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 Beginner's Guide.
- For those who wish to explore the details of each feature, please refer to Winmostar User Manual.
- Those who wish to practice the contents of this manual are encouraged to attend a training session.
  - Winmostar Introductory Training Session:This guide only introduces the operation methods of the Basic Tutorial.
  - Winmostar Basic Training Session: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.
  - Individual Training Session: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 Frequently asked questions.
- If your issue is not resolved through the Frequently Asked Questions, for the purpose of information accumulation and management, please contact us using Contact page. Attach files generated at the time of the issue and provide steps to reproduce the problem.
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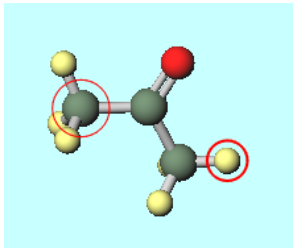
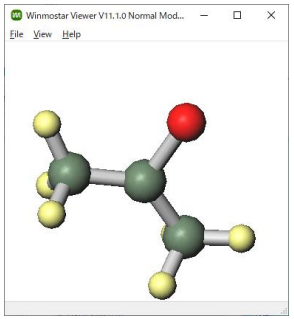
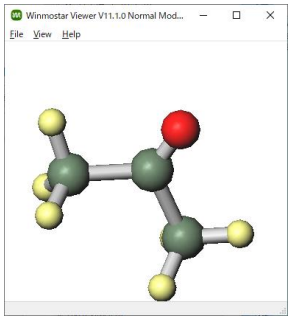
Overview

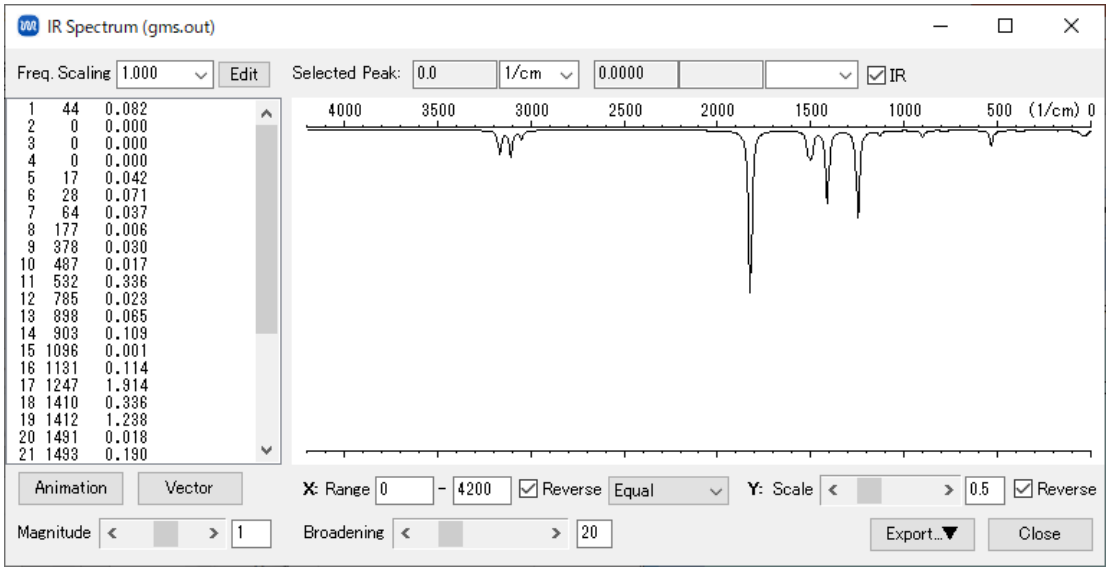
Using the PCM (Polarizable Continuum Model) method, we will perform structure optimization and IR calculations for an acetone molecule in aqueous solution at the B3LYP/6-31G* level. The PCM method approximates solvent effects by surrounding the solute molecule with a continuous dielectric medium that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







