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Winmostar tutorial
GAMESS/Gaussian/NWChem Basics
V9.4.0

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Nov 11, 2019

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Summary

- Quantum chemical calculations of styrene molecules are performed using GAMESS, Gaussian or NWChem. First, structure optimization is performed, and vibration spectrum (IR, Raman), NMR spectrum, and UV-Vis spectrum are calculated for the optimized structure. Also displays molecular orbitals and electrostatic potential.

Notes:

- This tutorial uses relatively low-precision basis functions and calculation methods so that various calculations can be performed in a short time.
- In normal research, the same calculation conditions are used as much as possible for structure optimization and physical property calculation, but in this tutorial, for the sake of convenience, only DFT is used instead of HF for UV-Vis calculation.
- The GAMESS NMR spectrum calculation procedure is not shown here.
- Since it takes time to display ESP, the potential distribution obtained from the point charge after population analysis that can be easily obtained is displayed here as the electrostatic potential.

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Configuration

-GAMESS
See Quantum GAMESS install manual
https://winmostar.com/en/manual_en/installation/GAMESS_install_manual_en_win.pdf

-Gaussian
Install Gaussian according to the instructions provided by the vendor.

-NWChem
See NWChem install manual page.
https://winmostar.com/en/nwchem4wm_en.html

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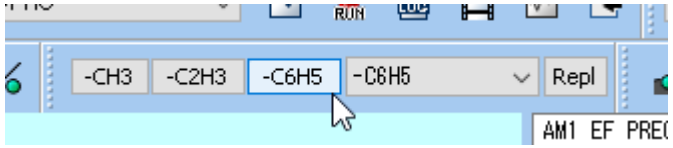
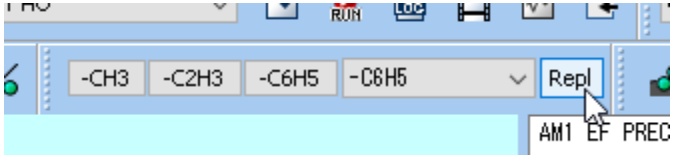
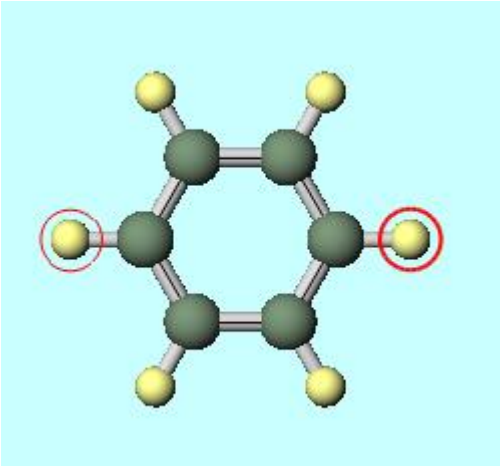
I. Creating the Model

1. Click the **-C6H5** button at the top of the screen.
2. Click the **Repl** button to create a benzene molecule.







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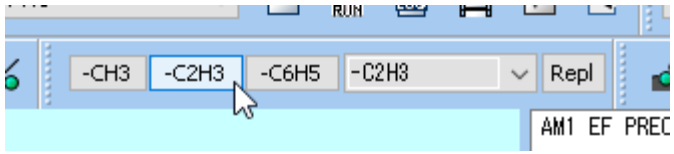
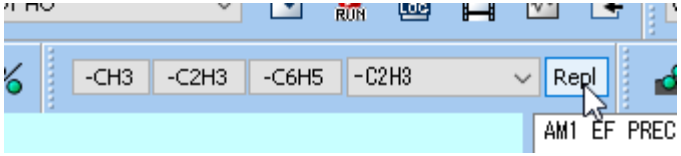
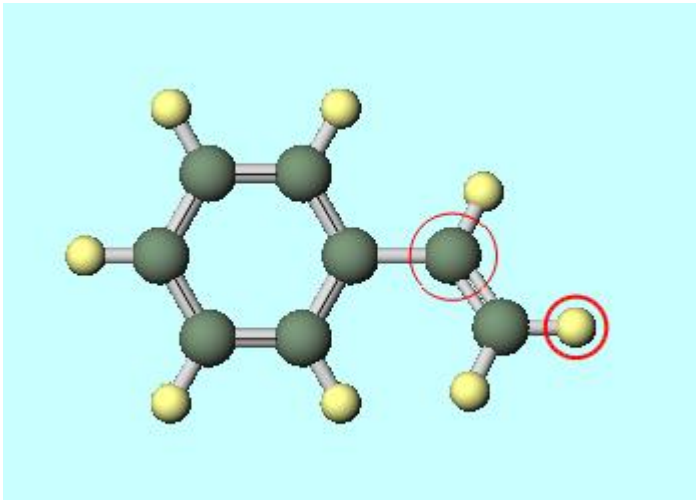
I. Creating the Model

1. Click the **–C2H3**.
2. Click the **Repl** button to create a styrene molecule.







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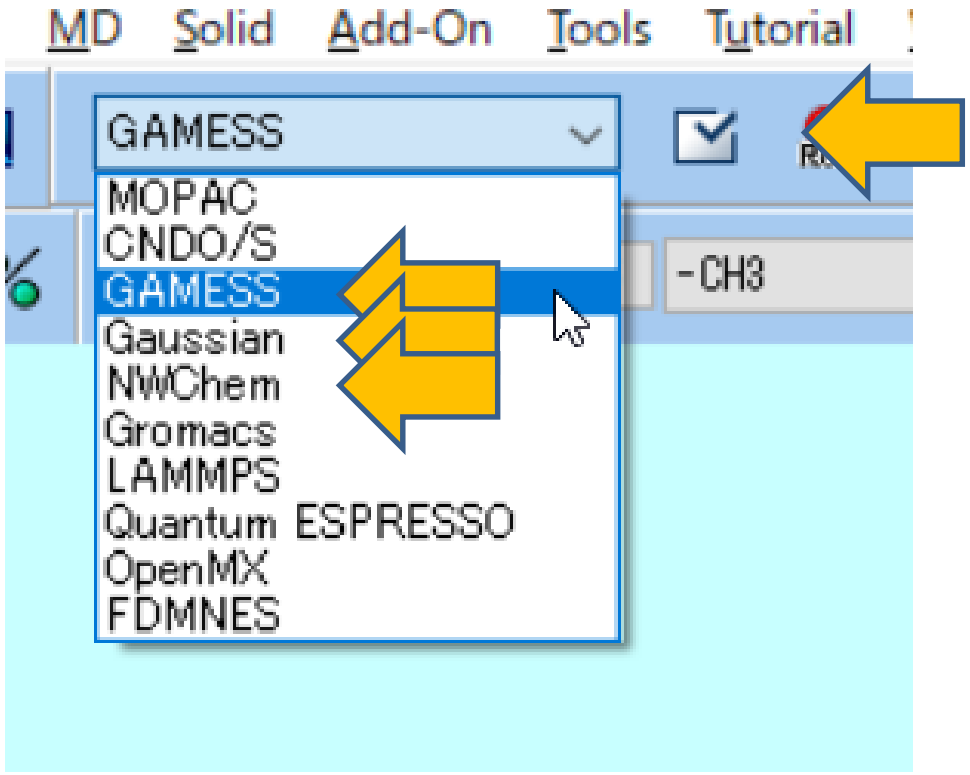
II. Structural optimization calculation

