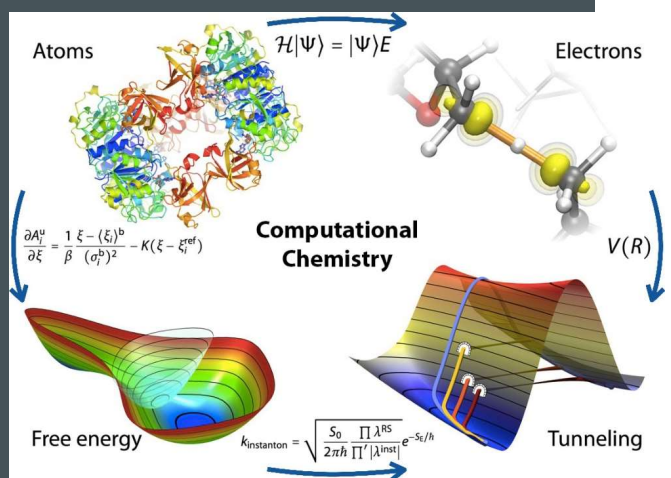


PRAKTIKUM/RISET KIMIA KOMPUTASI

VIRTUAL LABORATORY



SOFTWARE PRAKTIKUM DAN RISET KIMIA KOMPUTASI

1. GAUSSIAN + GAUSSVIEW (KOMERSIAL, WINDOWS/LINUX)
2. HYPERCHEM STUDENT VERSION (KOMERSIAL, WINDOWS)
3. CHEMOFFICE/CHEMDRAW 3D (KOMERSIAL, WINDOWS)
3. SOFTWARE OPEN SOURCE: JMOL, AVOGADRO, MARVIN SUITE, CHEMSCKETCH, NANOTUBE MODELER, MOLDEN, DRAGON, GABEDIT, MATERIAL STUDIO DLL

ONLINE SOFTWARE:

1. CHEMCOMPUTE (GAMESS)
2. NWCHEM ONLINE / EMSL
3. JMOL ONLINE

4. OFFLINE SOFTWARE: JMOL, AVOGADRO, MARVIN SUITE, CHEMSCKETCH, NANOTUBE MODELER, MOLDEN, DRAGON, GABEDIT, MATERIAL STUDIO DLL



SOFTWARE OPEN SOURCE:

1. NWCHEM (LINUX)
2. ORCA (LINUX, WINDOWS, 64 BIT)
3. JMOL, AVOGADRO, MARVIN SUITE, CHEMSCKETCH, NANOTUBE MODELER, MOLDEN, DRAGON, GABEDIT, MATERIAL STUDIO DLL

<https://sites.google.com/mail.unnes.ac.id/kimiakomputasi/> = <https://s.id/kimiakomputasi>

HTTPS://CHEMCOMPUTE.ORG/

Computational chemistry software for undergraduate teaching and research.

All without the hassle of compiling, installing, and maintaining software and hardware. Login or register at the top right to get full access to the system, or learn more about using ChemCompute in your class teaching.

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.

Equalizing STEM education with supercomptuers: <https://youtu.be/jaXuG2QGdl0>

Frontpage ChemCompute

The screenshot shows the ChemCompute website frontpage for GAMESS. The browser address bar shows chemcompute.org/gameass. The navigation bar includes links for ChemCompute, GAMESS, TINKER, NAMD, Psi4/Jupyter, Datasets (beta), Simulations, and Help. On the right side of the navigation bar, the 'Login / Register' link is circled in red. A dropdown menu for 'GAMESS' is open, showing options: 'Information & Experiments', 'Submit a job' (highlighted), and 'Get Job Results'. The main content area is divided into two columns. The left column features the 'GAMESS' title, a description of the system as a quantum chemistry package maintained by the Gordon research group at Iowa State University, and a call to action to create an account or login with Google or a university. Below this is a section titled 'How does GAMESS work?' with a four-step numbered list. The right column is titled 'GAMESS Experiments (11)' and contains a list of experiment categories: Physical Chemistry, General Education Chemistry, General Chemistry, Organic Chemistry, and General Instructions, each with a plus icon. The footer includes the Perri Group (Sonoma State University) logo, a link to 'Policies, Credits and Acknowledgements', and logos for SENTRY and XSEDE (Extreme Science and Engineering Discovery Environment).

chemcompute.org/gameass

ChemCompute GAMESS TINKER NAMD Psi4/Jupyter Datasets (beta) Simulations Help

Login / Register

GAMESS

Information & Experiments

Submit a job

Get Job Results

GAMESS(The General Atomic and molecular Electronic Structure System) is a quantum chemistry package maintained by the members of the Gordon research group at Iowa State University. This website allows you to submit your GAMESS jobs to our servers. Our hope is that this eases the process of quantum chemistry calculations.