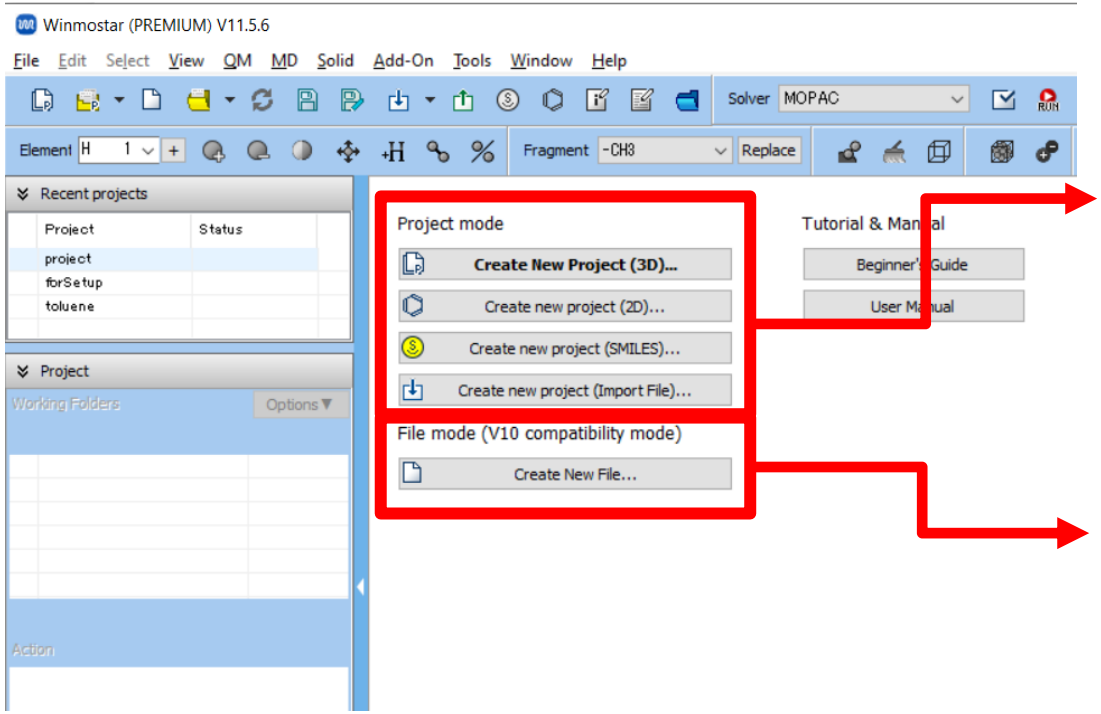


Preference of Operating Environment

- For GAMESS:
  - Please install GAMESS according to GAMESS Installation Manual available at https://winmostar.com/en/manual_en/installation/GAMESS_install_manual_en_win.pdf

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.



Project Mode **New Features in V11**

Users can manage jobs without having to manage individual files.
We generally recommend using this mode.

File Mode

Users explicitly create and manage individual files.
The operational procedure is the same as from V10 and earlier versions.

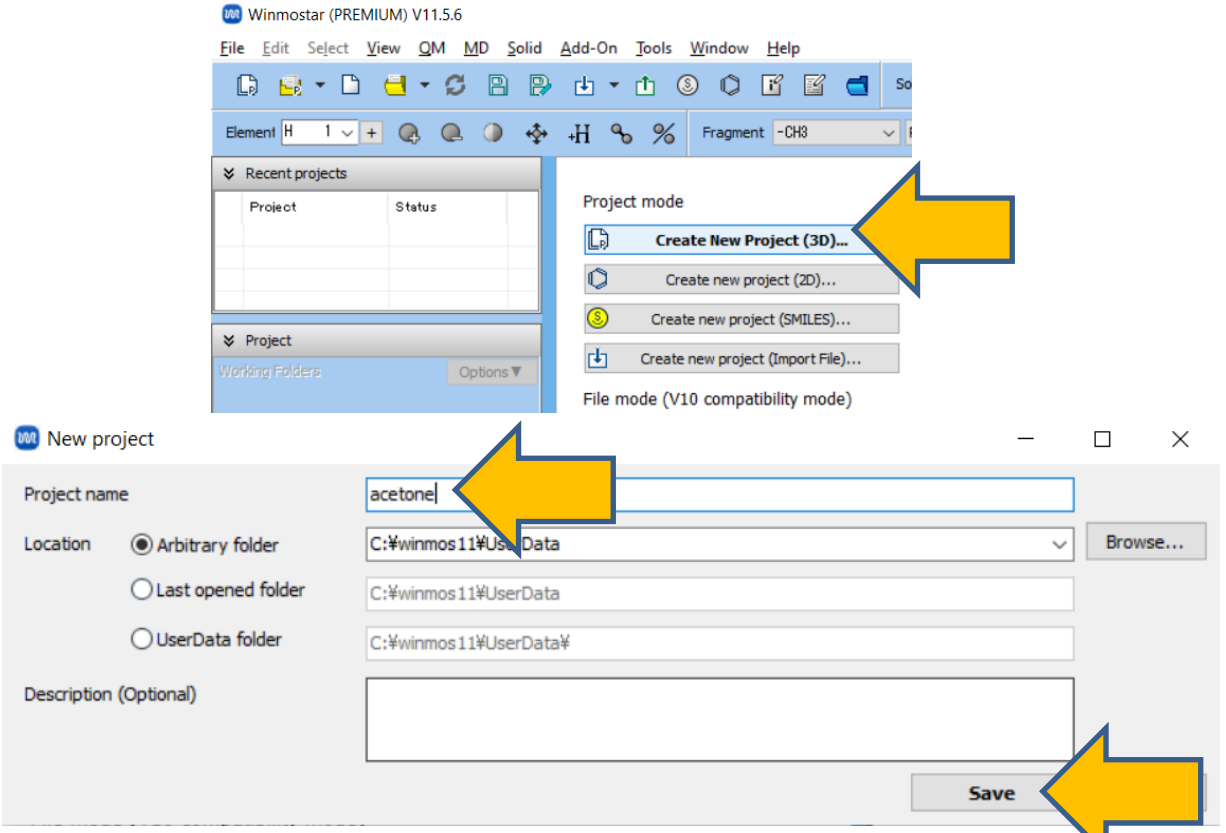
When creating a continuation job in File Mode or versions before V10, you must display the final structure of the original job each time. In Project Mode, this final structure is automatically inherited.