1. Select **GAMESS**, **Gaussian** or **NWChem** from the solver list.
2. Click **Configure**.



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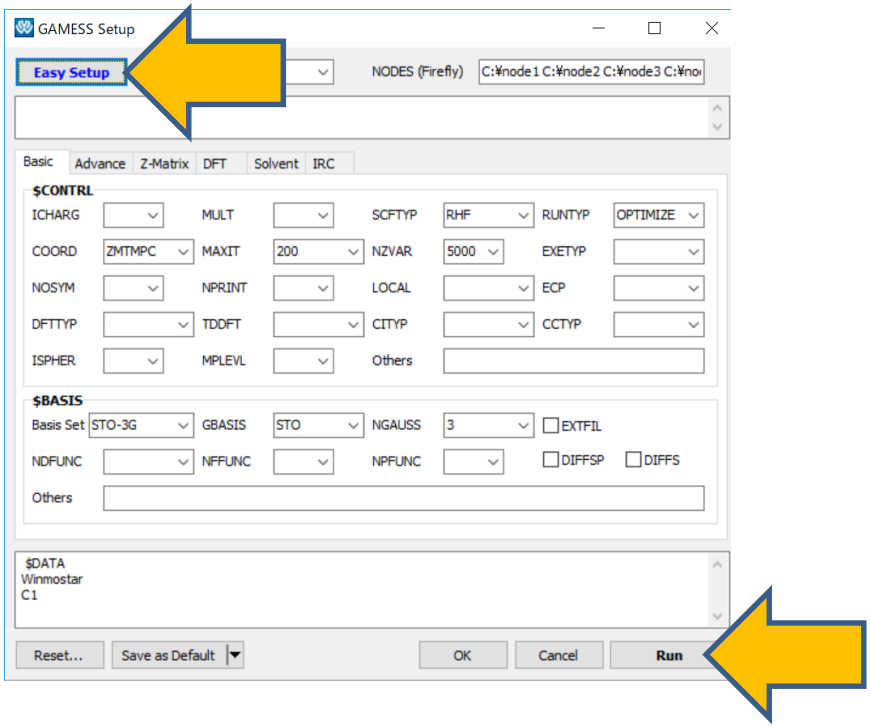
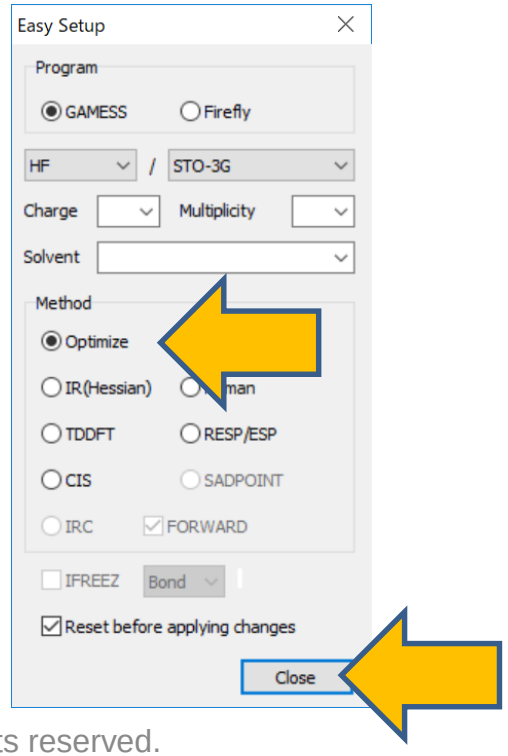
II. Structural optimization calculation

When **GAMESS** is selected in the solver list

1. Click **EasySetup** at the top of the GAMESS Setup window.
2. Select **Optimize** from **Method** in the Easy Setup window.
3. Click **Close** below.
4. Then click **Run** at the bottom of the GAMESS Setup window.





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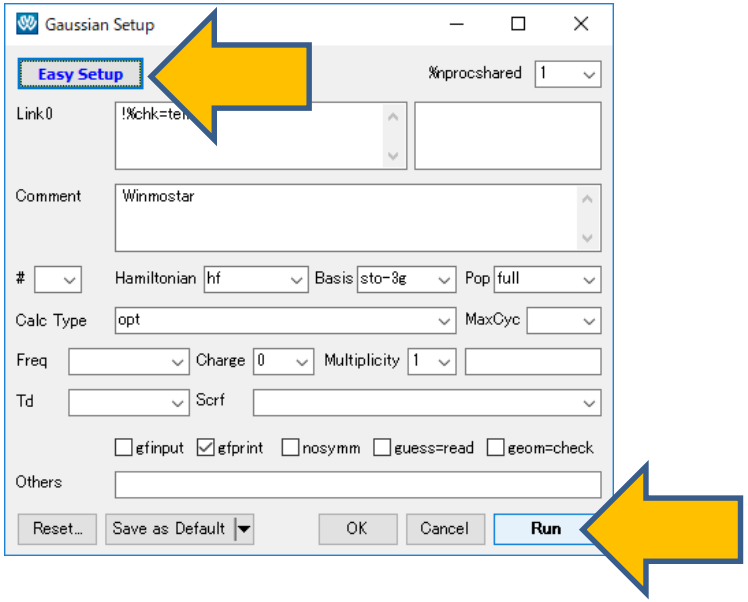
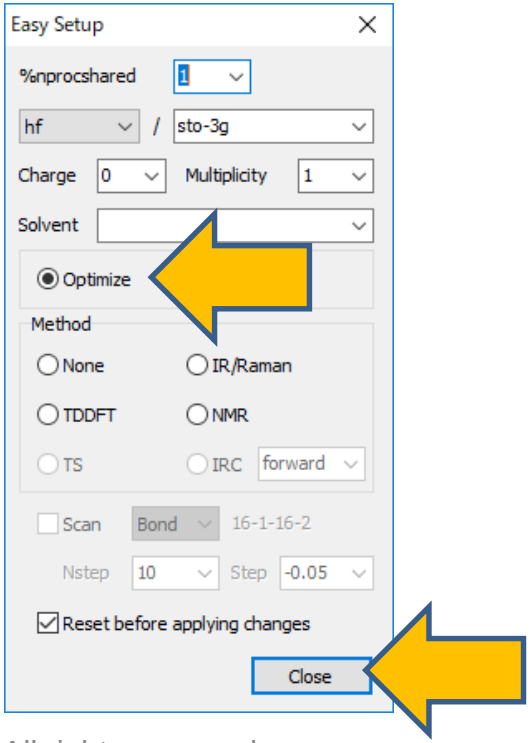
II. Structural optimization calculation

When **Gaussian** is selected in the solver list

1. Click **EasySetup** at the top of the Gaussian Setup window.
2. Select **Optimize** in the Easy Setup window.
3. Click **Close** below.
4. Then click **Run** at the bottom of the Gaussian Setup window.





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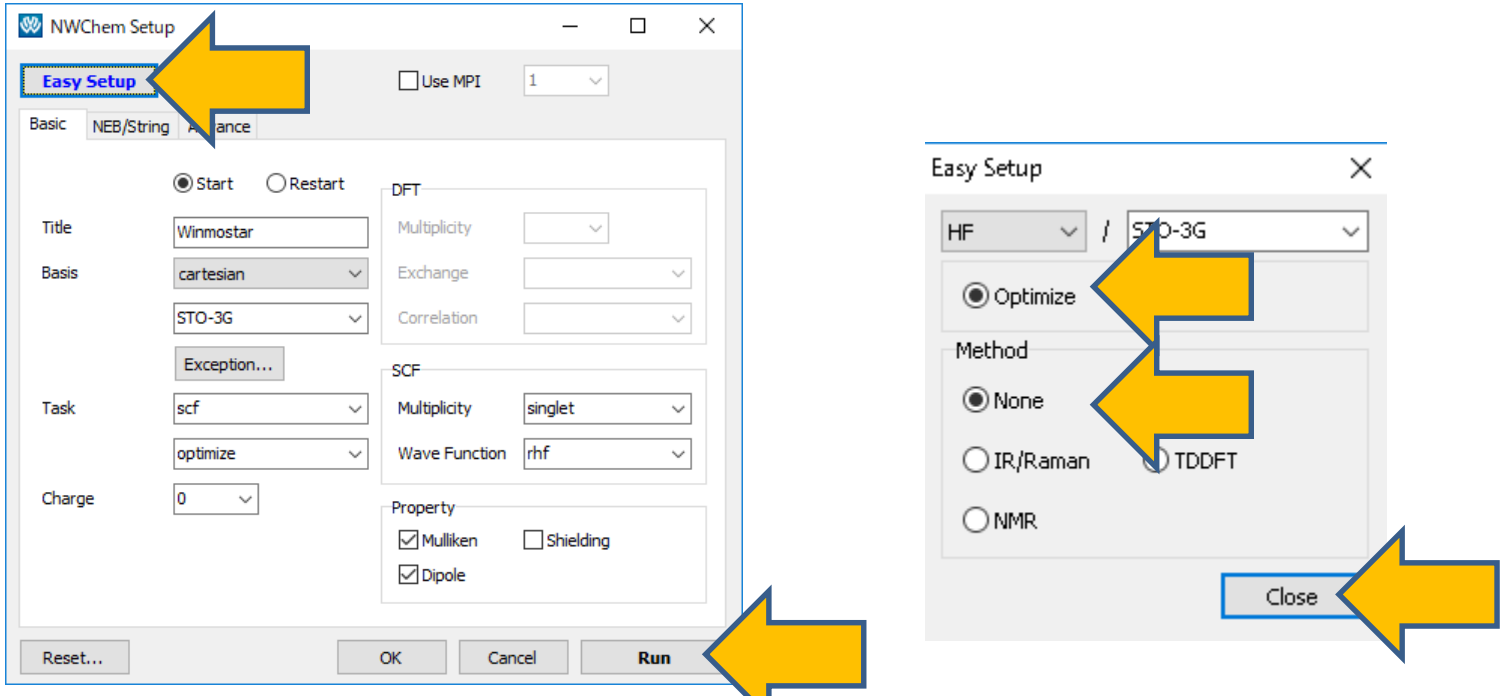
II. Structural optimization calculation

When **NWChem** is selected in the solver list

1. Click **EasySetup** at the top of the NWChem Setup window.
2. Select **Optimize** and **None** from **Method** in the Easy Setup window.
3. Click **Close** below.
4. Then click **Run** at the bottom of the NWChem Setup window.