Create an account or login with Google or your University to get access to the full functionality of ChemCompute, including saving experiment submissions.

How does GAMESS work?

- 1 Pick an experiment below or [skip straight to submitting a job](#)
- 2 Read the Background Theory
- 3 Complete the Prelab
- 4 Start the lab experiment or select Submit (Guided. Instructions appear

GAMESS Experiments (11)

- Physical Chemistry
- General Education Chemistry
- General Chemistry
- Organic Chemistry
- General Instructions

Perri Group (Sonoma State University)

Policies, Credits and Acknowledgements

<https://chemcompute.org/gameass/submit>

SENTRY XSEDE
Extreme Science and Engineering
Discovery Environment

Submit Input

Instructions

Download

(1) General Instructions

Before you begin please fill out this [survey](#) to help us improve (and help out future students)!

Instructions on how to build a molecule, submit a job, and view the results.

1. Make sure you are logged in.
Registered users are allocated more computational power.
2. Click the next button to begin!

Survey

Next

3D Panel

☒ Advanced Options☒ Label Atoms☒ Use Symmetry C1

On the 3D model:

☐ enantiomer☐ diastereomer in a C☐ Manually alter coordinates☐ Move atoms by dragging☒ optimize geometry automatically☐ delete atoms by clicking on them

Load from a database:

☒ NCI ☐ PubChem ☐ PDB

name of the molecule or PDB ID:

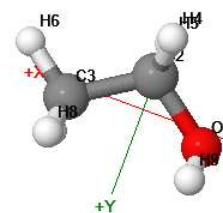
ethanol

Retrieve

Recalculate Hydrogens

Advanced Options 3D Panel

Done Symmetrizing



ethanol

JSmol

Instructions

Download

(1) General Instructions

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2. Click the next button to begin!

Survey

Next

3D Panel

☐ Advanced Options☒ Label Atoms☒ Use Symmetry C1

Resymmetrize

Draw Point Group Elements

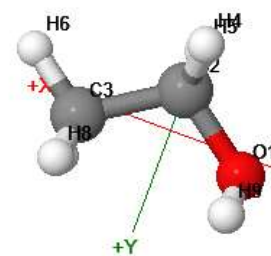
Optimize structure in 3D

(Several times may be needed)

Delete All hydrogens

Report Wrong Search Result

Done Symmetrizing



ethanol

JSmol

Next

Instructions

Download

(1) General Instructions

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Survey

Next

Set Parameters for Quantum Mechanical Calculation

Reset Settings to Default

Name for input file: ethanol

Comment: Optimasi geometri struktur ethanol

Charge: 0

Multiplicity: 1

Type: ☐ Single-Point Energy ☒ Geometry Optimization ☐ Saddle Point SearchAdd-Ons: ☒ IR ☐ UV-Vis ☐ NMR ☐ Thermodynamics ☐ ΔH_f (g3mp2) ☐ NBO ☐ NoneBasis Set: ☐ AM1 ☐ PM3 ☐ PM6 ☐ STO-3G ☐ 3-21G ☒ 6-31G* ☐ 6-311G** ☐ 6-311G**+ ☐ aug-cc-pVDZ ☐ SPK-DZPMolecular Orbital Method: ☒ RHF ☐ ROHF ☐ UHFDFT Functional: ☐ None ☒ B3LYP ☐ PBE0 ☐ M06 ☐ wB97X-D

ChemCompute GAMESS TINKER NAMD Psi4/Jupyter Datasets (beta) Simulations Help

HOME / GAMESS / SUBMIT

Hide Instructions

Instructions Download

(1) General Instructions

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2. Click the next button to begin!