A. System Modeling

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

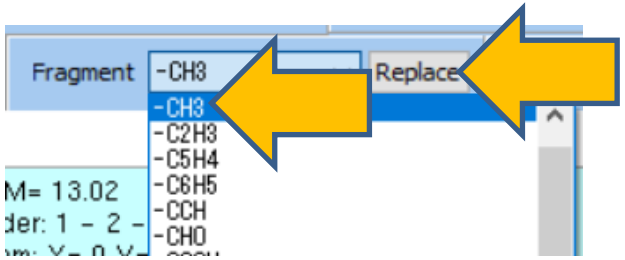
A. Launch Winmostar and click **Create New Project (3D)**. If Winmostar is already running, first click **File | Close**.

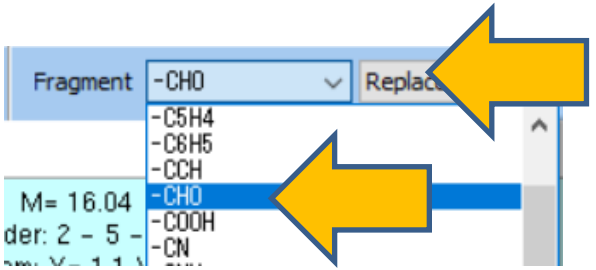
B. Enter 'acetone' for **Project name** and click **Save**.

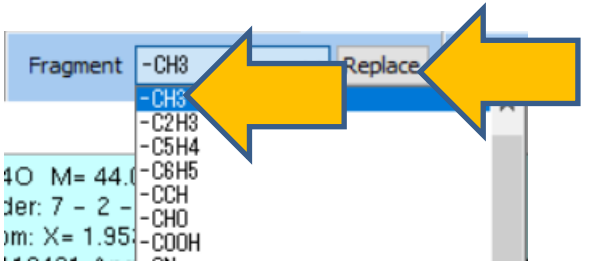


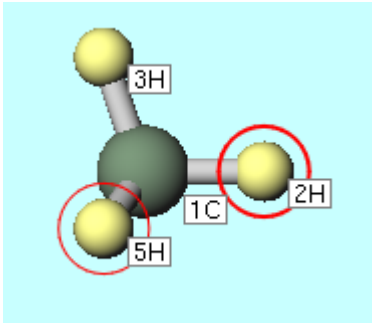
A. System Modeling

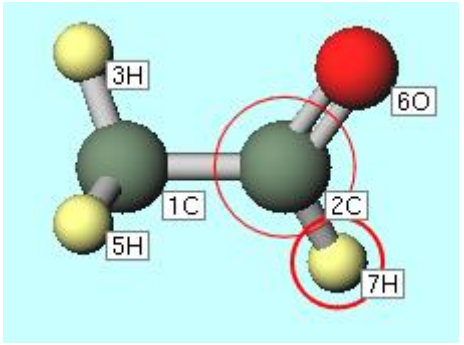
A. Select **-CH3** from **Fragment** at the top of Main Window and click **Replace** once to create methane.
B. Select **-CHO** from **Fragment** and click **Replace** once to create acetaldehyde.
C. Select **-CH3** again and click **Replace** once to create acetone.

