#### **M** winmostar tutorial

# **GAMESS Solvent Effects**

V11.5.6

29 January 2024 X-Ability Co., Ltd.

#### **About This Manual**

- This manual is a tutorial demonstrating use cases for Winmostar V11.
- For those using Winmostar V11 for the first time, please consult <u>Beginner's Guide</u>.
- For those who wish to explore the details of each feature, please refer to <u>Winmostar User Manual.</u>
- Those who wish to practice the contents of this manual are encouraged to attend a training session.
  - <u>Winmostar Introductory Training Session</u>: This guide only introduces the operation methods of the Basic Tutorial.
  - <u>Winmostar Basic Training Session</u>: We will cover the theoretical background, explanations on interpreting results, operational methods of the Basic Tutorial, and procedures for some tutorials beyond the basic level.
  - <u>Individual Training Session</u>: You can freely customize the training content according to your preferences.
- If you are unable to proceed with the operations as outlined in this manual, please first consult <u>Frequently asked questions</u>.
- If your issue is not resolved through the Frequently Asked Questions, for the purpose of information accumulation and management, please contact us using <u>Contact page</u>. Attach files generated at the time of the issue and provide steps to reproduce the problem.
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#### **Overview**

Using the PCM (Polarizable Continuum Model) method, we will perform structure optimization and IR calculations for an acetone molecule in aqueous solution at the B3LYP/6-31G\* level. The PCM method approximates solvent effects by surrounding the solute molecule with a continuous dielectric medium that possesses the dielectric constant of the solvent.

For comparison, we will also carry out similar structure optimization and IR calculations in vacuum at the B3LYP/6-31G\* level. We will observe how the stretching vibrations of the hydrophilic C=O group and the bending motions of the hydrophobic C-H group change.



### **Preference of Operating Environment**

- For GAMESS:
  - Please install GAMESS according to GAMESS Installation Manual available at <a href="https://winmostar.com/en/manual\_en/installation/GAMESS">https://winmostar.com/en/manual\_en/installation/GAMESS</a> install manual en win. <a href="https://winmostar.com/en/manual\_en/installation/gamess">pdf</a>

### **Operating Modes of Winmostar V11**

V11 offers two operating modes: **Project Mode** and **File Mode**. This manual focuses on operations in Project Mode. For operations in File Mode, please refer to tutorial for version 10.



When creating a continuation job in File Mode or versions before V10, you must display the final structure of the original job each time. In Project Mode, this final structure is automatically inherited.

### A. System Modeling

For basic operation methods, please refer to GAMESS Foundation Tutorial.

- A. Launch Winmostar and click **Create New Project (3D)**. If Winmostar is already running, first click **File | Close**.
- B. Enter 'acetone' for **Project name** and click **Save**.

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### A. System Modeling

- A. Select -CH3 from Fragment at the top of Main Window and click Replace once to create methane.
- B. Select -CHO from Fragment and click Replace once to create acetaldehyde.
- C. Select -CH3 again and click Replace once to create acetone.



### **B. Execution of Calculation**

- A. Select **GAMESS** from **Solver** and click **Workflow Setup**.
- B. In GAMESS Workflow Setup window, change Preset to Optimize+IR.
- If you want to reduce computational accuracy to finish calculations faster, change **Basis set** to **STO-3G**.
- C. Click + in # of Jobs.



#### **B. Execution of Calculation**

- A. Uncheck the box for **Same conditions as previous job** for the newly displayed **2nd job**.
- B. Change **Solvent** for **2nd job** to **WATER (PCM)**.
- C. Click OK.

 $\cdot$  1st job will be the structure optimization and IR calculation in vacuum, and 2nd job will be the structure optimization and IR calculation in aqueous solution.

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#### **B. Execution of Calculation**

A. Set **# of MPI Procs** according to the number of cores in your computer. When running on a remote machine, also configure settings such as the profile.

Β.	Click <b>Run</b> .	阙 Job Setting		_		×				
		Run local job								
		Program	GAMESS (1) V							
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- A. After the calculation is completed and the status of work2\_GMS\_OPT-IR folder in Working Folders changes to END or END(-), click on work1\_GMS\_OPT-IR in Working Folders.
- B. Confirm that Action () has changed to work1\_GMS\_OPT-IR, then click on **IR/Raman** to display **IR Spectrum** window for the vacuum condition.

