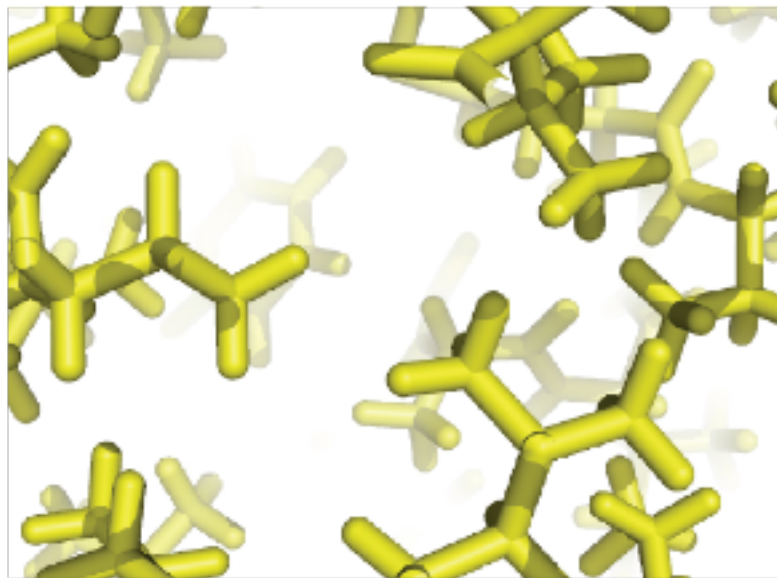


Ant Thermodynamic Cycle for Absolute ΔG of Binding

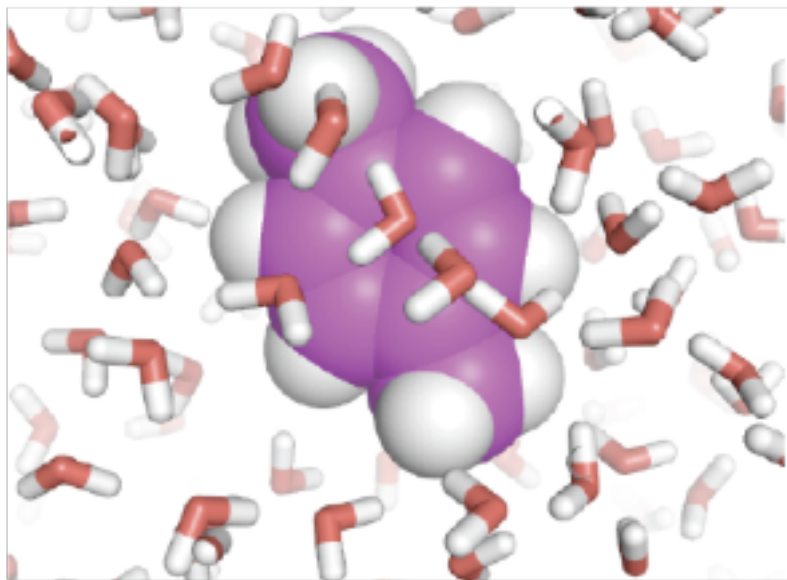
Cycle: Boresch et al., J. Phys. Chem. B
107:9535 (2003)

See also Gilson, Biophys J. 1997.

From [1]

