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...Understanding how life emerges from cosmic and planetary precursors

Theoretical Study of Autocatalytic Mechanisms and Homochirality

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- Gather understanding on the kinetic models describing the Soai Reaction
- Verify the performance of the kinetic models
- Analyze and quantify the nonlinear behavior associated with these models (limit cycles, chaos) in order to have predictions to experimentally validate.

Homochirality in Biomolecules

- Most essential molecules associated with life exhibit homochirality

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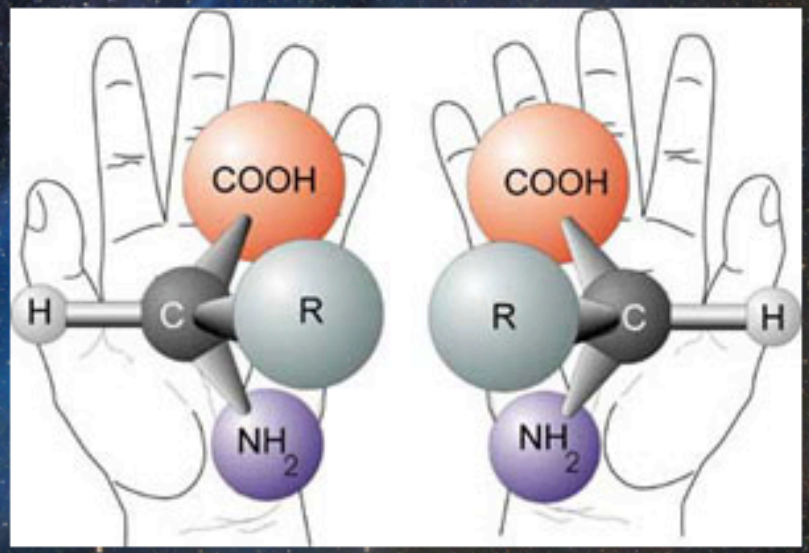

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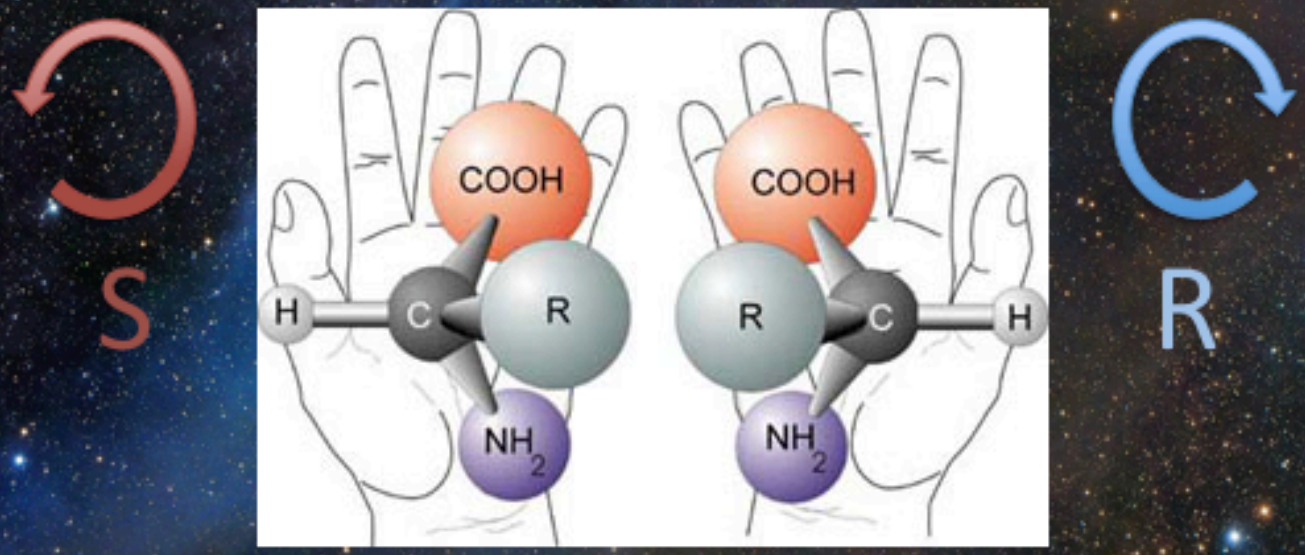

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$$A + B \longrightarrow 2B$$

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Simple Autocatalytic Reaction

