Kinetic Characterization of a Chemical Model System with Chiral Symmetry Breaking

by

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Abstract

Investigations were undertaken which characterized the parameter space of a novel computational chemical model system that demonstrates chiral symmetry breaking under several sets of conditions. The model described is completely symmetrical with no thermodynamic or kinetic advantage in place. The model displays chiral symmetry breaking after a quasi-equilibrium state and quick amplification of the initial break to near homochirality. Using two different computational programs, we performed temperature scans to find an optimal temperature for the model as well as investigated the governing equations and ratios in order to predict whether or not the model would display chiral symmetry breaking. These results were demonstrated in both the stochastic and deterministic programs. Our computational model of chiral symmetry breaking suggests a signature for the evolution of life on Earth and elsewhere. Our better understanding allows us to make connections to other theories of origins life.

Introduction

Many biological molecules display chirality, a property that describes the three-dimensional shape of molecules such that one form is non-superimposable with its mirror image. The two different forms are called enantiomers. For chiral molecules, the molecular formulas are the same, however the structures and therefore the shapes are different, which can lead to the chiral molecules having different biological properties (chemical and physical properties of enantiomers are identical). Chirality is denoted in several different ways: one notation relates to optical activity and another relates to the absolute 3-D structure. The notation, R or S, is used to designate handedness (3-D structure) of enantiomers while $_{D}$ and $_{L}$ denote the optical activity of the enantiomer. In ordinary chemical reactions, both chiral forms –

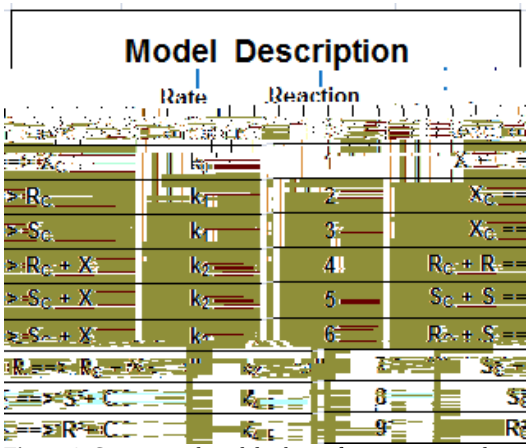

Figure 1: Symmetrical model scheme for computational programs; X is a prochiral precursor to R or S, C is an interactive surface to which X, R, or S can bind and k's are rate constants.

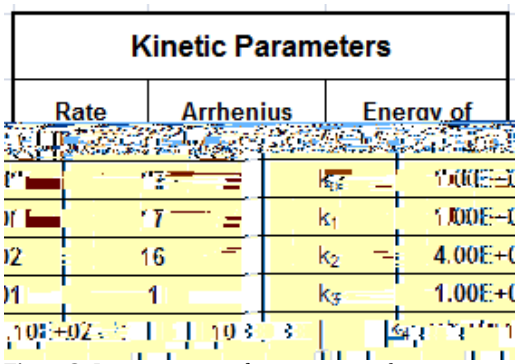

Figure 2: Input parameters for computational programs.

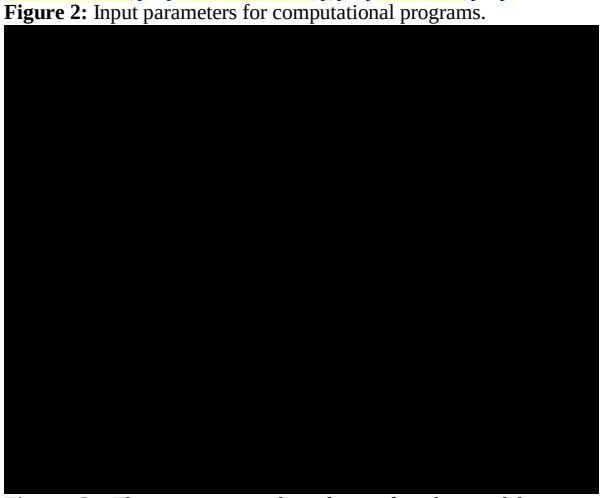

Figure 3: The temperature boundaries for the model were investigated for several sets of different initial conditions. The output of the temperature boundary analysis for the conditions R = S = 0M, X = 1M C = 1 M (held constant) and all intermediates are 0M are shown in Figure 3.

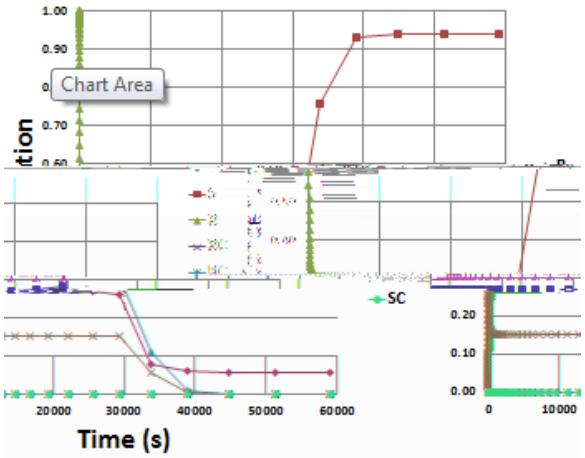

Figure 4: A typical output from Kintecus for the model under the conditions R = S = 0M, X = 1M C = 1 M (held constant) and all intermediates are 0M is shown.

hurdle for the evolution of life and is possibly the signature for life.

We previously concluded that a perfectly

Acknowledgements

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References

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