

*This guide is only meant as a practical checklist. For theory, background, and detailed methodology, consult the manuscript and SI.*

## Workflow Instructions: Thermodynamic Modeling of Amino Acid Synthesis on Titan

This archive contains all data and code used in the study “Prebiotic Chemistry Insights for Dragonfly: Thermodynamics of amino acid synthesis in Selk-sized craters on Titan” (Madan et al.). The goal of this document is to provide step-by-step guidance for reproducing or learning from the workflow, especially for reviewers and early-stage students.

### Overview of Workflow

1. Collect/estimate Gibbs free energy data.
2. Polynomial fitting to generate coefficients.
3. YAML input file setup.
4. Cantera Equilibrium Models.
5. Data collection/analysis.

### File Inventory

- Gibbs energy data: Gibbs\_Energies\_All.csv
- Gibbs energy estimator: Gibbs\_Energy\_Estimator\_298K.ipynb
- Polynomial Fitting: Polynomial\_Fitting.ipynb
- YAML data: yaml\_entry\_all.yaml
  - *Note:* This is a culmination of species entries, not a directly runnable input file. Individual YAML input files must be created per simulation.
- YAML example input file: Alanine\_Example\_Input.yaml
  - This is an example of how to structure the input files.
- Cantera Model Example: Cantera\_Equilibrium\_Skeleton.ipynb

### Step-by-Step Workflow

1. Collect/estimate Gibbs free energies.
  - a. Reference Gibbs\_Energies\_All.csv for all the Gibbs data we collected or estimated.
  - b. For estimation of a molecule of your choice, you can run Gibbs\_Energy\_Estimator\_298K.ipynb as per the instructions in the notebook. The

caveat is that for any molecule lacking published data, you will need to run a quantum chemical simulation (OPT, then FREQ at 298 K) using the level of theory, basis set, and solvation model defined in the manuscript.

2. Fit NASA9 polynomials.
  - a. Open Polynomial\_Fitting.ipynb and fit Gibbs energy vs. T curves.
  - b. You will obtain the two 9-term coefficient sets that will go into the species entry in the yaml input files.
3. Build YAML input files.
  - a. Use Alanine\_Example\_Input.yaml as a template.
  - b. Copy species entries from yaml\_entry\_all.yaml as needed for each model.
4. Run equilibrium models
  - a. Open Cantera\_Equilibrium\_Skeleton.ipynb and run as per the instructions.
5. Collect and analyze results.
  - a. You can print out the results or export to a csv format for easier processing later on.