Chem Compute Quickstart

Chem Compute is maintained by Mark Perri at Sonoma State University and hosted on Jetstream at Indiana University. The Chem Compute URL is https://chemcompute.org/. We will use Chem Compute as the frontend for running electronic structure calculations with *The General Atomic and Molecular Electronic Structure System*, GAMESS (http://www.msg.ameslab.gov/gamess/). Chem Compute also provides access to other computational chemistry resources including PSI4 and the molecular dynamics packages TINKER and NAMD, though we will not be using those resource at this time.

Follow this link, https://chemcompute.org/gamess/submit, to directly access the Chem Compute GAMESS guided submission interface. If you are a returning Chem Computer user, please log in now. If your University is part of the InCommon Federation you can log in without registering by clicking Login then "Log In with Google or your University" – select your University from the dropdown list. Otherwise if this is your first time working with Chem Compute, please register as a Chem Compute user by clicking the "Register" link in the top-right corner of the page. This gives you access to all of the computational resources available at ChemCompute.org and will allow you to maintain copies of your calculations in your user "Dashboard" that you can refer to later. Registering also helps track usage and obtain the resources needed to continue providing its service.

When logged in with the GAMESS-Submit tabs selected, an instruction section appears on the left side of the page with instructions for several different kinds of calculations. The following instructions illustrate the use of Chem Compute in "Submit (Guided)" mode. You can also submit your own input files from "Submit Your Own Files" tab, which provides increased flexibility. (See the online documentation for Chem Compute and GAMESS for more detailed information.)

- In the "Choose your Molecule" panel, you can define a molecule using the "Search for a molecule" box by entering the name or formula of the molecule. If the molecule is found in the database, it will appear in the 2D window and in the 3D windows below. You can also define a molecule by drawing it directly in the 2D window or by importing it from a previous calculation input or output file. When you click the "Transfer" button the 3D window will automatically add any hydrogens necessary to complete all valences. If you do not wish to automatically add hydrogens, uncheck the "Add hydrogens automatically" then click "Transfer".

- After searching for a molecule in the database or drawing the 2D representation and clicking Transfer your molecule will be automatically optimized (using a simple algorithm) and symmetrized. If you wish, you can unselect the "Automatically Optimize and Symmetrize Molecule" box to disable this feature.

- If you would like to alter the coordinates of atoms (e.g. to generate a potential energy surface), selecti the 3D Panel "Advanced Options" box then select the "Manually alter coordinates". You can also try "move atoms by dragging".

- In the "Set Parameters for Quantum Mechanical Calculation", you must input a file name. You can also include a comment or note about the calculation. Enter the overall charge and the multiplicity of the atom, molecule, or ion. (Multiplicity can be determined by adding one to the number of unpaired electrons present the atom, molecule, or ion.) If you want GAMESS to optimize the molecular structure, select the "Geometry Optimization" button. Select "Single-Point Energy" instead if you want to calculate the energy of the specific optimized geometry that you are submitting. Choose the information

that you want the program to report in "Add-Ons". Chose the appropriate "Basis Set", "Molecular Orbital Method" and "DFT Functional". Those parameters will be specified for the work related to this experiment. If you are doing the calculation for an isolated molecule then choose "None" in "PCM Solvent". The small jobs we are running for this experiment can be run on "Jetstream" so you are safe using whatever the default value is for "Processor Cores" and "Computer Cluster". More information is provided about each option by hovering your mouse pointer over the question mark on the right of each option line.

- You can submit the job at this point or, for finer control of the calculation you can directly edit the input file in the "Input File" window to provide customized GAMESS parameters. Start by clicking "Optional: Edit input file". For example, if you are doing single point calculations and want to specify bond lengths and angles you can edit the geometry in the $DATA section of the input file. By default, Cartesian coordinates are used to specify the molecular geometry but alternatively you can specify the molecular geometry using a z-matrix in the $DATA section which can simplify specifying and tracking bond lengths and bond angles. If you wish to use a theoretical model that is supported by GAMESS but not included among the Chem Compute guided submission options, you can add the keyword in the $CONTRL section of the input file. Thus, to use second order *Møller-Plesset Perturbation Theory*, MP2, you would add the keyword "MPLEVL=2" to other options between $CONTRL and the following $END in the input file. Note that some options should not be used together such as "MPLEVEL=2" and "DFTTYP=B3LYP". See the GAMESS documentation at http://www.msg.ameslab.gov/gamess/documentation.html for complete details about GAMESS input. An example of setting up an MP2 calculation in Chem Compute can be viewed on YouTube at: https://youtu.be/Q_PsdTUcmXQ. Be careful – MP2 calculations take up a lot of disk space. If your calculation is killed for going over the limit please retry on Comet or Bridges, which have more space and RAM.

- Click "Submit Job" when your input file is ready. You will be taken to the "Results" tab where you can view the results of your calculation when it finishes.

- When the calculation finishes an image of your molecule will appear in the Results tab viewer window along with a table of molecular orbital energies (and vibrational energies if calculated). Use the "Energy Units" pull down to select your preferred units. Click on a molecular orbital energy in the table to view the corresponding molecular orbital in the viewer. Clicking and dragging in the viewer window allows you to rotate the molecule. If you requested a vibrational calculation you can click on a vibrational energy to view the corresponding vibrational motion in the viewer. Note that the first five (for linear molecules) or six (for nonlinear molecules) energies in the vibrational table are related to translations and rotations of the whole molecule. You can also view the dipole moment vector, bond dipoles, electrostatic potential surface, UV-Vis and IR spectral simulations, and thermochemical data by clicking the corresponding boxes. Bond lengths can be viewed in the viewer window by *double-clicking* the first atom then *hovering* the pointer over the second atom in the bond. Similarly, bond angels can be viewed by *double clicking* on the first atom, *single clicking* the second atom, and *hovering* over the third atom. Dihedral angles work similarly by *single clicking* the third atom and *hovering* over the fourth. Other viewing options can be selected by *right-clicking* in the viewer window and selecting an option from the drop-down menu. All of the above information and more is available in the GAMESS output file that can be downloaded and viewed by clicking the "Download Output File" box.

- To start a new If you would like start a new calculation just go back to the "Submit (Guided)" tab at the top of the screen. If you would like to run a new calculation beginning with the calculated results of the current calculation clicking the "Do More Calculations" box will open the settings dialog. This will take

you back to the “Submit (Guided)” tab and automatically insert the molecule that you have just calculated. If your molecule doesn't appear then just click "Load from Output". "Load from Input" can be used if your calculation resulted in an error and you want to resubmit with different settings. This is useful when you want to do an optimization followed by a single point calculation with a more complex basis set. To ensure that you maintain the original optimized bond lengths and angles, you should uncheck “automatically Optimize and Symmetrize Molecule”. You can also choose NBO to calculate “Natural Bond Orbitals” (molecular orbitals cast in the form of typical hybrid orbitals).

- If you wish, you can explore the capabilities of GAMESS on Chem Compute on other molecules. If you would like to compute “large” molecules (more than 10 atoms, and heavy (third period) atoms, use the servers Comet and Bridges and increase the number of cores and wall time. From your dashboard (available at the top right) you can request more time and more cores if needed.