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Key Points:

- We explore how the topologies of atmospheric chemical reaction networks of Solar System bodies are distinct from one another
- The Earth's atmospheric chemical reaction network appears the most nonrandom and, in some metrics, resembles biological networks
- We hypothesize that a network-based biosignature may be developed for exoplanet characterization to complement existing biosignature methods

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Toward Network-Based Planetary Biosignatures: Atmospheric Chemistry as Unipartite, Unweighted, Undirected Networks

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Abstract Previous examinations of astrophysical chemical reaction networks found that Earth's atmospheric network was distinct in its hierarchical organization and scale-free nature. If Earth's unique atmospheric network structure is due to the coevolution between the biosphere and atmosphere, it may hint at a novel planetary-scale biosignature. Here, we use updated chemical reaction networks of planetary atmospheres and explore their topologies using a plethora of diagnostic techniques from network science and graph theory, including global metrics, centrality metrics, community detection, and cluster analysis methods. We show that the topologies of atmospheric chemical reaction networks of different planetary bodies in the Solar System are distinct from one another. While we find that model networks of Earth's atmosphere do not display scale-free topology, Earth's chemical reaction network is nonetheless distinguishable from those of other Solar System atmospheres through various other metrics. Earth's network has the most nonrandom topology of all the planetary networks and, in some global metrics, is more similar to biological networks than are the other planetary networks. Finally, we discuss how further investigations of atmospheric chemical networks using more advanced network representations and novel network metrics may lead to the development of a network-based biosignature applicable to exoplanets.

Plain Language Summary Atmospheric chemistry can be represented in graphical form by networks where nodes are chemical species and links are reactions. We show that the structures of atmospheric chemical reaction networks of different planetary bodies in the Solar System are distinct from one another. Of those examined, Earth's network is the most nonrandom planetary network. In certain metrics, Earth's network resembles the topologies of biological networks. We hypothesize that over billions of years of coevolution between biosphere and atmosphere, life may produce predictable patterns expressed in planetary-scale chemistry; if so, a network-based biosignature may be developed for exoplanet characterization to complement existing biosignature methods, providing a novel agnostic technique for identifying life as we do and do not know it. Testing this hypothesis will require extensive modeling of an ensemble of planetary atmospheres, combined with more advanced network representations and analysis.

1. Introduction

In the upcoming years and decades, astronomical observatories will characterize the chemical compositions of terrestrial exoplanet atmospheres and search for signs of life. However, the science of remote biosignature detection remains incomplete due in large part to a lack of a comprehensive understanding of how life emerges, evolves, and integrates into a planet's geochemical systems. Thus, a major challenge in astrobiology is to develop a theory of life that predicts signatures unique to life and that are universal across planetary contexts.

In life, information plays a fundamental role in structuring the flows of matter and energy (Bartlett & Wong, 2020; Walker, 2014; Walker & Davies, 2013; Wong & Prabhu, 2023). Because biological systems exhibit information-rich structures, it is thought that system complexity can be a metric by which to measure the living state (Bartlett & Beckett, 2019; Bartlett et al., 2022; Walker et al., 2018, 2020). Information flows continuously between life and its environment: life shapes its planet's atmosphere through the exchange of metabolic gases, and in turn atmospheric composition influences the evolution of life (Yung et al., 2014). This coevolution of the biosphere and atmosphere impacts the broader planetary system, making biology a planetary-scale phenomenon that may be quantifiable by looking at atmosphere's chemical reaction network holistically, rather than by detecting the presence and inferring the fluxes of individual molecules.

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In network science, complex systems are represented by graphical networks and quantified using metrics that describe the network's topology—e.g., how well-connected, heterogeneous, or scale-invariant the network is. Network science has been used to gain new insights and identify universal trends across complex phenomena, from biology (Kim et al., 2019; Leuenberger et al., 2017; West & Brown, 2005) to mineralogy (Hazen et al., 2019; Moore et al., 2022; Morrison et al., 2017, 2020). Here, we leverage network science to address key questions in atmospheric chemistry, comparative planetology, biosignature detection, and astrobiology (Fisher et al., 2022).

Solé and Munteanu (2004) first suggested that the chemical network of the Earth's atmosphere is topologically distinct from that of other Solar System atmospheres. Their chemical networks represented species as *nodes* and reactions as *edges* between nodes. The number of edges a node has is its *degree*. Their study showed that exponential curves fit the degree distributions of the atmospheres of Venus, Mars, and Titan. However, Earth's network, sourced from a textbook (Yung & DeMore, 1999), followed a power law, which is highly suggestive of life given that many living networks also follow power-law (or "scale free") distributions (Jeong et al., 2001)—though this claim has been challenged in recent years (Smith et al., 2021).

While intriguing, the complexity analysis pioneered in 2004 by Solé and Munteanu (2004) requires further development. In this contribution, we utilize a broader suite of network analysis techniques to reexamine Solé and Munteanu (2004)'s claim. We compare Earth's atmosphere to a larger collection of planetary atmospheres, whose properties are known better now than they were in 2004. Because exoplanetary atmospheres are unlikely to be characterized to "textbook-level" knowledge in the near term, we compare both the textbook reaction network and networks from models of Earth's atmosphere, but focus primarily on comparing the Earth model network to the model networks of other worlds.

In the spirit of Sagan et al. (1993), we examine our own planet in comparison with other worlds, knowing that Earth represents the only confirmed planet with a biosphere, to seek potentially biological anomalies that conform to our tentative criteria for life (Cleland, 2019a, 2019b). Ultimately, we find that the atmospheric chemistries of different Solar System bodies can be distinguished from one another in an abstract network-theoretic way. Although this does not provide conclusive evidence that the topology of Earth's atmospheric chemistry distinctly reflects the influence of biology, the possibility for developing a new kind of agnostic biosignature and a richer understanding of life at the planetary scale remains open.

2. Atmospheric Networks

In this study, we source our planetary networks from published studies simulating the photochemistry of Solar System atmospheres using the Caltech–JPL photochemistry–transport model KINETICS (Allen et al., 1981). This state-of-the-art model has been well-validated against decades of planetary data and has also been used to predict the photochemistry of ancient Solar System bodies (Wong et al., 2015; Wong, Charnay, et al., 2017) and exoplanetary atmospheres (Gao et al., 2015; Line et al., 2011). We compare the atmospheric networks of Venus (Zhang et al., 2012), Modern Earth (Yung et al., 1980, 2019), Mars (Nair et al., 1994), early Mars/Earth (Adams et al., 2021), Jupiter (Moses et al., 2005), Titan (Willacy et al., 2016), and Pluto (Wong, Fan, et al., 2017). All these planetary networks have been well validated against Solar System data, save for the early Mars/Earth network, for which we have no direct observations and is therefore a geochemically informed theoretical representation of CO_2-N_2-H_2O-dominated secondary atmospheres on young terrestrial bodies.

For direct comparison to the work of Solé and Munteanu (2004), we choose to represent these networks as unipartite, unweighted, and undirected graphs. Each graph G is composed of N nodes and E edges. In this representation, nodes represent different chemical species in the network, two nodes are connected when they are linked by a chemical reaction that contains one as a reactant and the other as a product, and there is no directionality to the edge. This simple representation has obvious limitations that can be improved upon in future work (see Section 6).

We visualize our networks with a Kamada-Kawai force-directed layout (Kamada & Kawai, 1989) using NetworkX's graphing functions (Hagberg et al., 2008). Nodes are arranged in 2-D space by spring forces between all linked pairs of nodes. When the graph relaxes to its minimum energy state, it creates a visually pleasing and intuitive diagram where nodes of high degree and centrality are clustered near the middle of the graph, with less well-connected nodes occupying the periphery.

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In Figure 1, we display these force-directed graphs with two additional data dimensions: *degree* (node color) and *betweenness centrality* (node size). Degree measures the number of other nodes to which a node is connected. Betweenness centrality is the fraction of shortest paths between other nodes in the network that travel through the node in question.

The overall structures of the network diagrams in Figure 1 are informative. The topology of a graph is determined by the presence and absence of components and connections, which allows patterns in connectivity to be revealed through network visualizations. For example, the networks of Titan and Pluto are highly symmetric and centered upon a few hub-like nodes; as distance from the center increases, degree and betweenness centrality tend to decrease in a monotonic fashion. On the other hand, the atmospheres of the terrestrial planets are less symmetric and not dominated by a single center, but multiple nodes of high degree and betweenness centrality.

By visual inspection of Figure 1, one can immediately identify the most salient nodes in each atmospheric network and their chemical relationships with respect to each other and the rest of the atmospheric constituents. In general, the nodes with the highest degree and betweenness centralities are highly reactive radical species created through photolysis of a major atmospheric component. The highly reducing worlds—Jupiter, Titan, and Pluto—are largely symmetric and centered upon the H radical, sourced from H_2 and CH_4 photolysis. This reflects the outsized importance of reactions involving H to the photochemistry of these atmospheres. Jupiter gains some heterogeneity from P and O chemistry, which Titan and Pluto do not have. Venus's network is structured around various S-, Cl-, and O-containing radicals—the four highest-degree nodes being O, SO, Cl, and OH. Figure 1a shows that O and SO are close to each other but distant from Cl and OH. The fact that O and SO are distant from Cl is unsurprising (they have different photolysis parents, SO_2 and HCl, respectively) but one might have naïvely expected OH and O to be closer (both being the photolysis products of H_2O); this demonstrates the value of network visualizations as a tool for identifying patterns that reveal which compounds are similar or dissimilar in terms of chemical connectivity. On Earth, Cl (from HCl photolysis), OH (from H_2O photolysis), and NO_2 (formed by the oxidation of NO, which is produced by lightning in Earth's N_2-O_2-rich atmosphere, as well as anthropogenic emissions) play dominant roles.

Nodes of low degree (bluish purple in color) but high betweenness centrality (large in size) are deceptively important "outliers" that play important roles in connecting different parts of the network despite not being hubs of high connectivity themselves. For example, in Jupiter's atmosphere, OH and NH_2 have moderate degrees but play important roles in connecting the O- and N-bearing parts of the graph, respectively, to other regions of the network.

In Figure 2a, we graph Earth's full atmospheric network, taken from Yung and DeMore (1999), using the same conventions as in Figure 1: unipartite, unweighted, undirected, nodes colored by degree, and nodes sized by betweenness centrality. In Figure 2b–2e, we show subsets of the full modern Earth atmosphere. The subsets that exclude CFCs (Figure 2b) or fluorine (Figure 2c) may be representative of Phanerozoic atmosphere, prior to the onset of human activity. The full Earth atmosphere (Figure 2a) clearly shows hub-and-spoke structures—most notably the CFCs that radiate from HCl, Cl, H_2O, and OH—that are indicative of the power-law degree distribution that Solé and Munteanu (2004) first noted.