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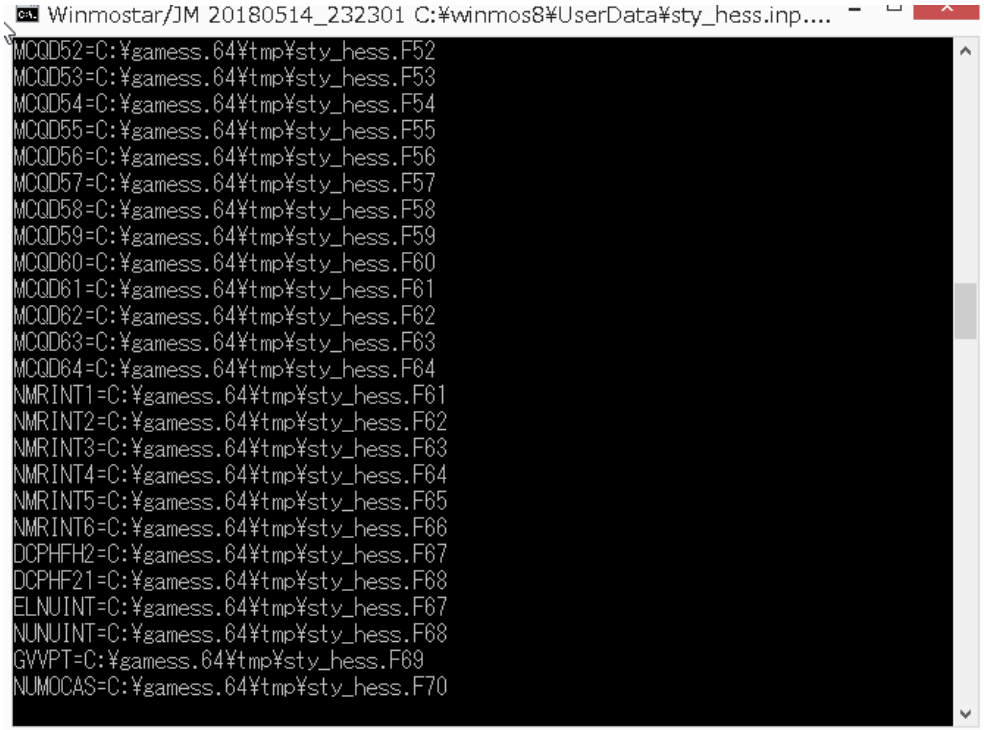
II. Structural optimization calculation

When the file save dialog opens, enter the file name. (Eg “**sty_opt**”)
When you click **Save**, the **Winmostar Job Manager** and command prompt window will appear, and the calculation will start.



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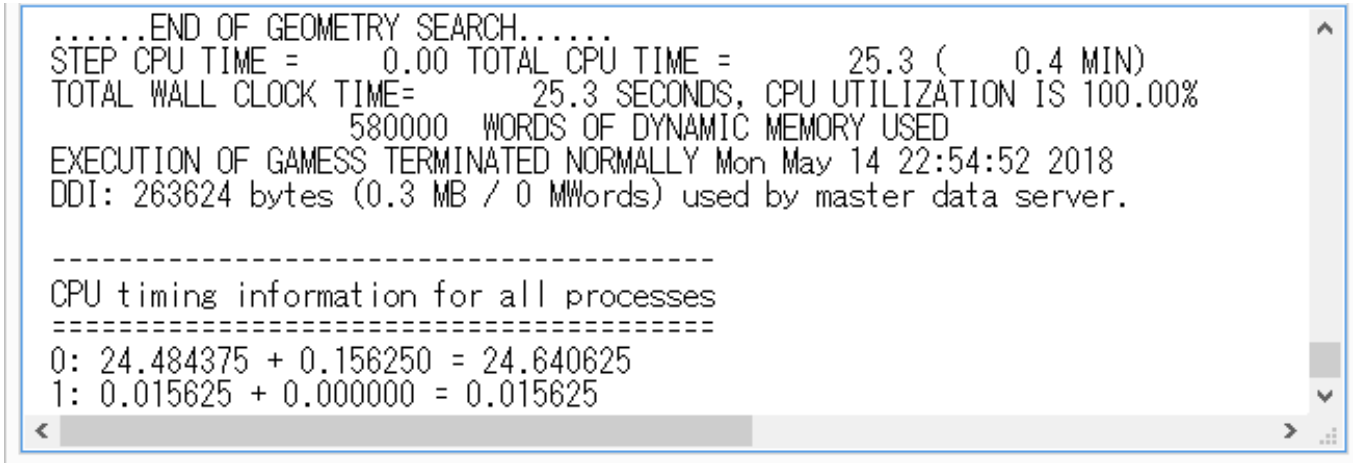
II. Structural optimization calculation

When **GAMESS** is selected in the solver list

1. After completing the calculation, click (**Open Log File**) in the main window.
2. Open the file selected by default in the dialog.
3. As the log file opens, check for a message indicating that the calculation ended normally, such as " **EXECUTION OF GAMESS TERMINATED NORMALLY...** ". This must be done after every calculation.



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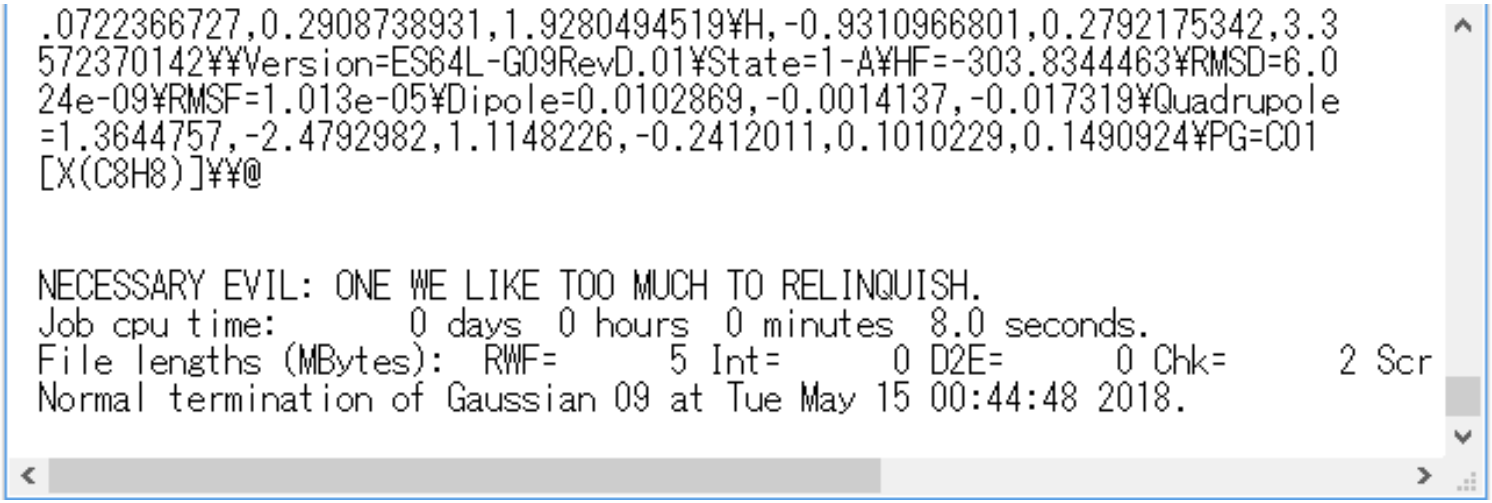
II. Structural optimization calculation

When **Gaussian** is selected in the solver list

1. After completing the calculation, click (**Open Log File**) in the main window.
2. Open the file selected by default in the dialog.
3. As the log file opens, check for a message indicating that the calculation ended normally, such as " **Normal termination of Gaussian 09...** ". This must be done after every calculation.



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II. Structural optimization calculation

When **NWChem** is selected in the solver list

1. After completing the calculation, click (**Open Log File**) in the main window.
2. Open the file selected by default in the dialog.
3. As the log file opens, check for a message indicating that the calculation ended normally, such as " **Optimization converged** ". This must be done after every calculation.

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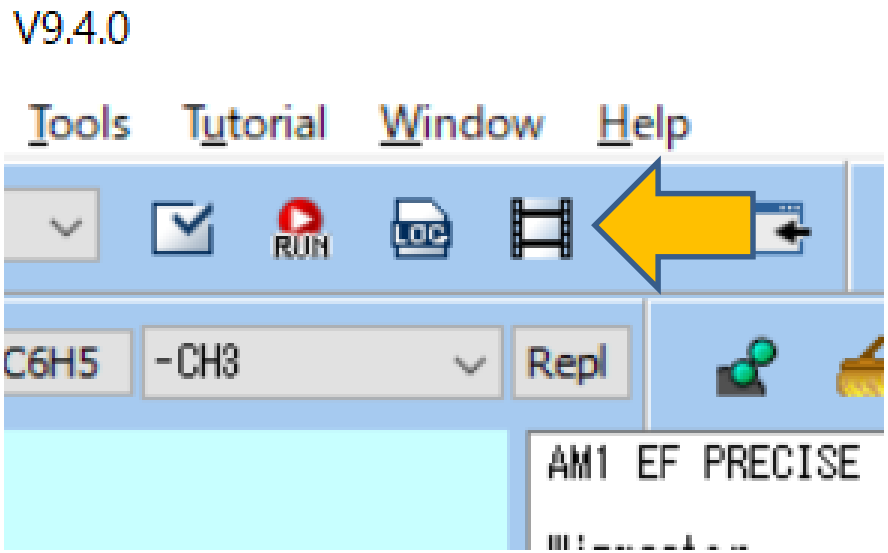
II. Structural optimization calculation

1. After completing the calculation, click (Animation) at the top of the main window.
2. In the dialog that opens, open the file selected by default.