	℅ Project		
Working Folders (acetone) Options V	Working Folders (acetone)	Options ▼	
• work1_GMS_OPT-IR	• work1_6MS_0PT-IR	END	📖 IR Spectrum (gms.out) — 🗆 🗙
work2_GMS_0PT-IR	work2_GMS_OPT-IR	END	Freq. Scaling 1.000 V Edit Selected Peak: 0.0 1/cm V 0.0000 V V IR
	6	>	1 44 0.082 2 0 0.000 3 0 0.000 4 0 0.000 5 17 0.042 6 28 0.071 7 64 0.037 8 177 0.068
Action (work2_GMS_OPT-IR)	Action (work1_GMS_OPT-IR)		9 378 0.030 10 487 0.017 11 532 0.338 12 785 0.023
Coordinate (Initial)	🔁 Coordinate (Initial)		13 836 0.005 14 903 0.109 15 1096 0.001
🔁 Coordinate (Final), Charge & Dipole	Coordinate (Final), Charge & D	Dipole	16 1131 0.114 17 1247 1.914 19 1440 0.920
🚾 Log	🚾 Log		18 1410 0.336 19 1412 1.238 20 1431 0.018
Log (Extracted)	Log (Extracted)		Animation Vector X: Range 0 - 4200 Vector Y: Scale > 0.5 Vector
Animation	Animation		Magnitude (
📑 MO & Charge	MO & Charge		
📑 IR/Raman	📑 IR/Raman		
Show in Explorer	Show in Explorer		

Check the C=O stretching vibration and C-H bending vibration in vacuum. If calculated using B3LYP/STO-3G, the values will be different.

- A. Click on the 24th peak at 1824cm<sup>-1</sup> and then click **Animation**, **Winmostar Viewer** will start. This peak is identified as the stretching vibration of the C=O part.
- B. Click on the 18th peak at 1410cm<sup>-1</sup> or the 19th peak at 1413cm<sup>-1</sup> and then click **Animation**, **Winmostar Viewer** will start, showing that these are the bending vibrations of the C-H part.

C=O Stretching Vibration



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C-H Bending Vibration

- A. Click on work2\_GMS\_OPT-IR folder in Working Folders.
- B. Confirm that Action () has changed to work2\_GMS\_OPT-IR and then click on **IR/Raman** to display **IR Spectrum** window for the aqueous solution.



Confirm the C=O stretching vibration and C-H bending vibration in aqueous solution.

- A. Click on the 24th peak at 1788cm<sup>-1</sup> and then click **Animation**. **Winmostar Viewer** will start, showing that this peak corresponds to the C=O stretching vibration.
- B. Click on either the 18th peak at 1405cm<sup>-1</sup> or the 19th peak at 1412cm<sup>-1</sup> and then click **Animation**. **Winmostar Viewer** will start, indicating that these peaks correspond to the C-H bending vibrations.



#### C=O Stretching Vibration



C-H Bending Vibration



In the stretching motion of the hydrophilic C=O part, there is a difference of 36 cm-1 between in vacuum and in water solution, while the bending vibration of the hydrophobic C-H part shows a difference of less than 5 cm-1. By performing calculations that include solvent effects, it is possible to understand from the calculations which parts are significantly affected by the solvent.

Vibrational Frequencies of Acetone (cm<sup>-1</sup>)

	In Vacuum	In Aqueous Solution
C=O Stretching Vibration	1824	1788
C-H Bending Vibration	1410 1413	1405 1412

## Finally

• For detailed information on each feature, please refer to Winmostar User Manual.





#### Winmostar User Manual

Scenes from Winmostar Training Session

- If you wish to practice the contents of this guide, please consider attending <u>Winmostar Introductory Training Session</u>, <u>Winmostar Basic Training Session</u>, or <u>Individual Training Session</u>. (See page 2 for details.)
- If you are unable to proceed as instructed in this guide, please first consult <u>Frequently asked questions</u>.
- If FAQs do not resolve your issue, for the purposes of information accumulation and management, please contact us through <u>Contact page</u>, detailing the steps to reproduce the issue and attaching any generated files at that time.