C8862
Free Energy Calculations exercise

4. Statistical Thermodynamics – Ideal Gas

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Excercise I

1. Determine composition of equimolar mixture of H_2O and D_2O (in gas or liquid state). At this time, assume that O-H and O-D bonds have the same energy.

Result: $H_2O:D_2O:HDO=1:1:2$

2. How the composition changes if you consider difference between O-H and O-D bonds (evaluate at qualitative level).

Exercise II

1. Calculate standard changes of thermodynamic properties such as H, S, and G describing dimerization of acetic acid in gas phase (ideal gas model) at standard conditions. Compare ΔG with the change of potential energy. What is the contribution of ZPE from vibrations?

Notes:

- all calculations will be done in Gaussian
- first, calculate all data at semiempirical level of theory (PM6)
- if all is OK, then use higher level of theory such as PBE0/def2-TZVPP with D3BJ dispersion correction (start from geometries optimized on PM6)