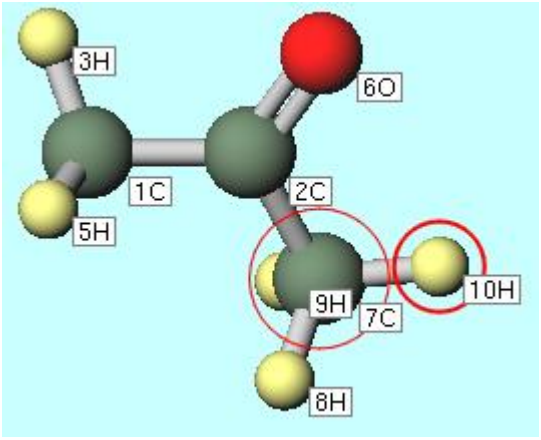












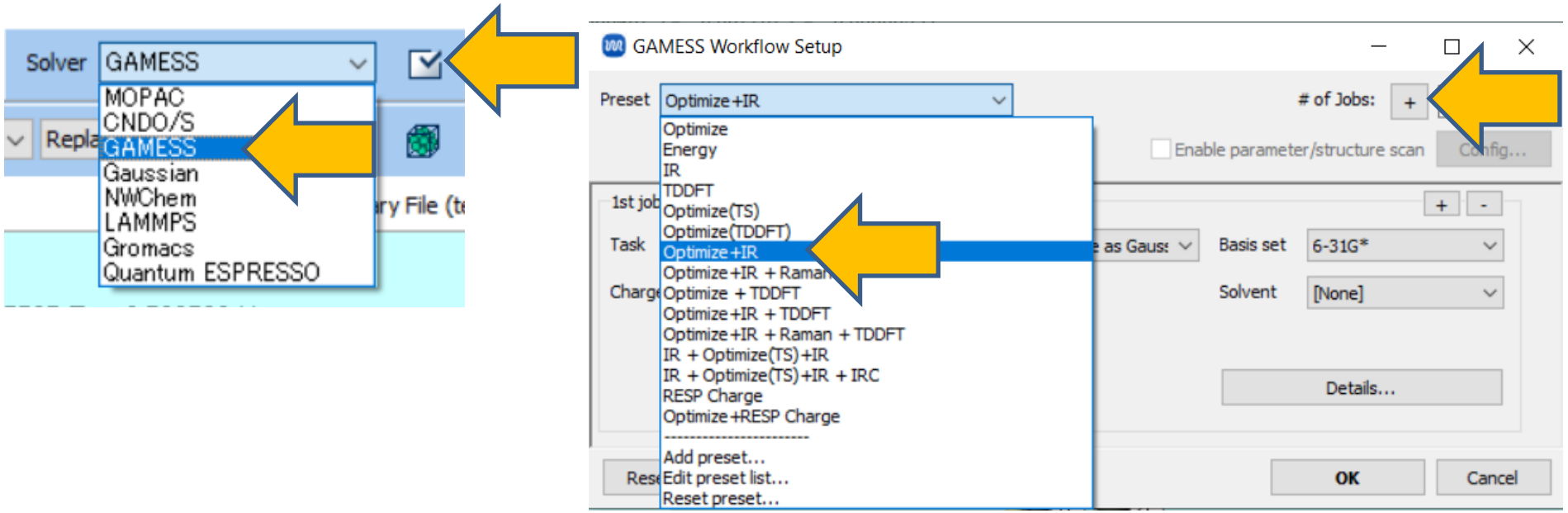
B. Execution of Calculation

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**.



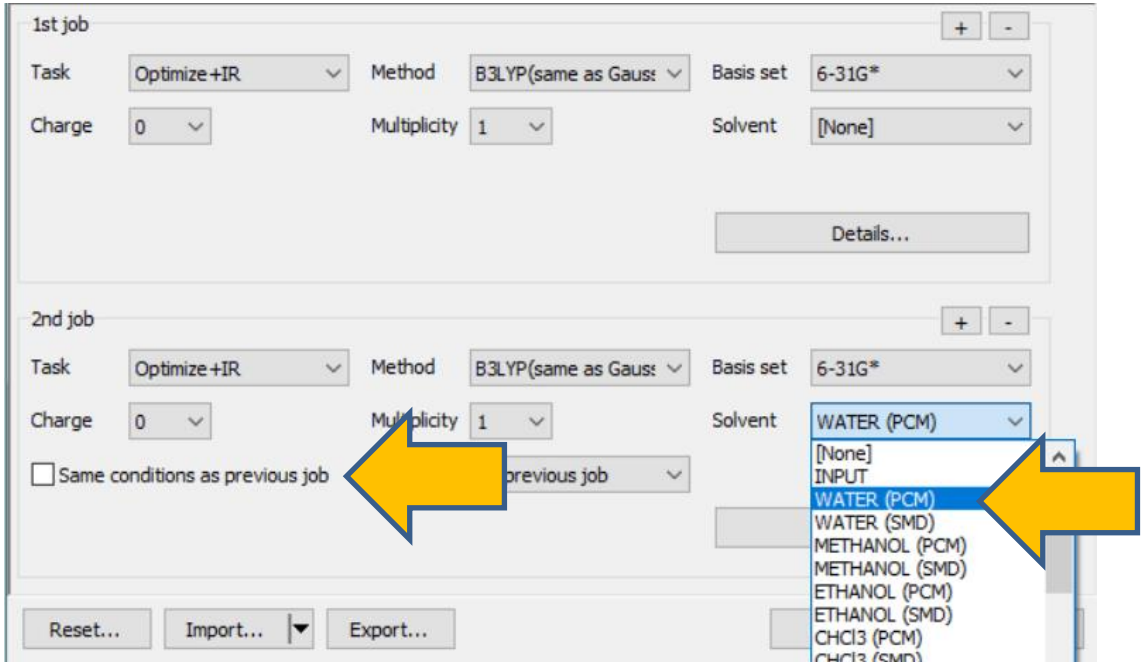
B. Execution of Calculation

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**.

