Study of a theoretical model for the origin of molecular complexity based on network science

Marcos Martínez[1,3], Izaskun Jiménez-Serra[1], Raúl Guantes[2] and Jacobo Aguirre[1,3]

[1]Centro de Astrobiología (CAB), CSIC-INTA, Torrejón de Ardoz, Madrid, Spain
[2]Instituto 'Nicolás Cabrera', Facultad de Ciencias, Universidad Autónoma de Madrid, 28049 Cantoblanco, Madrid, Spain
[3]Grupo Interdisciplinar de Sistemas Complejos (GISC), Madrid, Spain

Despite the recent detection of an increasing number of complex organic molecules in outer space [1], the origins of this molecular complexity are still unclear. Traditional astrochemical models predict the evolution of molecular abundances in astrophysical environments by taking into account all chemical reactions that are possible in these environments. However, these models suffer from overparameterization and rely on uncertain estimations of kinetic rates [2], suggesting a need for alternative models that can explain the emergence of complexity from first principles. The NetWorld framework, a recently developed computational environment based on complex networks in interaction, has shown promising results in the study of the emergence of molecular complexity [3]. NetWorld simulates astrochemical environments through the evolution of abstract network structures that can join or be divided at different rates, producing an artificial chemistry of networks that is able to reproduce important properties related to the origin of complex molecules with potential prebiotic interest.

In this work we developed a new version of the NetWorld computational framework that is more efficient and closer to real chemistry, as well as an analytic approximation based on molecular kinetics and ODEs. We used the computational and analytic versions of NetWorld to characterize this framework in more detail, studying the effect of different parameters on abundance dynamics and equilibria. Our results suggest that the new versions of NetWorld can act as good approximations of real astrochemical environments despite their extremely simplified kinetics and lack of realistic reaction mechanisms. Furthermore, NetWorld was able to predict relations between abundance and network properties that were later generalized to the abundances of real molecules in space.

References

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