However, we are unlikely to be able to characterize exoplanetary atmospheres to "textbook-level" detail; instead, atmospheric models will be constructed to reproduce the known physical parameters and sparse chemical data of the exoplanet in question. Also, because we still do not know the other Solar System atmospheres to the exquisite level of detail at which we know Earth's atmosphere, it is perhaps unfair to compare the textbook network of modern Earth's atmosphere from Yung and DeMore (1999) against the networks from models of the other Solar System bodies. Thus, the remainder of this study will focus primarily on comparing the Earth model network (Figure 1c, rather than Figure 2a) to other planetary models. While species and reactions are undoubtedly missing from all of these photochemical models, their validation against planetary data, and their foundation in experimental work in chemical kinetics, means that they do in fact capture the "essence" of each body's atmospheric chemistry to the best of our knowledge at present.

3. Network Metrics

Network metrics are mathematical tools for quantifying the structures of graphs. These may be assessed at the level of the whole network (global metrics) or at the level of individual nodes (centrality metrics); the latter

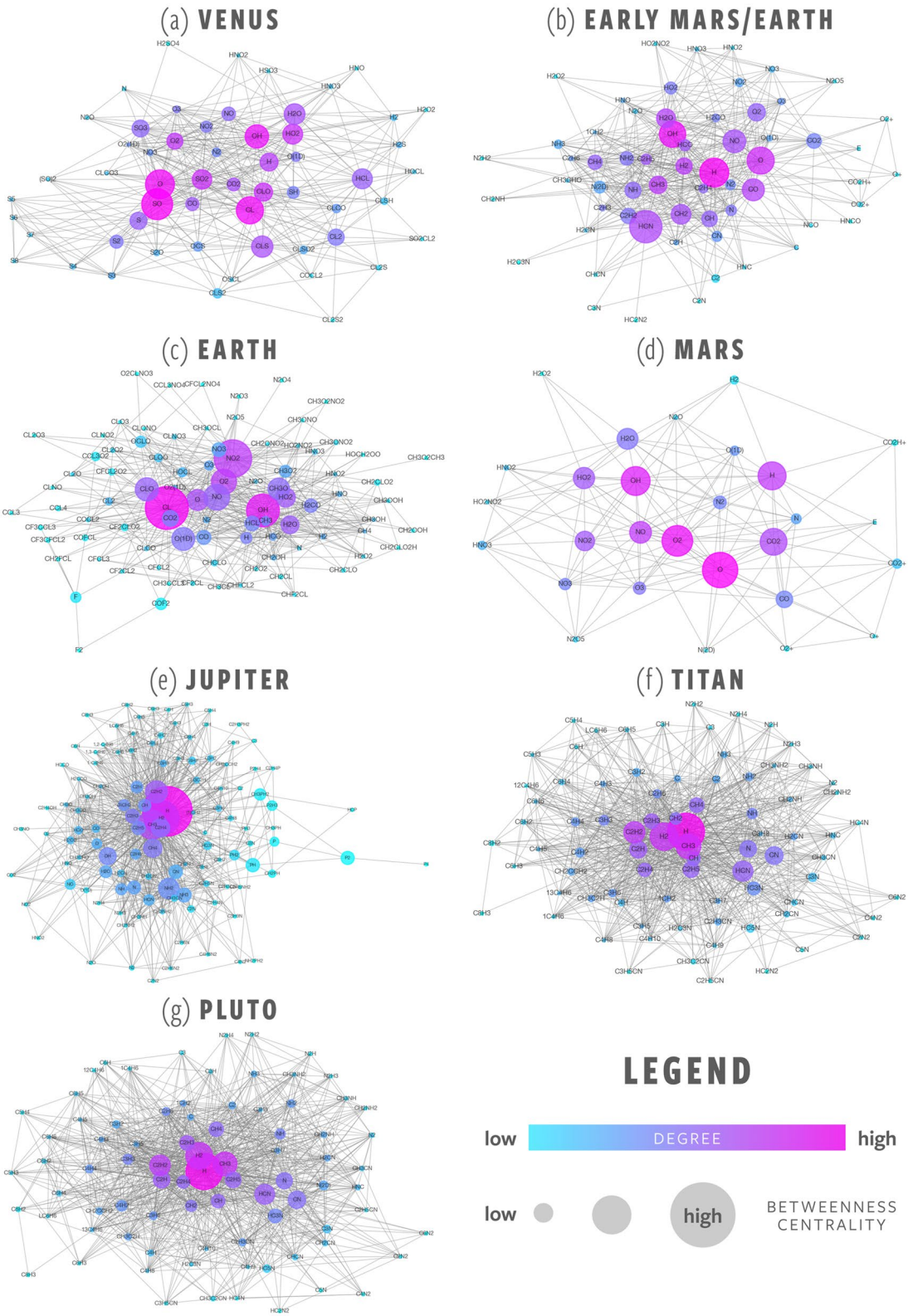

Figure 1. Solar System atmospheric networks (models). These diagrams represent the chemistry of planetary atmospheres as force-directed, unipartite, unweighted, undirected graphs. Nodes are colored by their degree and sized by their betweenness centrality. The color scale is semi-qualitative because each network is scaled to its own range of degree values.

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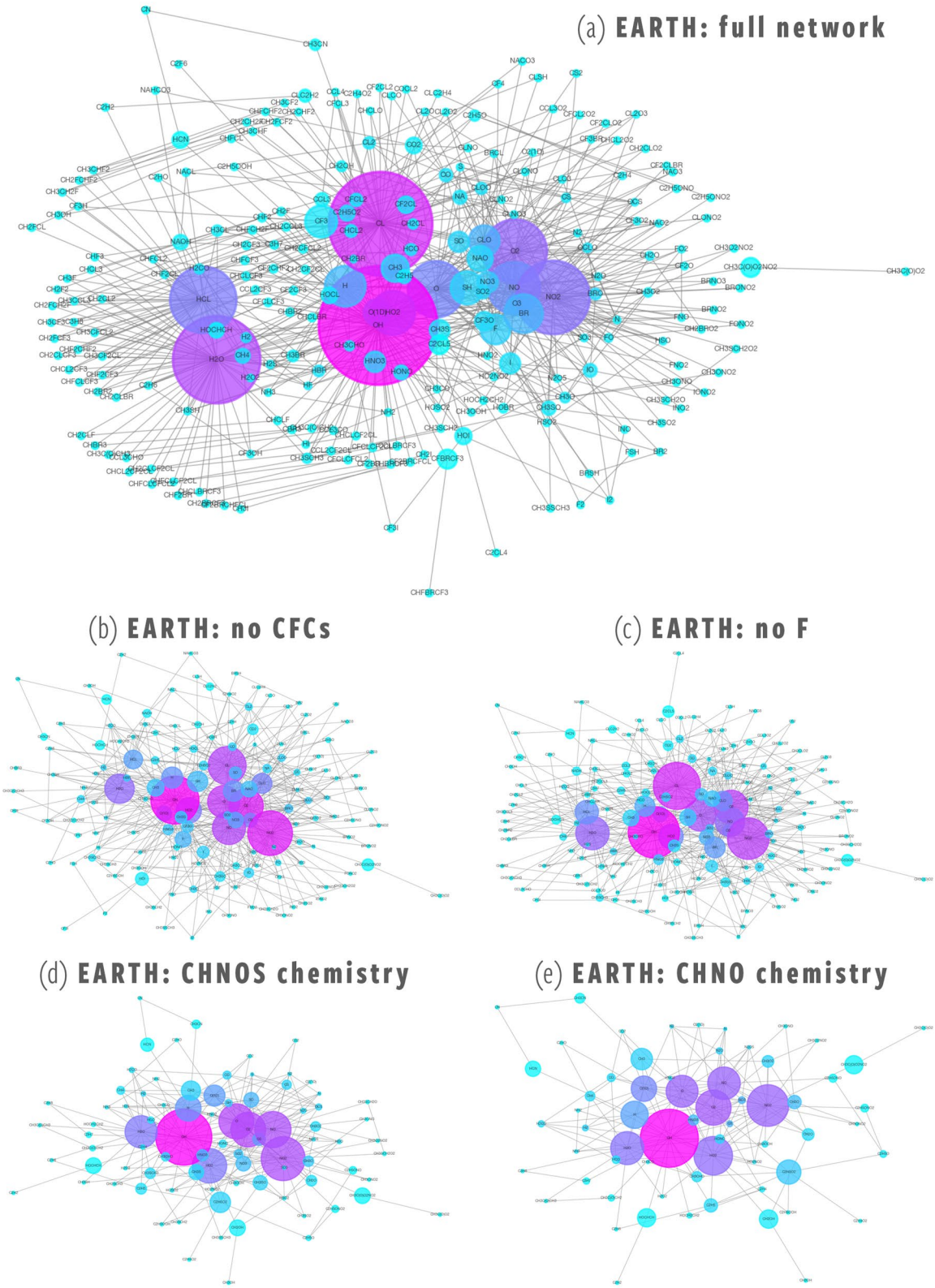

Figure 2. Earth's atmospheric network (textbook). (a) Earth's atmospheric chemical network; data from the reaction list in Yung and DeMore (1998). (b–e) Subsets of this atmosphere with certain chemistry excluded. Nodes are colored by their degree and sized by their betweenness centrality. The color scale is semi-qualitative because each network is scaled to its own range of degree values.

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produces a distribution of values that characterize the network. In some applications of network science, network metrics give proxies for the statistical similarity between different ensembles of components. However, in the case of a chemical network, where the components (molecules) physically interact via links (reactions), chemical networks are literally network data. Thus, in this study, the network metrics we present are actual statistical metrics of how the interactions among units differ from one assemblage to another, helping us characterize the behavior of different planetary atmospheres. We calculate global metrics (Section 3.1), degree distributions (Section 3.2), and centrality metrics (Section 3.3) for our chemical reaction networks using NetworkX's built-in algorithms (Hagberg et al., 2008).

3.1. Global Metrics

Global metrics summarize macroscopic features and trends of complex networks in single numbers. For example, the *degree assortativity* characterizes whether nodes tend to be connected to nodes of similar or dissimilar degree; in other words, it is a measure of how homogeneous or heterogeneous a network is (Newman, 2003). Networks whose architectures feature distinct hubs, each linked to many spokes that rarely connect to one another, are extremely heterogeneous and have low degree assortativity values.

Other global metrics of interest include the *average shortest path length* between pairs of nodes in G as well as measures of clustering. There are two common ways to calculate a network's clustering: via the *clustering coefficient* and the *transitivity*. Both essentially ask: How common is it for the neighbors of any given node to be neighbors of each other? In other words, if u is linked to v and v is linked to w, does that imply that u is linked to w? Both the clustering coefficient and the transitivity are valid formulations; subtle differences arise from the fact that transitivity is calculated directly at the global level, whereas the clustering coefficient is the global average of a local-scale metric (and hence can become dominated by nodes with a low degree). High clustering is common in social networks (a friend of a friend is a friend; actors appear in films with a tight circle of colleagues; scientists collaborate in coordinated research networks, Newman, 2018), forming densely connected regions known as *cliques*. In contrast, biological and technological networks tend to have low transitivity.

