

Boltzmann_Population_Calculator

Description

This Python script calculates the Boltzmann population distribution for a set of molecular conformations based on their energies. It's specifically designed to work with the output from the "Print_Information_Gaussian.py" script, which should be available in the same repository.

Features

- Reads energy data from a user-specified text file
- Calculates relative Boltzmann populations based on molecular energies
- Displays results sorted by population percentage

How it works

1. The script prompts the user to enter the name of the input file containing molecular energies.
2. It reads the file, extracting molecule names and their corresponding energies in Hartree.
3. Using the Boltzmann distribution formula, it calculates the relative population of each molecular conformation at a specified temperature (default is 298.15 K or 25°C).
4. The results are displayed, showing each molecule's name, energy, and relative population percentage, sorted from highest to lowest population.

Input File Format

The input file should be a text file with each line containing:

molecule_name,energy_in_Hartree

For example:

i01_A.log,-2820.251500

i01_B.log,-2820.247356

...

This format is compatible with the output generated by the "Print_Information_Gaussian.py" script.

Usage

1. Ensure you have Python 3 installed on your system.
2. Run the script:

./Boltzmann_Population_Calculator.py

3. When prompted, enter the name of your input file (e.g., "Search_results.txt").
4. The script will display the calculated Boltzmann populations for each molecule.

Constants

- Gas constant (R): 0.008314 kJ/(mol·K)
- Default temperature (T): 298.15 K (25°C)
- Conversion factor: 1 Hartree = 2625.5 kJ/mol

Note

This script assumes that the molecular energies are in equilibrium and that there are no significant interactions between molecules other than those reflected in their energies.

Dependencies

This script uses only Python standard libraries and does not require any additional installations.