# Guide for calculations of water corrected IR spectra with time-averaging approximation to simulate motional narrowing.

(Grahnen, Amunson & Kubelka JPCB 2010, 114, 13011; Auer & Skinner JCP 2007, 127, 104105)

## Programs:

* FORTRAN77

(all FORTRAN programs are essentially based on **hypep** and associated scripts)

preppsi.f prepares driving script for hypsi.f or chpsi.f or scpsi.f

hypsi.f reads tinker frames and calculates and saves WATER only individual electrostatic potential values for 6 amide atoms for each Tinker frame

chpsi.f reads tinker frames and calculates and saves individual WATER + CHARGED SIDE-CHAINS (D, E, K, R) + TERMINI electrostatic potential values for 6 amide atoms for each Tinker frame

scpsi.f reads tinker frames and calculates and saves individual WATER + ALL SIDE-CHAINS (ignoring backbone) electrostatic potential values for 6 amide atoms for each Tinker frame. Needs additional input CHARGES.INP with AMBER partial charges for all atom types.

prepfften.f prepares script for calculations of FF and TEN from the (averaged - see below in MATLAB code part) PSI files (by program psipep)

prepten.f prepares script for calculation of un-averaged .TEN files for the first frame of each averaging window.

psipep.f reads coordinates (SMALL, BIG), FF and TEN (SMALL) from vacuum calculations and atom table (CCT.INP) and calculates FF and TEN corrected for elstat potential in PSI files.

new5a.f like new5 (calculates intensities from TEN and F.INP output of new4) from two.TEN files (average and initial time, for details see references). It also reads two F.INP files (F.INP and F2.INP), but those should be the same (some early ideas, just didn’t get around to get rid of the second F.INP from the program)

Scripts for calculating TABS are again prepared using MATLAB program (below)

* MATLAB

psiav.m averages the electrostatic potential over a given number of frames

avscript.m prepares the script for calculating spectra (.TAB) from X, FTRY.INP, FF and two(!) .TEN files

## Instructions:

1. Run Tinker MD simulation, vacuum spectra calculation. Get all necessary files (Tinker frames, SMALL.X, SMALL.FC, SMALL.TEN, CCT.INP, BIJ.SCR, HYPEP.OPT). If all side-chain partial charges desired, CHARGES.INP will also be needed (it contains AMBER partial charges for all atom types, with the backbone ones set to zeros).

2. In **preppsi.f** select whether you will use **hypsi** (just water), **chpsi** (ionizable group charges) or **scpsi** (all side-chain AMBER partial charges). Compile **preppsi.f.**

3. Make NAMES.LST, which lists the filenames of Tinker frames.

4. Prepare script (‘**gopsi**’) using **preppsi**.

5. Run **gopsi**. It will save all the electrostatic potential files (.PSI)

6. In MATLAB, open **psiav.m** and edit the *filename, number of frames, number of averages* and *step* The MATLAB script has comments as to what is what. Run **psiav** and get averaged potentials (again extensions .PSI)

7. While you are at it, edit **avscript.m** so that the filenames and number of averages correspond to those is **psiav.m**. Then run **avscript**, it will produce file “**gotabs**”, which is the script for calculating spectra (.TAB files)

8. Make a different NAMES.LST, which lists the filenames of averaged potential (PSI) files.

9. Pepare script (‘**gofften**’) using **prepfften**.

10. Run **prepfften.** It will save all the .FF and .TEN files for each (averaged) electrostatic potential using program **psipep** (psipep calculates the FF and APT corrections using electrostatic potential from PSI)

11. Make yet another NAMES.LST file, which lists all .TEN files for the first frame of each averaging window. *The number on these files should correspond to those assigned to FILE2.TEN in the* ***gotabs*** *script*. For example, if you are doing averages of 59 frames taking a *step* of ten (see **avscript.m** for details), first average will be 1st-59th frame, the next 11th-69th, then 21st-79th etc. . The files corresponding to the *first frame of each averaging window* will be 0001, 0011, 0021 …etc. Check the **gotabs,** it should have them all calculated**.** If you are doing the average with step 1 it is less of an issue (they will be 0001,0002, 0003) you only have to worry about where they end.

12. run **prepten** to get the script **goten**.

13. Run **goten** to generate the .TEN files.

14. Run **gotabs** to get .TAB files.

15. Create TAB.LST (list of .TAB files) and use **jointab** to get everything into one .TAB file.

Examples of all scripts are included.