The clustering coefficient C of graph G is defined as the average of the local clustering coefficients C_u,

$$C = \frac{1}{N}\sum_{i=1}^{N} C_u, \tag{1}$$

where

$$C_u = \frac{2t_u}{k_u(k_u - 1)}, \tag{2}$$

t_u is the number of triangles that pass through u, and k_u is the degree of u.

A similar parameter, the *transitivity*, represents the fraction of all possible triangles in G that are realized:

$$T_G = 3\frac{\#\text{ of triangles}}{\#\text{ of triads}}, \tag{3}$$

where a triad is defined as two edges with a shared vertex.

Figure 3 compares these global metrics across planetary atmospheres in this study and three archetypal biological networks spanning a range of scales in life—a metabolic network, a neural network, and a marine food web network. We show global metric values for both the model Earth and textbook Earth networks because the model Earth network is more aptly compared to the other model planetary networks, whereas the textbook Earth network is more aptly compared to the archetypal biological networks, due to the level of detail at which those have been studied. Comparing the textbook Earth network with biological networks, it is evident that Earth's network is similar to biological networks in that it has a low degree assortativity, a low clustering coefficient, a low transitivity, and a high average shortest path length. The model Earth network is less like the biological networks and less distinct from planetary networks. Yet, the model Earth network still systematically deviates from the rest of the planetary networks in a manner that is consistent (in direction, though not magnitude) with the textbook Earth network. The fact that the global metrics of model Earth's network shows small but suggestive differences from those of other model planetary networks motivates the exploration of other network metrics.

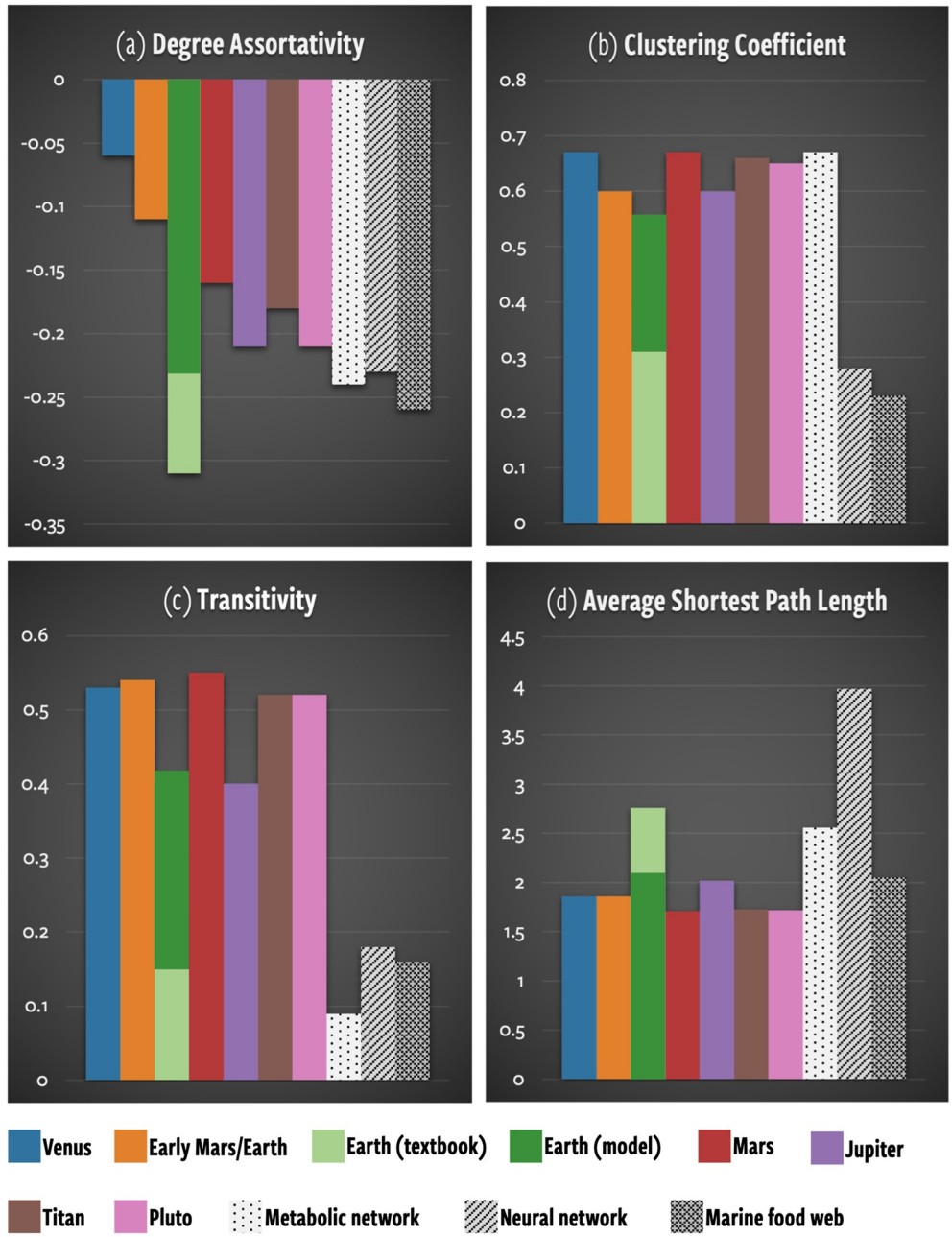

Figure 3. Global metrics of the planetary atmospheres and three representative biological networks. (a) Degree assortativity, (b) clustering coefficient, (c) transitivity, (d) average shortest path lengths between pairs of nodes in the network. See text for details. Biological networks taken from Table 10.1 of Newman (2018) and references therein.

3.2. Degree Distributions

A major claim of Solé and Munteanu (2004) is that Earth's network can be distinguished from those of other Solar System bodies via their degree distributions: Earth's network follows a power-law (scale-free) degree distribution; other networks' degree distributions follow exponential (random) distributions. We reproduce their finding that Earth's network as described by the reaction list in Yung and DeMore (1999) can indeed be plausibly described by a power-law degree distribution, in contrast to those of other planetary atmospheres (Figure 4).

However, we also find that the degree distribution of Earth's network as described by the KINETICS photochemical model does not follow a power-law distribution (Figure 4c). Instead, it is well-matched by a log-normal

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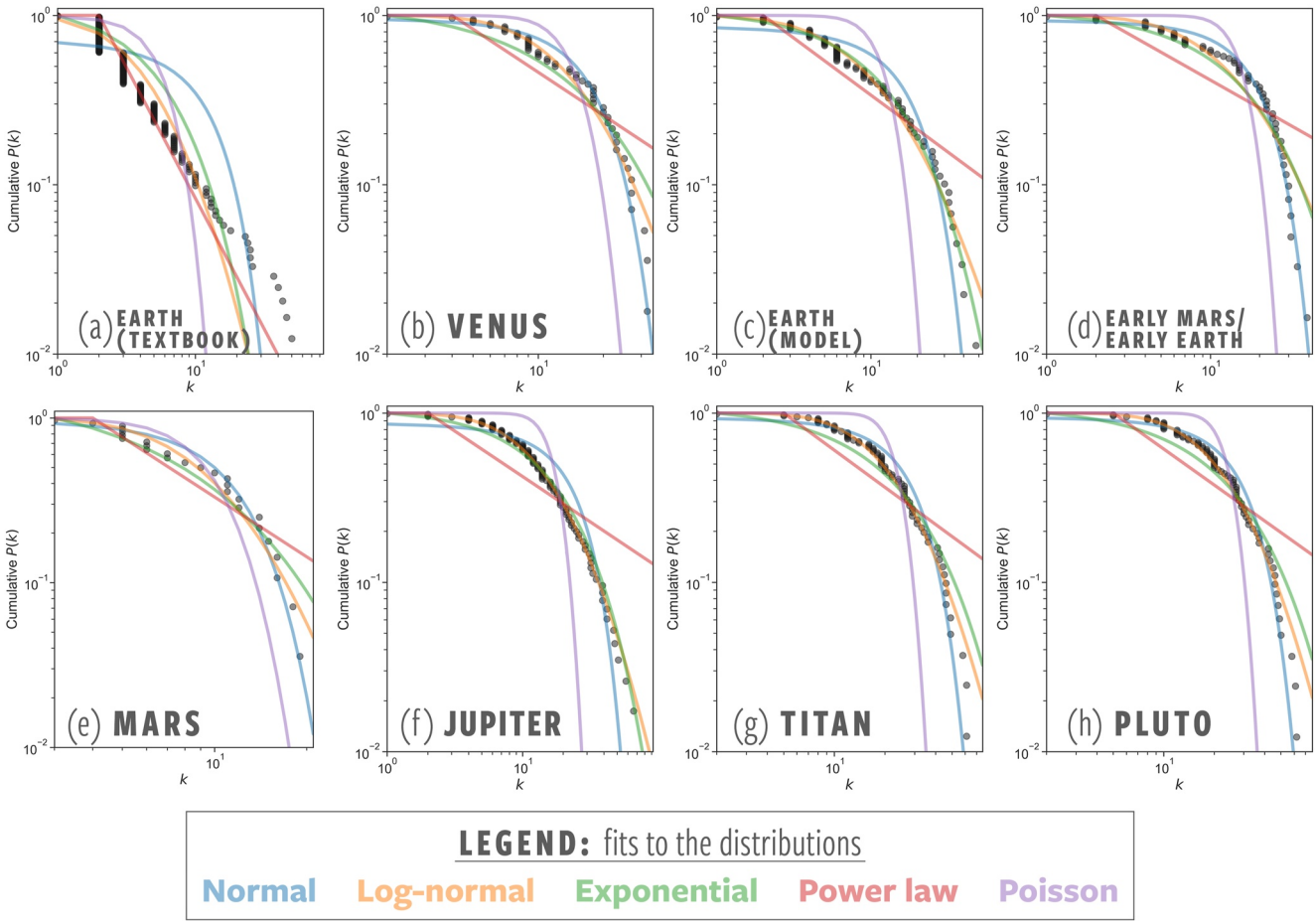

Figure 4. Fits to the cumulative degree distributions of various atmospheric chemical networks. (a) Earth (textbook), (b) Venus, (c) Earth (model), (d) early Mars/ Earth, (e) Mars, (f) Jupiter, (g) Titan, (h) Pluto. All of the degree distributions of these planetary networks are better fit by log-normal, normal, or exponential distributions over power-law or Poisson distributions. Consistent with Solé and Munteanu (2004), Earth's network from the Yung and DeMore (1998) textbook is well-matched by a power-law (scale-free) distribution, as evinced by its linear trend in log-log space. The other networks, including the Earth's network from the KINETICS model, do not display power-law distributions.

distribution, which is compatible with (Broido & Clauset, 2019)'s claim that scale-free networks are rare, and many real-world networks are better fit with log-normal distributions. All of the degree distributions of the planetary networks sourced from KINETICS models are better fit by log-normal, normal, or exponential distributions over power-law (scale-free) or Poisson (random) distributions.