Reaction	Step
$A \longrightarrow R$	I
$A \longrightarrow S$	II
$A + R \longrightarrow 2R$	III
$A + S \longrightarrow 2S$	IV
$R + S \longrightarrow RS$	V

Autocatalysis

- Simplest form of autocatalysis
- F. C. Frank found a theoretical model for a autocatalytic, enantio-selective reaction
- Quantifying homochirality

$$A + B \longrightarrow 2B$$

enantiomeric excess

$$ee = \frac{R - S}{R + S} \times 100\%$$

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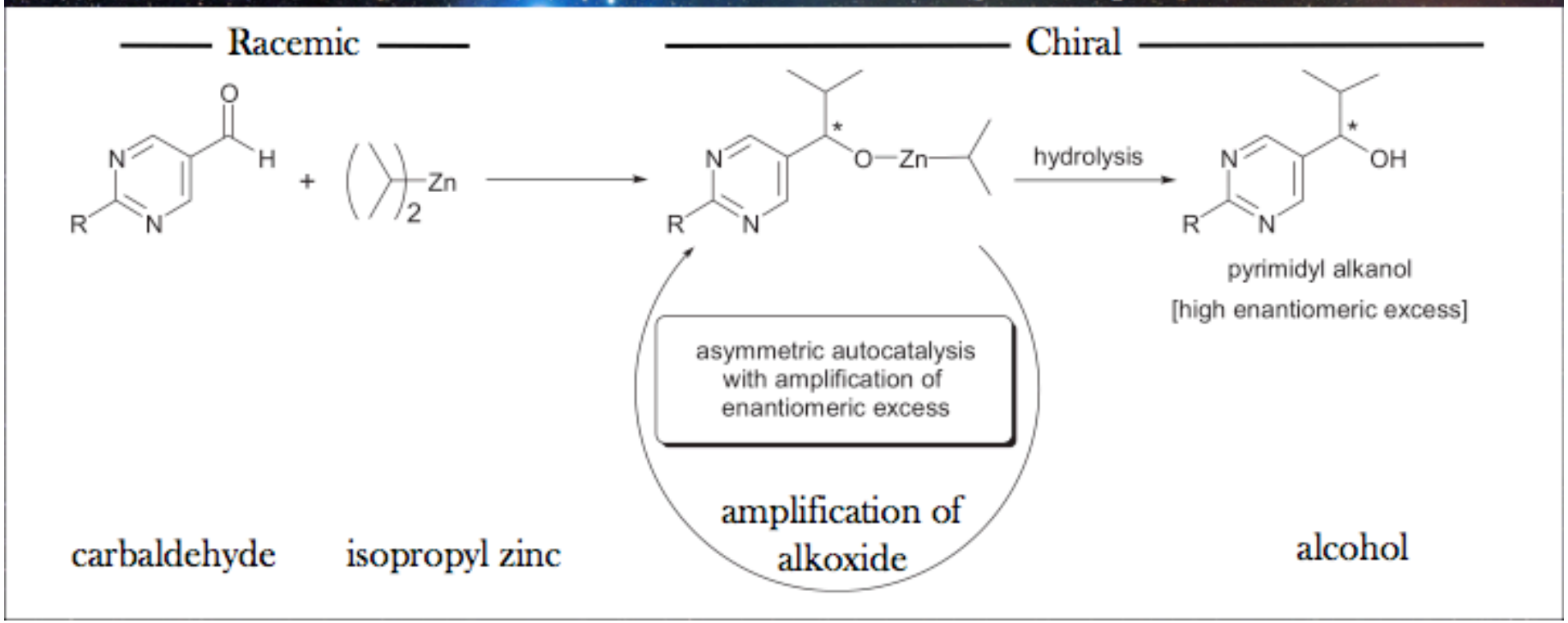
The Soai Reaction

- First example of a chiroselective autocatalysis in an organic reaction system. 1995
- It can start from an achiral set of initial concentrations and produce up to 100% ee.

diagram adapted from Buhse et al (2005)



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- Proposed kinetics uncertain
  - Islas et al (2005) model 1
    - Simplified model that demonstrates enantio-selectivity
  - Buhse/Micskei (2008) model
    - Complex model with potentially exotic dynamic behavior

Let's Study: Simple Model

- Autocatalytic model, based on F.C. Frank, 1953

Islas Reactions for model 1 (2005)