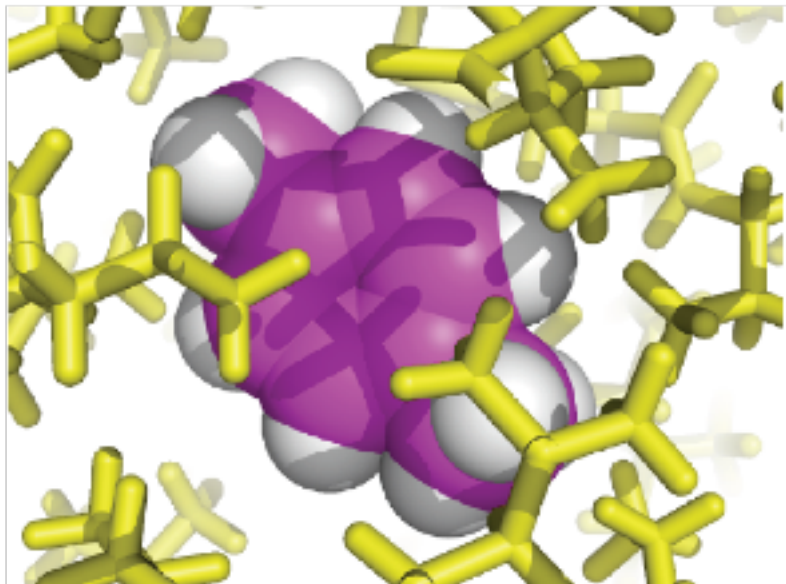




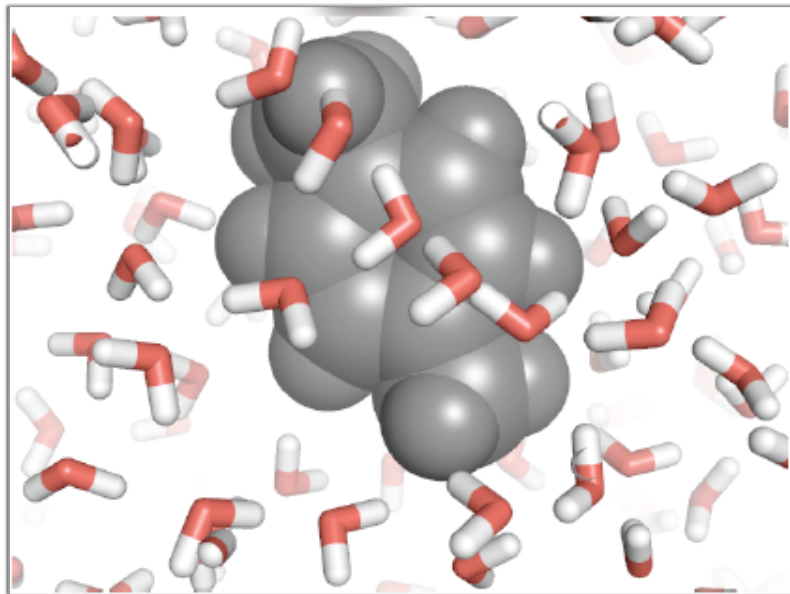


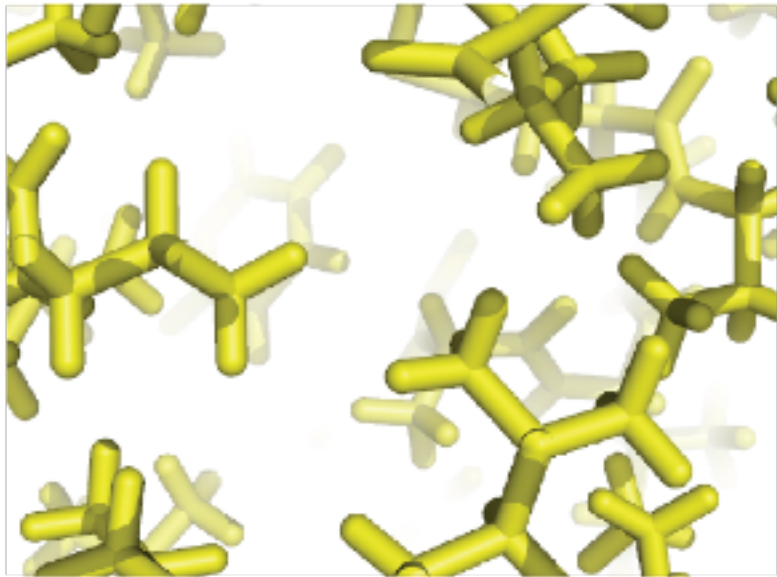
ΔG°



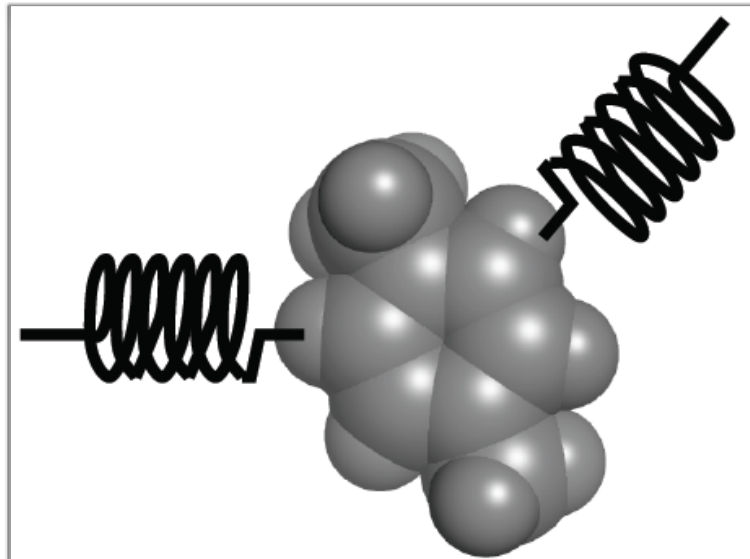




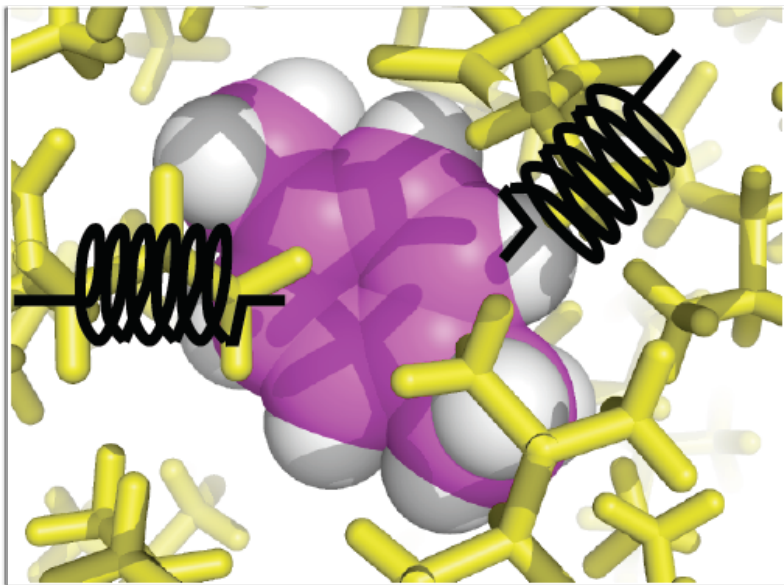


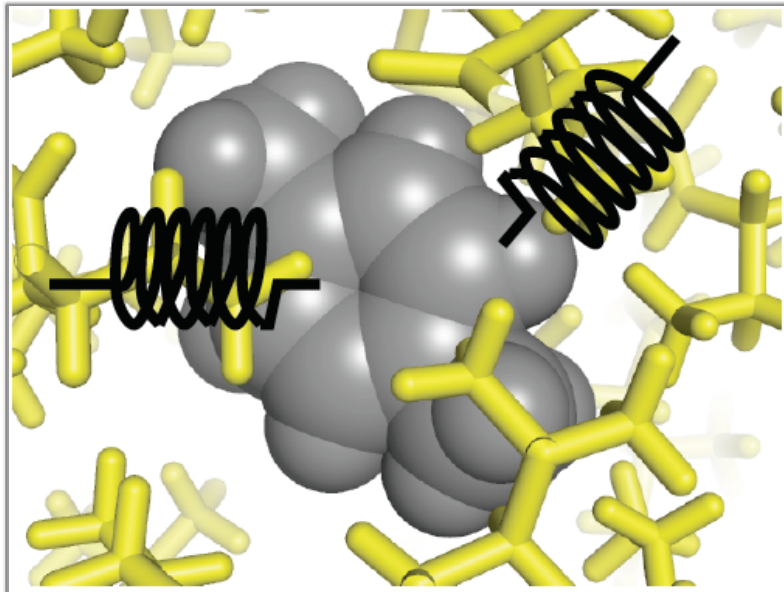


+



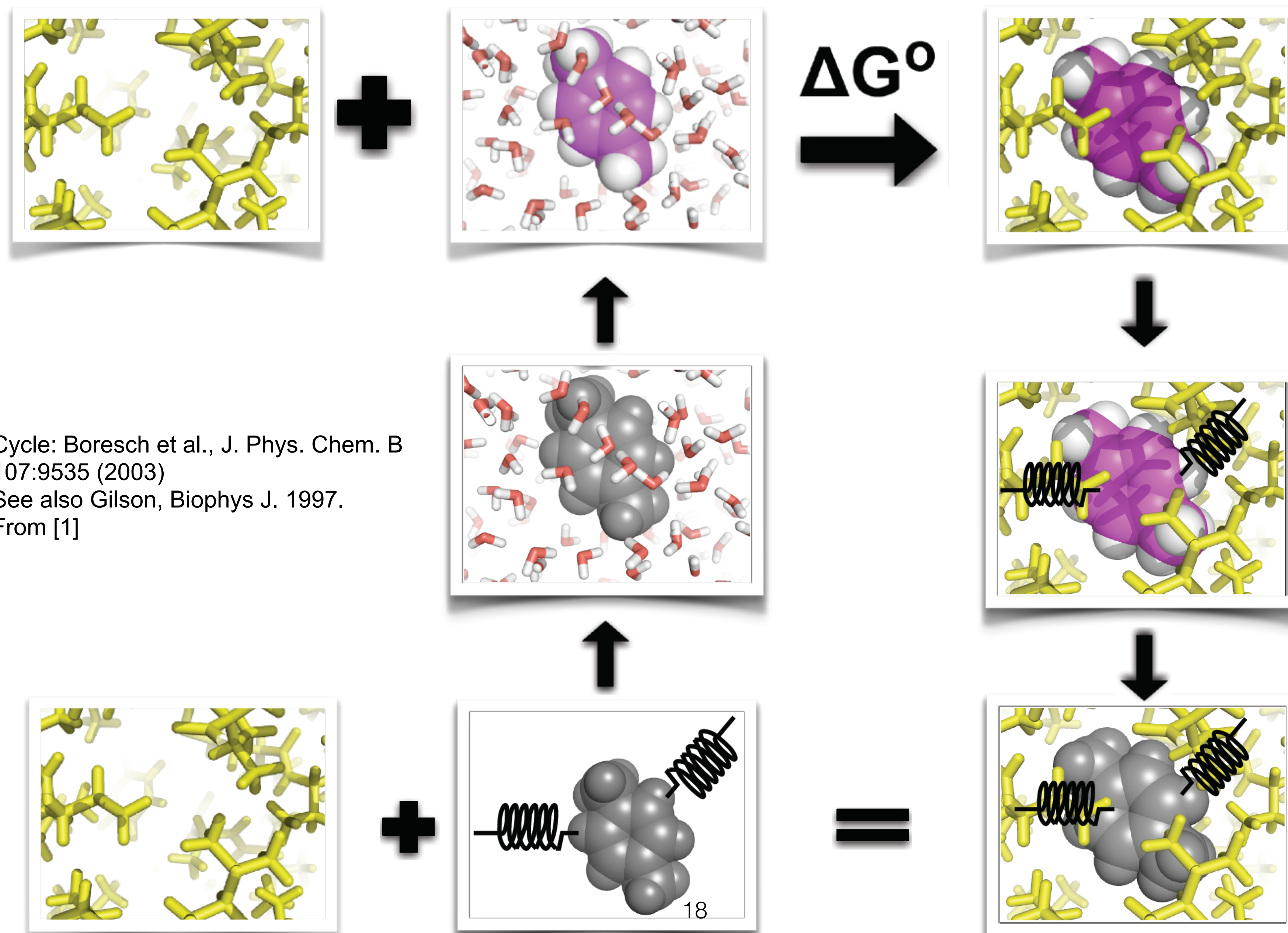
=







A Thermodynamic Cycle for Absolute ΔG of Binding



Cycle: Boresch et al., J. Phys. Chem. B
107:9535 (2003)
See also Gilson, Biophys J. 1997.
From [1]

References

- [1] Many parts of today's lecture were adapted from a lecture by David Mobley (https://github.com/MobleyLab/drug-computing/tree/master/uci-pharmsci/lectures/free_energy_basics) under the CC BY 4.0 license. The lecture is part of the Drug Discovery Computing Techniques course (PharmSci 175/275) at UC Irvine.
- [2] Zwanzig, R. High-Temperature Equation of State by a Perturbation Method. I. Nonpolar Gases. *Journal of Chemical Physics* 1954, 22 (8), 1420.
- [3] Bennett, C. H. Efficient Estimation of Free-Energy Differences from Monte Carlo Data. *Journal of Computational Physics* 1976, 22 (2), 245–268.
- [4] Shirts, M. R.; Chodera, J. D. Statistically Optimal Analysis of Samples from Multiple Equilibrium States. *Journal of Chemical Physics* 2008, 129 (12), 124105.