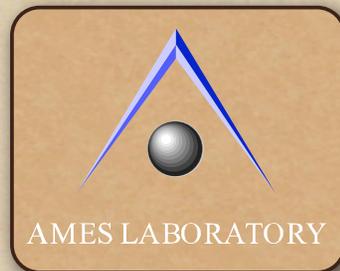


GAMESS and MacMolPlt

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GAMESS and MacMolPlt

This morning we discussed what GAMESS is and its capabilities. This talk will introduce the mechanical details of how to create input files, run GAMESS, and interpret output files for GAMESS.

GAMESS

- ◆ GAMESS runs on
 - ◆ Any Unix-based system available in the U.S.
 - ◆ Any Linux based system
 - ◆ Any Macintosh
 - ◆ Windows based system using WinGAMESS or PCGAMESS
- ◆ Obtained from www.msg.ameslab.gov

GAMESS

- ◆ GAMESS is a back-end program, ie no GUI.
- ◆ Typically it is run via a script
- ◆ Input is taken from a file (usually .inp)
- ◆ Output appears in .log file (stdout)
 - ◆ This is intended to be human readable
- ◆ MO Vectors, coordinates, hessians, etc appear in .dat file. Can be used for restarts.
- ◆ IRC and DRP data and numerical hessian restart information appear in .irc file.
- ◆ These are all ASCII text.

GAMESS Input file

- ◆ The input file is mostly free-format (ie flexible spacing) except:
 - ◆ '\$' sign specifying group must be in column 2!
 - ◆ All groups must terminate with a \$END (this '\$' can be anywhere except column 1).
 - ◆ anything in column 1 indicates a comment line

MacMolPlt

- ◆ While you can easily read the computed energy and exit status from the output interpreting the orbitals, normal modes and the movement of the atoms is harder for most people to interpret.
- ◆ MacMolPlt was designed by and for GAMESS users primarily as a tool to interpret GAMESS output.
- ◆ It has evolved some input generation capability as well.

MacMolPlt

- ◆ For the first 10+ years it has been a Macintosh only program.
- ◆ Now available on Macintosh, Linux and Windows.
- ◆ <http://www.scl.ameslab.gov/~brett/MacMolPlt/>

MacMolPlt Capabilities

- ◆ Directly reads GAMESS log files.
- ◆ Visualizes molecular geometries, orbitals, total electron densities, molecular electrostatic potentials, normal modes.
- ◆ Produces animations of normal modes, optimizations, IRCs, DRCs, etc.
- ◆ Rudimentary input generation.

MacMolPlt Capabilities

- ◆ It does not offer:
 - ◆ A point and click molecular builder
 - ◆ Ability to generate complete GAMESS input files for all run types
 - ◆ Automated background execution of GAMESS.
- ◆ These are planned additions in the (hopefully) near future.

Lab Demo #1

- ◆ Compute the Raman spectra for water
 - ◆ Make an initial guess at the structure, then optimize.
 - ◆ Compute a Hessian for the optimized structure.
 - ◆ Compute the Raman intensities.
 - ◆ Visualize the results!

Lab exercise #1

- ◆ Optimize NH_3

Lab exercise #2

- ◆ Optimize Planar NH_3
- ◆ Compute its Hessian
 - ◆ Verify there is one imaginary mode

Lab exercise #3

- ◆ Consider $\text{H} + \text{CH}_4 \rightarrow \text{H}_2 + \text{CH}_3$
- ◆ Optimize the reactants and the products using HF +MP2
- ◆ Make a guess at the transition state and run a hessian to see if it has an imaginary mode. If not, modify guess and try again.
- ◆ Do a saddle point search
- ◆ Do an IRC.