Lab5

Thermochemistry

- Enthalpy and free energy

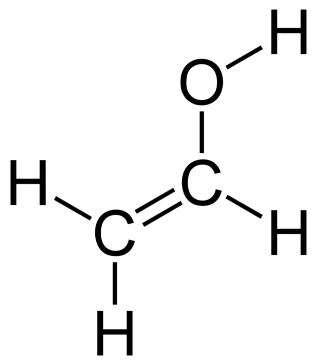
  https://gaussian.com/wp-content/uploads/dl/thermo.pdf

Hands-on - transition state

- What are the two isomers of vinyl alcohol and their respective transition state (do frequency calculations to confirm the nature, transition state or a local minimum?

  Coordinates:

  https://www.dropbox.com/scl/fo/drz05o8c3mubzkssb5ycs/h?rlkey=lpmk31x7vb374rbqscxcp01lh&dl=0

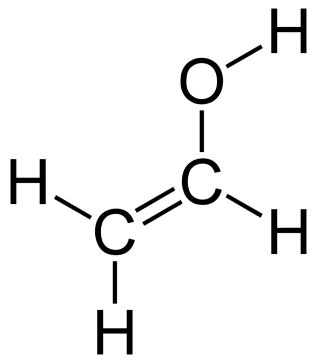


Hands-on - thermochemistry

- What is the stability trend of vinyl alcohol isomers across a temperature range of 0 to 500 K, in intervals of 50 K (you need to compute free energies)?

  Coordinates:

  https://www.dropbox.com/scl/fo/drz05o8c3mubzkssb5ycs/h?rlkey=lpmk31x7vb374rbqscxcp01lh&dl=0



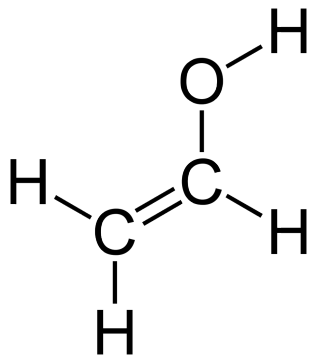
Hands-on - thermochemistry

- Compute the solvation free energy of vinyl alcohol at 298 K? Learn about the appropriate keywords from the gaussian manual.

  Coordinates:

  https://www.dropbox.com/scl/fo/drz05o8c3mubzkssb5ycs/h?rlkey=lpmk31x7vb374rbqscxcp01lh&dl=0

  Equation: $\Delta G_{sol} = G_{298K,sol} - G_{298K}$, gas-phase



References

1. https://avogadro.cc/
2. https://gaussian.com/gaussian16/
3. https://gaussian.com/wp-content/uploads/dl/thermo.pdf