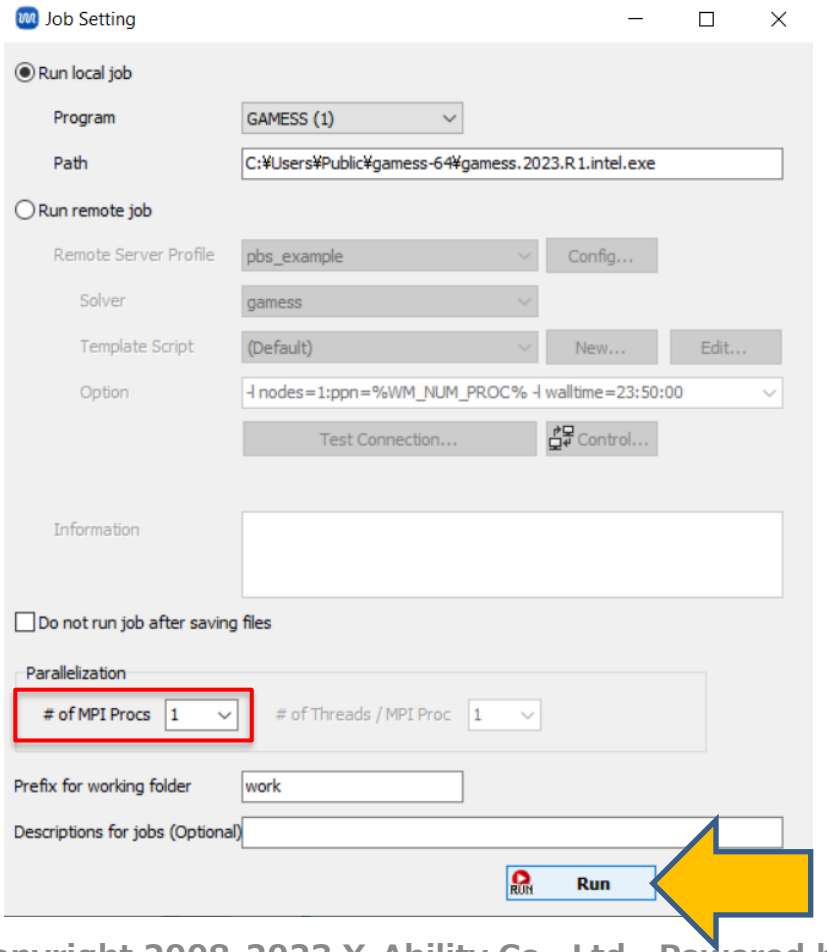
・1st job will be the structure optimization and IR calculation in vacuum, and 2nd job will be the structure optimization and IR calculation in aqueous solution.



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.

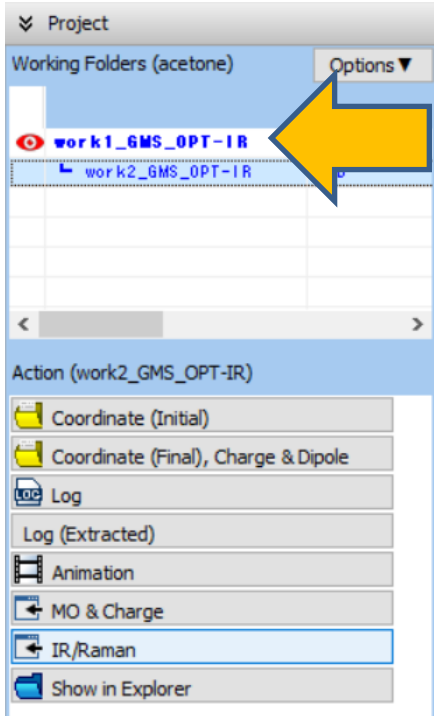
B. Click **Run**.