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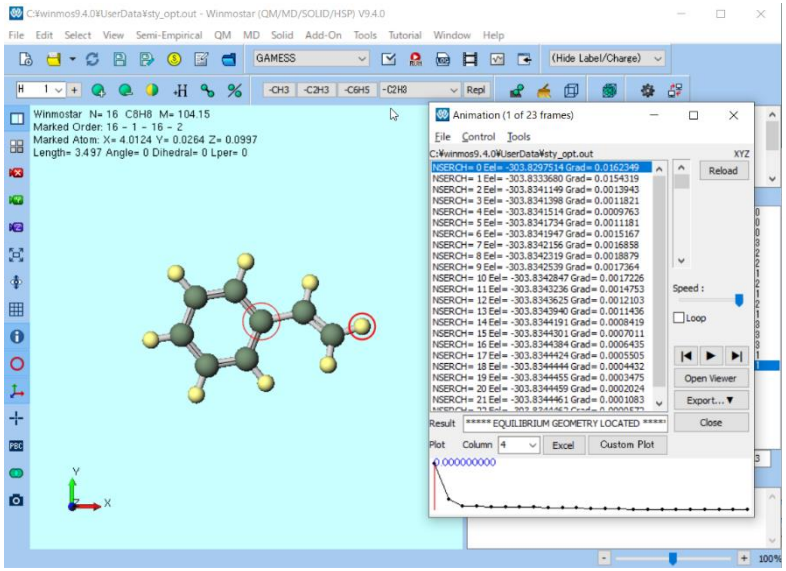
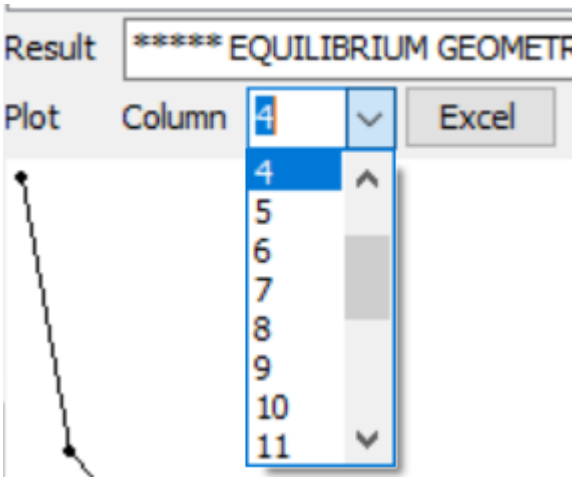
II. Structural optimization calculation

1. Click ▶ button at the bottom right of the **Animation** window to play the structure optimization animation (by default, playback ends in an instant).
2. At the bottom of the **Animation** window, a graph of the data in the column selected in **Column** among the numerical data of each step in the middle of the window is displayed.
3. Finally, close the **Animation** window with the final frame structure selected and displayed.

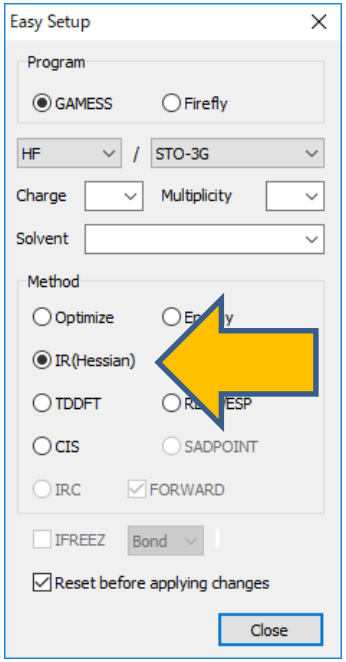




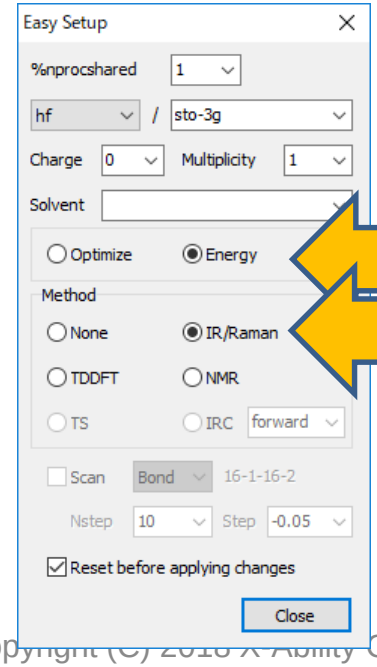
III. Calculation of vibration spectrum

1. Open **EasySetup** in the keyword setting window again.
2. For **GAMESS**, select **IR (Hessian),** click **Close** and **Run**.
   For Gaussian, select **Energy** and **IR / Raman**, click **Close** and **Run**.
   For NWChem, select **Energy** and **IR / Raman**, click **Close** and **Run**.
3. Save the file with a different file name from the structural optimization calculation such as **sty_hess**, and start the calculation.

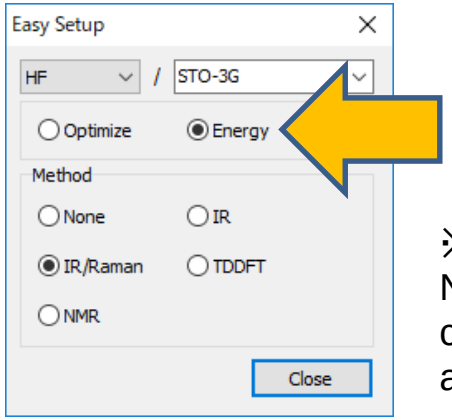
GAMESS



Gaussian



NWChem



※ In the case of NWChem, this calculation may take about 30 minutes.

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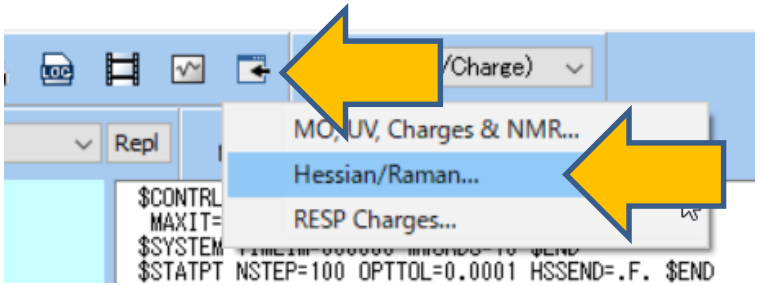
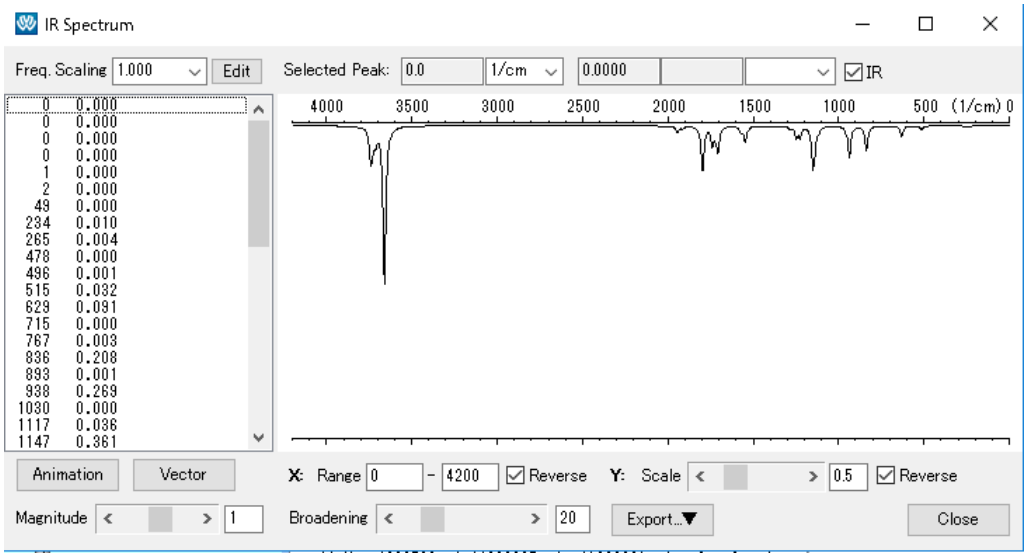
III. Calculation of vibration spectrum

1. After the calculation, click on the **Hessian/Raman, Freq** or **Frequencies/Ranman** of (**Analysis**).
2. When you select a file selected by default in the dialog, the **IR Spectrum** window appears. In the case of **Gaussian** and **NWChem**, a blue Raman spectrum is also drawn.
3. The scaling factor for each calculation method and basis function is selected by **Freq Scaling** as necessary.