Reaction	Rate Parameter	Value	Step
$A \longrightarrow R$	k_0	$1.0 \times 10^{-6}\ s^{-1}$	I
$A \longrightarrow S$	k_0		II
$A + R \longrightarrow 2R$	k_1	$1.0\ M^{-1}s^{-1}$	III
$A + S \longrightarrow 2S$	k_1		IV
$R + S \longrightarrow RS$	k_2	1.0×10^{2}	V

Corresponding Nonlinear ODEs

$$\frac{dA}{dt} = -2k_0A - k_1AR - k_1AS$$

$$\frac{dR}{dt} = k_0A + k_1AR - k_2RS$$

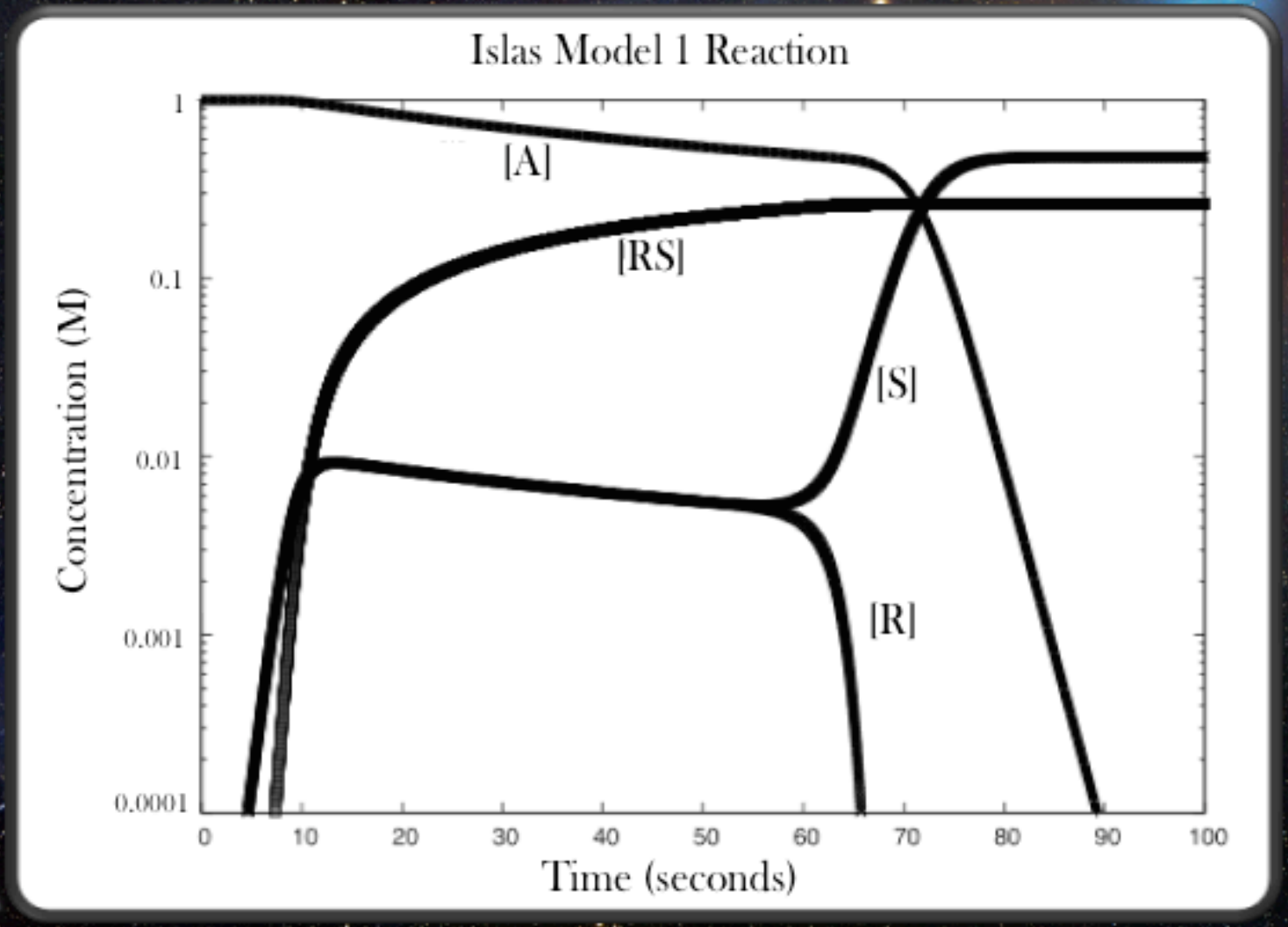
$$\frac{dS}{dt} = k_0A + k_1AS - k_2RS$$

