Materials List for:

Computation of Atmospheric Concentrations of Molecular Clusters from *ab initio* Thermochemistry

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Materials

Name	Company	Catalog Number	Comments
Avogadro	https://avogadro.cc		Open-source molecular visualization program
Gaussian [09/16] Software	http://www.gaussian.com/		Commercial ab initio electronic structure program
MOPAC 2016	http://openmopac.net/MOPAC2016.html		Open-source semi-empirical program
OGOLEM Software	https://www.ogolem.org		Genetic algorithm-based global optimization program
OpenBabel	http://openbabel.org/wiki/Main_Page		Open-source cheminformatics library
calcRotConsts.py	Shields Group, Department of Chemistry, Furman University		Python script to compute rotational constants
calcSymmetry.csh	Shields Group, Department of Chemistry, Furman University		Shell script to calculate symmetry number of a molecule given Cartesian coordinates
combine-GA.csh	Shields Group, Department of Chemistry, Furman University		Shell script to combine energy and rotational constants from different GA directories
combine-QM.csh	Shields Group, Department of Chemistry, Furman University		Shell script to combine energy and rotational constants from different QM directories
gaussianE.csh	Shields Group, Department of Chemistry, Furman University		Shell script to extract Gaussian 09 energies
gaussianFreqs.csh	Shields Group, Department of Chemistry, Furman University		Shell script to extract Gaussian 09 vibrational frequencies
getrotconsts	Shields Group, Department of Chemistry, Furman University		Executable to calculate rotational constants given a molecule's Cartesian coordinates
getRotConsts-dft-lb.csh	Shields Group, Department of Chemistry, Furman University		Shell script to compute rotational constants for a batch of large basis DFT optimized structures
getRotConsts-dft-lb-ultrafine.csh	Shields Group, Department of Chemistry, Furman University		Shell script to compute rotational constants for a batch of ultrafine DFT optimized structures
getRotConsts-dft-sb.csh	Shields Group, Department of Chemistry, Furman University		Shell script to compute rotational constants for a batch of small basis DFT optimized structures
getRotConsts-GA.csh	Shields Group, Department of Chemistry, Furman University		Shell script to compute rotational constants for a batch of genetic algorithm optimized structures

global-minimum-coords.xyz	Shields Group, Department of Chemistry, Furman University		Cartesian coordinates of global minimum structures of gly-(h2o)n, where n=0-5
make-thermo-gaussian.csh	Shields Group, Department of Chemistry, Furman University		Shell script to extract data from Gaussian output files and make input files for the thermo.pl script
ogolem-input-file.ogo	Shields Group, Department of Chemistry, Furman University		Ogolem sample input file
ogolem-submit-script.pbs	Shields Group, Department of Chemistry, Furman University		PBS batch submission file for Ogolem calculations
README.docx	Shields Group, Department of Chemistry, Furman University		Clarifications to help readers use the scripts effectively
runogolem.csh	Shields Group, Department of Chemistry, Furman University		Shell script to run OGOLEM
run-pw91-lb.csh	Shields Group, Department of Chemistry, Furman University		Shell script to run a batch of large basis DFT optimization calculations
run-pw91-lb-ultrafine.csh	Shields Group, Department of Chemistry, Furman University		Shell script to run a batch of ultrafine DFT optimization calculations
run-pw91-sb.csh	Shields Group, Department of Chemistry, Furman University		Shell script to run a batch of small basis DFT optimization calculations
run-thermo-pw91.csh	Shields Group, Department of Chemistry, Furman University		Shell script to compute the thermodynamic corrections for a batch of DFT optimized structures
similarityAnalysis.py	Shields Group, Department of Chemistry, Furman University		Python script to determine unique structures based on rotational constants and energies
symmetry	Shields Group, Department of Chemistry, Furman University		Executable to calculate molecular symmetry given Cartesian coordinates
symmetry.c	(C) 1996, 2003 S. Patchkovskii, Serguei.Patchkovskii@sympatico.ca		C code to determine the molecular symmstry of a molecule given Cartesian coordinates
template-marcy.pbs	Shields Group, Department of Chemistry, Furman University		Template for a PBS submit script which uses OGOLEM
template-pw91.com	Shields Group, Department of Chemistry, Furman University		Template Gaussian 09 input
template-pw91-HL.com	Shields Group, Department of Chemistry, Furman University		Template Gaussian 09 input for ultrafine DFT optimization
thermo.pl	https://www.nist.gov/mml/csd/chemical-informatics-research-group/products-and-services/program-computing-ideal-gas		Perl open-source script to compute ideal gas thermodynamic corrections
gly-h2o-n.xlsx	Shields Group, Department of Chemistry, Furman University		Excel spreadsheet for the complete protocol
table-1.xlsx	Shields Group, Department of Chemistry, Furman University		Excel spreadsheet
table-2.xlsx	Shields Group, Department of Chemistry, Furman University		Excel spreadsheet
table-3.xlsx	Shields Group, Department of Chemistry, Furman University		Excel spreadsheet
table-4.xlsx	Shields Group, Department of Chemistry, Furman University		Excel spreadsheet
water.xyz	Shields Group, Department of Chemistry, Furman University		Cartesian coordinates of water
glycine.xyz	Shields Group, Department of Chemistry, Furman University		Cartesian coordinates of glycine