) \end{aligned}$$

Define $E_{r_0} = E_{r_n}(\tilde{R})\mathcal{A}_{r_n r_{n-1}} \ldots \mathcal{A}_{r_2 r_1}\mathcal{A}_{r_1 r_0}$, where $\mathcal{A}_{r_1 r_0} = T_1(L_{s^1_1})$, $\mathcal{A}_{r_k r_{k-1}} = T_k(C_{s^1_k})$, $k = 2, \ldots, n-1$, and $\mathcal{A}_{r_n r_{n-1}} = T_n((Z_{(s^1_n)^*})^a)$, where

$$a = \begin{cases} 1 & \text{if } [j_0, \ldots, j_{n-2}, j_{n-1}, i] = (s^1_n)^*, \\ -1 & \text{if } [j_0, \ldots, j_{n-2}, i, j_{n-1}] = (s^1_n)^*. \end{cases}$$

Since $\mathbf{R}_i = E_{r_0}(1, 0, \ldots, 0)^T$ we have

$$\mathbf{R}_i = (\tilde{\mathbf{e}}_0, \tilde{\mathbf{e}}_1, \ldots, \tilde{\mathbf{e}}_n) \begin{pmatrix} 1 \\ C_{s^1_2} L_{s^1_1} \\ C_{s^1_3} S_{s^1_2} L_{s^1_1} \\ \vdots \\ C_{s^1_n} S_{s^1_{n-1}} \ldots S_{s^1_2} L_{s^1_1} \\ a S_{(s^1_n)^*} S_{s^1_{n-1}} \ldots S_{s^1_2} L_{s^1_1} \end{pmatrix}.$$

This is clearly a well-defined smooth function of (E,γ). We need to check that $R_{s^1_{n-1}}$ is geometrically independent. Certainly $R_{s^0_{n-2}}$ is geometrically independent, since $s^0_{n-2} \in \tilde{\Gamma}^{n-2}$ and $\tilde{R} \in \tilde{\mathcal{D}}_C$. The parts of the above expression for $\mathbf{R}_i$ which depend on $\tilde{\mathbf{e}}_0, \ldots, \tilde{\mathbf{e}}_{n-2}$ describe a point on the codimension two hyperplane in $\mathbb{R}^n$ containing $R_{s^0_{n-2}}$. Thus $R_{s^1_{n-1}}$ is geometrically independent if and only if the sum of the squares of the last two components of the above column vector is positive, i.e. $S^2_{s^1_{n-1}} \ldots S^2_{s^1_2} L^2_{s^1_1} > 0$. This follows from the fact that $\gamma \in \mathcal{D}_P$. Thus, finally, the smooth map ζ is defined on all $\mathcal{P} \times \mathcal{D}_P$ and takes values in $\mathcal{D}_C$. Furthermore it is immediate that ζ is the inverse of η: certainly this is true for $\tilde{\zeta}$ and $\tilde{\eta}$, but also the above expressions for the Cartesian coordinates of $\mathbf{R}_i$ in terms of polyspherical coordinate exactly invert our definitions of those polyspherical coordinates in terms of Cartesian coordinates. This finishes the proof that η is a diffeomorphism.

The map η certainly induces a bijection $\hat{\eta}\colon G_a \backslash \mathcal{D}_C \to \mathcal{D}_P$, which is independent of the choice of the root site r. Since the left action of G_a on $\mathcal{D}_C$ is fixed point free and proper, $G_a \backslash \mathcal{D}_C$ is a smooth manifold, and the projection mapping $\rho\colon \mathcal{D}_C \to G_a \backslash \mathcal{D}_C$ as well as the mapping $\hat{\eta}\colon G_a \backslash \mathcal{D}_C \to \mathcal{D}_P$ are smooth (see Proposition 4.1.23 on page 266 of [2]). A smooth inverse to $\hat{\eta}$ can be found by composing ζ and the

projection map, and then factoring this through the projection $\mathcal{P} \times \mathcal{D}_P \to \mathcal{D}_P$. Thus $\hat{\eta}$ is a diffeomorphism. □

Thus the orbit space $G_a \backslash \mathcal{D}_C$ acquires the structure of a principal fibre bundle with abelian structure group $(S^1)^{\Gamma_*^n}$, a fact which is not so obvious from the definition of $\mathcal{D}_C$.

The mapping η of the previous theorem is the composition of the two upper mappings from the following commutative diagram.

$$\begin{array}{ccccc} \mathcal{D}_C(\Gamma) & \xrightarrow{(E_r,\rho)} & \mathcal{P} \times [G_a \backslash \mathcal{D}_C(\Gamma)] & \xrightarrow{1\times\hat{\eta}} & \mathcal{P} \times \mathcal{D}_P(\Gamma) \\ \rho \downarrow & & \downarrow \pi_2 & & \downarrow \pi_2 \\ G_a \backslash \mathcal{D}_C(\Gamma) & \xrightarrow{1} & G_a \backslash \mathcal{D}_C(\Gamma) & \xrightarrow{\hat{\eta}} & \mathcal{D}_P(\Gamma) \end{array}$$

The left rectangle shows that choice of a root site r determines a local trivialization in the principal bundle $\rho\colon \mathcal{D}_C(\Gamma) \to G_a \backslash \mathcal{D}_C(\Gamma)$. (Here we identify G_a and $\mathcal{P}$ in the obvious way.)

Let $\mathcal{B} \subset (\mathbb{R}^n)^{\mathcal{N}}$ consist of those R whose isotropy subgroup is trivial, or equivalently, the mapping $G_a \to (\mathbb{R}^n)^{\mathcal{N}}\colon g \mapsto g \cdot R$ is one-to-one (necessarily surjective) onto the orbit $G_a \cdot R$. Let $\rho\colon \mathcal{B} \to G_a \backslash \mathcal{B}\colon R \mapsto G_a \cdot R$ be the projection mapping. ρ will define a principal bundle with structure group G_a provided the base space $G_a \backslash \mathcal{B}$ is a manifold and we can cover $\mathcal{B}$ with smooth G_a-equivariant local trivializations. To begin, we assert that $\mathcal{D}_C(\Gamma) \subset \mathcal{B}$ for every Z-system Γ. To see this, suppose $R \in \mathcal{D}_C(\Gamma)$. Since $N \geq n \geq 2$ there is at least one $s \in \Gamma^{n-1}$. Also R_s is geometrically independent. Let $g = (\mathbf{b}, A)$ be in the isotropy subgroup of R. Then $\mathbf{b} + A\mathbf{R}_i = \mathbf{R}_i$ for all $i \in s$. Thus for $i, j \in s$, $i \neq j$, we have $A(\mathbf{R}_i - \mathbf{R}_j) = \mathbf{R}_i - \mathbf{R}_j$. Thus the eigenspace of A for the eigenvalue 1 is at least $n-1$ dimensional. If $(\mathbf{e}_1, \ldots, \mathbf{e}_n)$ is a positively oriented orthonormal basis of $\mathbb{R}^n$ such that $A\mathbf{e}_i = \mathbf{e}_i$ for $i = 1, \ldots, n-1$ then we must have $A\mathbf{e}_n = \mathbf{e}_n$. Thus $A = I$ and consequently $\mathbf{b} = \theta$. Since the isotropy subgroup of R is trivial, we have that $R \in \mathcal{B}$.

If we define $\mathcal{B}_r = \{R \in (\mathbb{R}^n)^{\mathcal{N}} \mid R_{s_{n-1}(r)} \text{ is geometrically independent}\}$, where $r \in \mathcal{N}^n$ is *nonredundant* (i.e $s_{n-1}(r) \in \binom{\mathcal{N}}{n}$), then by a similar argument as given above $\mathcal{B}_r \subset \mathcal{B}$, and the mapping $(E_r, \rho)\colon \mathcal{B}_r \to \mathcal{P} \times [G_a \backslash \mathcal{B}_r]\colon R \mapsto (E_r(R), G_a \cdot R)$ defines a smooth G_a-equivariant local trivialization of the principal bundle $\rho\colon \mathcal{B} \to G_a \backslash \mathcal{B}$. When (Γ, r) is a rooted Z-system, we certainly have $\mathcal{D}_C(\Gamma) \subset \mathcal{B}_r$.

Thus our results so far provide us with a family, indexed by Γ, of smooth coordinate charts $\hat{\eta}$ on $G_a \backslash \mathcal{B}$, and a family indexed by nonredundant n-tuples r of G_a-equivariant local trivializations. It remains to see if the domains of these charts and trivializations cover all of $\mathcal{B}$.

Theorem. *Suppose $N \geq n \geq 2$ and $R \in \mathcal{B}$. Then there exists an n dimensional Z-system Γ on the set $\mathcal{N}$ such that $R \in \mathcal{D}_C(\Gamma)$.*

Proof. Without loss of generality let $\mathcal{N} = \{1, 2, \ldots, N\}$. Let $V = \operatorname{span}\{\mathbf{R}_2 - \mathbf{R}_1, \ldots, \mathbf{R}_N - \mathbf{R}_1\}$. If the dimension of V is less than or equal to $n-2$ then let $(\mathbf{e}_1, \ldots, \mathbf{e}_n)$ be a positively oriented orthonormal basis of $\mathbb{R}^n$ such that $V \subset \operatorname{span}\{\mathbf{e}_1, \ldots, \mathbf{e}_{n-2}\}$. By defining a nontrivial rotation in the plane $\operatorname{span}\{\mathbf{e}_{n-1}, \mathbf{e}_n\}$, and extending it to be the identity on $\operatorname{span}\{\mathbf{e}_1, \ldots, \mathbf{e}_{n-2}\}$, we obtain a nontrivial $A \in \mathrm{SO}(n)$ which is the identity on V. Then $(\mathbf{R}_1 - A\mathbf{R}_1, A)$ is a nonidentity element of the isotropy subgroup of R. Thus when $R \in \mathcal{B}$ we have that the dimension of V is greater than or equal to $n-1$. Hence there is a $n-1$ simplex $s_n \in \binom{\mathcal{N}}{n}$

such that R_{s_n} is geometrically independent. Without loss of generality assume that $s_n = \{1, \ldots, n\}$ and $\{\mathbf{R}_1, \ldots, \mathbf{R}_n\}$ is geometrically independent. We intend to define $\Gamma^{n-1} = \{s_n, s_{n+1}, \ldots, s_N\}$, and then extend it to an entire Z-system; if $N = n$ then Γ^{n-1} is now defined; otherwise we have only defined the first element of Γ^{n-1}.

If s is any $n-1$ simplex such that R_s is geometrically independent, and if for any k simplex $t \subset s$ we denote by $\text{span}\,(R_t)$ the k dimensional affine subspace of $\mathbb{R}^n$ containing R_t (and $\text{span}\,(\emptyset) = \emptyset$), then we claim that $\text{span}\,(R_{t_1}) \cap \text{span}\,(R_{t_2}) = \text{span}\,(R_{t_1 \cap t_2})$. Clearly we have $\text{span}\,(R_{t_1 \cap t_2}) \subset \text{span}\,(R_{t_1}) \cap \text{span}\,(R_{t_2})$. Now suppose $\tilde{\mathbf{R}} \in \text{span}\,(R_{t_1}) \cap \text{span}\,(R_{t_2})$, i.e. $\begin{pmatrix} 1 \\ \tilde{\mathbf{R}} \end{pmatrix} = \sum_{i \in t_1} \alpha_i \begin{pmatrix} 1 \\ \mathbf{R}_i \end{pmatrix} = \sum_{i \in t_2} \beta_i \begin{pmatrix} 1 \\ \mathbf{R}_i \end{pmatrix}$. Then $\sum_{i \in t_1 \setminus t_2} \alpha_i \begin{pmatrix} 1 \\ \mathbf{R}_i \end{pmatrix} + \sum_{i \in t_1 \cap t_2} (\alpha_i - \beta_i) \begin{pmatrix} 1 \\ \mathbf{R}_i \end{pmatrix} - \sum_{i \in t_2 \setminus t_1} \beta_i \begin{pmatrix} 1 \\ \mathbf{R}_i \end{pmatrix} = \begin{pmatrix} 0 \\ \boldsymbol{\theta} \end{pmatrix}$. Since $t_1 \cup t_2 \subset s$, the set $\{\begin{pmatrix} 1 \\ \mathbf{R}_i \end{pmatrix} \mid i \in t_1 \cup t_2\}$ is linearly independent, and hence we have that $\alpha_i = 0$ for $i \in t_1 \setminus t_2$, $\beta_i = 0$ for $i \in t_2 \setminus t_1$, and $\alpha_i = \beta_i$ for $i \in t_1 \cap t_2$. This implies that $\tilde{\mathbf{R}} \in \text{span}\,(R_{t_1 \cap t_2})$, and hence the claim is established. An immediate consequence of the claim is that $\cap_{i \in s} \text{span}\,(R_{s \setminus \{i\}}) = \emptyset$.