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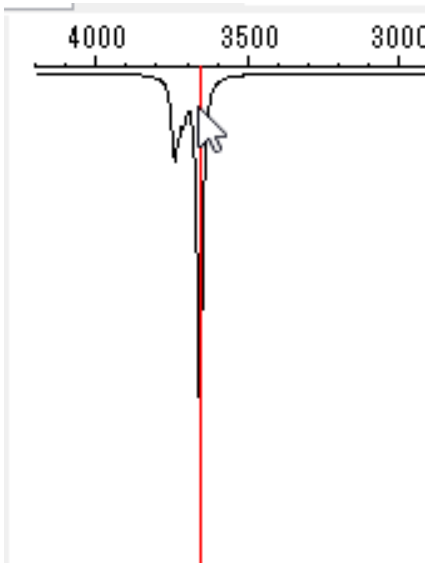
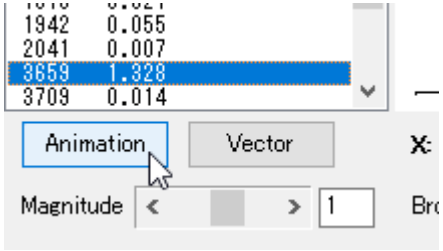
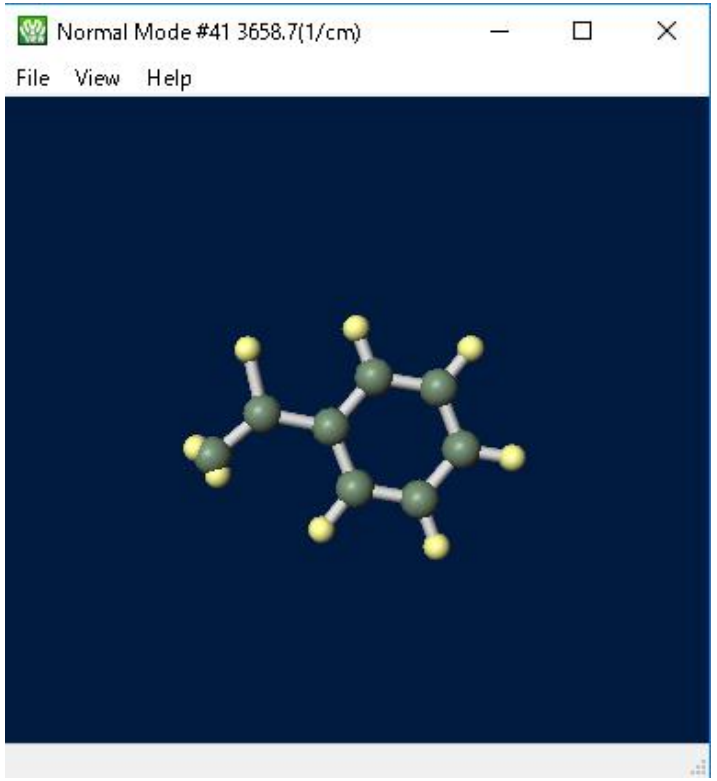
III. Calculation of vibration spectrum

1. Click near 3650 cm^{-1} on the **IR Spectrum** window to select a spectrum with red lines.
2. Then when you click the **Animation** button, **Winmostar Viewer** is started, animation you move the spectrum vibration direction to an atom in the vicinity of 3650 cm^{-1} appears.







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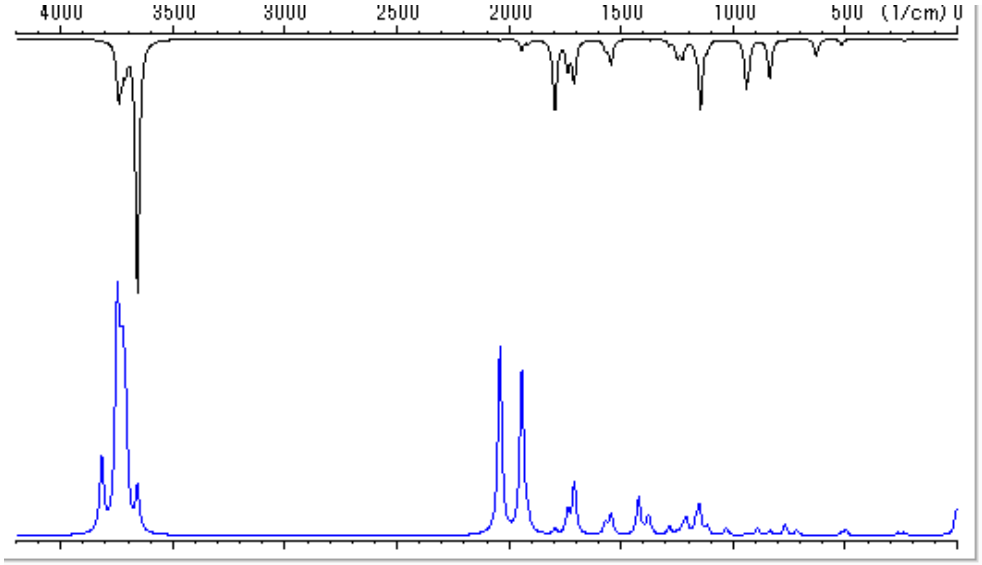
III. Calculation of vibration spectrum

When calculating the Raman spectrum with GAMESS

1. Without closing the **IR Spectrum** window, select Raman in **EasySetup** of the keyword setting window, and click **Close** and **Run** to calculate.
2. Save the file name as something different from when you select **IR (Hessian)** such as **sty_raman**.
3. After completing the calculation, click (**Analysis**) | **Hessian/Raman**.
4. When the file selected by default is opened again, a window with both IR and Raman spectra drawn appears.



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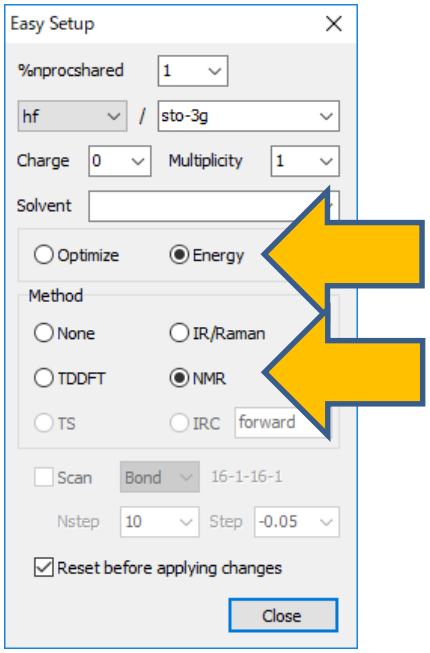
IV. NMR spectrum calculation

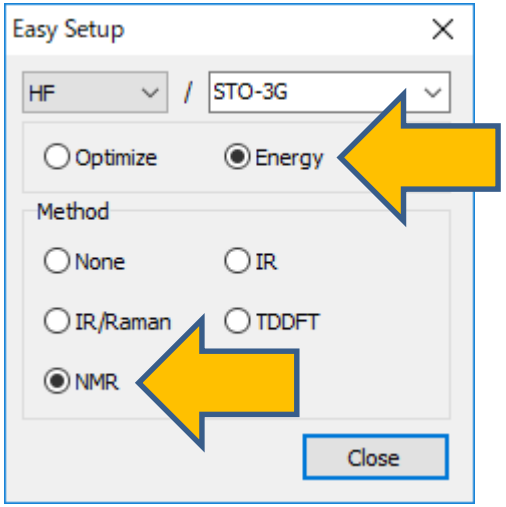
(In case of GAMESS, proceed to “V. UV-Vis spectrum calculation”.)

1. Close the **IR Spectrum** window.
2. Open **Configure| EasySetup** again, select **Energy** and **NMR**, click **Close** and **Run**. Enter the file name as **sty_nmr** and save to start the calculation.

