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

- 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
```

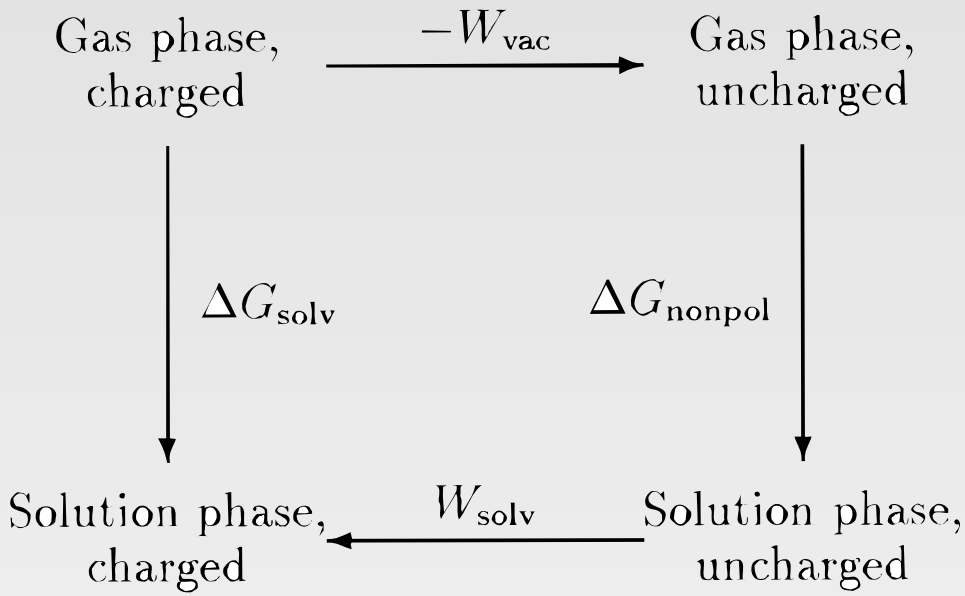
thermochemistry differences

effects of solvation:

2698 *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:

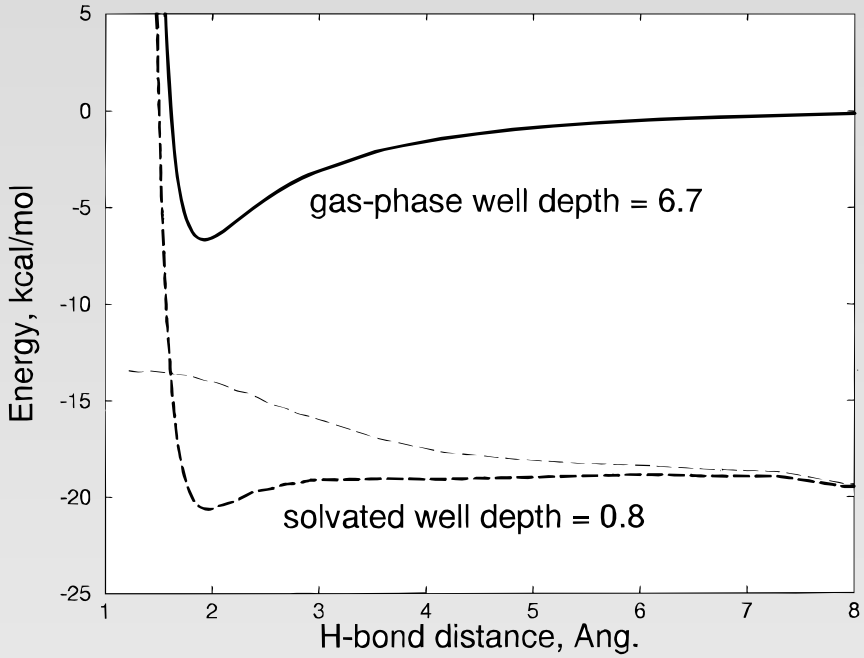


Figure 2. Energy profiles for formation of a linear dimer of formamides. Solid curve: gas-phase profile. Light dashed curve: solvation contribution from continuum model. Heavy dashed curve: net profile in water.

```
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
```

alanine-dipeptide dimer:

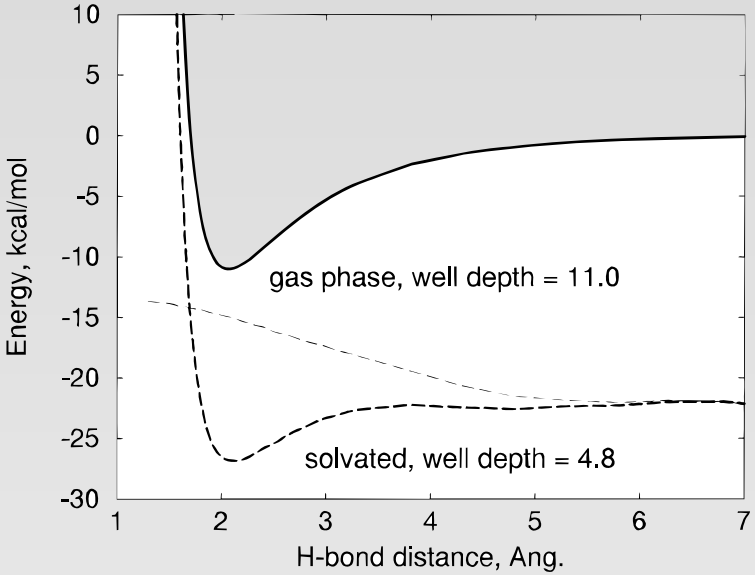


Figure 3. Energy profiles for formation of a linear dimer of alanine dipeptides. Solid curve: gas-phase profile. Light dashed curve: solvation contribution from continuum model. Heavy dashed curve: net profile in water.