Suppose $N \geq n+1$ and $n-1$ simplices $s_n, s_{n+1}, \ldots, s_{N-1}$ have been defined such that $R_{s_n}, R_{s_{n+1}}, \ldots, R_{s_{N-1}}$ are all geometrically independent, and $\{j\} = s_j \setminus s_{j-1}$ for all $j = n+1, \ldots, N-1$. Since $\cap_{i \in s_{N-1}} \text{span}\,(R_{s_{N-1} \setminus \{i\}}) = \emptyset$ there is an $i \in s_{N-1}$ such that $\mathbf{R}_N \notin \text{span}\,(R_{s_{N-1} \setminus \{i\}})$. Thus define $s_N = (s_{N-1} \setminus \{i\}) \cup \{N\}$. Clearly R_{s_N} is geometrically independent, and $\{N\} = s_N \setminus s_{N-1}$. Furthermore $s_j \cap (s_{l+1} \setminus s_l) = \emptyset$ for all $n \leq j \leq l \leq N-1$. Define n simplices $\tau_{n+1}, \ldots, \tau_N$ by the rule: $\tau_j = s_{j-1} \cup s_j$, $j = n+1, \ldots, N$. Define $\Gamma^{n-1} = \{s_n, \ldots, s_N\}$ and $\Gamma^n = \{\tau_{n+1}, \ldots, \tau_N\}$. $(\Gamma^{n-1}, \Gamma^n, \sigma)$ clearly defines a linear tree.

We need to show that these can be extended to a Z-system Γ. For this we will use the following construction. Let $\tau_1, \ldots, \tau_m$ be k simplices and $s_0, s_1, \ldots, s_m$ be distinct $k-1$ simplices, where $\tau_j = s_{j-1} \cup s_j$ for $j = 1, \ldots, m$, and $s_j \cap (s_{l+1} \setminus s_l) = \emptyset$ for all $0 \leq j \leq l \leq m-1$. We call this family $(s_0, \tau_1, s_1, \ldots, \tau_m, s_m)$ a *fence* of *order* k and of *length* m (see Figure 5). A fence of order k and of any length will be called a k-fence. If this k-fence of length $m \geq 1$ consists of simplices from a Z-system and if $k \geq 2$ then the Z-system would also contain the $k-2$-simplices $s_{j-1} \cap s_j$ for all $j = 1, \ldots, m$, but these need not all be distinct. So define $k_0 = 1$ and $k_{j+1} = \min\{k_j < l \leq m \mid s_{k_j - 1} \cap s_{k_j} \neq s_{l-1} \cap s_l\}$, for all $j \geq 0$ for which the minimum is over a nonempty set. Let k_J be the last one defined in this manner. Define $t_j = s_{k_j - 1} \cap s_{k_j}$ for $j = 0, 1, \ldots, J$. Then we claim that $(t_0, s_{k_1 - 1}, t_1, \ldots, s_{k_J - 1}, t_J)$ is a $k-1$-fence of length J, where $0 \leq J \leq m-1$. First we need to check that $t_0, t_1, \ldots, t_J$ are distinct $k-2$-simplices. Since s_{l-1} and s_l are distinct $k-1$-simplices contained in the k simplex τ_l, we see that $s_{l-1} \cap s_l$ is a $k-2$ simplex. Suppose $1 \leq j < l \leq m$ are such that $s_{j-1} \cap s_j = s_{l-1} \cap s_l$. Then we claim that $s_{j-1} \cap s_j = s_j \cap s_{j+1} = \cdots = s_{l-2} \cap s_{l-1} = s_{l-1} \cap s_l$. To see this, suppose $i \in s_{j-1} \cap s_j = s_{l-1} \cap s_l$. Since $s_{j-1} \cap (s_{l-1} \setminus s_{l-2}) = \emptyset$ and both $i \in s_{j-1}$ and $i \in s_{l-1}$ it follows that $i \in s_{l-2}$. In a similar way i is a member of all the intervening $s_{k'}$. Thus $s_{j-1} \cap s_j \subset s_{k'-1} \cap s_{k'}$ for all $j \leq k' \leq l$. Since both sets have $k-1$ elements, they must be equal as sets. Thus $t_0, t_1, \ldots, t_J$ are distinct $k-2$-simplices. Next we show that $t_j \cup t_{j+1} = s_{k_{j+1} - 1}$ for $j = 0, 1, \ldots, J-1$. To see this note that by definition $t_{j+1} = s_{k_{j+1} - 1} \cap s_{k_{j+1}}$ so clearly $t_{j+1} \subset s_{k_{j+1} - 1}$. Also

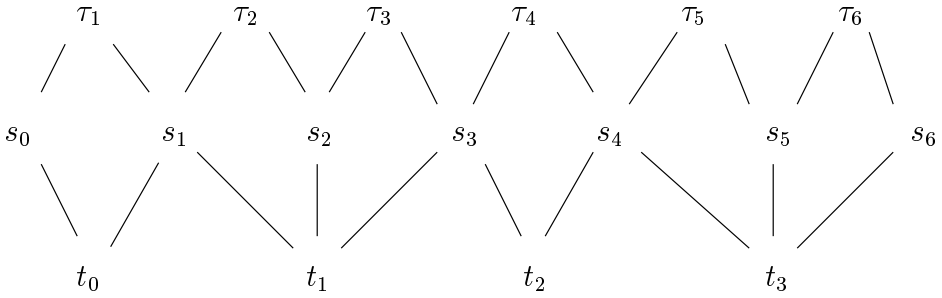

FIGURE 5. A k-fence of length $m = 6$ with its $k-1$-fence. In this example we have $k_0 = 1, k_1 = 2, k_2 = 4, k_3 = 5, J = 3$.

from the definition of k_{j+1} we have $t_j = s_{k_j-1} \cap s_{k_j} = s_{k_{j+1}-2} \cap s_{k_{j+1}-1}$, and hence $t_j \subset s_{k_{j+1}-1}$. Thus $t_j \cup t_{j+1} \subset s_{k_{j+1}-1}$. Since both t_j and t_{j+1} have $k-1$ elements and are distinct, the union must have at least k elements. Thus $t_j \cup t_{j+1} = s_{k_{j+1}-1}$ as claimed. Finally we check that $t_j \cap (t_{l+1} \setminus t_l) = \emptyset$ for all $0 \le j \le l \le J-1$. Suppose by way of contradiction that $i \in t_j \cap (t_{l+1} \setminus t_l)$. Since $k_{l+1} \ge k_l + 1 \ge k_j + 1$ we have $i \in s_{k_j-1}$ and $i \in s_{k_{l+1}-1}$ but $i \notin s_{k_l-1} \cap s_{k_l} = s_{k_{l+1}-2} \cap s_{k_{l+1}-1}$. Thus $i \notin s_{k_{l+1}-2}$, and hence $i \in s_{k_j-1} \cap (s_{k_{l+1}-1} \setminus s_{k_{l+1}-2})$, contradicting the assumption that $(s_0, \tau_1, s_1, \ldots, \tau_m, s_m)$ is a k fence. Thus if a Z-system contains a k-fence of length m then it also contains a $k-1$-fence of length $0 \le J \le m-1$ by the above construction.

If $s_0, s_1, \ldots, s_m$ are the k-simplices of a $k+1$-fence then we know that $s_j \cap (s_{l+1} \setminus s_l) = \emptyset$ for all $0 \le j \le l \le m-1$. However a reflected disjointness condition also holds: $(s_{j-1} \setminus s_j) \cap s_l = \emptyset$ for all $1 \le j \le l \le m$. The statement is trivial when $l = j$, and when $l = j+1$ we have $(s_{j-1} \setminus s_j) \cap s_{j+1} \subset s_{j-1} \cap (s_{j+1} \setminus s_j) = \emptyset$. The general case is proved by induction on l, for if $(s_{j-1} \setminus s_j) \cap s_l = \emptyset$ and $a \in (s_{j-1} \setminus s_j) \cap s_{l+1}$ then $a \in s_{j-1} \cap (s_{l+1} \setminus s_l) = \emptyset$, a contradiction.

We have already seen that $(s_n, \tau_{n+1}, s_{n+1}, \ldots, \tau_N, s_N)$ is an n-fence of length $N-n$. Using the above construction we can inductively define a sequence of fences of decreasing orders and lengths. Each of the k-simplices in these fences will be members of Γ^k for $k = 1, \ldots, n$. The last fence in this sequence is either of order 1 or of length 0 (or possibly both). For example when $N = n$ we have a single n-fence (s_n) with length 0. Let $(\Gamma_k^{k-1}, \Gamma_k^k)$ denote the fence of order k, where Γ_k^{k-1} is the set of $k-1$-simplices and Γ_k^k is the set of k-simplices. If the last fence $(\Gamma_k^{k-1}, \Gamma_k^k)$ is of order k and of length 0, then Γ_k^{k-1} has a single element $\mathcal{N}_k$ and $\Gamma_k^k = \emptyset$. It is always possible to choose sets $\Gamma_k^0, \Gamma_k^1, \ldots, \Gamma_k^{k-2}$ such that $(\Gamma_k^1, \ldots, \Gamma_k^{k-1}, \Gamma_k^k)$ is a k dimensional Z-system on a set $\mathcal{N}_k$ of k elements, where $\Gamma_k^0 = \binom{\mathcal{N}_k}{1}$ and $\Gamma_k^{k-1} = \{\mathcal{N}_k\}$. (This can be done by choosing spanning trees in line graphs as in section 2.) Of course if $k = 1$ there is nothing to do. If $k = 2$ then $\mathcal{N}_k = \{a, b\}$ is a 1 simplex, and $\Gamma_k^0 = \{\{a\}, \{b\}\}$. If $k \ge 3$ then there are some choices to make.

Our strategy beyond this point is to extend the sets $\Gamma_k^0, \Gamma_k^1, \ldots, \Gamma_k^k$ by adding leaves to each of the trees involved to obtain the sets $\Gamma_{k+1}^0, \Gamma_{k+1}^1, \ldots, \Gamma_{k+1}^k$. Then we adjoin the set Γ_{k+1}^{k+1} to this list, so that the top level tree is a linear chain. We assume that $\mathcal{N}_k = \cup_{s \in \Gamma_k^0} s \subset \{1, \ldots, N\}$ and $\Gamma_k^j \subset \binom{\mathcal{N}_k}{j+1}$, $j = 0, 1, \ldots, k$. We also assume that $(\Gamma_k^{j-1}, \Gamma_k^j, \sigma)$ is a tree for $j = 1, \ldots, k$ and whenever $s, s' \in \Gamma_k^j$ are such

that $s \cup s' \in \Gamma_k^{j+1}$ then $s \cap s' \in \Gamma_k^{j-1}$. This situation arises when the last fence has order k and length 0 as in the previous paragraph. It also makes sense when the last fence has order $k = 1$. But it also represents any of the intermediate stages of our construction of the Z-system Γ. This extension involves using information from the $k+1$-fence $(\Gamma_{k+1}^k, \Gamma_{k+1}^{k+1})$. There is a mapping $g\colon \Gamma_{k+1}^k \backslash \Gamma_k^k \to \Gamma_k^{k-1}$ defined as follows. Let $\Gamma_{k+1}^k = \{s_0, s_1, \ldots, s_m\}$; we use the notation introduced above to define the fence of one lower order. $s_0 \in \Gamma_{k+1}^k \setminus \Gamma_k^k$ and it gets mapped to $g(s_0) = t_0 = s_0 \cap s_1$. Also $s_m \in \Gamma_{k+1}^k \setminus \Gamma_k^k$, and it gets mapped to $g(s_m) = t_J = s_{m-1} \cap s_m$. Also if $0 \leq j \leq J-1$ is such that $k_{j+1} - 2 \geq k_j$ and $k_j \leq l \leq k_{j+1} - 2$ then $s_l \in \Gamma_{k+1}^k \setminus \Gamma_k^k$, and it gets mapped to $g(s_l) = t_j$. If $s \in \Gamma_{k+1}^k \setminus \Gamma_k^k$ then we always have $t = g(s) \subset s$. Let $s \setminus g(s) = \{i(s)\}$. We will be able to insure that we are always adding leaves provided we can show that $i(s)$ is not a member of $\mathcal{N}_k$, and furthermore the elements $i(s)$, $s \in \Gamma_{k+1}^k \setminus \Gamma_k^k$, are all distinct from one another.

This is a consequence of the disjointness of our fences. To see this suppose $s_0 \setminus g(s_0) = \{i\}$. Then i is not a member of $g(s_0) = s_0 \cap s_1$ or of s_j for $j = 1, \ldots, m$. Thus certainly it is not a member of $\mathcal{N}_k$. A similar argument works for s_m. If $s_m \setminus g(s_m) = \{i\}$ then i is not a member of $s_{m-1} \cap s_m$ nor of s_j for $j = 0, 1, \ldots, m-1$. Thus again $i \notin \mathcal{N}_k$. Finally suppose $0 \leq j \leq J-1$ is such that $k_{j+1} - 2 \geq k_j$ and $k_j \leq l \leq k_{j+1} - 2$, and $s_l \setminus g(s_l) = \{i\}$. Since $g(s_l) = t_j = s_{l-1} \cap s_l = s_l \cap s_{l+1}$ we have that $i \notin t_j$, and $i \notin s_j$ for all $j \neq l$. Thus $i \notin \mathcal{N}_k$. The above disjointness arguments are also strong enough to show that the elements $i(s)$, $s \in \Gamma_{k+1}^k \setminus \Gamma_k^k$, are all distinct from one another.