Our analysis indicates that degree distribution may not be a useful tool for identifying signs of Earthlikeness or life on other worlds: while modern Earth's chemical reaction network may indeed have a power-law degree distribution, it is unlikely that we would construct a model that reflects this attribute of atmosphere using exoplanetary data in the near future. This begs the question whether Earth's atmosphere, as represented in photochemical models, can be distinguished from other atmospheres using network metrics besides degree distribution. The rest of Sections 3–5 are devoted to exploring this question.

3.3. Centrality Metrics

Centrality metrics quantify the "importance" of individual nodes within a network. Importance is an ambiguous concept—there are many different ways to estimate importance depending on what kind of connectivity one values the most—hence, myriad centrality metrics have been developed. Table 1 lists the centrality metrics employed in our analysis. Figure 5 shows the distributions of centrality values for the planetary atmospheres in this study.

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Table 1
Descriptions of the Centrality Metrics Employed in Our Analysis

	Degree centrality	Closeness centrality	Betweenness centrality	Information centrality	Subgraph centrality	Harmonic centrality	Average neighbor degree
Question	How many nodes is this node directly linked to?	What is the average distance between this node and every other node?	How many shortest paths between nodes in this network pass through this node?	How can this node affect other nodes using all possible paths?	How many closed walks start and end at this node?	What is the reciprocal of the sum of the shortest-path distances from all other nodes?	What is the degree of this node's neighbors?
Measure of importance	Popularity	Distance	Control	Influence	Cycles	Distance	Proximity to popularity
$C_u =$	$\frac{k_u}{N}$	$\frac{1}{\sum_v d_{uv}}$	$\sum_{v,u\neq u} \frac{\sigma_{vw}(u)}{\sigma_{vw}}$	$\frac{N}{\sum_v \frac{1}{I_{uv}}}$	$\sum_{k=0}^{\infty} \frac{\mu_k(u)}{k!}$	$\sum_v \frac{1}{d(u,v)}$	$\frac{1}{\lvert N(u)\rvert} \sum_{v\in N(u)} k_v$

Note. See text for further details.

Classic centrality metrics include degree centrality, closeness centrality, and betweenness centrality. For a unipartite, undirected graph, the *degree centrality* of node u is simply the fraction of all nodes within the network that u is connected to (equivalently, the degree k_u divided by the total number of nodes N in graph G). This metric measures importance by an individual's popularity and is often useful in social or epidemiological networks to measure, for example, the risk a person has of catching a disease or the number of followers an individual has on social media. The distribution of a network's degree centrality values is essentially the same as the distribution of its degrees, examined in the previous subsection. The *closeness centrality* of node u is the reciprocal of the average shortest-path distance d between u and all other nodes in the network. It equates node importance to its closeness to all the other nodes in the network. The *betweenness centrality* of node u is the fraction of shortest paths σ between other nodes in the network that pass through u. This metric was developed to characterize the control of communication in a social network (Freeman, 1977). Hence, betweenness centrality equates importance to control; u is important if it bridges the gaps between many other nodes.

While useful for certain purposes, these classic metrics may not always be the most enlightening for characterizing chemical reaction networks. Indeed, as Figures 6a and 6b show, the closeness and betweenness centrality distributions of Solar System atmospheres are not particularly revealing. Additionally, each of the classic centrality metrics described above suffers from conceptual drawbacks. Degree centrality is a highly local metric; it is not significantly influenced by the greater graph structure, placing outsized importance on a node's nearest neighbors. Meanwhile, closeness centrality and betweenness centrality make the implicit assumption that influence only travels along shortest path lengths—an assumption that may not always hold true.

In chemical reaction networks, catalytic cycles often play an important role in forming molecules from precursors. A prime example of this influence is the role that HO_x, SO_x, ClO_x, and NO_x chemistry have in recombining CO + O into CO_2 in terrestrial planet atmospheres (Gao et al., 2015; Yung & Demore, 1982). CO_2 is photolyzed to CO + O by ultraviolet photons of wavelength $\lesssim$200 nm. The direct recombination reaction, $CO + O \rightarrow CO_2$, is a spin-forbidden reaction, and CO_2 is primarily reconstituted on Mars via a HO_x cycle:

$$CO + OH \rightarrow CO_2 + H$$

$$H + O_2 + M \rightarrow HO_2 + M$$

$$\frac{O + HO_2 \rightarrow O_2 + OH}{\text{net} : CO + O \rightarrow CO_2}$$

where M is a third body (usually a background gas molecule) that does not participate in the reaction but is required to carry away excess energy to stabilize the photochemical product.

Using centrality metrics that only capture influence through shortest paths would therefore miss the contribution of a very important but indirect path $O \rightarrow OH \rightarrow CO_2$ (the fact that O, originally liberated from CO_2, can find itself back in CO_2 by way of OH).

For the reasons outlined above, we choose to utilize centrality metrics that are better suited for the task of characterizing the complex tangle of interactions in a chemical reaction network. One such metric is *information centrality* (Stephenson & Zelen, 1989). Information centrality was developed to model interaction in social networks and treats nodes as agents that can propagate signals between each other via the edges that link them. Signals propagate between nodes u and v not only via the shortest path between them, but by *all possible paths* that connect them. Each path $P_{uv}(s)$ has an information value $I_{uv}(s)$ proportional to its distance; for an unweighted graph, $I_{uv}(s) = 1/d_{uv}$, where d_{uv} is the distance between u and v. That is, longer paths between u and v suffer a penalty associated with greater "noise" or "resistance" and therefore transmit information poorly. Hence, information centrality is also known as *current flow closeness centrality* (Brandes & Fleischer, 2005). The total information between nodes u and v is $I_{u,v} = \sum_s I_{u,v}(s)$, and the information centrality of node u in graph G is defined as

$$\mathrm{IC}_u = \frac{N}{\sum_v \frac{1}{I_{u,v}}}. \tag{4}$$

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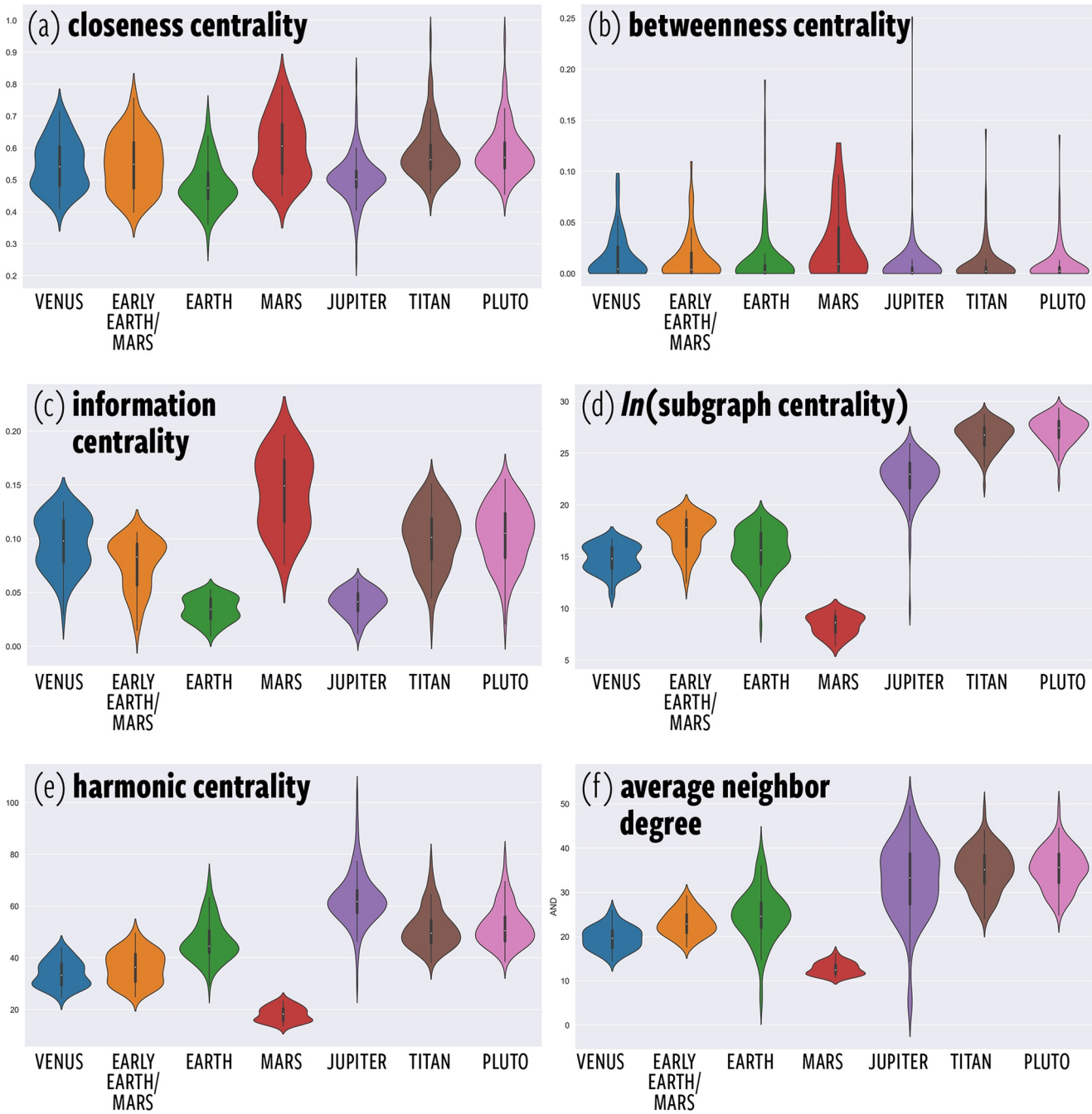

Figure 5. Violin plots showing the distributions of centrality metrics for nodes in each atmospheric network. (a) Closeness centrality, (b) betweenness centrality, (c) information centrality, (d) natural log of the subgraph centrality, (e) harmonic centrality, (f) average neighbor degree. See text and Table 1 for details about each metric. Each violin plot shows the kernel density estimation of the underlying data as well as a miniature box-and-whisker plot giving the median (white dot), upper and lower quartiles (box), and extent of distribution (whiskers).

On living worlds, if the atmosphere is tightly coupled to the biosphere through the exchange of atmospheric gasses, then functional (Hazen et al., 2007) or semantic (Kolchinsky & Wolpert, 2018) information may be expressed in the atmospheric system, and information centrality may be a key parameter with which to assess this information flow.