Gaussian



NWChem



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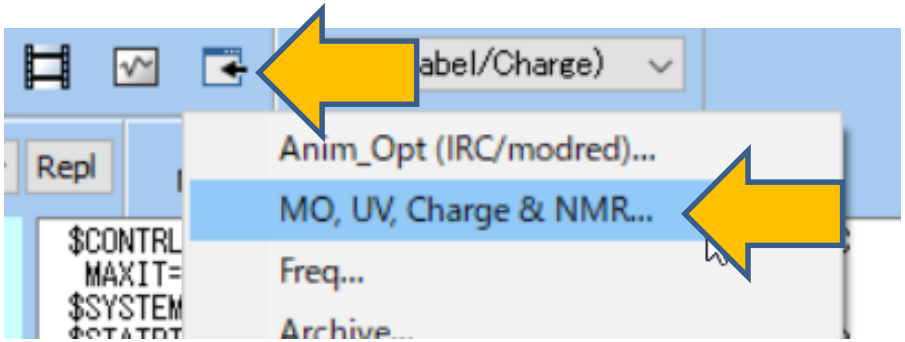
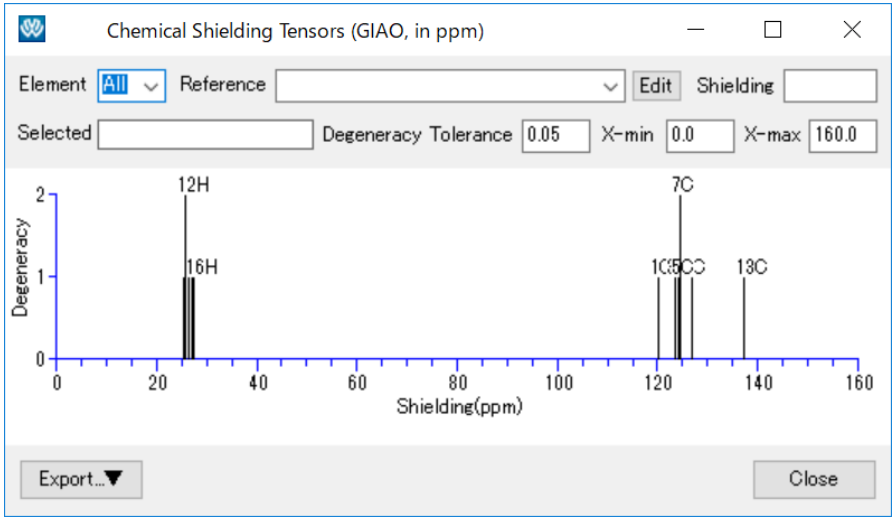
IV. NMR spectrum calculation

1. After the calculation, select **MO, UV-Vis, Charge, & NMR**… from  (Analysis).
2. Open the file selected by default in the dialog. **Chemical Shielding Tensors** window opens with the other windows, and the NMR spectrum is drawn.





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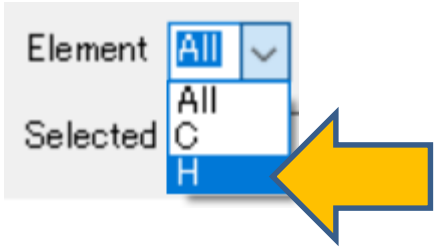
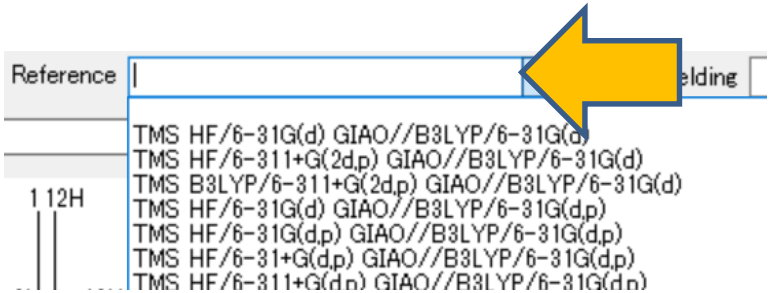
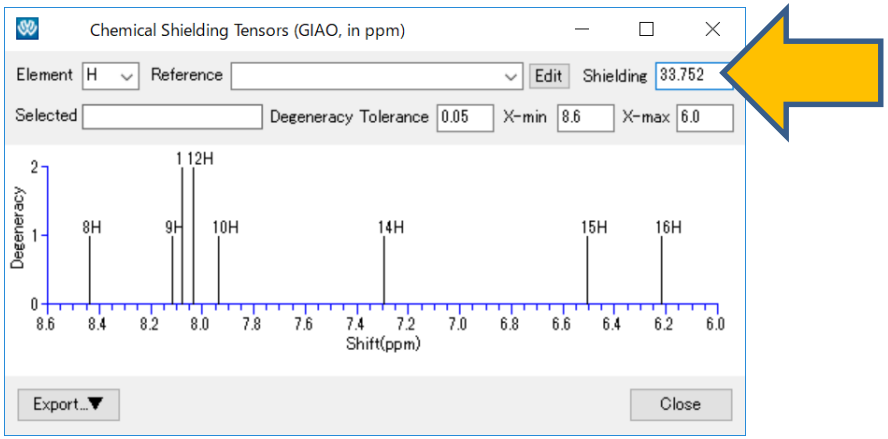
IV. NMR spectrum calculation

1. To display for each element, select the element in **Element**.
2. When you select reference data in **Reference** or enter a shielding constant in **Shielding**, the horizontal axis changes and chemical shifts are displayed.
3. How to add reference data is shown in the supplement of this tutorial.
4. After confirmation, close the window and the **MO Plot** window.







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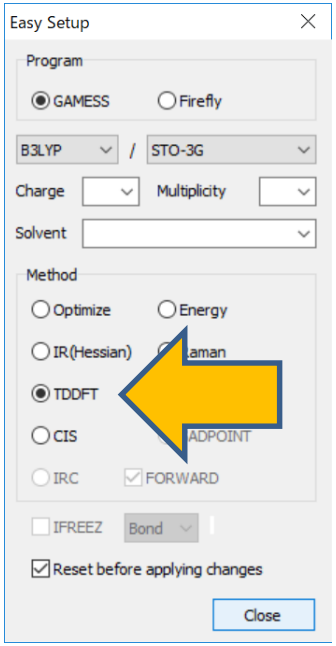
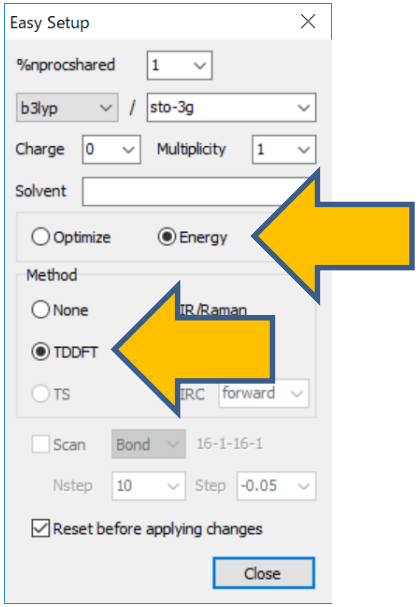
V. UV-Vis spectrum calculation

1. Open **Configure| EasySetup** again.
2. Select **TDDFT** for **GAMESS, Energy** and **TDDFT** for **Gaussian** or **NWChem**.
3. Click **Close** and **Run**.
4. Specify the file name **sty_uvvis** and start the calculation.

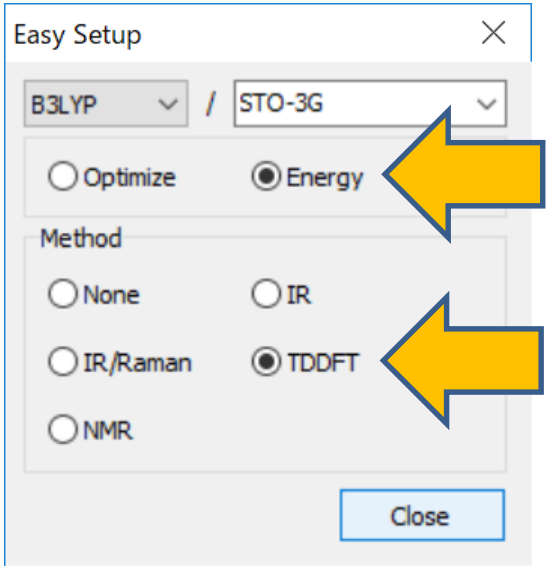
GAMESS



Gaussian



NWChem



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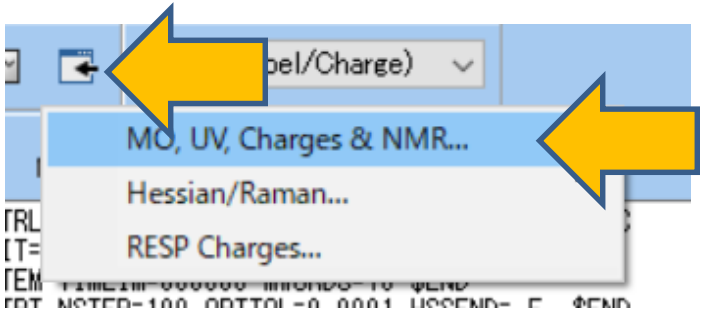
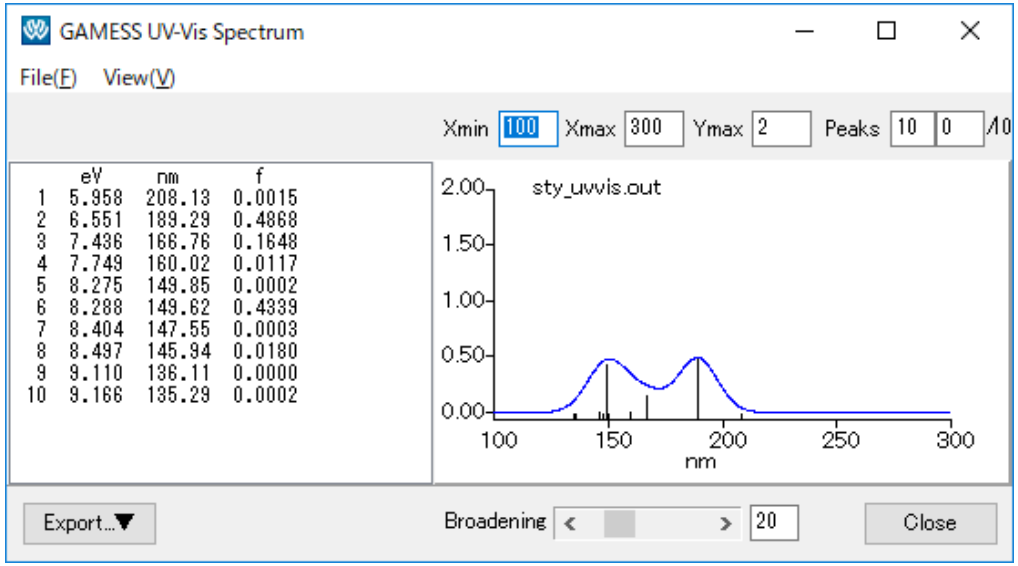
V. UV-Vis spectrum calculation

1. After the calculation is completed, select **MO, UV, Charge & NMR** from  (Analysis) button.
2. Open the file selected by default in the dialog.
3. The **UV-Vis Spectrum** window opens with the other windows, and the UV-Vis spectrum is drawn.