So for any $s \in \Gamma_{k+1}^k \setminus \Gamma_k^k$ and $t^{k-1} = g(s) \in \Gamma_k^{k-1}$ we can choose (in an arbitrary manner) a sequence $t^0 \subset t^1 \subset \cdots \subset t^{k-1}$ such that $t^j \in \Gamma_k^j$ for $j = 0, 1, \ldots, k-1$. (Let us agree that $t^{-1} = \emptyset$.) If $s \setminus t^{k-1} = \{i\}$ then $\{i\} \subset t^0 \cup \{i\} \subset \cdots \subset t^{k-2} \cup \{i\} \subset s$ is a sequence of simplices which are distinct from any in Γ_k^j, $j = 0, 1, \ldots, k$. Thus we define

$$\Gamma_{k+1}^j = \Gamma_k^j \cup \{t^{j-1} \cup \{i(s)\} \mid s \in \Gamma_{k+1}^k \setminus \Gamma_k^k\},$$
$$\mathcal{N}_{k+1} = \mathcal{N}_k \cup \{i(s) \mid s \in \Gamma_{k+1}^k \setminus \Gamma_k^k\}.$$

When the new tree $(\Gamma_{k+1}^{j-1}, \Gamma_{k+1}^j)$ is compared with the old tree $(\Gamma_k^{j-1}, \Gamma_k^j)$ we see that new vertices $t^{j-2} \cup \{i(s)\}$ have been added, and new edges $t^{j-1} \cup \{i(s)\}$ have also been added connecting the new vertices to the old vertices t^{j-1} (which depend implicitly on arbitrary choices made for each s). Thus the addition of these new simplices are in every case the addition of leaves, with the consequence that after these additions we have trees at each level. Hence $\Gamma_{k+1}^0, \ldots, \Gamma_{k+1}^{k+1}$ is an extended system of sets satisfying the same hypotheses that $\Gamma_k^0, \ldots, \Gamma_k^k$ satisfied.

Thus we ascend the hierarchy of fences, using each one as the basis of an extension as we have described. When completed we have the sets $\Gamma_n^0, \Gamma_n^1, \ldots, \Gamma_n^n$, which is a Z-system (orient the n simplices in an arbitrary manner) on the set $\mathcal{N}_n$. Since $\Gamma_n^{n-1} = \Gamma^{n-1}$ and $\Gamma_n^n = \Gamma^n$, we must have $\mathcal{N}_n = \{1, \ldots, N\}$. Clearly then we have defined a Z-system Γ such that $R \in \mathcal{D}_C(\Gamma)$. □

Thus Z-systems index coordinate charts in the manifold $G_a \backslash \mathcal{B}$, over which $\mathcal{B}$ is a principal bundle with structure group G_a. General arguments could have been given to show that $G_a \backslash \mathcal{B}$ is a smooth manifold, so the main interest here is the explication of the domain of applicability of the totality of Z-system style

polyspherical coordinates. For other mathematical results on the principal bundle $\rho\colon \mathcal{B} \to G_a\backslash\mathcal{B}$ see [25], [42].

5. Z-Matrices

Z-systems are mathematical objects which contain the minimal amount of information to specify a polyspherical coordinate system on its coordinate domain (provided we do not require an ordering of the coordinates). In order to store a Z-system in a computer, additional information must be specified which is extraneous to defining the coordinate system and which if retained will lead to objects with complicated rules of manipulation. Nevertheless, these objects can be easily stored and displayed, and so are important.

Definition. An (unlabelled) n-dimensional *Z-matrix* on the set $\mathcal{N}$ is a mapping

$$\alpha\colon \{(i,j) \in \mathbb{Z}^2 \mid 0 \le j \le n, j < i \le N\} \to \mathcal{N},$$

where $N = |\mathcal{N}| \ge n$, with the following properties:

(1) $\mathcal{N} = \{\alpha(i,0) \mid 1 \le i \le N\}$.
(2) For every $1 \le k \le n$ and for every $k < i \le N$ there exists $k \le i' < i$ such that $\{\alpha(i,j) \mid 1 \le j \le k\} = \{\alpha(i',j) \mid 0 \le j \le k-1\}$.

An example of an unlabelled 3-dimensional Z-matrix on the set $\mathcal{N} = \{C, O, H_1, H_2, H_3, H\}$ is as follows.

	$j=0$	$j=1$	$j=2$	$j=3$
$i=1$	C			
$i=2$	O	C		
$i=3$	H_1	C	O	
$i=4$	H_2	C	O	H_1
$i=5$	H_3	C	O	H_1
$i=6$	H	O	C	H_1

This Z-system is for the molecule methanol, so refer to Figures 1 and 2. Z-matrices were first used in the 3 dimensional case by the chemist J. Pople as a means of entering a molecular geometry into quantum chemistry computer programs [36], [56], [24], [14]. The precise mathematical definition of the n dimensional Z-matrix (even the 3 dimensional case) is apparently new to this work.

The question naturally arises about the exact relation between Z-matrices and Z-systems.

Theorem. *Every Z-matrix α on $\mathcal{N}$ determines a Z-system $\Gamma(\alpha)$ by the rule:*

$$\Gamma^k(\alpha) = \{\{\alpha(i,j) \mid 0 \le j \le k\} \mid k+1 \le i \le N\}, \qquad 1 \le k \le n,$$
$$\Gamma^n_*(\alpha) = \{[\alpha(i,0), \ldots, \alpha(i,n)] \mid n+1 \le i \le N\}.$$

α also determines a site $r_\alpha = (\alpha(1,0), \alpha(2,0), \ldots, \alpha(n,0))$ in Γ, and a leaf-picking order λ_α in the rooted tree $(\Gamma^{n-1}(\alpha), \Gamma^n(\alpha), \subset, s_{n-1}(r(\alpha)))$. Conversely, if (Γ, r, λ) is a triple where Γ is a Z-system, r is a site of Γ, and λ is a leaf-picking order in the rooted tree $(\Gamma^{n-1}, \Gamma^n, \subset, s_{n-1}(r))$, then a Z-matrix $\alpha(\Gamma, r, \lambda)$ is uniquely determined such that $\Gamma^k = \Gamma^k(\alpha(\Gamma, r, \lambda))$ for all $1 \le k \le n$, $r = r(\alpha(\Gamma, r, \lambda))$, and $\lambda = \lambda(\alpha(\Gamma, r, \lambda))$. Also $\alpha(\Gamma(\alpha), r(\alpha), \lambda(\alpha)) = \alpha$ for every Z-matrix α.

Proof. Assume that α is a Z-matrix. To demonstrate that $\Gamma(\alpha)$ is a Z-system we first verify the following: for all $1 \leq j \leq n$ and for all $j < i \leq N$ there exists $1 \leq i' < i$ such that $\alpha(i,j) = \alpha(i',0)$. This result is a consequence of condition (2) if $j = 1$, so suppose it is true for $1 \leq j \leq j' - 1 \leq n - 1$. Since by condition (2) $\{\alpha(i,1), \ldots, \alpha(i,j')\} = \{\alpha(i',0), \ldots, \alpha(i',j'-1)\}$ we can apply the induction hypothesis to obtain $1 \leq i'' < i'$ such that $\alpha(i,j') = \alpha(i'',0)$. Thus the result is true for $j = j'$ as well.

Next we must show that $\{\alpha(i,j) \mid 0 \leq j \leq k\}$ is always an abstract k simplex, i.e. it cannot have fewer than $k+1$ elements. Let $2 \leq i \leq N$ be the first row in which repetitions occur (assuming by way of contradiction that they occur somewhere). Let $j \geq 0$ be as small as possible such that $\alpha(i,j) = \alpha(i,k)$ for some $j < k \leq n$. If $j = 0$ then since $k \geq 1$ we must have $\alpha(i,k) \in \{\alpha(i',0) \mid 0 \leq i' < i\}$, a contradiction with condition (1). If $j \geq 1$ then by condition (2) $\{\alpha(i,1), \ldots, \alpha(i,k)\} = \{\alpha(i',0), \ldots, \alpha(i',k-1)\}$ for some $i' < i$, and a repetition must have occurred on an earlier row, a contradiction of the choice of i.

Now suppose $\{\alpha(i,j) \mid 0 \leq j \leq k\} \in \Gamma^k$ is a k simplex. It is incident on two $k-1$ simplices, namely $\{\alpha(i,j) \mid 0 \leq j \leq k-1\}$ and $\{\alpha(i,j) \mid 1 \leq j \leq k\}$. We need to show that it is incident on no other $k-1$ simplex. Suppose $s \in \Gamma^{k-1}$ is a $k-1$ simplex on which $\{\alpha(i,j) \mid 0 \leq j \leq k\}$ is incident. We have $s = \{\alpha(i',j) \mid 0 \leq j \leq k-1\}$ for some $k \leq i' \leq N$. $i' > i$ is impossible since then $\alpha(i',0) = \alpha(i'',0)$ for some $i'' \leq i < i'$ contradicting condition (1). If $i' = i$ then s is one of the two $k-1$ simplices we already know about. So suppose $i' < i$. s is obtained from $\{\alpha(i,j) \mid 0 \leq j \leq k\}$ by omitting a single element, which must be $\alpha(i,0)$ since otherwise $\alpha(i,0) \in s$ and hence $\alpha(i,0) = \alpha(i'',0)$ for some $i'' \leq i' < i$, contradicting condition (1). Thus $s = \{\alpha(i,j) \mid 1 \leq j \leq k\}$, which is the other of the $k-1$ simplices that we already knew about.

Since each k simplex is incident on exactly two $k-1$ simplices, $(\Gamma^{k-1}, \Gamma^k, \sigma)$ is a graph. It is easy to see that this graph is connected, since every $k-1$ simplex (vertex) appears on a row of the Z-matrix defining a k simplex (edge) connecting it to a $k-1$ simplex (vertex) appearing on a previous row. This can only end if the previous vertex is the first $k-1$ simplex specified, namely $\{\alpha(k-1,0), \ldots, \alpha(k-1,k-2)\}$. A connected graph with one fewer edges than vertices must be a tree. Finally it is clear that the intersection of the two $k-1$ simplices $\{\alpha(i,j) \mid 0 \leq j \leq k-1\}$ and $\{\alpha(i,j) \mid 1 \leq j \leq k\}$ is the $k-2$ simplex $\{\alpha(i,j) \mid 1 \leq j \leq k-1\} \in \Gamma^{k-2}$ by condition (2). Thus $\Gamma = (\Gamma^1, \ldots, \Gamma^n_*)$ is a Z-system.

We claim that $r = (\alpha(1,0), \alpha(2,0), \ldots, \alpha(n,0))$ is a site for the Z-system Γ. Clearly $\{\alpha(1,0), \alpha(2,0)\} = \{\alpha(2,0), \alpha(2,1)\} \in \Gamma^1$. Suppose $\{\alpha(i,0) \mid 1 \leq i \leq k\} = \{\alpha(k,j) \mid 0 \leq j \leq k-1\}$ for some $2 \leq k < n$. Then $\{\alpha(k+1,j) \mid 1 \leq j \leq k\}$ must equal $\{\alpha(k,j) \mid 0 \leq j \leq k-1\}$ by condition (2), and by the induction hypothesis this must equal $\{\alpha(i,0) \mid 0 \leq i \leq k\}$. Adding the element $\alpha(k+1,0)$ to both sets shows that $\{\alpha(i,0) \mid 1 \leq i \leq k+1\} = \{\alpha(k+1,j) \mid 0 \leq j \leq k\} \in \Gamma^k$. Thus r is a site of Γ.

Note that $\{\alpha(N,j) \mid 0 \leq j \leq n-1\} \in \Gamma^{n-1}$ is of degree one in the graph $(\Gamma^{n-1}, \Gamma^n, \sigma)$, since no n simplex other than $\{\alpha(N,j) \mid 0 \leq j \leq n\} \in \Gamma^n$ can contain the element $\alpha(N,0)$. Thus the Z-matrix determines a *leaf-picking order* for the rooted tree $(\Gamma^{n-1}, \Gamma^n, \sigma)$, in the sense that the vertices of this tree are ordered (assigned numbers n through N) starting at the root vertex $s_{n-1}(r) = \{\alpha(1,0), \ldots, \alpha(n,0)\} = \{\alpha(n,0), \ldots, \alpha(n,n-1)\}$ with number n, such that for

every $n < k \leq N$ the vertex $\{\alpha(k,0),\ldots,\alpha(k,n-1)\}$ is a leaf of the tree subgraph of $(\Gamma^{n-1},\Gamma^n,\sigma)$ induced by the set of vertices numbered n through k.