Another alternative centrality metric that takes into account each node's relationship to the entire graph structure is *subgraph centrality* (Estrada & Rodríguez-Velázquez, 2005). Subgraph centrality has been shown to

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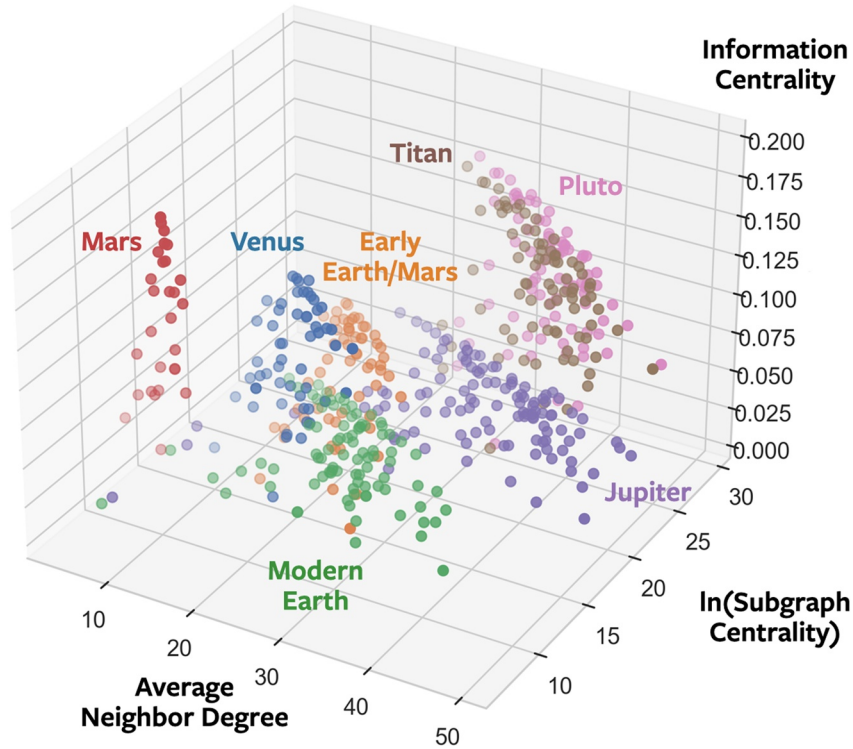

Figure 6. Three-dimensional scatter plot of network centrality metrics for the seven planetary atmospheres considered in this study. Each point represents a node in a network.

differentiate nodes whose classic centrality metrics (degree, closeness, betweenness, etc.) are identical. This metric characterizes a node's importance via the number of closed walks μ (or subgraphs) in the network that starts and ends at that node:

$$\mathrm{SC}_u = \sum_{k=0}^{\infty} \frac{\mu_k(u)}{k!}, \tag{5}$$

where k are powers of the adjacency matrix of G (see Estrada & Rodríguez-Velázquez, 2005 for the derivation). For an unweighted network, these walks are weighted such that their importance to the node's centrality decreases as the length of the walk increases (i.e., smaller subgraphs have higher importance). In this way, subgraph centrality is sensitive to catalytic cycles in a chemical network, be they triangles, squares, or otherwise.

We also consider *harmonic centrality* (Boldi & Vigna, 2014). The harmonic centrality of node u is similar in form to closeness centrality in that it uses distance as a measure of importance. But instead of being the reciprocal of the sum of the shortest-path distances from all other nodes to u, it is the sum of the reciprocal of the shortest-path distances from all other nodes to u:

$$\mathrm{HC}_u = \sum_{v} \frac{1}{d(u,v)}. \tag{6}$$

This metric is attractive from a network science perspective because it satisfies Boldi and Vigna (2014)'s three axioms for centrality, whereas closeness centrality satisfies none.

Finally, we consider the *average neighbor degree* (Barrat et al., 2004): the average degree of all of a node's neighbors, defined as follows:

$$\mathrm{AND}_u = \frac{1}{|N(u)|} \sum_{v \in N(u)} k_v. \tag{7}$$

This metric represents a node's proximity to well-connected nodes. For example, if u only has three edges but all of those edges connect to hub nodes that have dozens of edges each, u's centrality would be high according to its

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average neighbor degree; on the other hand, if u is a hub that connects to many spoke nodes, each of which rarely connects to anything else, u's centrality would be relatively low despite having a large degree.

Figure 6 is a three-dimensional plot that combines three centrality metrics: information centrality, subgraph centrality, and average neighbor degree. Each point in this diagram corresponds to a node in an atmospheric network. Using such a multidimensional centrality-metric space, we can differentiate between various planetary atmospheres, which occupy distinct (but overlapping) regions of this parameter space. This higher-dimensional view allows us to break degeneracies that occur when using only one centrality metric (e.g., Earth and Jupiter's similar distributions of information centrality).

4. Community Detection and Clustering

Community detection and clustering algorithms are powerful tools for characterizing the relationships among nodes and among groups of nodes within complex networks (Fortunato, 2010; Girvan & Newman, 2002). In general, community detection algorithms quantitatively determine the mesoscopic properties of network structure (Yang et al., 2016). With regard to our atmospheric reaction networks, community detection and clustering allow us to understand what chemical attributes contribute most to this structure.

4.1. Louvain Community Detection

Louvain community detection employs a heuristic method based on modularity optimization to extract the community structure of large networks (Blondel et al., 2008). Briefly, this method identifies community members iteratively in two phases: (a) starting with each node being its own distinct community, small communities are formed at a local level by maximizing the modularity of certain nodes; (b) each small community is aggregated into one "super node" to form a new "super node network" and the first step is repeated until there are no changes in the network and the modularity has been optimized (Blondel et al., 2008; de Meo et al., 2011). As an unsupervised algorithm, the Louvain modularity approach does not require a user to specify the number of clusters in a data set a priori and solves for the optimal number of clusters itself, thus removing some of the bias associated with many other clustering algorithms.

Figure 7 shows the results of community detection via the Louvain method on the force-directed graphs from Figure 1. The Mars network shows the presence of three distinct communities, while atmospheric networks for Venus, Titan, Pluto, early Earth/Mars have four communities each. Atmospheric networks for Jupiter and Modern Earth show a higher complexity in terms of community detection and contain at least six communities.

The Louvain method determines a network's communities based on graph structure alone, with no influence from the chemical composition of the nodes. Nonetheless, the algorithm tends to form communities based around common chemistries. For instance, the four communities in the Venus network can be classified as S_x-SO_x chemistry, Cl-S chemistry, H-bearing chemistry, and SO_x-NO_x chemistry. For Titan and Pluto, the community breakdown consists of hydrocarbon (C_xH_y) chemistry where $x \geq y$, hydrocarbon (C_xH_y) chemistry where $x \leq y$, nitrile (CN) chemistry, and CH_x-N_xH_y chemistry. Jupiter's communities are as follows: two hydrocarbon (C_xH_y) groups, nitrile (CN) chemistry, NH_x chemistry, O-bearing chemistry, and P-bearing chemistry. Although Jupiter's network is similar to those of Titan and Pluto in that it is dominated by high-centrality, high-degree H_x and CH_x nodes, the detection of NH_x-, O-, and P-themed communities speaks to the additional complexity brought by the existence of ammonia (NH_3), phosphine (PH_3), and water (H_2O) in Jupiter's highly reducing atmosphere.

Earth's network contains six communities. Three are dominated by high-degree nodes NO_2, OH, and Cl. Another encompasses the O_2-O_3-O Chapman chemistry as well as some of the ClO_x and NO_x compounds that are known to interact with this stratospheric cycle. Finally, there are two other communities of CH_2-bearing chlorine compounds and F_2-bearing chlorofluorocarbons, pointing to the added complexity that anthropogenic activity has imparted upon our atmosphere.

4.2. Distance Heatmaps

Heatmaps are frequently utilized to summarize the full extent of a data set in a visual form that is often easily interpreted by the human eye. Each occurrence of a variable or phenomenon in a data set is visualized using colors

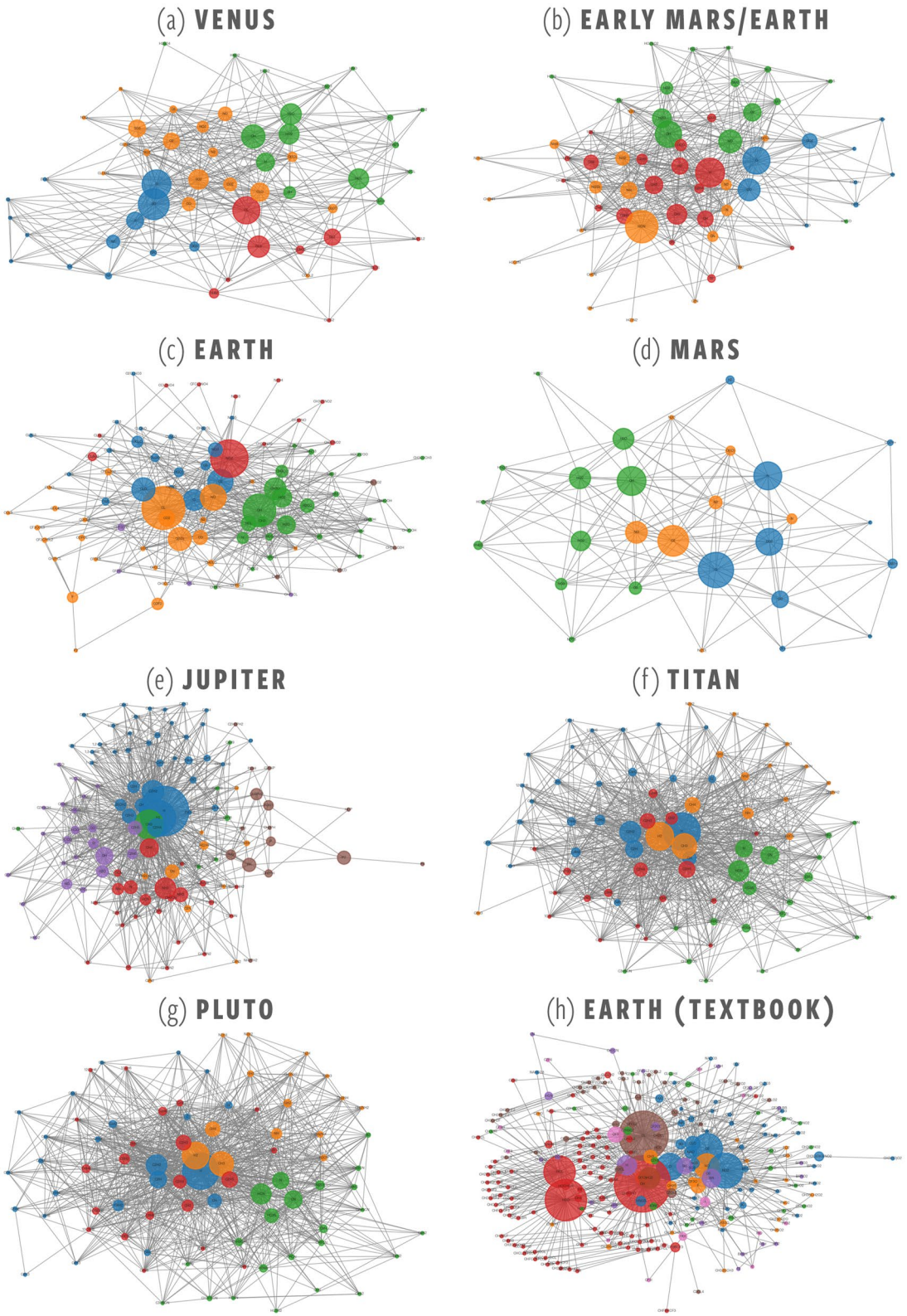

Figure 7. Network diagrams where nodes are colored by Louvain community assignment. Nodes are sized by betweenness centrality, as in Figures 1 and 2. (a) Venus: 4 communities, (b) Early Mars/Earth: 4 communities, (c) Earth: 6 communities, (d) Mars: 3 communities, (e) Jupiter: 6 communities, (f) Titan: 4 communities, (g) Pluto: 4 communities, (h) Earth (textbook): 7 communities.