Survey Next

Add-Ons: ☒ IR ☐ UV-Vis ☐ NMR ☐ Thermodynamics ☐ ΔH_f (g3mp2) ☐ NBO ☐ None

Basis Set: ☐ AM1 ☐ PM3 ☐ PM6 ☐ STO-3G ☐ 3-21G ☒ 6-31G* ☐ 6-311G** ☐ 6-311G**+ ☐ aug-cc-pVDZ ☐ SPK-DZP

Molecular Orbital Method: ☒ RHF ☐ ROHF ☐ UHF

DFT Functional: ☐ None ☒ B3LYP ☐ PBE0 ☐ M06 ☐ wB97X-D

PCM Solvent: ☒ None ☐ Water ☐ Methanol ☐ Ethanol ☐ Acetone ☐ THF

Computer Cluster: ☐ auto ☒ jetstream

Processor Cores: ☒ 1

Time Limit: ☒ 1 hour

Optional: Edit input file

You may edit the data in the box below. Do not make changes to the atoms in any way if using symmetry. Use Manually alter coordinates instead.

Submit Job

BAGIAN BAWAH

TANPA REGISTRASI DAN LOGIN

Instructions

Download

(1) General Instructions

Before you begin please fill out this [survey](#) to help us improve (and help out future students)!

Instructions on how to build a molecule, submit a job, and view the results.

1. Make sure you are logged in.
Registered users are allocated more computational power.
2. Click the next button to begin!

Survey

Next

Type: ☐ Single-Point Energy ☒ Geometry Optimization ☐ Saddle Point Search

Add-Ons: ☒ IR ☐ UV-Vis ☐ NMR ☐ Thermodynamics ☐ ΔH_f (g3mp2) ☐ NBO ☐ None

Basis Set: ☐ AM1 ☐ PM3 ☒ PM6 ☐ STO-3G ☐ 3-21G ☐ 6-31G* ☐ 6-311G** ☐ 6-311G**+ ☐ aug-cc-pVDZ
☐ SPK-DZP

Molecular Orbital Method: ☒ RHF ☐ ROHF ☐ UHF

DFT Functional: ☐ None ☒ B3LYP ☐ PBE0 ☐ M06 ☐ wB97X-D

PCM Solvent: ☒ None ☐ Water ☐ Methanol ☐ Ethanol ☐ Acetone ☐ THF

Computer Cluster: ☐ auto ☐ jetstream ☐ comet ☒ bridges2

Processor Cores: ☐ 1 ☐ 6 ☐ 24 ☒ 128

Time Limit: ☐ 1 hour ☒ 6 hour

Optional: Edit input file

**REGISTRASI DAN
LOGIN**

Submit Job

HOME / GAMESS / STATUS

[Hide Instructions](#)

Instructions

[Download](#)

(1) General Instructions

Before you begin please fill out this [survey](#) to help us improve (and help out future students)!

Visualize Your Results

1. Write down your job number (6 digit number at the left). Wait for the job to finish.
2. Under visualizations choose to view orbitals or vibrations (if calculated in the previous step)
3. Measurements can be made by double clicking on an atom to start and stop a measurement. Single click on intermediate atoms to measure angles
4. To perform additional calculations using this molecule click "Do More"

[Background Info](#)[Submit \(Guided\)](#)[Submit Your Own Files](#)[Results](#)

Job Number: 278338

[Download Input File](#)[Download Output File](#)[Summary](#)[Real Time Output](#)

in progress...

Job 278338 (Bridges2) ACTIVE

ethanol OPTIMIZE + HESSIAN 6-311G** B3LYP neutral singlet

GAMESS supplementary output files will be written to /ocean/projects/cda170005p/ccompute/prod/2
Copying input file 278338.inp to your run's scratch directory...

ChemCompute GAMESS TINKER NAMD Psi4/Jupyter Datasets (beta) Simulations Help labkim's Dashboard

HOME / GAMESS / STATUS Hide Instructions

Instructions

Download

(1) General Instructions

Before you begin please fill out this [survey](#) to help us improve (and help out future students)!