Now we will show the converse of this, namely that a rooted Z-system (Γ,r) with a choice λ of leaf-picking order for the top level rooted tree determines a Z-matrix $\alpha(\Gamma,r,\lambda)$. The key ideas for how the Z-matrix is determined have already been explained in the proof of the main theorem. We obviously should define $\alpha(1,0),\ldots,\alpha(n,0)$ so that the root site is given by $r = (\alpha(1,0),\alpha(2,0),\ldots,\alpha(n,0))$. Also we must define $\alpha(2,1) = \alpha(1,0)$, so that $\{\alpha(2,0),\alpha(2,1)\} = s_1(r) \in \Gamma^1$. If $S \subset \Gamma^0$ then define $\Gamma^k_S = \{s \in \Gamma^k \mid s \subset S\}$. Notice that $\Gamma^0_{s_1(r)} = \{\{\alpha(1,0)\},\{\alpha(2,0)\}\}$ and $\Gamma^1_{s_1(r)} = \{\{\alpha(2,0),\alpha(2,1)\}\}$. Now suppose the first k rows of the Z-matrix have been defined for $2 \leq k \leq n-1$ such that for all $0 \leq h \leq k-1$ we have $\Gamma^h_{s_{k-1}(r)} = \{\{\alpha(i,j) \mid 0 \leq j \leq h\} \mid h+1 \leq i \leq k\}$. Define $s^1_k = s_k(r) = \{\alpha(1,0),\ldots,\alpha(k+1,0)\} \in \Gamma^k$. s^1_k is incident on two $k-1$ simplices, one of which is $s^0_{k-1} = s_{k-1}(r) = \{\alpha(1,0),\ldots,\alpha(k,0)\} \in \Gamma^{k-1}$, and the other we denote by s^1_{k-1}. Note that $\alpha(k+1,0) \in s^1_{k-1}$. As in the proof of the main theorem we define $s^0_{k-2} = s^0_{k-1} \cap s^1_{k-1}$, and let s^1_{k-2} be the $k-2$ simplex on which s^1_{k-1} is incident besides s^0_{k-2}. Note again that $\alpha(k+1,0) \in s^1_{k-2}$. Continuing this procedure as in the proof of the main theorem we end up with two 0 simplices: $s^1_0 = \{\alpha(k+1,0)\}$ and s^0_0. We define $\alpha(k+1,1),\ldots,\alpha(k+1,k)$ such that $s^0_h = \{\alpha(k+1,1),\ldots,\alpha(k+1,h+1)\}$ for $h = 0,1,\ldots,k-1$.

$$
\begin{array}{rccccccc}
 & s^0_0 = & \{\alpha(k+1,1)\} & & & & & \\
 & s^0_1 = & \{\alpha(k+1,1), & \alpha(k+1,2)\} & & & & \\
 & \vdots & \vdots & \vdots & \ddots & & & \\
 & s^0_{k-1} = & \{\alpha(k+1,1), & \alpha(k+1,2), & \ldots & \alpha(k+1,k)\} & & \\
s^1_k = & \{\alpha(k+1,0), & \alpha(k+1,1), & \alpha(k+1,2), & \ldots & \alpha(k+1,k)\} & & \\
\vdots & \vdots & \vdots & \vdots & & & & \\
s^1_2 = & \{\alpha(k+1,0), & \alpha(k+1,1), & \alpha(k+1,2)\} & & & & \\
s^1_1 = & \{\alpha(k+1,0), & \alpha(k+1,1)\} & & & & & \\
s^1_0 = & \{\alpha(k+1,0)\} & & & & & &
\end{array}
$$

Since $s^0_0 \subset s^0_1 \subset \cdots \subset s^0_{k-1} = s_{k-1}(r)$ we have that $s^0_h \in \Gamma^h_{s_{k-1}(r)}$ for $h = 0,1,\ldots,k-1$, and by the induction hypothesis this means that $s^0_h = \{\alpha(i,j) \mid 0 \leq j \leq h\}$ for some $h+1 \leq i < k+1$, verifying condition (2) for row $k+1$ of the Z-matrix. Note also that $s^1_h = \{\alpha(k+1,0),\alpha(k+1,1),\ldots,\alpha(k+1,h)\}$ for $h = 0,1,\ldots,k$. Thus $\Gamma^h_{s_{k-1}(r)} \cup \{s^1_h\} \subset \Gamma^h_{s_k(r)}$. Thus these two sets will be equal if we can show that $|\Gamma^h_{s_k(r)}| = k-h+1$, since $|\Gamma^h_{s_{k-1}(r)}| = k-h$. As we argued in the proof of the lemma in section 2 $(\Gamma^{l-1}_{s_k(r)},\Gamma^l_{s_k(r)},\sigma)$ is an acyclic subgraph of the tree $(\Gamma^{l-1},\Gamma^l,\sigma)$, and hence $|\Gamma^{l-1}_{s_k(r)}| \geq |\Gamma^l_{s_k(r)}| + 1$. Since $\Gamma^k_{s_k(r)} = \{s^1_k\}$, and hence $|\Gamma^k_{s_k(r)}| = 1$, we have $|\Gamma^l_{s_k(r)}| \geq k-l+1$ for all $l = 0,1,\ldots,k$. But then $k+1 \leq |\Gamma^0_{s_k(r)}| \leq |s_k(r)| = k+1$. Thus $k-l+1 \leq |\Gamma^l_{s_k(r)}| \leq k-l+1$ for $l = 0,1,\ldots,k$, showing the desired result. This shows that $\Gamma^h_{s_k(r)} = \{\{\alpha(i,j) \mid 0 \leq j \leq h\} \mid h+1 \leq i \leq k+1\}$ for $h = 0,1,\ldots,k$. This finishes the induction step, so that the first n rows of the Z-matrix are defined so that condition (2) is satisfied for these rows and moreover we have $\Gamma^h_{s_{n-1}(r)} = \{\{\alpha(i,j) \mid 0 \leq j \leq h\} \mid h+1 \leq i \leq n\}$ for $h = 0,1,\ldots,n-1$.

To define rows $n+1$ through N of the Z-matrix we need to use the leaf-picking order that has been chosen for the tree $(\Gamma^{n-1}, \Gamma^n, \sigma)$ with root $s_{n-1}(r)$. Thus the elements of Γ^{n-1} are assumed numbered n through N, the root vertex being numbered n, so that for all $n \leq k \leq N$ the vertex numbered k is a leaf in the subgraph of $(\Gamma^{n-1}, \Gamma^n, \sigma)$ induced by the set of vertices numbered n through k. Suppose rows 1 through k of the Z-matrix have been defined, where $n \leq k \leq N-1$, such that $\Gamma^h_{S(k)} = \{\{\alpha(i,j) \mid 0 \leq j \leq h\} \mid h+1 \leq i \leq k\}$ for $h = 0, 1, \ldots, n$, where $S(k) = \{\alpha(1,0), \ldots, \alpha(k,0)\}$. Assume that condition (2) is satisfied for each of these k rows. Also assume that for all $n \leq i \leq k$ that $\{\alpha(i,0), \ldots, \alpha(i,n-1)\}$ is element number i in Γ^{n-1}. Let s^1_{n-1} be element number $k+1$ in Γ^{n-1}, and since it is a leaf in the subgraph of $(\Gamma^{n-1}, \Gamma^n, \sigma)$ induced by the set of vertices numbered n through $k+1$, let the unique edge of this subgraph incident on s^1_{n-1} be denoted by $s^1_n \in \Gamma^n$. Let $s^0_{n-1} \in \Gamma^{n-1}$ denote the other vertex on which this edge is incident. It must be one of the vertices numbered n through k, and hence in $\Gamma^{n-1}_{S(k)}$. By the properties of Z-systems we have that $s^0_{n-2} = s^0_{n-1} \cap s^1_{n-1} \in \Gamma^{n-2}$. Also let $s^1_{n-2} \in \Gamma^{n-2}$ denote the other vertex besides s^0_{n-2} on which the edge s^1_{n-1} is incident. Continuing as in the proof of the main theorem we define s^1_h and s^0_h for $h = 0, 1, \ldots, n-1$. We define $\alpha(k+1, 0)$ such that $s^1_0 = \{\alpha(k+1, 0)\}$, and we define $\alpha(k+1, 1), \ldots, \alpha(k+1, n)$ such that $s^0_h = \{\alpha(k+1, j) \mid 1 \leq j \leq h+1\}$ for $h = 0, 1, \ldots, n-1$. We also have that $s^1_h = \{\alpha(k+1, j) \mid 0 \leq j \leq h\}$ for $h = 0, 1, \ldots, n$. We know that $|\Gamma^n_{S(k)}| = k - n$ by the induction hypothesis. $s^1_n \in \Gamma^n_{S(k+1)}$ is incident on element number $k+1$ of Γ^{n-1}, and hence is distinct from the edges in $\Gamma^n_{S(k)}$ which are incident on elements numbered n through k of Γ^{n-1}; so $|\Gamma^n_{S(k+1)}| \geq k - n + 1$. Using the fact that $(\Gamma^{h-1}_S, \Gamma^h_S, \sigma)$ is a subgraph of a tree, with the consequence that $|\Gamma^{h-1}_S| \geq |\Gamma^h_S| + 1$, we obtain after n applications that $|\Gamma^0_{S(k+1)}| \geq k+1$. Thus $|S(k+1)| = k+1$ and hence $\alpha(k+1, 0) \notin S(k)$. Furthermore we have that $|\Gamma^h_{S(k+1)}| = k - h + 1$, for $h = 0, 1, \ldots, n$. Thus $\Gamma^h_{S(k+1)} = \Gamma^h_{S(k)} \cup \{s^1_h\}$ for $h = 0, 1, \ldots, n$. Since $s^0_h \in \Gamma^h_{S(k)}$ for $0 \leq h \leq n-1$ we have that condition (2) is satisfied by row $k+1$ of the Z-matrix. This finishes the inductive definition of the Z-matrix. The first column of the Z-matrix has N distinct elements from the set $\mathcal{N}$, which has exactly N elements; so condition (1) is also satisfied.

The construction of the Z-matrix $\alpha(\Gamma, r, \lambda)$ obviously satisfies $\Gamma^k = \Gamma^k(\alpha(\Gamma, r, \lambda))$, $1 \leq k \leq n$, $r = r(\alpha(\Gamma, r, \lambda))$, and $\lambda = \lambda(\alpha(\Gamma, r, \lambda))$. Also if α is a Z-matrix and $\tilde{\alpha} = \alpha(\Gamma(\alpha), r(\alpha), \lambda(\alpha))$, then the Z-matrices α and $\tilde{\alpha}$ must coincide by a simple induction argument, similar to those already given; the reader is invited to generate this argument as an exercise. □

The orientations of the n simplices in $\Gamma^n_*(\alpha(\Gamma, r, \lambda))$ need not coincide with the orientations in Γ^n_*. Different choices of root site r and leaf-picking order λ for the Z-system will lead to different Z-matrices and hence to possibly different orientations of the n simplices. For example, suppose Γ is the Z-system for methanol given in Figure 1. Choose the root site $r = (C, O, H_1)$, and the leaf-picking order $\lambda = (\{O, C, H_1\}, \{O, C, H_2\}, \{O, C, H_3\}, \{O, C, H\})$. Then $\alpha(\Gamma, r, \lambda)$ is the same as the Z-matrix α given above for methanol. We have

$$\Gamma^3_*(\alpha) = \{[H_2, C, O, H_1], [H_2, C, O, H_1], [H, O, C, H_1]\},$$
$$\Gamma^3_* = \{[C, O, H_1, H_2], [C, O, H_1, H_3], [H, O, C, H_1]\}.$$

Since $[H_j, C, O, H_1] = [C, O, H_j, H_1] = -[C, O, H_1, H_j]$, $j = 2, 3$, we see that $\Gamma^3_*(\alpha) \neq \Gamma^3_*$.

Thus Z-systems can be understood as generalizations of Z-matrices in the sense that one merely forgets the root site and the leaf-picking order. Thus Z-matrices can be viewed as extremely compact presentations of Z-systems. The difficulty in manipulating Z-matrices can be understood as arising from both the high degree of compression of the information in the Z-system and from the presence of the extra information, namely the specific choice of the root site and the leaf-picking order. In the 3 dimensional case the iterated line graph picture (see Figure 2) provides a natural graphical way of presenting a Z-system which also makes manipulations surprisingly easy (see section 6 for examples).

The concept of a labelled Z-system has its counterpart in the concept of a labelled Z-matrix. If $\alpha\colon \{(i,j) \in \mathbb{Z}^2 \mid 0 \leq j \leq n, j < i \leq N\} \to \mathcal{N}$ is a Z-matrix, then a mapping $\beta\colon \{(i,j) \in \mathbb{Z}^2 \mid 1 \leq j \leq n, j < i \leq N\} \to \mathbb{R}$ is a labelling of the Z-matrix α if

(1) $\beta(i,1) > 0$ for $2 \leq i \leq N$;
(2) $0 < \beta(i,j) < \pi$ for $2 \leq j \leq n-1$, $j+1 \leq i \leq N$;
(3) $-\pi < \beta(i,n) \leq \pi$ for $n+1 \leq i \leq N$.