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or shapes to represent the frequency or magnitude of variables or to depict relationships among variables (Galili et al., 2018; Perez-Llamas & Lopez-Bigas, 2011). Heatmaps can, however, be overwhelming when the data set that is being represented is particularly large and pairing a heatmap with a clustering algorithm is a common approach to adding additional context to the final visualization (Dhariwal et al., 2017; McKenna et al., 2016).

In Figure 8, we use heatmaps, structured by an agglomerative hierarchical clustering algorithm, to visualize pairwise resistance distances between pairs of species in our chemical networks. To calculate resistance distance values, a network is modeled as junctions or utility boxes (the nodes in the graph) that are connected by a series of resistors (the edges in the graph) controlling the flow of information or electricity in the graph (Lukovits et al., 1999). Large pairwise resistance distance values are indicators of information not being easily communicated between two nodes and lower values describe nodes that allow information to easily pass between one another (van Dam et al., 2014). In this way, resistance distance is related to information centrality (see Section 3.3). In our atmospheric networks, a pair of species will have a low resistance distance value if they react directly with one another and are also well-connected topologically via many routes (e.g., when both are in a highly connected cluster at the dense core of a graph). On the other hand, a pair of species will have a high resistance distance value if they do not chemically interact with one another directly and the average shortest path between them is long (e.g., two species situated at opposite outskirts of a graph). The resistance distances of the atmospheric networks were calculated using the NetworkX resistance distance function (Hagberg et al., 2008).

We then used a complete linkage agglomerative hierarchical clustering algorithm to structure the atmospheric network heatmap visualizations. An agglomerative hierarchical clustering algorithm treats each observation in a data set as its own individual cluster and merges them sequentially based on the similarity of a distance metric supplied by a user until all observations are in a single cluster (Everitt et al., 2011; Yim & Ramdeen, 2015). Complete linkage is a robust approach to defining distance between clusters and uses further neighbors to produce clusters that are more compact (Everitt et al., 2011). The complete linkage agglomerative algorithm was implemented using the "hclust" function of the "stats" package in R (R Core Team, 2016). The agglomerative clustering process can be depicted graphically using a dendrogram that displays how clusters are grouped and also highlights the order in which clusters were merged based on the similarity of the raw resistance distance values. Dendrograms were generated using the "as.dendrogram" function in the "stats" package (R Core Team, 2016). The dendrograms and the resistance distance matrices were supplied to a function named "heatmaply" to produce the final clustered heatmap visualizations (Galili et al., 2018). The negative natural logs of resistance distances were displayed in the final visualizations (Figure 8), in an effort to ease identification of similarities and discrepancies within and across the atmospheric heatmaps. Matrix elements with a raw resistance distance value of zero generated infinite values after the natural log transformation; therefore, these values were replaced with the second largest values (i.e., the largest non-infinite value) in the matrix.

5. Comparison to Equivalent Random Networks

So far, we have demonstrated that Earth's atmospheric network is distinct from those of other planetary atmospheres using global network metrics, centrality metric distributions, and community detection and clustering analyses. Although all of the model networks considered in this study are well-validated against planetary data and capture the essence of each atmosphere's photochemistry, they are neither exhaustive nor complete. Each network omits certain species and reactions, either for simplicity or because they are unknown or highly unconstrained at present. Naturally, the atmospheric chemistry of other planets is less constrained than that of Earth. Therefore, a question remains: Could Earth's network appear distinct from those of the other Solar System bodies simply due to the unique number of nodes and edges in Earth's atmospheric network (i.e., due to greater knowledge of our own planet relative to others), rather than the structure of its network?

To explore this question, we compare the metrics for our atmospheric networks to the metrics of their *equivalent random networks*, defined as networks created using a random network generator with the same number of nodes N and edges E as their atmospheric reaction network counterparts. For each planetary network, we generated equivalent random networks using the Erdős-Rényi model (Erdős & Rényi, 1959), where edges between nodes are picked with a probability $p = E/\begin{pmatrix} n \\ 2 \end{pmatrix}$. Because there is some small variance in network topology between randomly generated networks of the same N and p, we generated 100 of them and compared their averaged global

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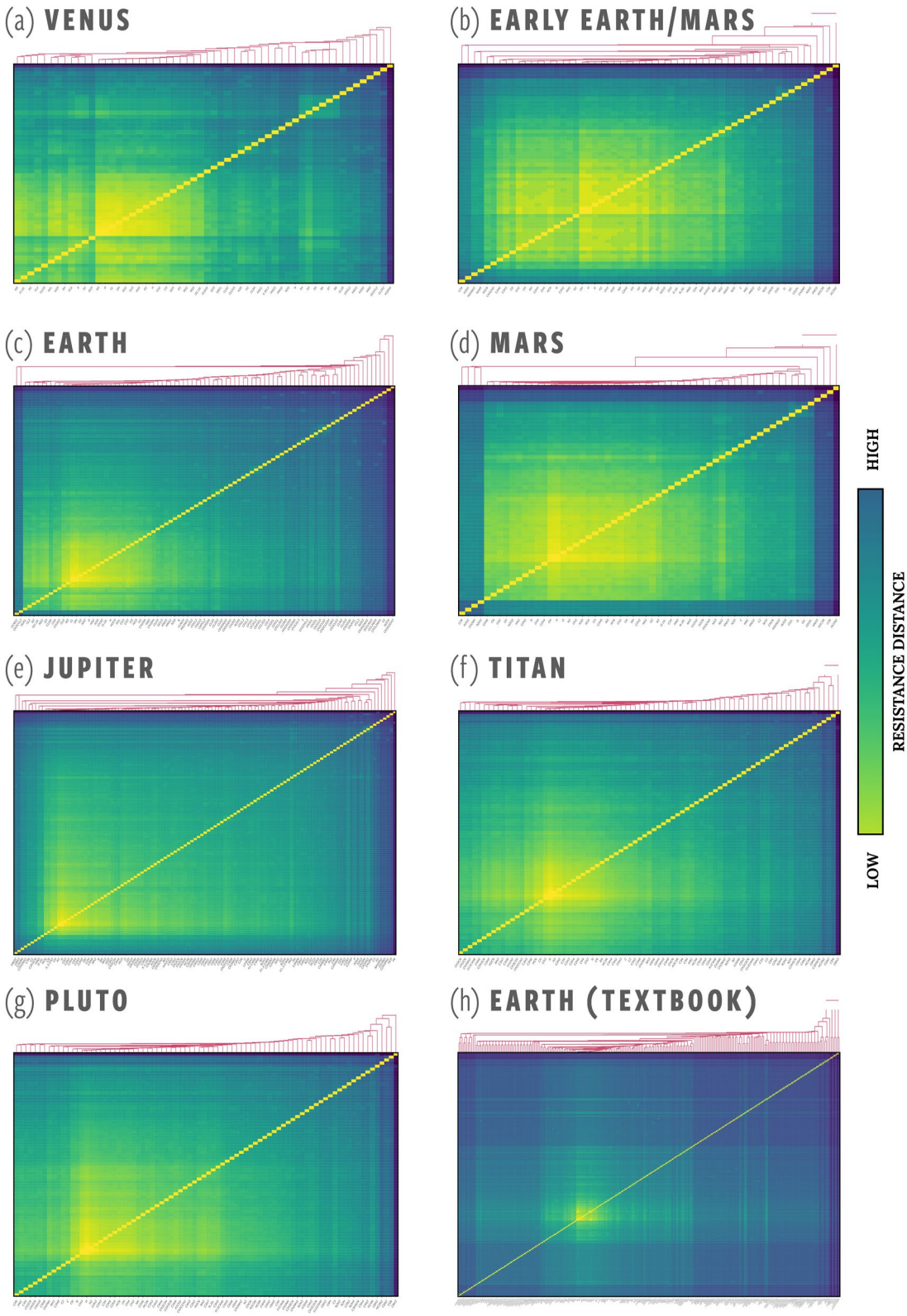

Figure 8.

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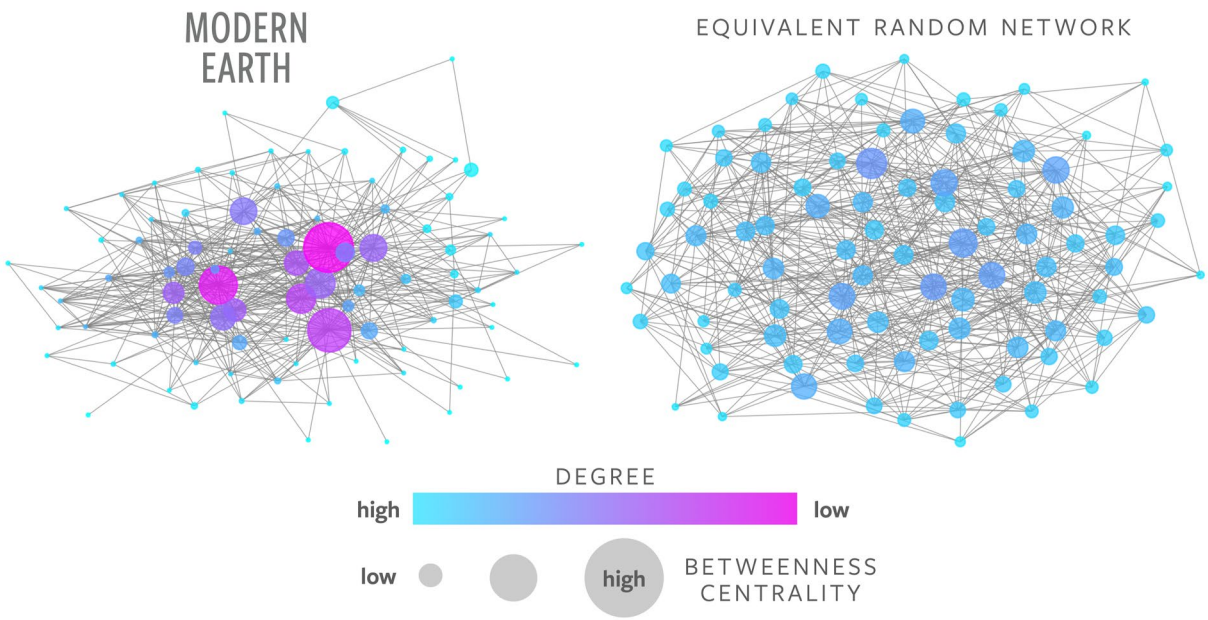

Figure 9. Earth's atmospheric chemical network (left) compared to its equivalent random network (right). Following the convention of Figures 1 and 2, node color represents degree and node size represents betweenness centrality.

metric values to their respective planetary networks. This method tended to produce much more homogenous graphs, as shown in Figure 9.