Visualize Your Results

1. Write down your job number (6 digit number at the left). Wait for the job to finish.
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3. Measurements can be made by double clicking on an atom to start and stop a measurement. Single click on intermediate atoms to measure angles
4. To perform additional calculations using this molecule click "Do More"

Background Info

Submit (Guided)

Submit Your Own Files

Results

Job Number: 278338

Download Input File

Download Output File

Summary

Real Time Output

Job 278338 (Bridges2) Success

ethanol OPTIMIZE + HESSIAN 6-311G** B3LYP neutral singlet

EXECUTION OF GAMESS TERMINATED NORMALLY Mon May 3 19:34:48 2021
TOTAL CPU TIME= 25.6 (0.4 MIN)
Wait for the gears to stop spinning at the bottom. Please save your output file instead of opening it.

HOME / GAMESS / STATUS

Hide Instructions

Instructions

Download

(1) General Instructions

Before you begin please fill out this [survey](#) to help us improve (and help out future students)!

Visualize Your Results

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2. Under visualizations choose to view orbitals or vibrations (if calculated in the previous step)
3. Measurements can be made by double clicking on an atom to start and stop a measurement. Single click on intermediate atoms to measure angles
4. To perform additional calculations using this molecule click "Do More"

Energy Units: kJ/mol

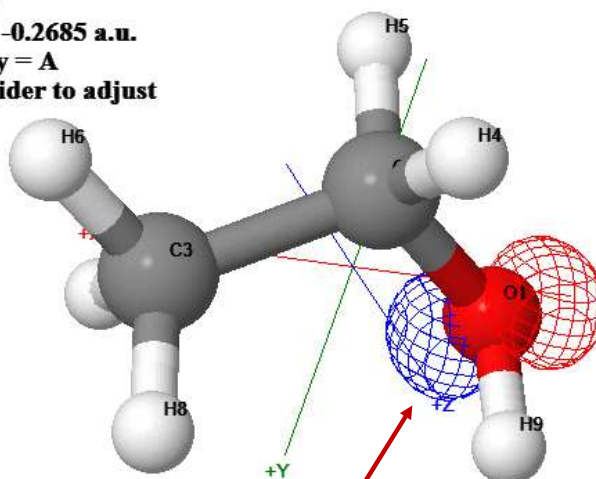
Electronic Energy = -406938.71 kJ / mol

MO 13/23

Energy = -0.2685 a.u.

Symmetry = A

Use the slider to adjust

☒ Label Atoms

Visualizations

Orbitals
kJ / molVibrations
cm⁻¹

15) 188.25 (A)	0.1
14) 97.41 (A)	0.07
13) -704.95 (A)	0.01
12) -849.09 (A)	7.32
11) -970.65 (A)	9.89
10) -1000.05 (A)	15.56
9) -1127.39 (A)	271.39
8) -1182.26 (A)	319.92
7) -1311.17 (A)	421.9
6) -1633.32 (A)	811.08

MO Cutoff

0.19

Solid

Mesh

JSmol

Do More Calculations

HOME / GAMESS / STATUS

Hide Instructions

Instructions

Download

(1) General Instructions

Before you begin please fill out this [survey](#) to help us improve (and help out future students)!

Visualize Your Results

1. Write down your job number (6 digit number at the left). Wait for the job to finish.
2. Under visualizations choose to view orbitals or vibrations (if calculated in the previous step)
3. Measurements can be made by double clicking on an atom to start and stop a measurement. Single click on intermediate atoms to measure angles
4. To perform additional calculations using this molecule click "Do More"

Electronic Energy = -406938.71 kJ / mol

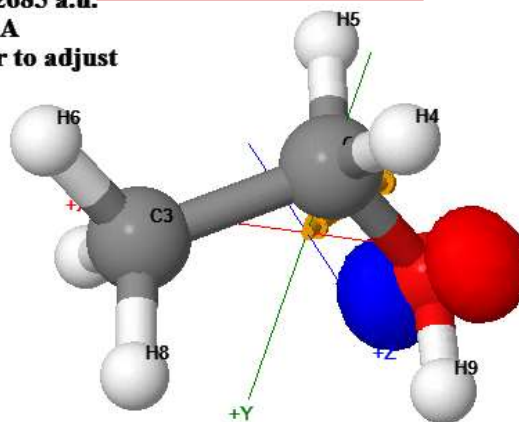
MO 13/23

Energy = -0.2685 a.u.