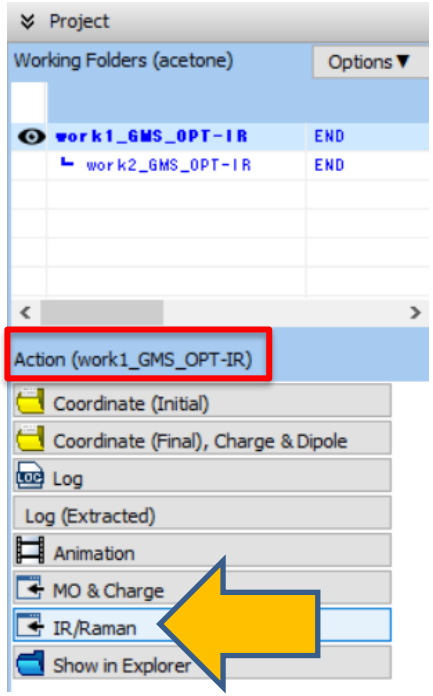


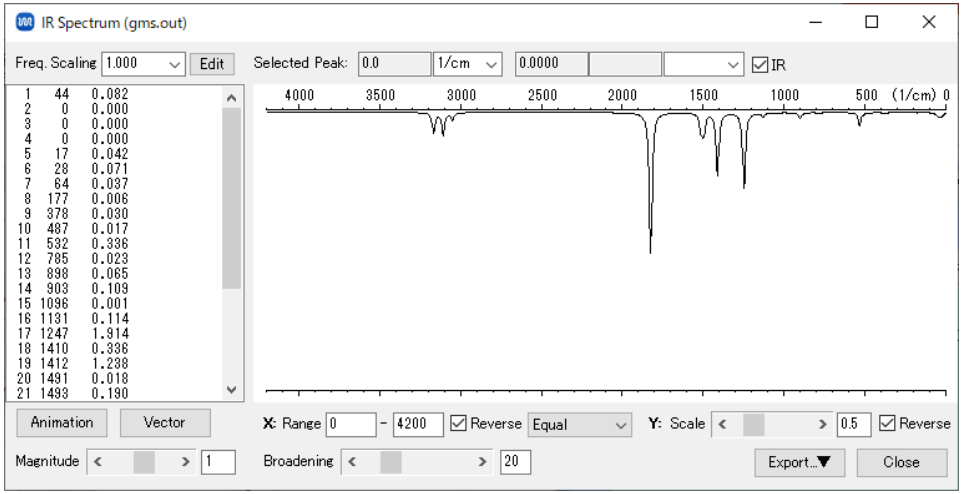
C. Results Analysis

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.







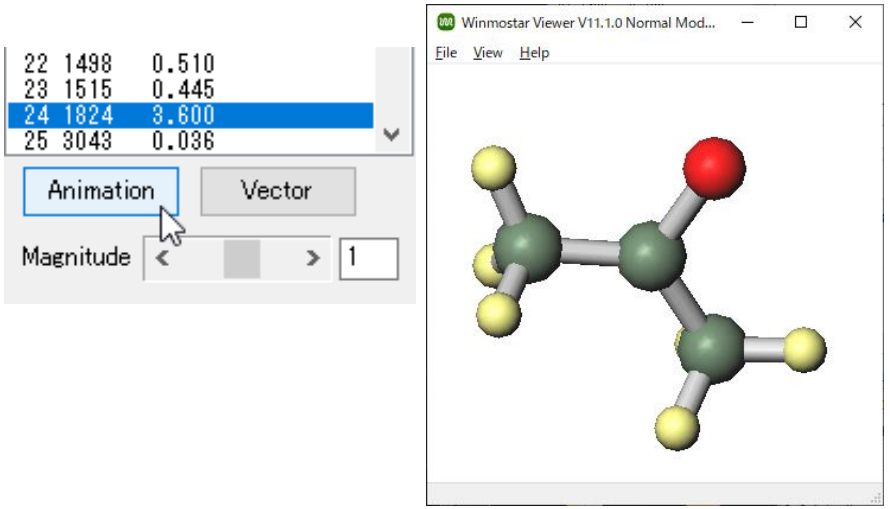
C. Results Analysis

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

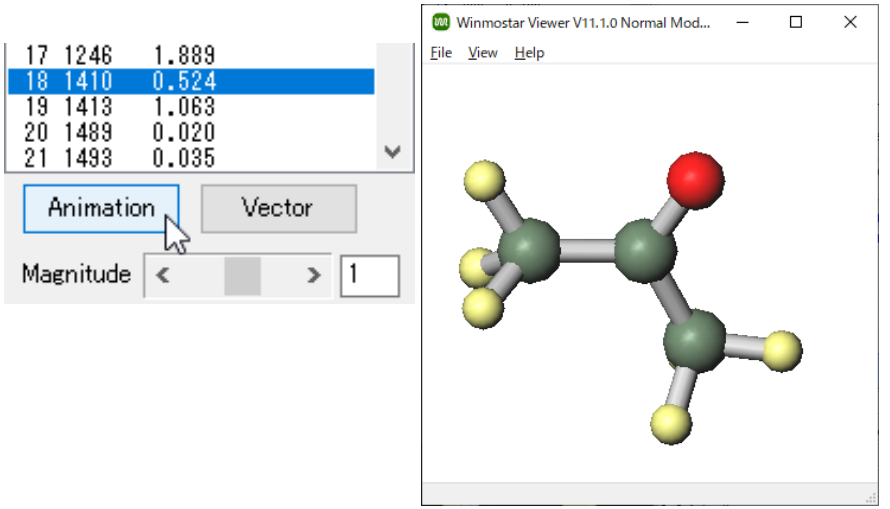
A. Click on the 24th peak at 1824cm^{-1} and then click **Animation**, **Winmostar Viewer** will start. This peak is identified as the stretching vibration of the C=O part.