Figure 10 displays a comparison between planetary networks and their equivalent random networks, showing that Earth's atmosphere stands out as the *least* random planetary chemical network. Each bar represents a ratio: the planetary network's value divided by the average value of its equivalent random networks. For instance, in Figure 10c, Earth's network has a transitivity ratio of 2.94 (the highest ratio of all the planetary networks), meaning that Earth's actual transitivity was 2.94 times the mean transitivity of its equivalent random networks. That no planetary network has a transitivity ratio of ≈1 (Mars is the closest at 1.52) shows that none of the planetary networks approximate random networks. Figure 10f displays the natural log of the Estrada index, a metric from chemical graph theory that was developed to describe the 3D "compactness" or folding of molecular structures, such as proteins (Estrada, 2000). While the Estrada Index may not have any physical meaning for a chemical reaction network, it is still interesting that Earth's network deviates from randomness more than any other planetary network for this metric, too. Earth, followed by Jupiter, systematically shows the greatest deviation from the randomness of all of the planetary networks across these six metrics. This analysis suggests that Earth's network stands out among its planetary companions, and not merely due to the unique number of nodes and edges in its network.

6. Discussion

We have shown numerous ways in which the atmospheric reaction networks of Solar System bodies are topologically distinct from one another, with evidence that suggests that Earth's network may be somewhat unique. The networks used in this study come from state-of-the-art photochemical models of planetary atmospheres built from species and reaction lists in the Caltech/JPL KINETICS database. Generally speaking, photochemical models are built with specific atmospheric chemistry questions in mind, ranging from reproducing spacecraft

Figure 8. Resistance distance heatmaps of species in each atmospheric network. (a) Venus, (b) early Mars/Earth, (c) Earth, (d) Mars, (e) Jupiter, (f) Titan, (g) Pluto, and (h) Earth (textbook). Bright yellow colors represent low pairwise resistance distance between molecules and dark purple colors represent high pairwise resistance distance between molecules. The red dendrograms above each heatmap depict the results of the agglomerative clustering algorithm calculated using the raw resistance distance values. Elements closer together in the dendrogram and that merge at similar heights in the hierarchy are more similar than those that are farther apart. Mars and early Earth/Mars for instance have very large degrees of similarity within each network heatmap since many molecules merge at a similar point within the network hierarchy, while Earth (textbook) shows the greatest amount of variation in the distribution of resistance distance values since many different molecules merge at varying heights and in irregular numbers. The color scale is semi-qualitative because each heatmap is scaled to its own range of resistance distance values.

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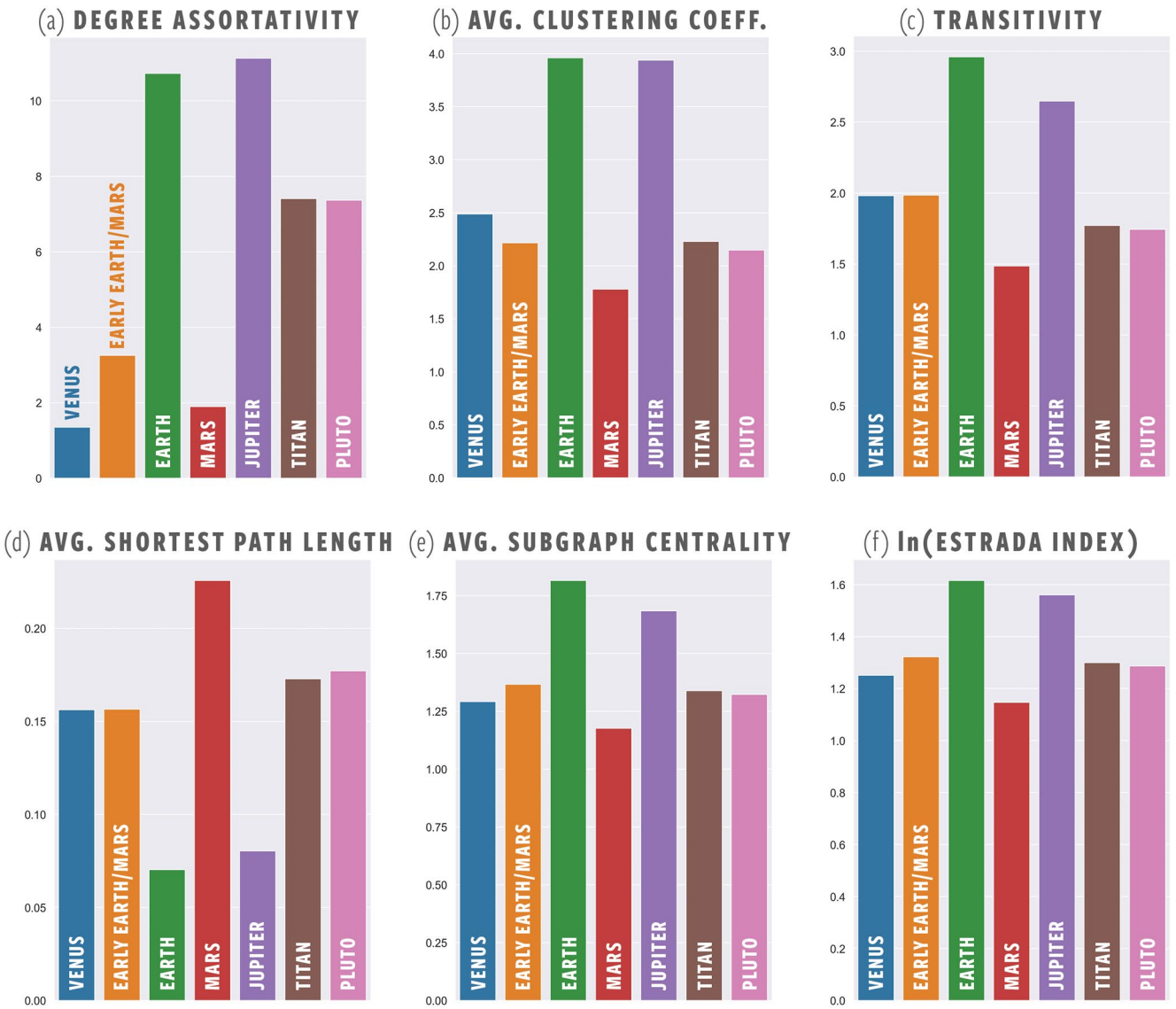

Figure 10. Bar graphs of global metric ratios between planetary networks and their equivalent random networks. For a description of metrics shown in (a–f), see main text. (a) Degree assortativity, (b) average clustering coefficient, (c) transitivity, (d) average shortest path length, (e) subgraph centrality, (f) the natural logarithm of the Estrada Index.

data to predicting the production of astrobiologically relevant molecules in paleoenvironments. Models will omit certain trace chemicals of negligible importance for the sake of computational simplicity and convergence. Thus, all photochemical models are *representations* of planetary atmospheres that do not contain every single known molecule or reaction and, of course, inevitably reflect gaps in present-day knowledge as well. That said, all of the chemical reaction networks in this study are well-validated by Earth and planetary observations save for one: early Earth/Mars. This network was taken from theoretical studies simulating CO_2-N_2-H_2O-dominated early atmospheres with minor amounts of CH_4 and H_2 and other trace CHNO species but omits important species, like S-bearing molecules (Adams et al., 2021; Wong, Charnay, et al., 2017). We envision that the network analysis in this contribution will be updated in the future as models increase in sophistication and knowledge of planetary atmospheres—both present and past—advances.

Across the various metrics we explored, the two most similar networks were Titan's and Pluto's. This result is to be expected as both are cold, N_2-dominated atmospheres, with CH_4 as the next most abundant component. Solar radiation and energetic particles destroy these major constituents, resulting in a cornucopia of hydrocarbon

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and nitrile chemistry that generates global atmospheric haze layers on both worlds (Cheng et al., 2017; Gao et al., 2017; Gladstone et al., 2016; Luspay-Kuti et al., 2017; Willacy et al., 2016; Wong, Fan, et al., 2017). Throughout our analysis, we find that Jupiter's chemical network also tends to stand out in a similar way to Earth's. We speculate that this similarity is due to the fact that Jupiter's chemical reaction network contains out-of-equilibrium species (e.g., CO) vertically mixed from depths at which they are thermochemically abundant or introduced via cometary material (Bézard et al., 2002; Prinn & Barshay, 1977). We conjecture that the inclusion of reaction rates and species abundances in future network analyses, via the use of weighted network representations, will more robustly distinguish Earth's network from Jupiter's.

6.1. Astrobiological Implications

The findings of this work invite the following astrobiological queries: How has the presence of life on Earth impacted the network structure of the atmosphere over billions of years of coevolution, and can an understanding of life's coevolution with atmospheric chemistry lead to the development of a novel agnostic biosignature?

We speculate that, in principle, it may be possible to use the topology of atmospheric chemical reaction networks as a sign of life. It is known that life on Earth exhibits common network structures across all scales, from biochemical to planetary (Kim et al., 2019). The modular hierarchical structure of biochemical networks hints at functionality, robustness, and error tolerance—attributes that would have been selected for via natural selection (Jeong et al., 2000, 2001; Ravasz et al., 2002). Just as the structures of biochemical networks have been honed by evolutionary processes to promote the survival of individual cells, it may be that any prolific, long-lived biosphere will evolve to exhibit persistence-enhancing features in its global-scale chemical networks.

Although the Earth as a whole is not evolving *Darwinianly* (i.e., through some form of planetary self-replication), the Earth as a complex adaptive system can evolve nonetheless (Lenton, 1998; Lenton and van Oijen, 2002). Evolution, in the broadest sense, can occur in any system where there are a large number of interacting agents, a way for those agents to access a variety of combinatorial states, and a selection mechanism (Hazen, 2009; Hazen & Eldredge, 2010). Many complex planetary systems, including atmospheric chemistry and the biosphere, satisfy these conditions. According to the theory of *persistence evolution*, the differential survival of non-reproducing, non-competing systems allows them to respond to natural selection and evolve toward greater robustness (Bouchard, 2008; Doolittle, 2017; Ford Doolittle, 2014). Many biological and social entities—from ecosystems to economic systems—are understood to evolve to maximize persistence through time; though these systems do not reproduce or form lineages, they can develop more resilient assemblages by establishing autocatalytic networks and functional redundancy (Dussault & Bouchard, 2017; Lenton et al., 2021). The biosphere, too, can be viewed as a complex adaptive system that, over time, would be incentivized to develop and strengthen homeostatic feedbacks that enhance its own self-perpetuation (Boyle & Lenton, 2022; Chopra & Lineweaver, 2016).