Suppose $\gamma \in \mathcal{D}_P$ is a labelling for the Z-system Γ, and suppose α is a Z-matrix associated to Γ for some choice of root site and leaf-picking order. Assume that the oriented n simplices in Γ^n_* are the same as those determined by the Z-matrix α. Then we define the labelling β of the Z-matrix associated to γ as follows.

(1) If $2 \leq i \leq N$ then define $\beta(i,1) = L_e$, where $e = \{\alpha(i,0), \alpha(i,1)\}$.
(2) If $2 \leq j \leq n-1$ and $j+1 \leq i \leq N$ then define $\beta(i,j) = \cos^{-1} C_e$, where $e = \{\alpha(i,h) \mid 0 \leq h \leq j\}$.
(3) If $n+1 \leq k \leq N$ then define $\beta(k,n) \in (-\pi, \pi]$ such that $e^{i(-1)^{n-1}\beta(k,n)} = Z_{e^*}$, where $e^* = [\alpha(k,0), \ldots, \alpha(k,n)]$.

The only unexpected aspect of this definition is the factor $(-1)^{n-1}$ appearing in the equation for $\beta(k,n)$. It reflects a discrepancy in even dimensional spaces between the interpretation of an oriented n simplex that is natural for Z-systems versus that which is conventional and natural for Z-matrices (see Figure 6). In Z-systems it is natural to interpret $[i_0, \ldots, i_n]$ in terms of a positive rotation of the half-hyperplane containing the codimension 2 subset Y (spanned by $\mathbf{R}_{i_0}, \ldots, \mathbf{R}_{i_{n-2}}$) and containing $\mathbf{R}_{i_{n-1}}$ into the half-hyperplane containing Y and $\mathbf{R}_{i_n}$. According to the usual conventions for Z-matrices this would be represented by the oriented n simplex $[i_{n-1}, i_0, \ldots, i_{n-2}, i_n]$. These two oriented n simplices are related by $n-1$ transpositions. Fortunately in 3 dimensions, where the Z-matrix convention is standard among chemists, the two conventions agree.

Labelled Z-matrices are very close to usual coordinate systems where the coordinates are all assumed to be real numbers and where a specific ordering of the coordinates is specified. However, even a labelled Z-matrix does not tell us whether the coordinates should be ordered by rows or by columns. In our discussion of Z-systems we have not assigned any importance to the ordering of coordinates; also we refused to make a choice of branch of the phase angle for an element of S^1, treating the complex number itself as the "coordinate". There is not a universally agreed upon file format for storing a labelled Z-matrix. The GAUSSIAN format [36], [24] lists the coordinate $\beta(i,j)$ right after the specification $\alpha(i,j)$, whereas the MOPAC format [14] lists all the coordinates between columns 0 and 1 of the

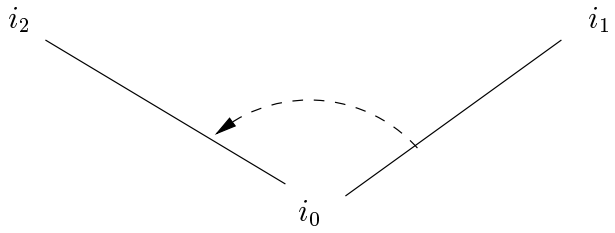

FIGURE 6. An oriented angle in the case $n = 2$. The Z-system convention would assign a positive angle to $[i_0, i_1, i_2]$. The Z-matrix convention would assign a positive angle to $[i_1, i_0, i_2]$.

Z-matrix. These details are of no mathematical interest, and consequently make no appearance in our mathematical description.

6. Biomolecular Conformation

The theory of n dimensional Z-systems has been described to provide perspective for the 3 dimensional theory, which can be applied to the study of the geometry of biological macromolecules. The 3 dimensional case is simpler in many ways than the n dimensional case, and so various alternatives to Z-system theory might be proposed for the 3 dimensional applications which would be inadequate in general. Hence it is with confidence that we claim that Z-systems are the "correct" tool for a mathematical study of biomolecular conformations. In this section we set $n = 3$ and discuss these motivating applications.

We begin by introducing some terminology natural in the context of molecules. We refer to the Z-system for methanol introduced in Figures 1 and 2, for which a related Z-matrix was given in the previous section. References to columns and rows are in relation to that Z-matrix. The one element sets in Γ^0 contain the names in the 1st column. It is natural to call elements of Γ^0 *atoms*. The two element subsets in Γ^1 of the associated Z-system contain the names listed in the 1st two columns excluding the 1st row, i.e. $\Gamma^1 = \{\{O, C\}, \{H_1, C\}, \ldots, \{H, O\}\}$. In this example each of the 1 simplices in Γ^1 consist of a pair of atom names which are covalently bonded in the molecule methanol. For this reason elements of Γ^1 are often called *bonds*. This terminology is slightly misleading because not every covalently bonded pair of atoms will always be a member of Γ^1, such as happens in molecules containing rings. Also we will see (in our discussion of five-membered rings) that it is sometimes convenient to include as an element in Γ^1 a pair of atom names corresponding to atoms which are not covalently bonded in the molecule. Such pairs can only be called "bonds" in some abstract sense. We will however use this terminology. The three element subsets in Γ^2 contain the first three entries of each row, excluding the first two rows. Hence $\Gamma^2 = \{\{H_1, C, O\}, \{H_2, C, O\}, \{H_3, C, O\}, \{H, O, C\}\}$. We will call the elements of Γ^2 *triangles*. Likewise the four element subsets (3 simplices) in Γ^3 contain all the entries of each row, excluding the first three rows. We will call the elements of Γ^3 *tetrahedra*. The order that the atom names are listed in each row (after the first three rows) determines the orientation of the 3 simplex; in this way the elements of Γ^3_* are determined.

The polyspherical coordinate system associated to the above example of a Z-system assigns coordinates to each element of each of the sets Γ^1, Γ^2, and Γ^3_*. The

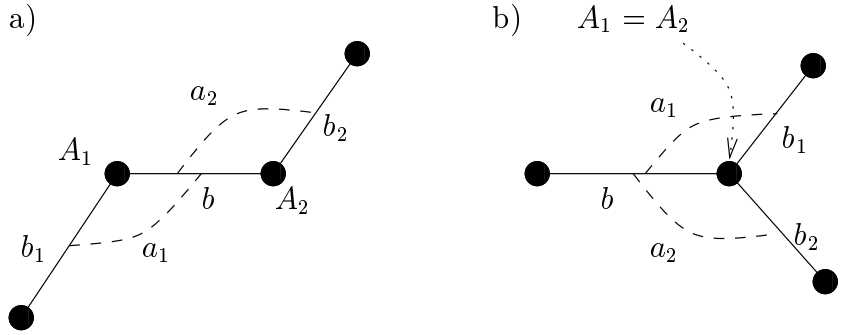

FIGURE 7. (a) $w = \{a_1, a_2\}$ is a dihedral. (b) $w = \{a_1, a_2\}$ is an improper. In both cases b is the common bond shared by a_1, a_2.

positive real number $L_b(R)$ assigned to each bond $b \in \Gamma^1$ is called the *bond length* of b in the configuration $R \in \mathcal{D}_C(\Gamma)$. Recall the lemma from section 2 defines a bijection β_2: edge $L(\Gamma^0, \Gamma^1, \sigma) \to \Gamma^2$. Thus every triangle $t \in \Gamma^2$ is associated via β_2 with a pair $\{b_1, b_2\}$ of bonds, where $b_1 \cap b_2 = A \in \Gamma^0$ is an atom. We call $a = \{b_1, b_2\}$ an *angle* and A is its *common atom*. b_1 and b_2 are the two 1-simplices on which the 2-simplex t is incident. The real number $C_t(R) \in (-1, 1)$ assigned to each triangle $t \in \Gamma^2$ is called the *bond angle cosine*, $\cos(\theta)$, being a measure of the angle θ between bonds b_1 and b_2 with vertex at atom A, in the configuration R. Similarly the bijection β_3: edge $L(\Gamma^1, \Gamma^2, \sigma) \to \Gamma^3$ allows us to associate with every tetrahedron $\tau \in \Gamma^3$ a pair $\{t_1, t_2\}$ of triangles where $t_1 \cap t_2 = b \in \Gamma^1$. We call $w = \{t_1, t_2\}$ a *wedge* and b is its *common bond*. t_1 and t_2 are the two 2-simplices on which the 3-simplex τ is incident. The unit modulus complex number $Z_{\tau^*}(R) = C_\tau(R) + iS_{\tau^*}(R) = e^{i\varphi}$ assigned to each oriented tetrahedron $\tau^* \in \Gamma^3_*$ is called a *wedge angle coordinate*, being a measure of the angle φ between the half-planes containing the triangles t_1 and t_2 measured in the plane perpendicular to the line containing the common bond b, in the configuration R. The sign of this angle depends on the chosen orientation of the tetrahedron τ. If $b = \{\tilde{A}, \tilde{A}'\}$ and $t_i \setminus b = \{\tilde{A}'_i\}$, $i = 1, 2$, and $\tau^* = [\tilde{A}, \tilde{A}', \tilde{A}'_1, \tilde{A}'_2]$, then the positive sense of φ is according to the right-hand-rule, where the axis of rotation is oriented from $\tilde{A}$ toward $\tilde{A}'$, and the half-plane of triangle t_1 is rotated into the half-plane of triangle t_2. If the oriented tetrahedron τ^* is kept fixed and we compare two configurations R and R' in which $Z_{\tau^*}(R') = \overline{Z_{\tau^*}(R)}$ (so that the corresponding angles φ are negatives of one another) we find that the geometric orientations of the resulting 3 simplices (not abstract) in the two configurations are reversed, i.e. they have opposite *chirality*.

According to the proof of the lemma from section 2 the only bonds which are subsets of a triangle are those in the associated angle. Hence the common bond b of a wedge must be part of both of the angles associated to t_1 and t_2. So triangle t_i is associated to angle $a_i = \{b, b_i\}$, $i = 1, 2$. Let A_i be the common atom of angle a_i, $i = 1, 2$; we always have $A_1, A_2 \subset b$. Tetrahedra (and also wedges) are classified into two disjoint categories. We say τ (or w) is a *dihedral* if $A_1 \neq A_2$ so that $b = A_1 \cup A_2$. We say τ (or w) is an *improper* if $A_1 = A_2$. This categorization of a tetrahedron as either a dihedral or an improper depends on the details of the Z-system; different Z-systems might cause the same tetrahedron to be categorized in opposite ways. In

the example of the Z-system for methanol, we have the dihedral $[H, O, C, H_1]$ and the impropers $[H_2, C, O, H_1]$ and $[H_3, C, O, H_1]$.

One important consequence of the dichotomy between dihedral and improper is their behavior in relation to orientations. There is a canonical way to assign an orientation to a tetrahedron (3-simplex) which is a dihedral. Let τ be a dihedral, where we adopt to notation above, and add the definitions $b_i = A_i \cup A'_i$, $i = 1, 2$. Then the canonical orientation of the tetrahedron τ is $[\tilde{A}'_1, \tilde{A}_1, \tilde{A}_2, \tilde{A}'_2]$, where $A_i = \{\tilde{A}_i\}$ and $A'_i = \{\tilde{A}'_i\}$, $i = 1, 2$. We say it is canonical because it does not depend on the ordering of the triangles t_1, t_2 forming the associated wedge, i.e. $[\tilde{A}'_1, \tilde{A}_1, \tilde{A}_2, \tilde{A}'_2] = [\tilde{A}'_2, \tilde{A}_2, \tilde{A}_1, \tilde{A}'_1]$ as one can easily check. We will call this the *canonical dihedral orientation*. Although it is not necessary to do so, it is the usual practice (although mostly unconscious) to always use the canonical dihedral orientation for any tetrahedron which is a dihedral when building a Z-system. When a dihedral tetrahedron is equipped with its canonical orientation it is called a *torsion*. As one can easily check, we have done this for the dihedral in our Z-system for methanol. The situation for impropers is quite different. An orientation needs to be chosen but neither of the two possibilities stands out as a better choice. Unlike dihedrals, the common bond b is oriented, from $A_1 = A_2$ toward the other atom $A_3 = \{\tilde{A}_3\}$. But since the two triangles are not ordered, no particular orientation is determined. If we add information to the tetrahedron τ which orders the two triangles as t_1, t_2, then an orientation consistent with this choice is $[\tilde{A}_1, \tilde{A}_3, \tilde{A}'_1, \tilde{A}'_2]$. But if we reverse the order of the two triangles then we get $[\tilde{A}_1, \tilde{A}_3, \tilde{A}'_2, \tilde{A}'_1]$, which is clearly the opposite orientation to that obtained from the other ordering. Even though there is no canonical orientation of an improper, a choice of an orientation of an improper is equivalent to a choice of an ordering of the two triangles forming the improper wedge.