Symmetry = A

Use the slider to adjust

Dipole = 1.654996 Debye

☒ Label Atoms

Visualizations

Orbitals
kJ / molVibrations
cm⁻¹

15) 188.25 (A)	0.1
14) 97.41 (A)	0.07
13) -704.95 (A)	0.01
12) -849.09 (A)	7.32
11) -970.65 (A)	9.89
10) -1000.05 (A)	15.56
9) -1127.39 (A)	271.39
8) -1182.26 (A)	319.92
7) -1311.17 (A)	421.9
6) -1633.32 (A)	811.08

MO Cutoff

0.19

Solid

Mesh

JSmol

Do More Calculations

Dipole Moment

Bond Dipoles

HOME / GAMESS / STATUS

Hide Instructions

Instructions

Download

(1) General Instructions

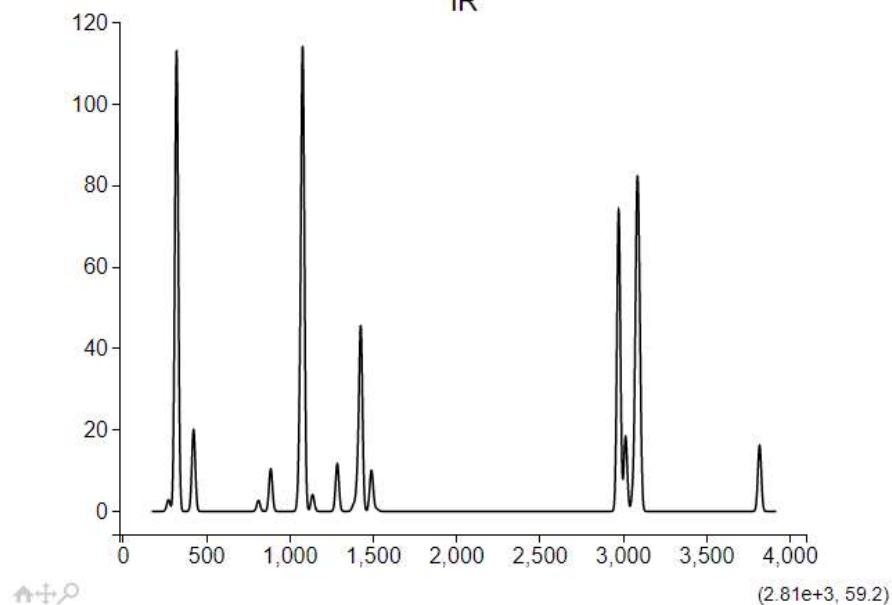
Before you begin please fill out this [survey](#) to help us improve (and help out future students)!

Visualize Your Results

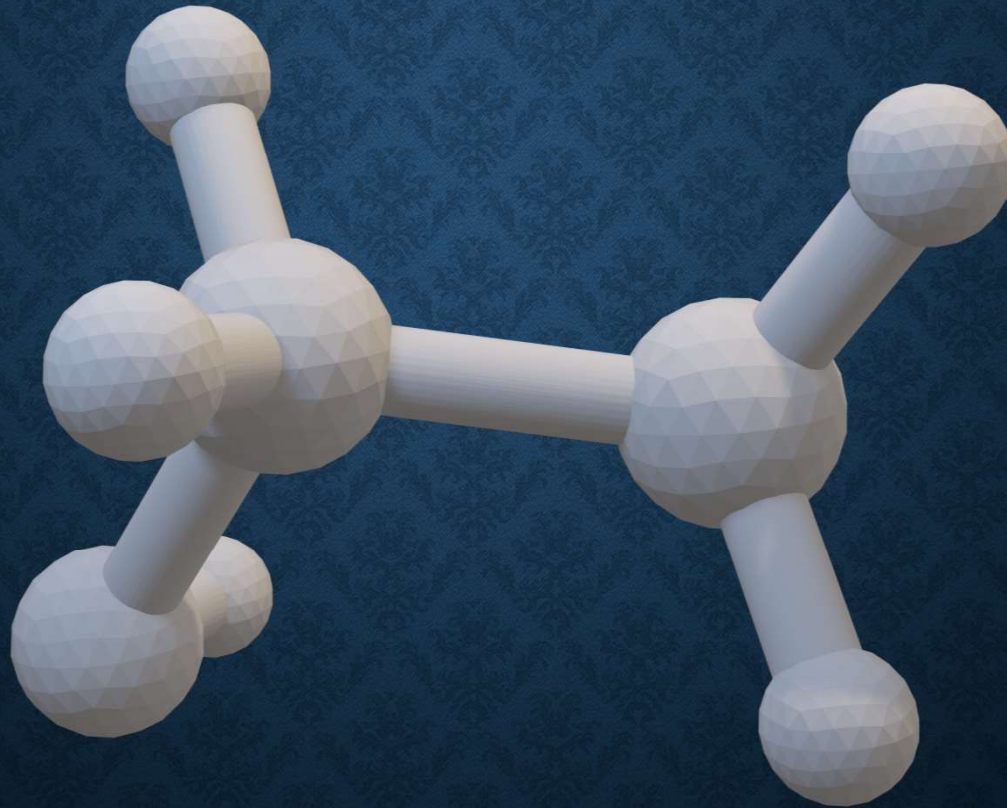
1. Write down your job number (6 digit number at the left). Wait for the job to finish.
2. Under visualizations choose to view orbitals or vibrations (if calculated in the previous step)
3. Measurements can be made by double clicking on an atom to start and stop a measurement. Single click on intermediate atoms to measure angles
4. To perform additional calculations using this molecule click "Do More"