B. Click on the 18th peak at 1410cm^{-1} or the 19th peak at 1413cm^{-1} and then click **Animation**, **Winmostar Viewer** will start, showing that these are the bending vibrations of the C-H part.

C=O Stretching Vibration



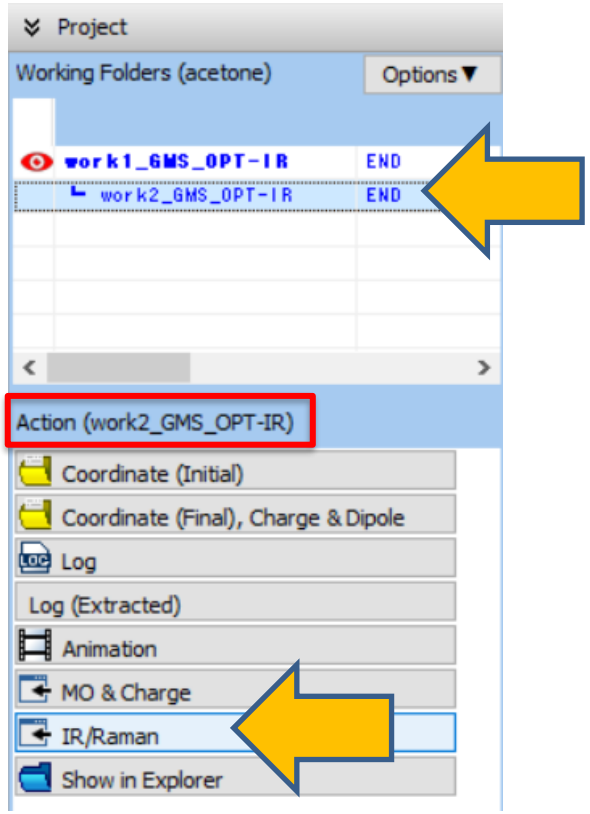
C-H Bending Vibration

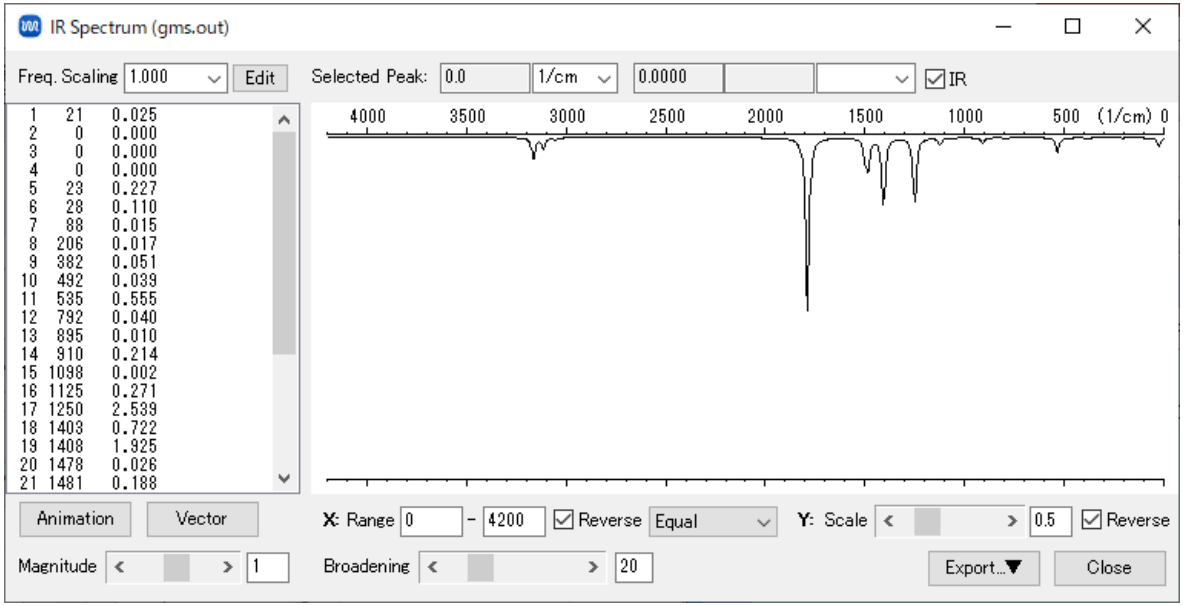


C. Results Analysis

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.