One practical difference between dihedrals and impropers arises from the nature of chemical forces. Since the Z-system Γ determines a coordinate system valid throughout the dense open set $\mathcal{D}_C(\Gamma)$, the potential energy of the molecule is a well-defined function on $\mathcal{D}_P(\Gamma)$. (We are assuming there are no external forces so that the potential energy is invariant under all rigid motions of the molecular configuration.) For biological molecules under most biologically relevant conditions such potential energies are not greatly elevated above their minimum possible values. Thus if the Z-system is chosen correctly we can expect that the bond lengths will be effectively constrained to be within one or two tenths of an angstrom of a minumum energy value. Likewise the bond angles are constrained to be within 0.5 to 1 degrees of a minimum energy value. Improper wedge angles are also constrained to be within 1 or so degrees of a minimum energy value. But dihedral wedge angles are not so strongly constrained under normal biologically important conditions [49]. Thus an interesting mathematical model of a biomolecule is obtained by exactly freezing the values of all the bond lengths, bond angles, and improper wedge angles, but allowing complete freedom for the dihedral wedge angles. However the clarity of this situation can be marred by a poor choice of Z-system, namely if there is an *overuse of dihedrals*. For example, consider the methyl group in methanol, namely the group of atoms C, H_1, H_2, H_3, which is attached to the rest of the molecule via the bond $\{C, O\}$. Under normal biologically relevant conditions the methyl group is well approximated as a rigid body whose primary degree of freedom is its ability to rotate about the axis of the bond $\{C, O\}$. This one degree of freedom should

correspond to a single free dihedral. Thus in our Z-system for methanol we use the single dihedral $\tau_1 = \{H, O, C, H_1\}$ to describe the orientation of the methyl group relative to the rest of the molecule, and we use the two impropers $\{H_2, C, O, H_1\}$ and $\{H_3, C, O, H_1\}$ to fix the shape of the methyl group as a rigid body. However it is mathematically possible (but chemically inadvisable) to replace these two impropers with the two dihedrals $\tau_2 = \{H_2, C, O, H\}$ and $\tau_3 = \{H_3, C, O, H\}$. The rigid body constraint would in this new coordinate system translate into constraints on the differences between pairs of dihedral angles: $\varphi_{\tau_2} - \varphi_{\tau_1} = 120^\circ$ and $\varphi_{\tau_3} - \varphi_{\tau_1} = -120^\circ$. Thus as the methyl group rotates three dihedral angles change, but would do so in concert. Clearly it is preferable to have only one angle change during this rotation. Thus, if when constructing a Z-system care is taken not to overuse dihedrals, then a biomolecule (excluding the covalently bonded rings of atoms) can be approximated as a system of linked rigid bodies whose primary independent degrees of flexibility are its torsion angles [28], [20], [58].

Chemical reactions give rise to interesting constructions on Z-systems. Suppose molecules described by Z-systems Γ and Λ approach one another in space and undergo a chemical reaction from which molecules described by Z-systems Σ and Ω emerge. When the reaction is viewed in this way, Γ and Λ describe the *reactants* and Σ and Ω describe the *products*. In order to describe the approach of the reactants toward one another in space and the early stages of the chemical reaction it is necessary to form a Z-system $\Gamma \oplus_\mu \Lambda$ for the *reactant supermolecule*. There are many ways this approach could be described, and a particular choice of how this will be done is represented by the information μ. Similarly there will be a *product supermolecule* described by a Z-system $\Sigma \oplus_\nu \Omega$. Both of the Z-systems $\Gamma \oplus_\mu \Lambda$ and $\Sigma \oplus_\nu \Omega$ should be able to describe the *transition state* configurations, i.e. all such configurations should be members of $\mathcal{D}_C(\Gamma \oplus_\mu \Lambda) \cap \mathcal{D}_C(\Sigma \oplus_\nu \Omega)$.

The operation of forming from Γ and Λ the new Z-system $\Gamma \oplus_\mu \Lambda$ using the information μ will be called *tethering*. (See Figure 8.) We assume that Γ is a Z-system on the set $\mathcal{N}$ of N elements, and Λ is a Z-system on the set $\mathcal{M}$ of M elements, where $\mathcal{N} \cap \mathcal{M} = \emptyset$. Then $\Gamma \oplus_\mu \Lambda$ will be a Z-system on the set $\mathcal{N} \cup \mathcal{M}$ of $N + M$ elements. Thus tethering conserves atoms. One simple way to specify the tethering information μ is to give two sites, one from Γ and the other from Λ. Thus we must specify a triple (i_0, i_1, i_2) of elements of $\mathcal{N}$ such that $\{i_0\} \in \Gamma^0$ (necessarily true), $\{i_0, i_1\} \in \Gamma^1$, and $\{i_0, i_1, i_2\} \in \Gamma^2$; this defines a site from Γ. Likewise we must specify a triple (j_0, j_1, j_2) of elements of $\mathcal{M}$ such that $\{j_0\} \in \Lambda^0$ (necessarily true), $\{j_0, j_1\} \in \Lambda^1$, and $\{j_0, j_1, j_2\} \in \Lambda^2$. Clearly we will have $(\Gamma \oplus_\mu \Lambda)^0 = \Gamma^0 \cup \Lambda^0$. We define $(\Gamma \oplus_\mu \Lambda)^1 = \Gamma^1 \cup \Lambda^1 \cup \{\{i_0, j_0\}\}$. The new bond $\{i_0, j_0\}$ is called the *tether*. Since $|\Gamma^1| = N - 1$ and $|\Lambda^1| = M - 1$ we have that $|(\Gamma \oplus_\mu \Lambda)^1| = (N - 1) + (M - 1) + 1 = N + M - 1$. Since the graph $((\Gamma \oplus_\mu \Lambda)^0, (\Gamma \oplus_\mu \Lambda)^1, \sigma)$ is obviously connected, it must be a tree. Also define $(\Gamma \oplus_\mu \Lambda)^2 = \Gamma^2 \cup \Lambda^2 \cup \{\{i_0, i_1, j_0\}, \{j_0, j_1, i_0\}\}$ and $(\Gamma \oplus_\mu \Lambda)^3 = \Gamma^3 \cup \Lambda^3 \cup \{\{i_0, i_1, i_2, j_0\}, \{i_0, i_1, j_0, j_1\}, \{j_0, j_1, j_2, i_0\}\}$. By similar counting arguments we see that both $((\Gamma \oplus_\mu \Lambda)^1, (\Gamma \oplus_\mu \Lambda)^2, \sigma)$ and $((\Gamma \oplus_\mu \Lambda)^2, (\Gamma \oplus_\mu \Lambda)^3, \sigma)$ are trees. The intersection condition is immediately verified. In regard to orientations we note that the central tetrahedron must be a dihedral, so we choose its orientation to be canonical, i.e. $[i_1, i_0, j_0, j_1]$. The other two tetrahedra could be either dihedrals or impropers, but we assign their orientations as follows: $[j_0, i_0, i_1, i_2]$ and $[i_0, j_0, j_1, j_2]$. In the dihedral case, this is the canonical orientation. But in the improper case we have

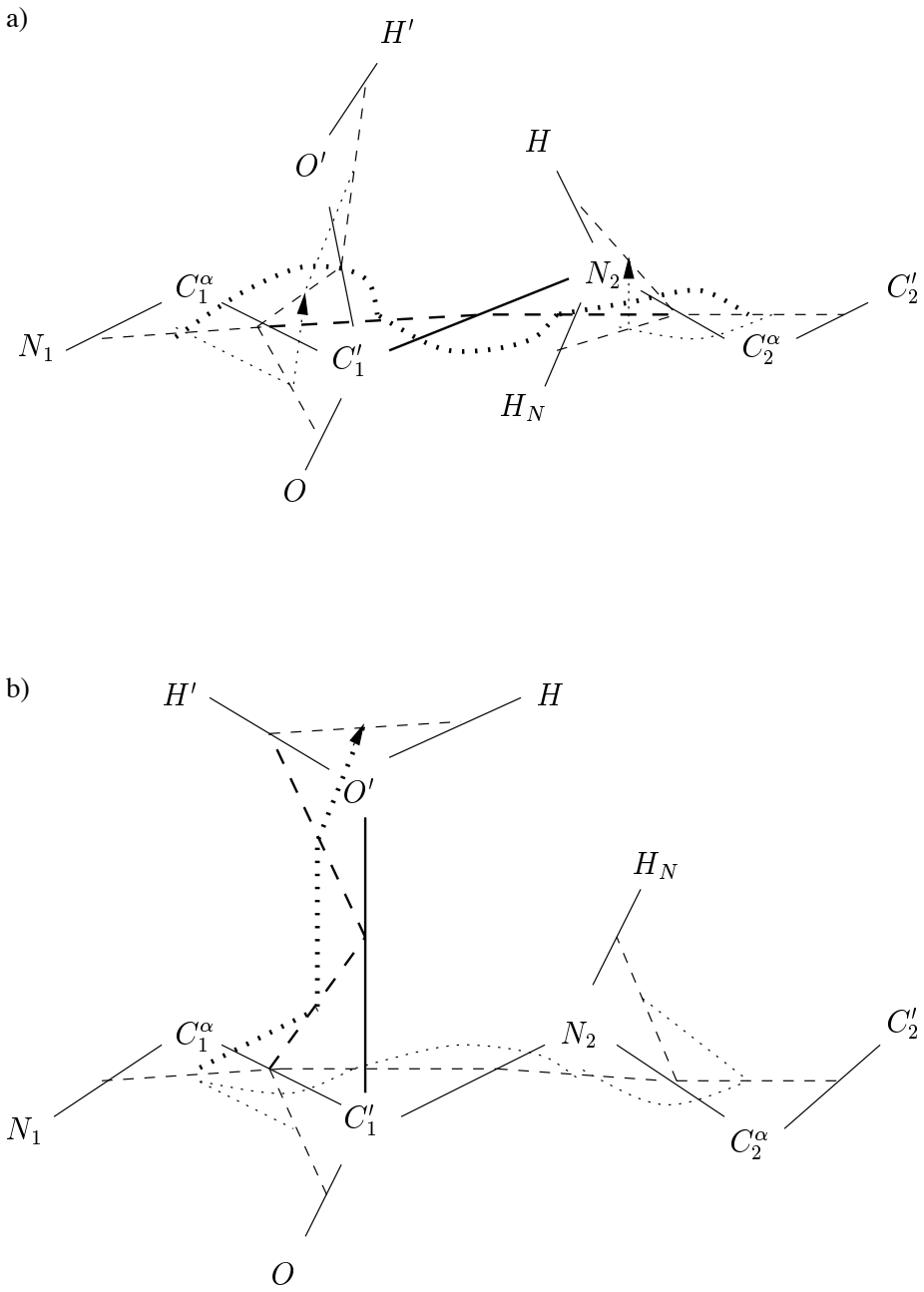

FIGURE 8. a) A tethered Z-system for the reactant supermolecule. Two amino acids approach one another. b) A tethered Z-system for the product supermolecule. A water molecule moves away from a dipeptide. The tethers (bonds) are shown as dark lines, the tether angles as dark dashed lines, and the tether wedges are shown as dark dotted curves or lines.

effectively decided that the new triangle gets rotated into the old triangle. Thus we define $(\Gamma \oplus_\mu \Lambda)^3_* = \Gamma^3_* \cup \Lambda^3_* \cup \{[j_0, i_0, i_1, i_2], [i_1, i_0, j_0, j_1], [i_0, j_0, j_1, j_2]\}$. Thus with $\mu = \{(i_0, i_1, i_2), (j_0, j_1, j_2)\}$ we have that $\Gamma \oplus_\mu \Lambda$ is a well-defined Z-system.

It should be clear that $\Gamma \oplus_\mu \Lambda = \Lambda \oplus_\mu \Gamma$. Furthermore if γ is a site in Γ, λ_1, λ_2 are sites in Λ, and δ is a site in another Z-system Δ, then we have an associative property:

$$\Gamma \oplus_{\{\gamma,\lambda_1\}} (\Lambda \oplus_{\{\lambda_2,\delta\}} \Delta) = (\Gamma \oplus_{\{\gamma,\lambda_1\}} \Lambda) \oplus_{\{\lambda_2,\delta\}} \Delta.$$

Tethering can also be done with labelled Z-systems, where the numerical labels of the six added simplices specify the relative position and orientation of the two molecules.