VISUALISASI SPEKTRA IR

IR



WRITE STL (3D PRINTING)



ANIMATE MINIMIZATION

ChemCompute — Free Compute x

chemcompute.org/games/status

Apps | Inbox (42) - labkim... | DAFTAR MAHASIS... | Bebas Laboratorium | Bebas Perpustakaa... | Memo Lembur Pen... | Self Assessment (Re... | LABORATORIUM KI... | Reading list

ChemCompute | GAMESS | TINKER | NAMO | Psi4/Jupyter | Datasets (beta) | Simulations | Help | labkim's Dashboard

HOME / GAMESS / STATUS | Hide Instructions

Instructions

Download

(1) General Instructions

Before you begin please fill out this survey to help us improve (and help out future students)

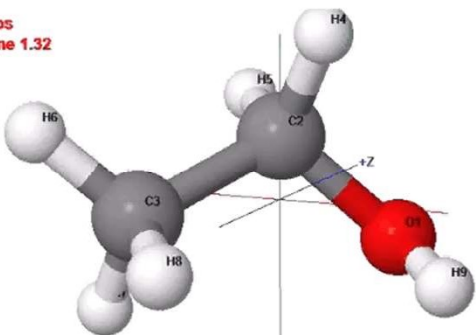
Visualize Your Results

1. Write down your job number (6 digit number at the left). Wait for the job to finish.
2. Under visualizations choose to view orbitals or vibrations (if calculated in the previous step)
3. Measurements can be made by double clicking on an atom to start and stop a measurement. Single click on intermediate atoms to measure angles
4. To perform additional calculations using this molecule click "Do More Calculations"
5. To perform calculations on a new molecule click the Submit Tab at the top.

Survey

Electronic Energy = -406938.71 kJ / mol

10 fps
Frame 1.32



Label Atoms

JSmol

Visualizations

Orbitals
kJ / mol

15) 188.25 (A)	15.56
14) 97.41 (A)	271.39
13) -704.95 (A)	319.92
12) -849.09 (A)	421.9
11) -970.65 (A)	811.08
10) -1000.05 (A)	884.74
9) -1127.39 (A)	1059.85
8) -1182.26 (A)	1076.64
7) -1311.17 (A)	1135.95
6) -1433.33 (A)	1200.05

Vibrations
cm⁻¹

15) 188.25 (A)	15.56
14) 97.41 (A)	271.39
13) -704.95 (A)	319.92
12) -849.09 (A)	421.9
11) -970.65 (A)	811.08
10) -1000.05 (A)	884.74
9) -1127.39 (A)	1059.85
8) -1182.26 (A)	1076.64
7) -1311.17 (A)	1135.95
6) -1433.33 (A)	1200.05

MO Cutoff 0.10

Solid Mesh

Do More Calculations

Dipole Moment	Bond Dipoles
Electrostatic Potential	UV-Vis
Thermo	IR
Animate Minimization	Write STL (3D Printing)
Reset Display	

