[Overview]
This is a program of ab initio molecular orbital method and the density functional theory. Specifically, the Hartree-Fock theory, the 2nd-order Møller-Plesset perturbation, and the Kohn-Sham method are implemented.

[Install]
Make sure that your Windows is a 64-bit version. This program does not work on 32-bit versions. Expand the compressed file (Zip format) into directly under your "Documents" folder. A folder named "Quantum_Chemistry" is created, and files are placed under it. Even if you expand the zip file into some other place, there is no problem in operation. However, in that case, icon of shortcuts will not be displayed correctly. If you mind it, please reset icons by yourself. You can change icon through the "property" in the right-click menu. Files for icon (with extension .ico) exist in the "Gui" folder. Do not change the name and relative location of the folders under the "Quantum_Chemistry". Otherwise, the program will not work properly.

[Uninstall]
Delete the folder "Quantum_Chemistry". That's it. The registry is not used at all.

[How to use]
Go to "Run" folder, and double-click a shortcut named "01_Quantum". A small window will open. Make appropriate settings there, and then click "Run" button at bottom of the window. Your calculation will starts, and files "structure_..." to write the results and logs, will be created in the "Run" folder. You can see progress of your calculation in a frame in the window. When the calculation is completed, you will see "Completed. Normal termination". Click "Close" button to end the program.

All the setting items and choices are given in the standard terms of quantum chemistry. If you don't understand them, please refer to books. Also, contents of the result file are usual, and can be understood intuitively. Cube format files for visualization can be viewed with an accepting software (Avogadro, Winmostar etc.). If you choose the MP2 theory, only the energy will be improved by the 2nd-order many-body perturbation. In other words, outputted molecular orbitals, electron densities, and partial charges are those in the Hartree-Fock(HF) theory. If you choose RPA (Random Phase Approximation) or TDA (Tamm-Dankoff approximation), after HF theory calculations (e.g. structure optimization), the electronic excited states are calculated by the time-dependent HF method, and the UV-visible absorption spectrum is output.

Structure optimization carry out an approxmate conjugate gradient method using only gradients. "Times" input specifies number of times of "gradient calculation + linear exploration". One time is set by default, but increase it as necessary. Although it depends on the structure entered, in general, this set must be done many times to fully optimize the structure. Vibration analysis should be executed at (near) the optimal structure for the theory and basis set used. In "Times" input, you can specify number of times of the optimization set to be performed before vibration analysis. One time is set by default, but change it as needed. Zero times can be specified. If you are confident that the input structure is close enough to the optimal structure for the theory and basis set, you can specify zero.

[Caution]
The calculation time varies greatly depending on the size of the molecule, the type of calculation, and the basis set. In fact, some calculations can be done in an instant, while others can take several hours. So, when you run a calculation for the first time after changing the settings, keep in mind that it may take long. In general, structure optimization and vibration analysis, which require the gradient calculation many times, needs lots of calculation and hence take a long time. So, you should be careful when you execute structure optimization or vibration analysis of a molecule which is not small, such as trying from the simplest STO-3G basis set or executing a gradient calculation in advance to estimate the time required.

[Arbitrary Molecule]
The shortcut "01_Quantum" can calculate only given specific molecules and atoms. If you want to calculate other molecules, use a shortcut named "02_Editor" instead. This program is an editor to create an input file to be passed to an executable file named "Molecule.exe", but you can also start a calculation directly from it.

At startup, an input for calculating Glycine is displayed as an example. As in this example, list into the bottom frame the symbols and coordinates of all the atoms that make up the molecule you want to calculate, one atom per line. This entry makes it possible to specify an arbitrary molecule. (Though, the number of atoms is limited to 200. Usable atoms are, up to Xe in the STO-3G and 3-21G basis sets, up to Kr(Ar) in the 6-31G type basis set without(with) diffusive basis, up to Ar in the 6-21G basis set.) The coordinates of the atoms should be specified in the Cartesian coordinates in the [Å] units. The Z-matrix format is not supported. Concerning the sequence of atomic symbols and coordinates, it is better to generate in a molecular editor such as the Avogadro, and then paste the sequence into the frame. There are several examples of the input file in the "Input" folder under the "Sample" folder.

After setting the necessary items, click "Save" button. An input file with an appropriate name will be created and saved in the "Run" folder. Then, move this to your calculation server, and give it as an argument to the "Molecule.exe" to execute your calculation. To fine tune the calculation, pass a parameter file as an additional argument. This is the procedure originally supposed. However, this requires the "Molecule.exe" separately on the calculation server.

By clicking "Submit" button instead of the "Save" button, you can start your calculation on the computer on which you are editing your input file, without preparing a calculation server (the saving is also done in advance). You may exit the editor after submitting. Your calculation continues even if the editor ends. Of course, you may save the input file once, and then run the "Molecule.exe" with it on the "Command-Prompt". Determine the completion of the calculation, based on the size of the output files or decrease in CPU usage. If you want to kill it, use "Task Manager".

Originally, the "Molecule.exe" is intended for general molecules which do not necessarily have symmetry. Therefore, even if the molecule has symmetry, this program does not use symmetry. Hence, the calculation takes longer. When you run the "Molecule.exe" on a personal computer, you had better to limit to relatively small molecules (up to about amino acids). For larger molecules (peptides and proteins), you had better not to run it on a personal computer, because it takes long time to complete.

[History]

July 17,	2023.	Calculation of UV-visible absorption spectrum is added.
May 09,	2022.	Calculation of polarizability and Raman scattering spectrum are added.
August 14,	2021.	Calculation of IR absorption spectrum is added.
November 12,	2020.	Implementation of basis set is changed. Recalculations in ERI are reduced.
October 03,	2020.	Structure optimization is improved. Various recalculations are reduced.
April 22,	2020.	Hybrid functionals are added. Diffusive basis are added.
January 04,	2020.	Several molecules are added.
November 26,	2019.	Vibration analysis is added.
October 28,	2019.	MP2 single point energy calculation is added.
September 10,	2019.	The first release candidate. This file is created.