Molecular simulations of biomolecules
Remote Lecture #5

comments on Homework #5
dealing with ligands

CCB 550, Spring 2020

Comments on your class project/term paper

course

- Choose a paper of interest to you that uses either quantum chemistry or force field modeling
- Design and carry out some sample computations that could reproduce or extent the reported results
- Paper will describe: background; results reported in the paper; discussion of your calculations; conclusions
- Paper is due in four weeks(!), on May 4.
- **Important:** before you begin computing or writing, you must send me email giving your choice of paper, and outlining the proposed calculations. I will approve and/or make suggestions, as appropriate

Comments on homework #5

Here's what I got after minimizing the structure of the formamide dimer with B3LYP/6-31G*:

SCF Done: E(RB3LYP) = -339.805525627 A.U. after

....

Sum of electronic and thermal Enthalpies= -339.701726

Sum of electronic and thermal Free Energies= -339.742469

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	64.543	24.576	85.751
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	39.405
Rotational	0.889	2.981	27.361
Vibrational	62.765	18.615	18.985

and from the same calculation on the monomer:

SCF Done: E(RB3LYP) = -169.888843121 A.U.

Sum of electronic and thermal Enthalpies= -169.838636

Sum of electronic and thermal Free Energies= -169.868893

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	30.913	10.923	63.680
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	37.339
Rotational	0.889	2.981	21.213
Vibrational	29.135	4.961	5.128

thermochemistry differences

ΔH = dimer $-$ 2(monomer) = $\begin{cases} -15.4 \\ -2.9 \end{cases}$ kcal/mol

ΔG = " "

$\Delta(-TS) = -298.15\,(39.405/1000) \Rightarrow -11.75$

trans $-2[$ " $37.399\ ] \Rightarrow 2(-13)$

translational $+10.5$

total $\Delta(-TS)$ S

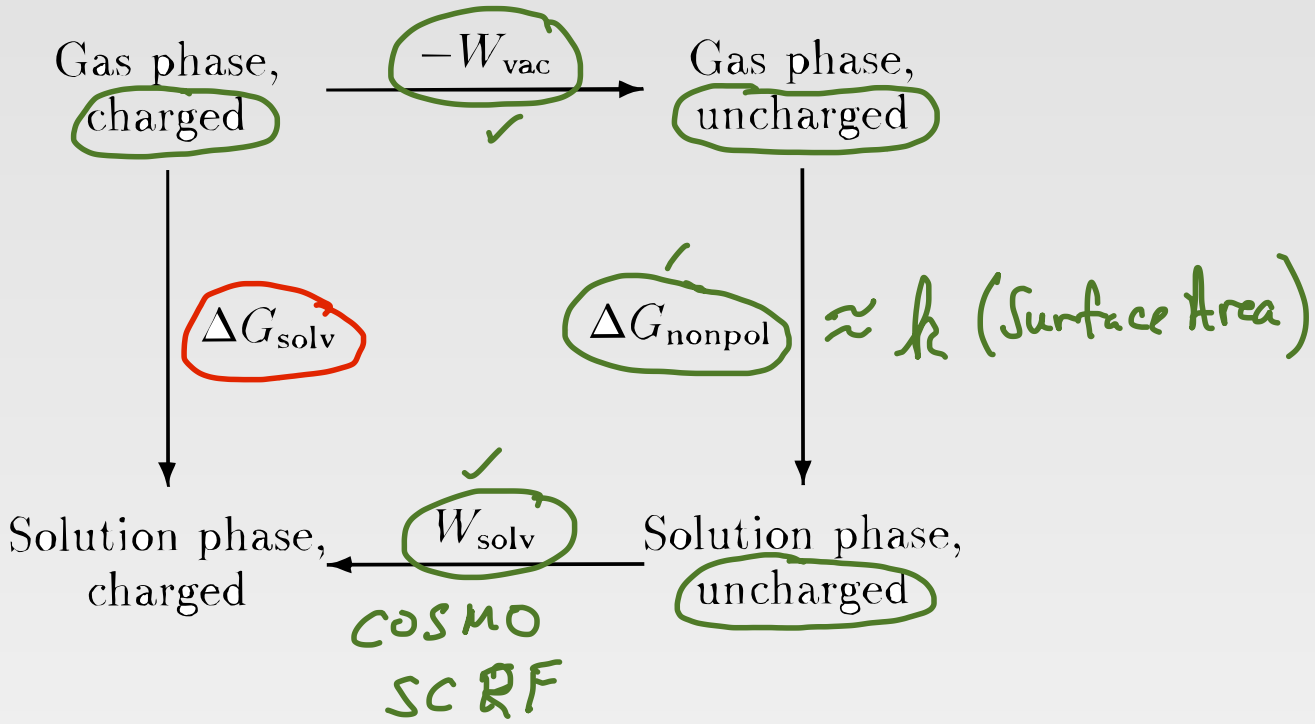
effects of solvation:

J. Phys. Chem. **1996,** *100,* 2698−2705

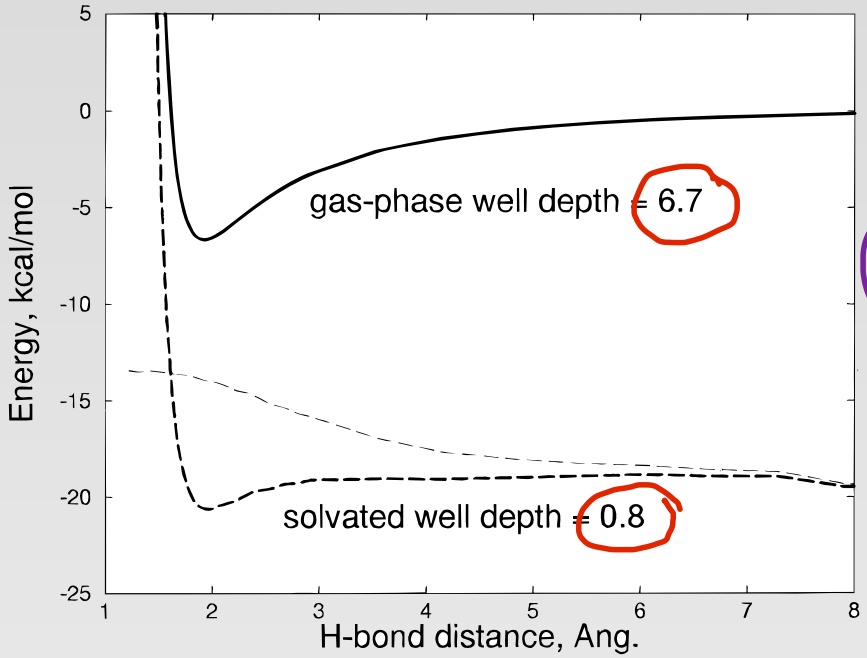
Dielectric Continuum Models for Hydration Effects on Peptide Conformational Transitions

K. Ösapay, W. S. Young, D. Bashford,* C. L. Brooks, III,* and D. A. Case*

Department of Molecular Biology, The Scripps Research Institute, La Jolla, California 92037



formamide dimer, back in 1995:



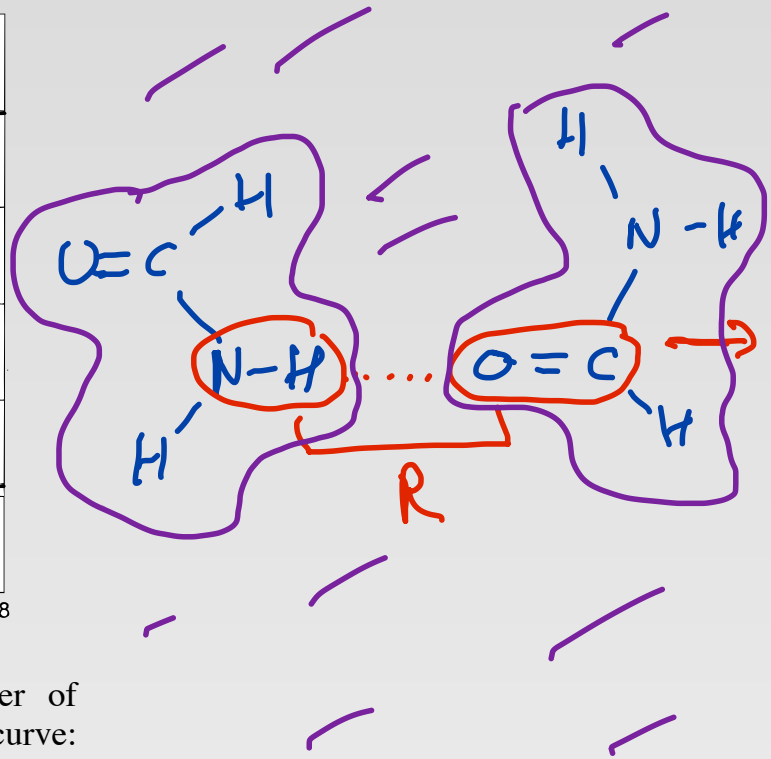


Figure 2. Energy profiles for formation of a linear dimer of formamides. Solid curve: gas-phase profile. Light dashed curve: solvation contribution from continuum model. Heavy dashed curve: net profile in water.