The fact that Earth's atmosphere has undergone major changes over geologic time does not preclude the evolution of homeostatic functions that involve the atmosphere. As the history of life demonstrates, living systems are generally stable against short-term perturbations but amenable to long-term evolution. Similarly, Earth's atmosphere may be both stable against short-term perturbations (e.g., solar flares) and amenable to slower changes that push it toward new attractors (e.g., the Great Oxidation Event) while not compromising short-term robustness. It would be of interest to test whether Earth's atmosphere has increased in robustness and resilience as the result of biological forcing over evolutionary history. While admittedly speculative, it may be that extraterrestrial civilizations that have consciously prioritized long-term homeostasis and wellbeing will purposefully affect their planets' atmospheric compositions such that they provide an even greater degree of stability (Frank et al., 2022; Wong & Bartlett, 2022).

Hence, examining the network topologies of planetary atmospheres may represent one plausible strategy for distinguishing abiotic worlds from those with mature biospheres (and potentially those with mature technospheres as well). Even if atmospheric network topology does not represent a standalone, definitive biosignature, it could contribute an independent line of evidence to life-detection frameworks (Green et al., 2021; Meadows et al., 2022), such as Bayesian approaches (Catling et al., 2018; Walker et al., 2018). For life on exoplanets, we may never be able to point to the highly evolved, non-random biochemical network of an extraterrestrial cell as a biomarker; however, we may be able to recognize the structural motifs of a highly evolved planetary atmosphere—regardless of what specific metabolisms emerged and gained prominence in that biosphere—as a sign of life. In

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other words, as far as exoplanets go, the detectable "unit of life" is not individuals, but the living planet itself. Others have made an analogy between the topology of cells and the large-scale organization of planets, most notably the vectorial nature of the thermodynamic driving force across cell membranes and the redox gradient between the interiors and exteriors of planets (Barge et al., 2017; Langmuir & Broecker, 2012; Russell, 2007). Perhaps such an analogy can be extended to include chemical network topology as well: Could it be that one universal hallmark of biology is the "rewiring" of flows of matter and energy into chemical networks—at all scales, from subcellular to atmospheric—that promote stability and facilitate information flow?

This line of reasoning presents us with a testable hypothesis: that biology should alter a planet's atmospheric chemistry in ways that enhance the system's stability against internal and external perturbations (e.g., from a solar flare or a sudden change in gas flux). Network functionality is best assessed through network dynamics (not explicitly assessed in this contribution), but certain aspects of dynamics may be reflected in network structure (examined here as unweighted graphs). In the case of the photochemical networks presented here, molecules are included in the networks based on their significance to the overall chemistry of the planetary atmosphere. For example, in the absence of methanogenic life, CH_4 and/or many of its photochemical derivatives might not be significant enough to appear in the modern Earth photochemical network, resulting in a different network topology that betrays a less biogeodynamic planet.

The relationships between network functionality, dynamics, and structure can be quantified through photochemical simulations, combined with a novel *weighted* representation of planetary reaction networks (Newman, 2004). Weighted representations probe far more information contained in atmospheric reaction networks than the unweighted graphs examined in this study. In a weighted representation, nodes and links may have weights corresponding to chemical abundances and the rates of reactions, respectively, allowing changes in species concentrations and chemical timescales to alter the network topology. Because the set of biogenic gasses overlaps significantly with the set of geologically derived gasses, the mere *presence* of a certain gas in a network is not a conclusive indicator of biology. (If searching for life on other planets were as easy as identifying a single molecular species, there would be no need for the more holistic approach we argue for here.) Instead, it is crucial to understand individual gas's relationships to other molecules in the photochemical network, using the context of chemical connectivity to derive the overall network's dynamics and functionality. Thus, weighted representations would be a significant advance toward enabling the discrimination between living and nonliving worlds, and we advocate for the development of weighted network representations of atmospheric chemical networks in future work.

Another pillar of living systems is information processing, which includes the transduction of raw internal or external data into "meaningful" information through functional context and causal coupling (Bartlett & Wong, 2020; Fields & Levin, 2020; Wong & Prabhu, 2023). As a global courier of matter and energy, a major player in all biogeochemical cycles, the regulator of climate, and the Earth's interface with exogenous radiation, an enormous amount of meaningful information may flow through the atmosphere at the planetary level (Frank et al., 2022). This could potentially be quantified using the tools of functional information (Hazen et al., 2007), semantic information (Kolchinsky & Wolpert, 2018), or some new formulation that takes into account atmospheric network topology. We leave this quantification to future research.

Identifying how and why the atmospheric networks of Solar System bodies differ from one another is merely the first step in developing a novel network-based exoplanet biosignature. Because the Solar System presents us with only a handful of planetary atmospheres—just one of which is known to reflect the influence of life—it is not reasonable to expect the present analysis to definitively reveal whether the network topologies of living worlds *in general* are distinguishable from nonliving ones. The coevolutionary history between life and planet on Earth represents but one trajectory in a potentially vast phase space of living worlds. Exoplanetary biospheres may produce atmospheric networks that do not have the exact same metrics as Earth's, though they are nonetheless highly evolved and resilient. Similarly, the atmospheric chemistries of the other Solar System worlds represent only a handful of (presumably) abiotic cases in a far larger phase space of nonliving worlds. That these abiotic Solar System networks do not always resemble each other is not surprising given the diversity of chemical constituents and redox states represented among the atmospheres of Venus, Mars, Jupiter, Titan, and Pluto. Our results are still consistent with the hypothesis that these other Solar System bodies belong to a much wider ensemble of nonliving worlds whose commonalities can be identified when a larger population is studied.

Thus, the development of a potential network-based planetary atmospheric biosignature will rely on modeling *ensembles* of biotic and abiotic worlds, with different initial conditions and evolutionary histories, through

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time. The statistically robust identification of network trends across these ensembles—using existing and future network theory tools (see Section 6.2)—may enable us to map out the network-metric phase space of living worlds, in contrast to that of nonliving worlds. Furthermore, if network metrics can robustly group stages of biological evolution across worlds with different geochemical contexts, then this approach may help uncover a possible universal connection between life and planetary complexity and shed light on a theory of life at the planetary scale. On the other hand, we cannot rule out the possibility that an ensemble approach will reveal that there is no network theoretic difference between planets with and without life. This "null-result" would be a fundamental contribution to astrobiology, as it would refute the working hypothesis that life adds additional complexity to a planetary system that can be detected remotely.

6.2. Network Science and Data Science Implications

Data-driven planetary science and astrobiology research offers new and promising data science challenges. Answering some of the most important questions in astrobiology and planetary science is contingent on solving these data science challenges and developing methods that can assimilate information stored in these data sets and identify hidden patterns and trends.

In the case of exploring planetary atmospheres, we need to develop methods that can characterize the atmospheric compositions of planets and distinguish the atmospheres of biotic and abiotic planets. Network science is the obvious choice to explore planetary atmospheric compositions because the data structure of its chemical reactions is the same as the edge list for a network. Additionally, network science explorations are ideally suited to explore and understand small- to medium-sized data sets. As shown in this paper, we have been able to explore network topologies for planetary atmospheres and identify distinctions between various Solar System atmospheric chemical networks.

However, to characterize the differences between the atmospheres of biotic and abiotic planets, we need to explore the relationships among planetary atmospheres as part of a single "network environment." There are a few ways to make this comparison, all of which require the development of new metrics and methods.

First, we need to be able to characterize the relationship among subgroups in the network while preserving the relationship with the whole network. For instance, after Louvain community detection identifies a certain number of communities within a network (Section 4.1), we want to understand not only the relationships among the individual groups but also how each group relates to the entire network structure (something that cannot be done with current methods). We are currently working to develop a set of network metrics that can be applied to a spectrum of network data, from one node to a group of nodes. These metrics will describe characteristics of the subgraph while maintaining its context and relationship with the larger network. We call such metrics *granular network metrics*. Such granular network metrics will help us explore a specific part of the planet's atmosphere and compare its impact on the whole of the atmosphere. For example, we can focus on characterizing the impact of Earth's biosphere on its atmosphere and compare that with the impact of Earth's technosphere on its atmosphere.

Second, we need to compare planetary atmospheres as a single data system to be able to extract underlying patterns and network motifs from these atmospheres. We propose the use of *multilayer networks* for this study (Kivelä et al., 2014). By combining innovations in granular network metrics and multilayer networks, we plan to study, compare, and find underlying patterns in the atmospheres of planets with biology and those without. We plan to do this by simulating the evolution of an ensemble of biological planets to create a set of biotic planetary atmospheres with different geochemical and biochemical inputs. Each biotic planetary atmosphere will be a single layer in our multilayer network setup. Similarly, we will study abiotic planetary atmospheres to see if we can extract the underlying patterns in those atmospheres. Our goal in this future study is to see if there are any motifs that emerge in biotic planetary atmospheres that are distinct from motifs in abiotic planetary atmospheres. As stated in the previous subsection, the impact of finding such motifs may be far reaching, helping us carve a path to identify planetary-scale biosignatures.

7. Conclusions

We have revisited the topologies of atmospheric chemical reaction networks as unipartite, unweighted, and undirected graphs following the work of a pioneering study by Solé and Munteanu (2004). We sourced our atmospheric

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networks from state-of-the-art photochemical models that reproduce the chemical profiles of Solar System atmospheres to high fidelity and consider atmospheres that were not available to Solé and Munteanu (2004) at the time of their work. Furthermore, we utilized a broader array of network science techniques to examine and compare our planetary networks, including visualization as Kamada-Kawai force-directed graphs (Section 2); additional centrality metrics, such as information centrality and subgraph centrality, which we argue are more appropriate than classic centrality metrics for understanding chemical reaction networks (Section 3.3); community detection, cluster analysis, and distance heatmaps (Section 4); comparison to equivalent random networks (Section 5).

Our exploration of the topologies of atmospheric chemical reaction networks has shown that one can distinguish the chemistries of Solar System atmospheres through the lens of graph theory. In certain metrics, Earth's network seems to resemble those of living networks. The working hypothesis that Earth may be distinct, in chemical network topology, from the ensemble of non-living worlds is not simply due to the unique number of nodes and edges in Earth's network; when compared to their equivalent random networks, Earth's atmospheric network appears to stand out amongst the other planetary networks in this study.

This finding invites future innovations in both astrobiology and data science. We suggest that long-lived biospheres will tend to construct atmospheric networks with robust and adaptive properties, and that learning to interpret the vast parameter space of network topologies of exoplanetary atmospheres may lead us to a novel biosignature. To test these hypotheses, larger populations of planets must be studied and more intricate network analyses must be developed and employed, including weighted and multilayer network representations and granular network metrics. We suggest that future work should take an ensemble approach to mapping out the network-metric phase space of living versus nonliving worlds to identify a potential planetary-scale biosignature.

Data Availability Statement

Data and code used in this study—including chemical reaction lists, code to read chemical reaction lists into a NetworkX environment, the resulting network edge lists, and the Louvain community detection code—are hosted on the project's GitHub repository (Wong, 2022).

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Erratum

In the originally published version of this article, the citation "Fisher et al., 2022" was omitted from the last sentence of the third paragraph of the Introduction. The sentence should read: "Here, we leverage network science to address key questions in atmospheric chemistry, comparative planetology, biosignature detection, and astrobiology (Fisher et al., 2022)." The full reference has been added to the reference section. This version may be considered the authoritative version of record.

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