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

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**Introduction:** Solé and Munteanu (2004) (S&M) first suggested that the chemical reaction network of Earth's atmosphere is topologically distinct from that of other planetary atmospheres. These authors speculated that the uniqueness of Earth's atmospheric network is due to a nonlinear coupling between the biosphere and the atmosphere through the exchange of gases, implying that the network topology of Earth's atmosphere reflects the presence of life. Furthermore, the coevolution of biosphere and atmosphere suggests that the network topologies of atmospheric chemical networks have the potential to serve as an *agnostic* biosignature, because such a description relies less on specific molecules but rather on the nature of the relationships among molecules. However, before atmospheric networks can be used as an astrobiological tool, their analysis requires further development. Here, we build upon S&M's work and explore a more diverse set of atmospheric networks using new graphical representations and topological metrics to classify the network topologies of planetary atmospheres.

**Methods:** We map the chemical reaction networks of Solar System atmospheres using reaction lists from the Caltech/JPL photochemical model KINETICS (Allen et al., 1981), a versatile and extensively validated code for simulating planetary atmospheric chemistry. Specifically, we analyze chemical reaction networks for: Venus (Zhang et al., 2012), Modern Earth (Yung et al., 2019, 1980), 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 et al., 2017). Our network visualizations and analyses are performed primarily using NetworkX (Hagberg et al., 2008).

**Results:** We visualize planetary atmospheres as force-directed unipartite networks, where nodes are chemical species linked by shared reactions. In Figure 1, node color denotes *degree* (the number of links it has) and node size denotes *betweenness centrality* (the number of shortest paths between other nodes in the network that pass through a node). This visualization allows us to qualitatively gauge network characteristics, such as symmetry, "hub" vs. "spoke" nodes, deceptively important nodes (low degree but high centrality), and node distance.

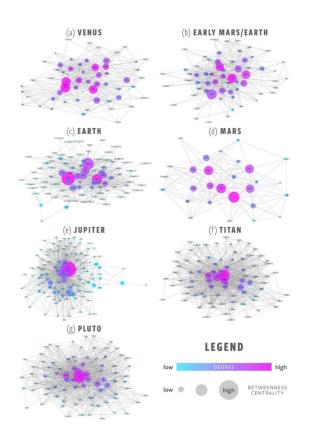
We quantify network structure using a panoply of well-established network metrics including but not limited to: transitivity, degree distribution, centrality distributions, community detection algorithms, and hierarchical clustering. We also compare the metrics of atmospheric networks to equivalent random networks generated using the Erdős-Rényi model (Erdős and Rényi, 1959).

While our modern Earth network does *not* follow a power-law degree distribution (contrasting with S&M's findings), Earth can be distinguished via different metrics. For example, Figure 2 shows that Earth's *degree assortativity*, a measure of whether nodes of similar degree are connected to one another, stands out against various planetary networks and is more similar to certain biological networks. This finding 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 still stands out amongst the other planetary networks in this study.

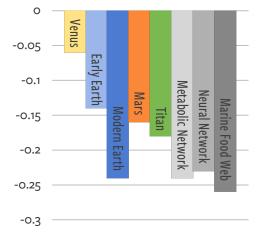
**Discussion:** We speculate that, in principle, it may be possible to use the topology of atmospheric chemical reaction networks as a sign of life. It is known that life on Earth exhibits common network structures across all scales, from biochemical to planetary (Kim et al., 2019). The modular hierarchical structure of biochemical networks hints at functionality, robustness, and error tolerance—attributes that would have been selected for via natural selection (Jeong et al., 2001, 2000; 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.

While informative, unipartite graphs offer a *minimal* description of chemical reaction networks because they lack any information about chemical abundances and reaction rates. Hence, we advocate for the use of *weighted* and *directed* network representations, which we plan to pursue in future work. Such representations will incorporate far more information about chemical networks, which are not merely characterized by whether species are present or absent, but also by their abundances and fluxes. If network metrics can robustly group stages of biological evolution across worlds with different geochemical contexts, this may help uncover a possible universal connection between life and planetary complexity and shed light on a theory of life at the planetary scale.



**Fig. 1** Solar System atmospheric networks. 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.

Network Degree Assortativity



**Fig. 2** Network degree assortativity for various planetary atmospheres and biological networks. The lower the assortativity, the more heterogeneous the network is. This is one example of how the topology of modern Earth's chemical network bears resemblance to that of biological networks.

## **References:**

- Adams D, Luo Y, Wong ML, et al. Nitrogen Fixation at Early Mars. Astrobiology 2021;21(8):968–980; doi: 10.1089/ast.2020.2273.
- Allen M, Yung YL and Waters JW. Vertical Transport and Photochemistry in the Terrestrial Mesosphere and Lower Thermosphere (50-120 Km). J Geophys Res 1981;86(A5):3617–3627; doi: 10.1029/JA086iA05p03617.
- Erdős P and Rényi A. On Random Graphs. Publ Math 1959;6(290).
- Hagberg AA, Schult DA and Swart PJ. Exploring Network Structure, Dynamics, and Function Using NetworkX. In: Proceedings of the 7th Python in Science Conference. (Varoquaux G, Vaught T, and Millman J. eds) Pasadena, CA USA; 2008; pp. 11–15.
- Jeong H, Mason SP, Barabási A-L, et al. Lethality and Centrality in Protein Networks. 2001.
- Jeong H, Tombor B, Albert R, et al. The Large-Scale Organization of Metabolic Networks. Nature 2000;407:651–654.
- Kim H, Smith HB, Mathis C, et al. Universal Scaling across Biochemical Networks on Earth. 2019.
- Moses JI, Fouchet T, Be B, et al. Photochemistry and Diffusion in Jupiter's Stratosphere: Constraints from ISO Observations and Comparisons with Other Giant Planets. J Geophys Res 2005;110:1–45; doi: 10.1029/2005JE002411.
- Nair H, Allen M, Anbar AD, et al. A Photochemical Model of the Martian Atmosphere. Icarus 1994;111(1):124–150; doi: 10.1006/icar.1994.1137.
- Ravasz E, Somera AL, Mongru DA, et al. Hierarchical Organization of Modularity in Metabolic Networks. Science (1979) 2002;297:1551–1555.
- Solé R V. and Munteanu A. The Large-Scale Organization of Chemical Reaction Networks in Astrophysics. Europhysics Letters 2004;68(2):170–176; doi: 10.1209/epl/i2004-10241-3.
- Willacy K, Allen M and Yung Y. A NEW ASTROBIOLOGICAL MODEL OF THE ATMOSPHERE OF TITAN. Astrophys J 2016;829(2):1–11; doi: 10.3847/0004-637X/829/2/79.
- Wong ML, Fan S, Gao P, et al. The Photochemistry of Pluto's Atmosphere as Illuminated by New Horizons. Icarus 2017;287:110–115; doi: 10.1016/j.icarus.2016.09.028.
- Yung YL, Long J, Jiang JH, et al. Effect of the Quasi-Biennial Oscillation on Carbon Monoxide in the Stratosphere. Earth and Space Science 2019;6(7):1273–1283; doi: 10.1029/2018EA000534.
- Yung YL, Pinto JP, Watson RT, et al. Atmospheric Bromine and Ozone Perturbations in the Lower Stratosphere. J Atmos Sci 1980;February:339–353.
- Zhang X, Liang MC, Mills FP, et al. Sulfur Chemistry in the Middle Atmosphere of Venus. Icarus 2012;217(2):714–739; doi: 10.1016/j.icarus.2011.06.016.