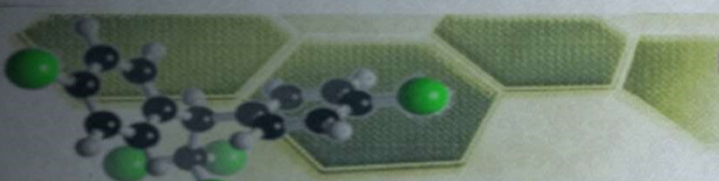
ONLINE SOFTWARE LAIN

NWCHEM ONLINE

EMSL Arrows is a revolutionary approach to materials and chemical simulations that uses NWChem and chemical computational databases to make materials and chemical modeling accessible via a broad spectrum of digital communications including posts to web APIs, social networks, and traditional email.

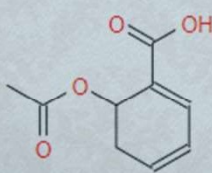
<https://arrows.emsl.pnnl.gov/api/expert>

The screenshot shows the EMSL Arrows 2D Molecular And Reaction Editor web interface. At the top, there is a navigation bar with links: 3D Periodic Editor, 3D Molecular And Reaction Editor, Expert Editor, Microsoft Quantum Editor, EMSL Aerosol Workshop Editor, and Manual. Below the navigation bar, the title "EMSL Arrows 2D Molecular And Reaction Editor" is displayed. A descriptive paragraph states: "EMSL Arrows is a revolutionary approach to materials and chemical simulations that uses NWChem and chemical computational databases to make materials and chemical modeling accessible via a broad spectrum of digital communications including posts to web APIs, social networks, and traditional email." Below this, statistics are shown: "391892 Arrows calculations carried out to date" and "59516 Molecular calculations in database to date". A prompt asks the user to "Enter an [esmls](#), [esmls reaction](#), or other Arrows input, then push the 'Run Arrows' button." Below the input field, there are buttons for "Run Arrows" and "Email Submit". A section for "Append SMILES from JSME Molecular Editor" includes a "Reaction on" dropdown set to "no html5" and a "Clear" button. Below this, a row of buttons for various computational methods is shown: theory(dft), theory(pspw), theory(pspw4), theory(mp2), theory(ccsd(t)), theory(pm3), basis(6-31G*), basis(6-311++G(2d,2p)), xc(lda), xc(pbe), xc(pbe0), xc(b3lyp), xc(b3lyp), xc(m06-2x), solvation_type(None), solvation_type(COSMO), solvation_type(COSMO-SMD), and water (default). Below these buttons, there are buttons for "charge" and "mult". At the bottom, there is a section for "Arrows input to JSME" with a dropdown menu and a set of chemical drawing tools including NEW, R, Z, C, F, G, and Y.



Desain Jmol untuk Penguatan Representasi Submikroskopis pada Perkuliahan Kimia

- MENU UTAMA
- EKSTENSI KOMPUTASI
- DATA STRUKTUR MOLEKUL
- SPEKTRA MOLEKUL
- REAKSI ORGANIK
 - Organic Reactions Introduction
 - Nucleophilic attack by hydride
 - Cyanohydrin Formation
 - Hydrolysis and Transesterification
 - SN¹ & SN² Reaction
 - Simple SN² Reaction
 - SN² Reaction
 - Organometallic Addition
 - Organolithium Reagent
 - Grignard Reagent
 - Eliminasi e₂
 - Pembentukan Acetal



<http://blogchem.com/jmol/>

Structure pasted.

NCI(small molecules) Search

Write down a molecule name, such as indigo, methane, trinitro toluene, PDB Id, and others, choose database and click Search. Below, write command(s) and click Console.

help Console 2D = 3D

JMOL/JSMOL PANEL

Draw a structure on the 2D panel, obtain 3D structure by clicking 3D

Convert: 2D = 3D Eugenol 3D Name It

Load PDB Load PDB by ID Load FILE Load SCRIPT

Change 2D panel to 3D panel:

Show Any MO. Enter *mo*, followed by a *number* (if you have *.log & *.

Pilihan file *.log & *.dat help Run

Examples, PDB File: Pilihan PDB ID File ()

Examples, Load in 2D panel: Flavonoid 3D panel: Indigo Eugenol

Save FILE Save STATE Save JPG Save PNG

Get information of the currently drawn 2D structure:

get the JME string

get the SMILES

get the MOL data