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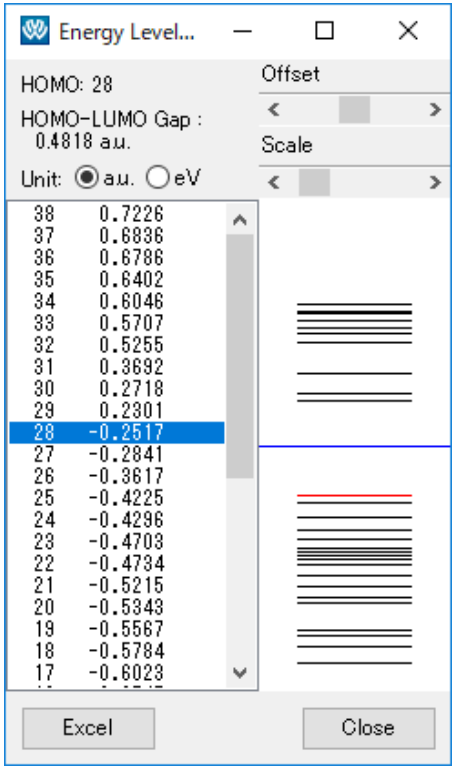
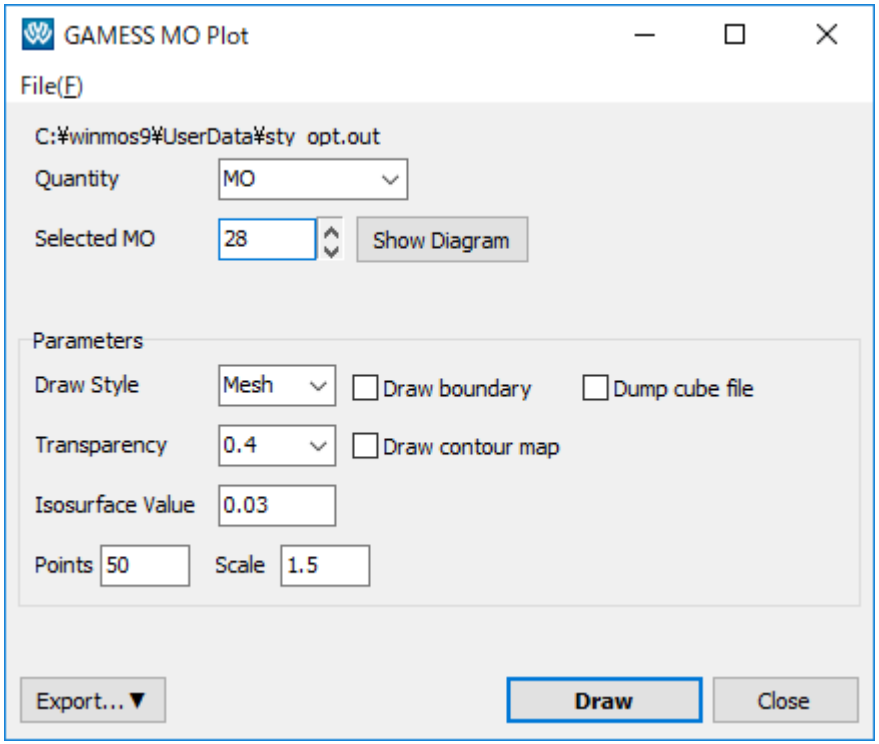
VI. Molecular orbital display

1. Select **MO, UV, Charge & NMR** from  (**Analysis**).
2. Open the structure optimization calculation log file (**sty_opt.out** or **sty_opt.log**).
3. The **Energy Level** Diagram window (vertical window) and the **GAMESS (Gaussian) MO Plot** window will open.





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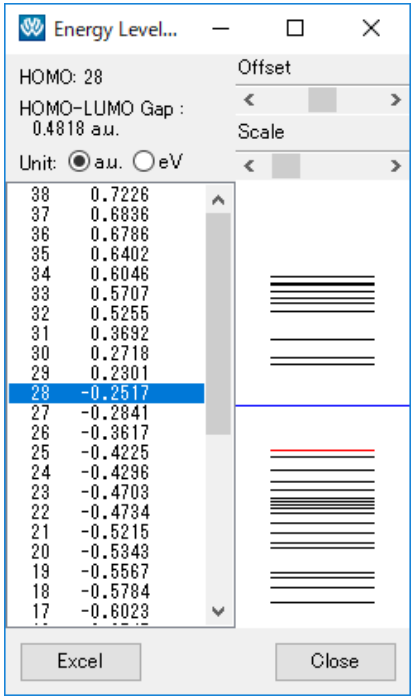
VI. Molecular orbital display

Energy Level Diagram window displays the calculated energy of each molecular orbital. In the initial state, the HOMO orbital is selected (28th orbital in the example shown).
At the top of the window, the **HOMO** orbit number, **HOMO-LUMO Gap** is displayed.



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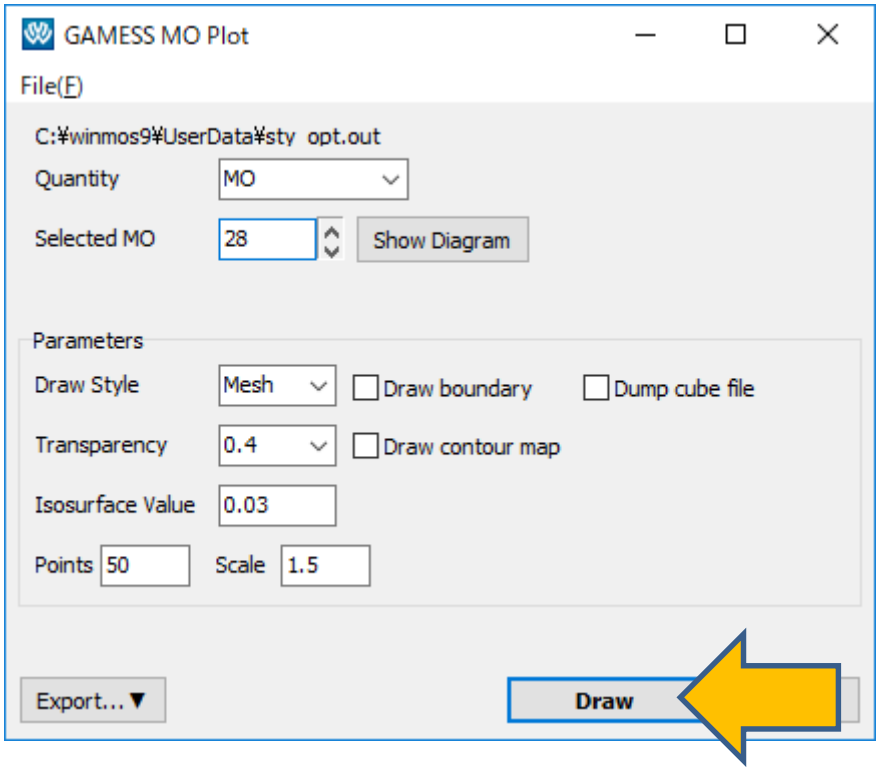
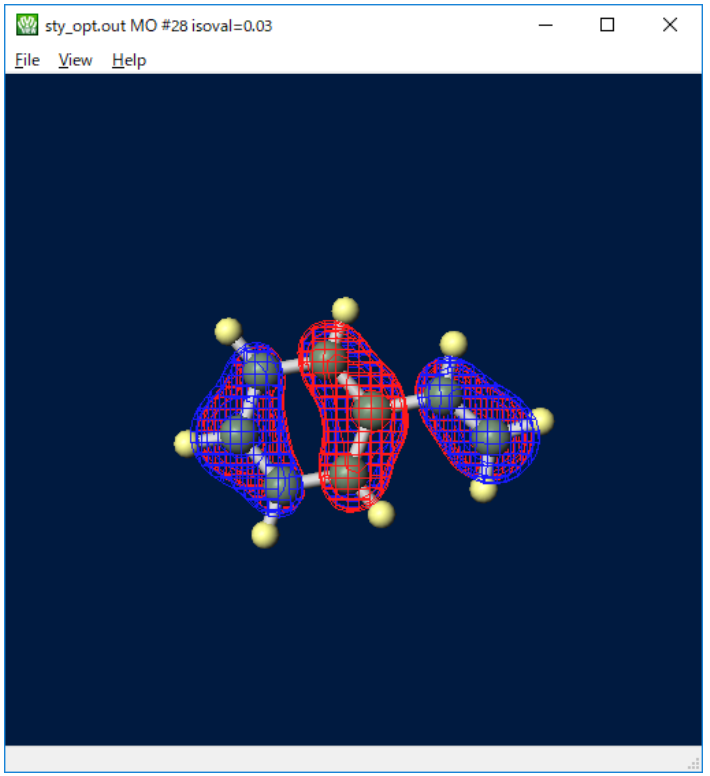
VI. Molecular orbital display

Clicking **Draw** button in the **MO Plot** window launches **Winmostar Viewer**, which displays the orbital selected in the list in **Energy Level Diagram** window (28th orbital in the example shown).