Z-systems for large biomolecules are extremely laborious to generate from scratch. As compact as a Z-matrix is, it nevertheless has one row for each atom, and biomolecules can easily have thousands of atoms. The details of the structure of these molecules cannot be neglected if a mechanistic understanding of biological processes is to be achieved [48], [51], [12], [65], [10], so we must find ways to deal with the huge quantity of information in large Z-systems. One idea is to build up large Z-systems from smaller Z-systems by gluing the smaller pieces together. Biomolecules lend themselves to this approach because they are polymers, synthesized from many copies of smaller molecules called monomers. But as we have seen, mimicking the chemical reactions involved in joining these monomers together is rather complicated in its detail. It is desirable to have a gluing operation which can bypass the chemical processes and go straight to the final result. In fact, when one builds plastic models of molecules one uses exactly such a gluing operation. It is interesting that Z-systems are perfectly suited to such an operation.

Suppose Z-systems Γ and Λ on disjoint sets $\mathcal{N}$ and $\mathcal{M}$ respectively, and with sites $\gamma = (i_0, i_1, i_2) \in \operatorname{vert} \mathcal{S}(\Gamma)$ and $\lambda = (j_0, j_1, j_2) \in \operatorname{vert} \mathcal{S}(\Lambda)$ are given. We require that $\{i_0\}$ is a leaf vertex in the tree $(\Gamma^0, \Gamma^1, \sigma)$, and that $\{j_0\}$ is a leaf vertex in the tree $(\Lambda^0, \Lambda^1, \sigma)$. We intend to define a new Z-system $\Gamma *_\mu \Lambda$, where $\mu = \{\gamma, \lambda\}$. It will be a Z-system on the set $\mathcal{L} = (\mathcal{N} \setminus \{i_0\}) \cup (\mathcal{M} \setminus \{j_0\})$, which (together with the mappings $\iota_\mathcal{N}, \iota_\mathcal{M}$) is the pushout of the following diagram:

$$\begin{array}{ccc} \{i_1, j_1\} & \xrightarrow{i_1 \mapsto j_0, j_1 \mapsto j_1} & \mathcal{M} \\ {\scriptstyle i_1 \mapsto i_1, j_1 \mapsto i_0}\downarrow & & \downarrow{\scriptstyle \iota_\mathcal{M}} \\ \mathcal{N} & \xrightarrow{\iota_\mathcal{N}} & \mathcal{L}. \end{array}$$

Given any set S and any mappings $f\colon \mathcal{M} \to S$, $g\colon \mathcal{N} \to S$ such that $f(j_0) = g(i_1)$ and $f(j_1) = g(i_0)$ there exists a unique mapping $h\colon \mathcal{L} \to S$ such that $f = h \circ \iota_\mathcal{N}$ and $g = h \circ \iota_\mathcal{N}$. This pushout property requires the definitions:

$$\iota_\mathcal{N}(i) = \begin{cases} i & i \in \mathcal{N} \setminus \{i_0\} \\ j_1 & i = i_0 \end{cases}, \qquad \iota_\mathcal{M}(j) = \begin{cases} j & j \in \mathcal{M} \setminus \{j_0\} \\ i_1 & j = j_0 \end{cases},$$

and hence $h(l) = \begin{cases} f(l) & l \in \mathcal{M} \setminus \{j_0\} \\ g(l) & l \in \mathcal{N} \setminus \{i_0\} \end{cases}$. (We describe these mappings in such an elaborate manner to indicate how the construction might be generalized to the case $n \neq 3$, where instead of gluing along a 1 simplex, one glues along an $n-2$ simplex. The upper horizontal and left vertical mappings of the pushout rectangle would be

required to be monomorphisms of Z-systems.) Now we define

$$(\Gamma *_\mu \Lambda)^1 = \{\iota_{\mathcal{M}}(b) \mid b \in \Gamma^1\} \cup \{\iota_{\mathcal{N}}(b) \mid b \in \Lambda^1\},$$
$$(\Gamma *_\mu \Lambda)^2 = \{\iota_{\mathcal{M}}(t) \mid t \in \Gamma^2\} \cup \{\iota_{\mathcal{N}}(t) \mid t \in \Lambda^2\},$$
$$(\Gamma *_\mu \Lambda)^3 = \{\iota_{\mathcal{M}}(\tau) \mid \tau \in \Gamma^3\} \cup \{\iota_{\mathcal{N}}(\tau) \mid \tau \in \Lambda^3\} \cup \{\{i_2, i_1, j_1, j_2\}\}.$$

We must show that these definitions satisfy the necessary properties to define a Z-system. Since $\{i_0\}$ is a leaf vertex in the tree $(\Gamma^0, \Gamma^1, \sigma)$ the bond $\{i_0, i_1\}$ is the only bond in Γ^1 incident on $\{i_0\}$. So if $b \in \Gamma^1 \setminus \{\{i_0, i_1\}\}$ then $\iota_{\mathcal{N}}(b) = b$. Likewise since $\{j_0\}$ is a leaf vertex in the tree $(\Lambda^0, \Lambda^1, \sigma)$ the bond $\{j_0, j_1\}$ is the only bond in Λ^1 incident on $\{j_0\}$. So if $b \in \Lambda^1 \setminus \{\{j_0, j_1\}\}$ then $\iota_{\mathcal{M}}(b) = b$. Clearly $\iota_{\mathcal{N}}(\{i_0, i_1\}) = \iota_{\mathcal{M}}(\{j_0, j_1\}) = \{i_1, j_1\}$. Thus $(\Gamma *_\mu \Lambda)^1 = (\Gamma^1 \setminus \{\{i_0, i_1\}\}) \cup (\Lambda^1 \setminus \{\{j_0, j_1\}\}) \cup \{\{i_1, j_1\}\}$. Since $(\Gamma *_\mu \Lambda)^0 = \binom{\mathcal{L}}{1}$ has $(N-1)+(M-1) = N+M-2$ elements, and $(\Gamma *_\mu \Lambda)^1$ has $(N-2)+(M-2)+1 = N+M-3$ elements, and the graph $((\Gamma *_\mu \Lambda)^0, (\Gamma *_\mu \Lambda)^1, \sigma)$ is connected, it must be a tree. The set $\{\iota_{\mathcal{M}}(t) \mid t \in \Gamma^2\}$ and the set $\{\iota_{\mathcal{N}}(t) \mid t \in \Lambda^2\}$ are disjoint, hence $(\Gamma *_\mu \Lambda)^2$ has $(N-2)+(M-2) = N+M-4$ elements. The graph $((\Gamma *_\mu \Lambda)^1, (\Gamma *_\mu \Lambda)^2, \sigma)$ is clearly connected, so it must be a tree. The union defining $(\Gamma *_\mu \Lambda)^3$ is a disjoint union, so $(\Gamma *_\mu \Lambda)^3$ has $(N-3)+(M-3)+1 = N+M-5$ elements. The tetrahedron $\{i_2, i_1, j_1, j_2\}$ connects the triangle $\iota_{\mathcal{N}}(\{i_0, i_1, i_2\}) = \{i_2, i_1, j_1\}$ to the triangle $\iota_{\mathcal{M}}(\{j_0, j_1, j_2\}) = \{i_1, j_1, j_2\}$, so the graph $((\Gamma *_\mu \Lambda)^2, (\Gamma *_\mu \Lambda)^3, \sigma)$ is connected and hence a tree. The intersection property is clearly satisfied. The mapping $\iota_{\mathcal{N}}$ and $\iota_{\mathcal{M}}$ take oriented 3 simplices into oriented 3 simplices in the obvious manner. Furthermore, the 3 simplex $\{i_2, i_1, j_1, j_2\}$ is a dihedral, with the canonical orientation $[i_2, i_1, j_1, j_2]$. Thus $(\Gamma *_\mu \Lambda)^3_*$ is defined. So $\Gamma *_\mu \Lambda$ is a Z-system.

This gluing operation on Z-systems can be illustrated by the example of combining methane and water to make methanol. Let

$$\begin{array}{llll} C & & & \\ H_* & C & & \\ H_1 & C & H_* & \\ H_2 & C & H_* & H_1 \\ H_3 & C & H_* & H_1 \end{array} \qquad\qquad \begin{array}{lll} O & & \\ H & O & \\ H^* & O & H \end{array}$$

be a Z-matrices Γ and Λ for methane and water respectively. As before we use a Z-matrix to define a Z-system, where we ignore the root site and the leaf-picking order. We choose the site $\gamma = (H_*, C, H_1)$ in methane, and the site $\lambda = (H^*, O, H)$ in water. We have $\mathcal{N} = \{C, H_*, H_1, H_2, H_3\}$ and $\mathcal{M} = \{O, H, H^*\}$ and the mappings

$$\iota_{\mathcal{N}}(l) = \begin{cases} C & l = C, \\ O & l = H_*, \\ H_1 & l = H_1, \\ H_2 & l = H_2, \\ H_3 & l = H_3, \end{cases} \qquad \iota_{\mathcal{M}}(l) = \begin{cases} O & l = O, \\ H & l = H, \\ C & l = H^*. \end{cases}$$

The result of gluing is the Z-system $\Gamma *_\mu \Lambda$ on the set $\mathcal{L} = \{C, H_1, H_2, H_3, O, H\}$, where

$$(\Gamma *_\mu \Lambda)^1 = \{\{C, H_1\}, \{C, H_2\}, \{C, H_3\}, \{O, H\}, \{C, O\}\}$$
$$(\Gamma *_\mu \Lambda)^2 = \{\{H_1, C, O\}, \{H_2, C, O\}, \{H_3, C, O\}, \{C, O, H\}\}$$

$$(\Gamma *_\mu \Lambda)^3_* = \{[H_2, C, O, H_1], [H_3, C, O, H_1], [H_1, C, O, H]\}.$$

This Z-system for methanol coincides with the one pictured in Figures 1 and 2 except that the orientations of the two impropers are reversed. As usual there are many Z-matrices one could write for this Z-system, such as the one given in section 5, but none of them are obtained from the two initial Z-matrices by a simple manipulation.

Labelled Z-systems can be glued as above to yield another labelled Z-system. The gluing information μ, in addition to the two sites γ and λ, must contain a bond length for the bond $\{i_1, j_1\}$ and a unit modulus complex number as the wedge angle coordinate for the oriented 3 simplex $[i_2, i_1, j_1, j_2]$. The other labels are carried over from the corresponding simplices of Γ or Λ. The bond length of $\{i_1, j_1\}$ is in practice determined by the element types of i_1 and j_1, since $\{i_1, j_1\}$ will almost always be a single bond (the formation of double or triple bonds usually involve more complex rearrangments than contemplated in this gluing construction). The (dihedral) wedge angle coordinate is usually not uniquely determined anyway at normal biological conditions, so this construction fits well with chemical reality. The gluing of labelled Z-systems provides a very convenient operation on this mathematical model of biomolecules [20].

The lack of a simple way of gluing Z-matrices has been an effective obstacle to their being adopted as the primary working data structure for biomolecules. The existence of many Z-matrices for the same molecule has also made the adoption of a standard Z-matrix for each biomolecule inadvisable. Z-systems correct both problems. Given the standard atom names and conformational variables already established in the references [37], [38], [39], it is a short step to choose standard Z-systems for all the important monomers of biopolymers. Z-systems for the polymers themselves can easily be constructed by gluing. Labelled Z-matrices can be used to manipulate conformations of biopolymers because computer software can mediate between molecular configurations (i.e. pdb files), Z-matrices and Z-systems. Already a computer program IMIMOL [18] developed by the author with a graphics programmer, Scott Johnson, with funding provided by the Industrial Mathematics Institute at the University of South Carolina, allows the user to build edit and manipulate (tether and glue) three dimensional Z-systems graphically and to write labelled Z-matrices. This makes manipulation of the geometry of biomolecules quite easy.

The significance of Z-systems as a means of biomolecular geometry description is best understood against the backdrop of previous efforts in this direction. There has been a good amount of careful work on describing molecular geometry and unique naming of three dimensional molecular structures by the stereochemist Andre Drieding and his collaborators [19], [72]. In particular the paper by Andreas Dress, Andre Dreiding and Hans Haegi [20] carefully lays out the mathematical scheme. However the approach taken in that paper to the problem of an "internal coordinate" description of molecular geometry is based on using only distances as coordinates (i.e. no angles) as in the book by Crippen and Havel [15]. This approach has attracted a lot of interest from specialists in "rigidity theory" [31], [66]. Here one relaxes the condition that $\Gamma = (\Gamma^0, \Gamma^1, \sigma)$ be a tree, but still labels each edge of this graph with a distance between the two atoms involved. The main question of "rigidity theory" is how to characterize the class of graphs Γ for which this collection of distances (together with some discrete "chirality" coordinates) gives a

coordinate chart on $G_a \backslash \mathcal{D}_C(\Gamma)$, where $\mathcal{D}_C(\Gamma)$ is some dense open subset of $(\mathbb{R}^3)^{\mathcal{N}}$. We should remark that even after this question is settled, the coordinate domain $\mathcal{D}_C(\Gamma)$ will probably be extremely difficult to characterize, not to mention the parameter domain $\mathcal{D}_P(\Gamma)$. Lingering uncertainty about where the singularities of a coordinate chart are is enough to limit the practical applicability of such internal coordinate systems.