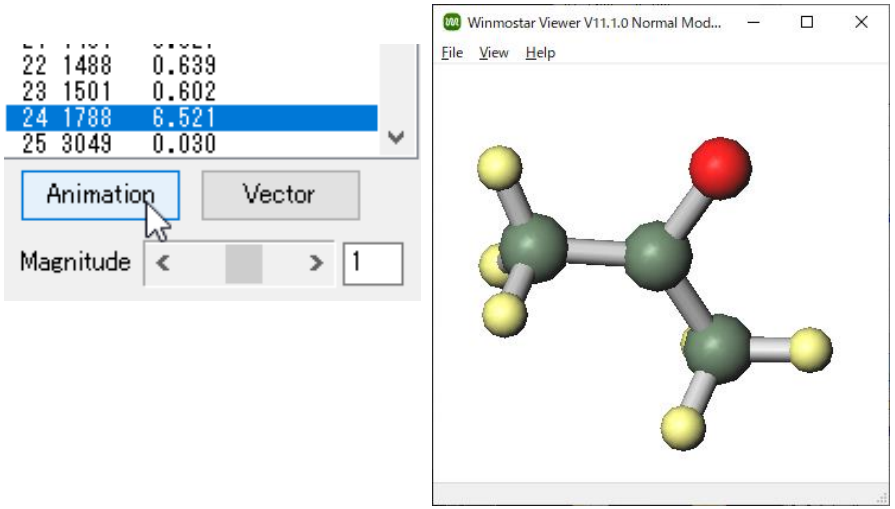
C. Results Analysis

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

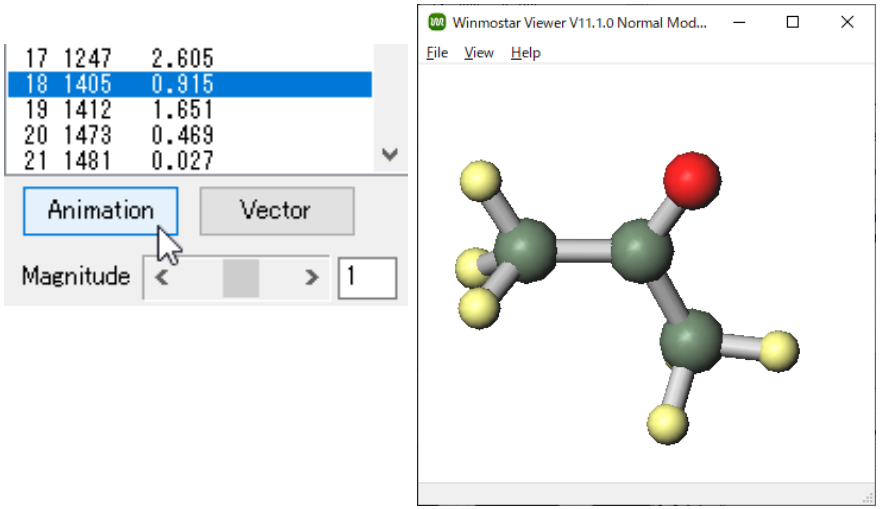
A. Click on the 24th peak at 1788cm^{-1} and then click **Animation**. **Winmostar Viewer** will start, showing that this peak corresponds to the C=O stretching vibration.

B. Click on either the 18th peak at 1405cm^{-1} or the 19th peak at 1412cm^{-1} 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



C. Results Analysis

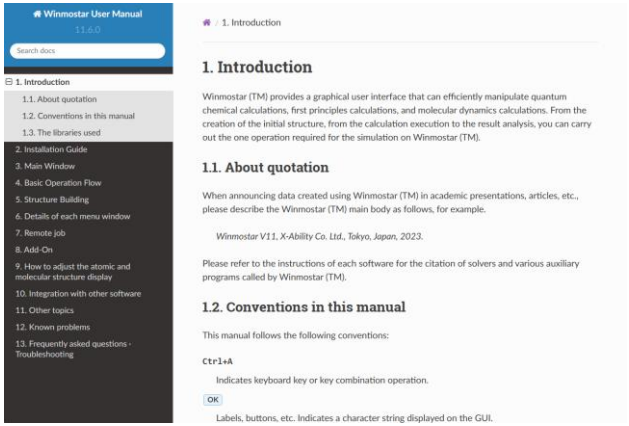
In the stretching motion of the hydrophilic C=O part, there is a difference of 36 cm-1 between in vacuum and in water solution, while the bending vibration of the hydrophobic C-H part shows a difference of less than 5 cm-1. By performing calculations that include solvent effects, it is possible to understand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

Vibrational Frequencies of Acetone (cm^{-1})

	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

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