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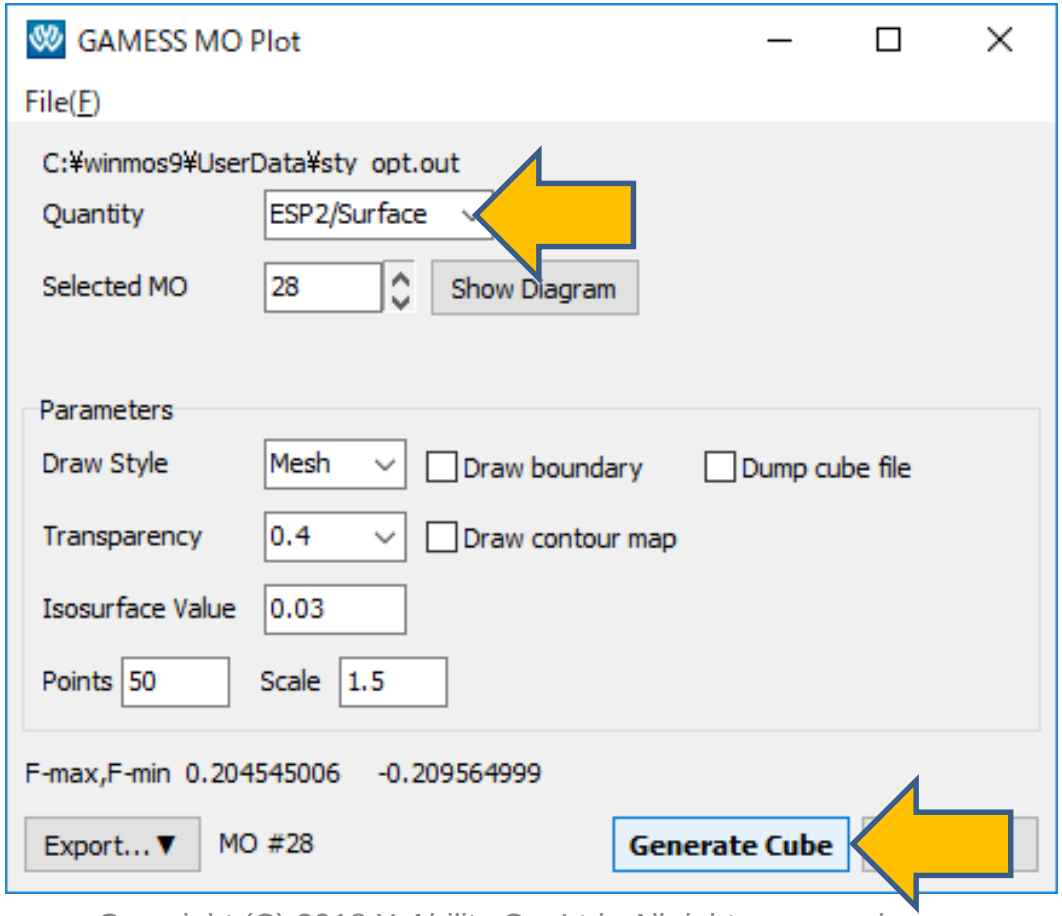
VII. Electrostatic potential display

Select **ESP2/Surface** from the pull down in the middle of the **MO Plot** window, Press **Generate Cube** button at the bottom.



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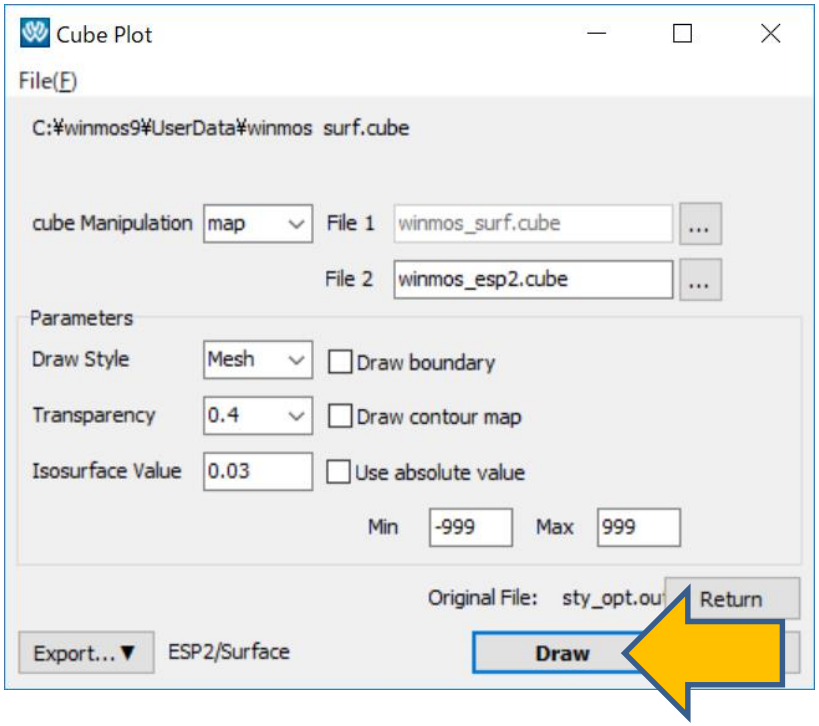
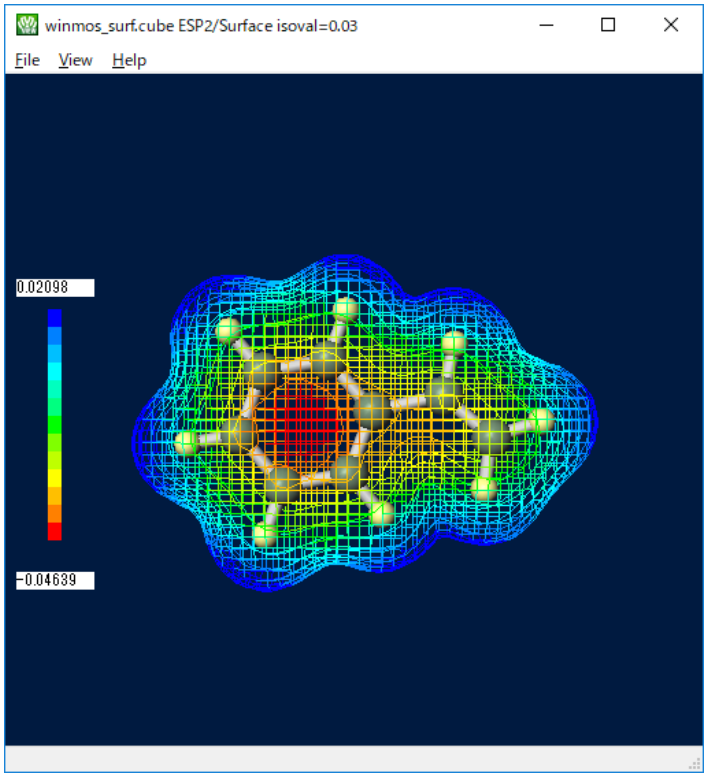
VII. Electrostatic potential display

When **Cube Plot** window appears and **Draw** button at the bottom is pressed, **Winmostar Viewer** is launched and the electrostatic potential calculated from the point charge after Population analysis with **Contour** appears on the molecular surface. (What displayed here is the so-called ESP not itself)





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Appendix: How to add NMR reference data

1. Optimize structures and acquire NMR spectra with molecules such as TMS.
2. Open **Chemical Shielding Tensors** window.
3. Left-click on the spectrum you want to reference. Then, in the upper left, “**13H 33.7549 ppm**” and the spectrum's shielding constant are displayed (see the figure below).
4. Click **Edit** to open **wm_nmr.ref** under **UserPref**.
5. If you add the line **“(element name) (Shielding constant obtained above)“ (name when displayed in Winmostar)** ”, you can select the shielding constant in Winmostar **Reference**.