Other authors, such as Walter Whiteley, have considered the possibility of using both distances and angles [69], [70]. But specifications of exactly which combinations of distances and angles are sufficient have not been rigorously justified. In fact in [69] Whiteley says the problem in 3-dimensions is too hard. This is surprising considering the long history of molecular physics and the obvious need to separate the overall positional and orientational degrees of freedom from the internal degrees of freedom [47], [43]. There has been a huge amount of study of the kinetic energy of a molecule in various internal coordinate systems, but the type of systems considered has been strongly influenced by the desire to treat high energy scattering processes; see e.g. [17] and [27]. Alexey Mazur and Ruben Abagyan have tackled this problem in the context of biomolecules, and have developed what they call the "BKS tree" [54]. Here one requires that $(\Gamma^0, \Gamma^1, \sigma)$ be a tree, but then one introduces a numbering of the atoms, the root atom being numbered 1, so that along paths starting at the root the atom numbers must increase. The tree defines a partial ordering $\prec$ of the atoms, where the $\prec$ predecessor of an atom A is the second atom along the path starting at A and ending at the root atom. Using this data one constructs a Z-matrix as follows: each atom A after the first is part of a bond with its $\prec$ predecessor B; each atom A two or more bonds away from the root is part of an angle with its $\prec$ predecessor B and with B's $\prec$ predecessor C; each atom A three or more bonds from the root is part of a dihedral with B, C, D, where B, C are as above and D is the $\prec$ predecessor of C. This prescription is attributed to Eyring [23]. However certain of the initial choices of the Z-matrix are not always settled by this prescription. Also, to avoid overuse of dihedrals, a modified rule is applied to all atoms $A_{i_1}, \ldots, A_{i_m}$, whose $\prec$ predecessor B is a branch point of the tree. If $i_1 < \cdots < i_m$, the atom A_{i_1} follows the above prescription. The atoms $A_{i_2}, \ldots, A_{i_m}$ are part of impropers with the atom A_{i_1}, where the "old" triangle involving A_{i_1} is rotated into the "new" triangle.

Most chemists and molecular physicists consider it to be obvious that such prescriptions define valid internal coordinate systems, and so a careful proof has apparently never been written down. However recently John Frederick and Clemens Woywod [26] have written down "guidelines" for the proper construction of "bond angle" coordinate systems. These are stated without proof, and they explicitly eschew a rigorous definition of the coordinate chart with its coordinate and parameter domains. One of their guidelines, "bond angle coordinates must all subtend two of the bond length coordinates present in a valid set", which is consistent with the structure of Z-systems, is nevertheless not necessary in order to obtain a coordinate chart with all the good properties listed in our main theorem. Consider a system with $\mathcal{N} = \{1, 2, 3, 4\}$ and $\Gamma^1 = \{\{1, 2\}, \{2, 3\}, \{3, 4\}\}$, where a bond length coordinate is associated with each bond in Γ^1. Assign bond angle coordinates to each of the angles $\{\{1, 2\}, \{2, 3\}\}$ and $\{\{1, 3\}, \{3, 4\}\}$. Assign a wedge angle coordinate to the data: $\{\{1, 2, 3\}, \{1, 3, 4\}\}$ and $[2, 1, 3, 4]$. Let Γ stand for all this data. Then $\mathcal{D}_C(\Gamma)$ consists of all configurations R such that the 2 simplices associated to $\{1, 2, 3\}$ and

$\{1,3,4\}$ are geometrically independent. $\mathcal{D}_P(\Gamma) = (0,\infty)^3 \times (-1,1)^2 \times S^1$. These coordinates define a diffeomorphism $G_a\backslash\mathcal{D}_C(\Gamma) \to \mathcal{D}_P(\Gamma)$ even though the angle $\{\{1,3\},\{3,4\}\}$ is incident on a bond $\{1,3\}$ whose bond length was not specified as a coordinate. This example shows the necessity of going beyond the chemists and physicists appeal to intuition and providing rigorous proof. Thus the question of exactly which combinations of bond lengths, bond angles, and wedge angles, are *necessary* and sufficient to obtain a diffeomorphism $G_a\backslash\mathcal{D}_C(\Gamma) \to \mathcal{D}_P(\Gamma)$ between coordinate and parameter domains defined as in section 3 is still open. However the second theorem of section 4 shows that Z-systems are adequate for all noncollinear molecular configurations, so the practical benefit of considering systems more general than Z-systems and yet with the same coordinate and parameter domains is not likely to be real.

An extensive amount of work has been done on the problem of automatically generating a suitable internal coordinate system from a given molecular configuration R (a list of Cartesian coordinates for each atom) [61], [7], [62]. These automatically generated systems are intended to simplify vibrational analysis, or to make the process of geometry optimization (finding the conformation of least potential energy) more efficient. Often linear combinations of bond length, bond angle, and/or wedge angle coordinates are introduced which lose clear geometric interpretation. Such coordinate systems are clearly unsuitable for our purposes, i.e. a mathematical study of biomolecular geometry. The torsion angle representation of molecules is popular in the field of rational drug design, [55], [44].

The most serious difficulty in using Z-systems in the study of biomolecular geometry is the presence of flexible covalently bound rings [64], [15], [16], [50], [21]. Five-membered rings are present in both proteins (i.e. proline) and in all nucleic acids (the furanose ring) [3], [45], [46], [1]. Larger flexible rings are frequently present (via disulfide bonds) in proteins, and constitute an important constraint on their conformational flexibility [40]. If $\mathcal{N} = \{0,1,2,3,4\}$ then the orbit space $G_a\backslash\mathcal{B}$ is $15-6=9$ dimensional. Because of the five covalent bonds of the ring, it is desirable to use those bond lengths as five of the nine coordinates. This clearly takes us outside the realm of Z-systems. A simple possibility (see Mazur [53]) is to use as additional coordinates the bond angles $\{\{0,1\},\{1,2\}\}$ and $\{\{1,2\},\{2,3\}\}$ and the dihedral wedge angles $[0,1,2,3]$ and $[1,2,3,4]$. The cosine of the angle $\{\{2,3\},\{3,4\}\}$ is found by solving a quadratic equation derived by imposing the distance constraint between atoms $\{0\}$ and $\{4\}$. There are obviously generically either two or zero real solutions, so these nine coordinates either do not determine any conformation or do not determine a unique conformation. If we always choose the larger of the two solutions of the quadratic equation, the coordinate domain (which cannot be dense) and the parameter domain still need to be characterized. Another more complex (yet more symmetrical) choice of the four coordinates supplementing the five bond lengths has been proposed and studied (Marzec Day [52]). This system has the benefit that the primary degree of flexibility of the ring is described by one of the coordinates, the so-called *pseudorotation phase angle*. However, the coordinate and parameter domains for this system have not been characterized.

An interesting alternative to these approaches can be based directly on Z-system theory. Consider the Z-system Γ on $\mathcal{N}$ with the Z-matrix (see also Figure 9)

$$\begin{array}{cccc} 1 & & & \\ 2 & 1 & & \\ 0 & 2 & 1 & \\ 3 & 0 & 2 & 1 \\ 4 & 3 & 0 & 2 \end{array}$$

This system has the "bonds" $\{0,2\}$ and $\{3,0\}$ which are not covalently bonded pairs of atoms. Nevertheless our main theorem gives us a diffeomorphism $\hat{\eta}\colon G_a\backslash\mathcal{D}_C(\Gamma) \to \mathcal{D}_P(\Gamma)$. As usual $\mathcal{D}_C(\Gamma)$ is the dense open set of all configurations $R \in (\mathbb{R}^3)^{\mathcal{N}}$ for which the three triangles $\{0,2,1\}, \{3,0,2\}, \{4,3,0\}$ represent noncollinear triangles. Also $\mathcal{D}_P(\Gamma) = (0,\infty)^{\Gamma^1} \times (-1,1)^{\Gamma^2} \times (S^1)^{\Gamma^3_*}$. Define

$$\begin{aligned} \Lambda^1 &= \{\{0,1\},\{1,2\},\{2,3\},\{3,4\},\{4,0\}\}, \\ \Lambda^2 &= \{a_1 = \{\{0,1\},\{1,2\}\}, a_4 = \{\{3,4\},\{4,0\}\}\}. \end{aligned}$$

Define the mapping $\xi'\colon (0,\infty)^{\Gamma^1} \times (-1,1)^{\Gamma^2} \to (0,\infty)^{\Lambda^1} \times (-1,1)^{\Lambda^2}$ by the rule $\xi(L',C') = (L,C)$, where

$$\begin{aligned} L_{\{0,1\}} &= \sqrt{(L'_{\{1,2\}})^2 + (L'_{\{0,2\}})^2 - 2L'_{\{1,2\}}L'_{\{0,2\}}C'_{\{0,2,1\}}} \\ L_{\{1,2\}} &= L'_{\{1,2\}} \\ L_{\{2,3\}} &= \sqrt{(L'_{\{0,2\}})^2 + (L'_{\{0,3\}})^2 - 2L'_{\{0,2\}}L'_{\{0,3\}}C'_{\{3,0,2\}}} \\ L_{\{3,4\}} &= L'_{\{3,4\}} \\ L_{\{4,0\}} &= \sqrt{(L'_{\{0,3\}})^2 + (L'_{\{4,3\}})^2 - 2L'_{\{0,3\}}L'_{\{4,3\}}C'_{\{4,3,0\}}} \\ C_{a_1} &= \frac{L'_{\{1,2\}} - L'_{\{0,2\}}C'_{\{0,2,1\}}}{L_{\{0,1\}}} \\ C_{a_4} &= \frac{L'_{\{4,3\}} - L'_{\{0,3\}}C'_{\{4,3,0\}}}{L_{\{4,0\}}} \end{aligned}$$

This mapping simply recoordinatizes each of the three triangles in Γ^2. Define $\Delta \subset (0,\infty)^{\Lambda^1} \times (-1,1)^{\Lambda^2}$ to be the range of ξ'. The new coordinatization for the triangle $\{0,2,3\}$ is in terms of the lengths of its three sides, and this entails a restriction on the possible triples of lengths. Hence

$$\begin{aligned} \Delta = \{(L,C) \mid\ & L\colon \Lambda^1 \to (0,\infty), C\colon \Lambda^2 \to (-1,1), \text{such that} \\ & [(L'_{\{0,2\}})^2 + (L'_{\{0,3\}})^2 - (L_{\{2,3\}})^2]^2 < 4(L'_{\{0,2\}})^2(L'_{\{0,3\}})^2, \\ & \text{where } (L'_{\{0,2\}})^2 = (L_{\{0,1\}})^2 + (L_{\{1,2\}})^2 - 2L_{\{0,1\}}L_{\{1,2\}}C_{a_1}, \\ & \text{and } (L'_{\{0,3\}})^2 = (L_{\{0,4\}})^2 + (L_{\{4,3\}})^2 - 2L_{\{0,4\}}L_{\{4,3\}}C_{a_4}\}. \end{aligned}$$

If ξ is equal to ξ' with its codomain restricted to Δ then ξ is a diffeomorphism (as the reader is invited to check by explicitly constructing its inverse mapping). If $\mathcal{D}_P(\Lambda) = \Delta \times (S^1)^{\Gamma^3_*}$, then $(\xi \times 1) \circ \hat{\eta}$ is a diffeomorphism between $G_a\backslash\mathcal{D}_C(\Gamma)$ and $\mathcal{D}_P(\Lambda)$. This is an internal coordinate system for the five-membered ring where both the coordinate and the parameter domains are explicitly identified. The coordinates are the five bond lengths $L_{\{0,1\}}, L_{\{1,2\}}, L_{\{2,3\}}, L_{\{3,4\}}, L_{\{4,0\}}$, the two bond-angle

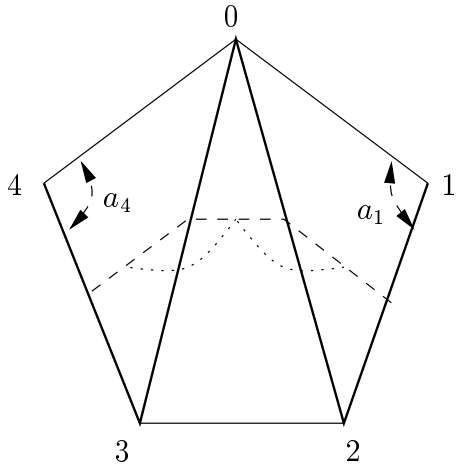

FIGURE 9. A Z-system Γ for a Five-Membered Ring.

cosines C_{a_1}, C_{a_4}, and the two wedge angles $\varphi_{[3,0,2,1]}, \varphi_{[4,3,0,2]}$. The two wedge angle coordinates are called *flap angle* coordinates in this case. Pseudorotation cycles form closed paths in the flap angle plane and in the bond angle plane. Flap angle coordinates have also appeared in the study of rings with more than five atoms [41], [34].

This result on five-membered rings suggests that there may be interesting generalizations of our main theorem where Λ is more general than a Z-system, and where $\mathcal{D}_P(\Lambda)$ is a semialgebraic set [11].

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