From the formamide dimer with SCRF:
Sum of electronic and thermal Enthalpies= -339.713215
From the formamide monomer, with SCRF:
Sum of electronic and thermal Enthalpies= -169.848956

$\Delta H_{gas} = -15.4/2$ $\Delta H = -9.7/2$

alanine-dipeptide dimer:

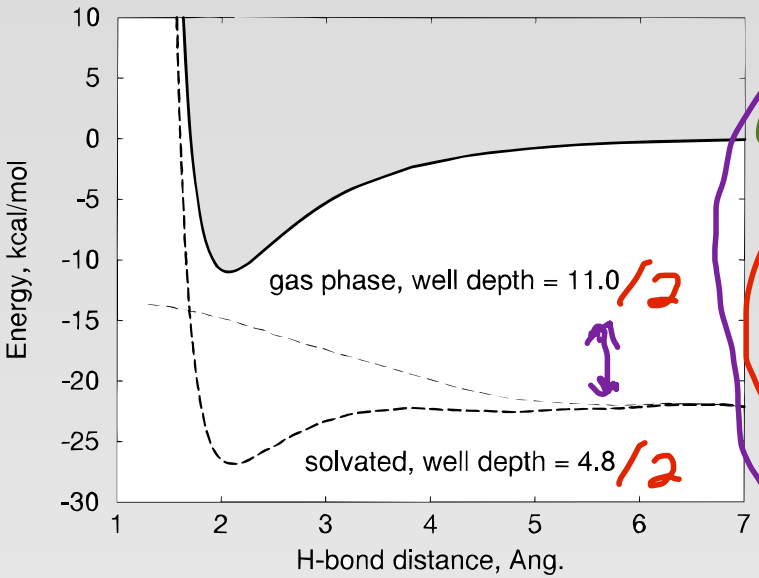
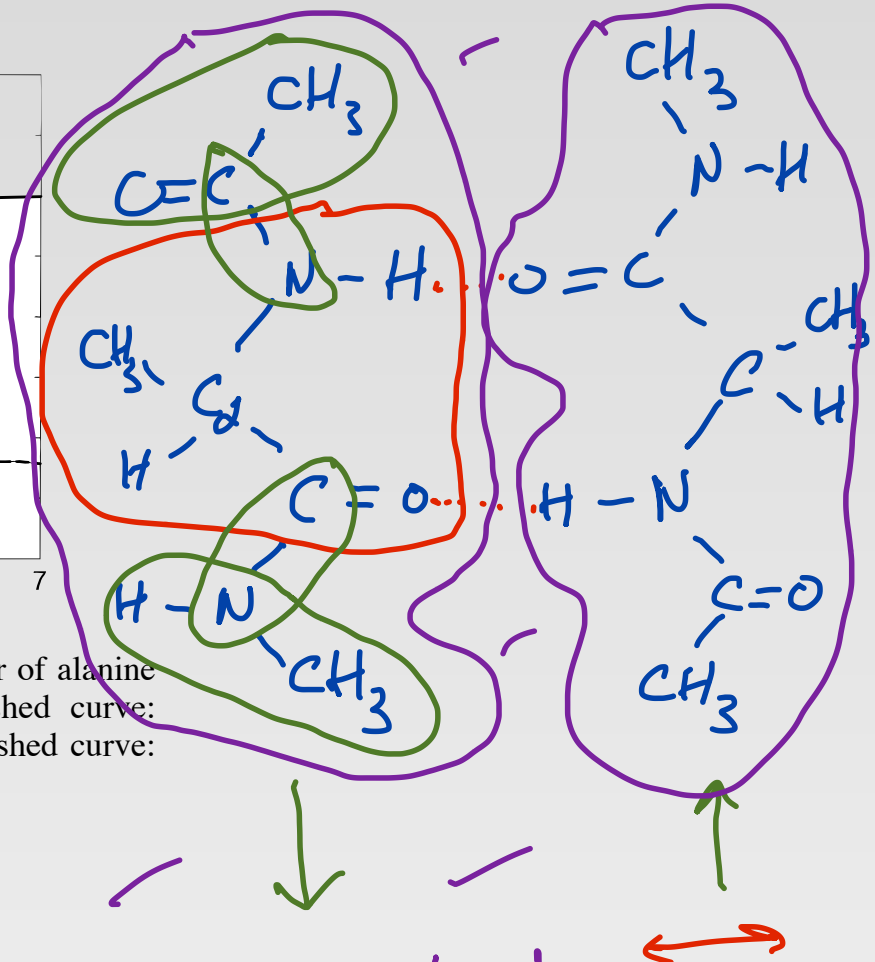


Figure 3. Energy profiles for formation of a linear dimer of alanine dipeptides. Solid curve: gas-phase profile. Light dashed curve: solvation contribution from continuum model. Heavy dashed curve: net profile in water.



H bond "strength" is very dependent on enviroment