$$\frac{d(RS)}{dt} = k_2RS$$

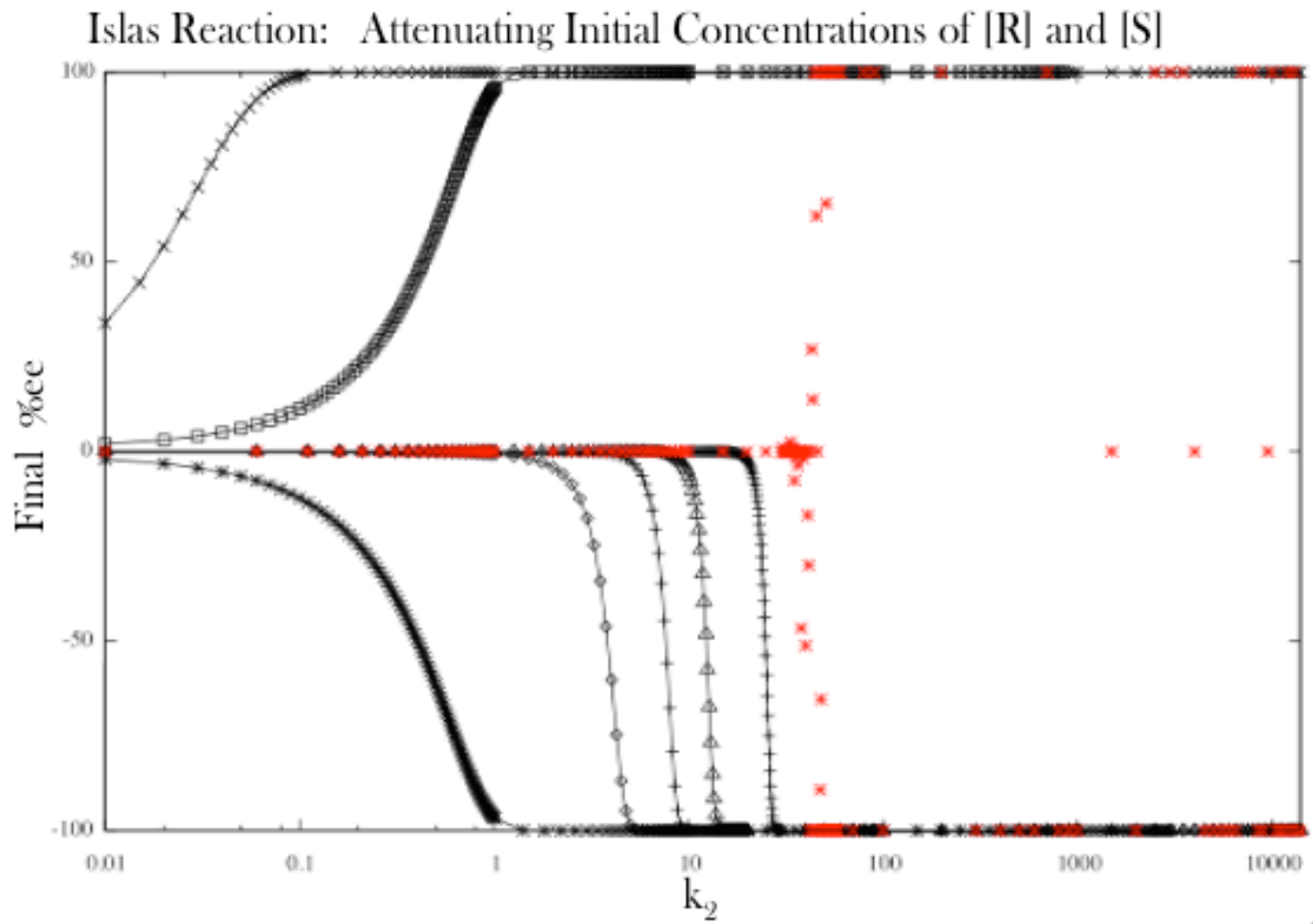
Islas et al (2005)

- Solved with GEAR algorithm for stiff systems

Reaction Characteristics: Mirror-symmetry Breaking



More Characteristics



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- Analyzing its Lyapunov spectra
  - Lends to quantifiable predictions on the system's chaotic/stable behavior
- Gathering predictions for experimental validation
  - Verifying a kinetic model for the Soai reaction

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