

# Maple Quantum Chemistry Toolbox

The [Maple Quantum Chemistry Toolbox from RDMChem](#), a separate add-on product to Maple, is a powerful environment for the computation and visualization of the electronic structure of molecules. In Maple 2025, this toolbox has significant new features and enhancements that enable: (1) Talking about molecular science with an updated AI-powered command Chat that now supports entire conversations, (2) Treating strong correlation in your density functional theory (DFT) calculations through an improved and faster generalized DFT algorithm, (3) Computing molecules with newly added basis sets, (4) Localizing molecular orbitals to analyze electron density and chemical bonding, (5) Obtaining atomic orbital integrals for both energies and properties, (6) Learning about quantum computing through a new lesson based on the Toolbox's symbolic quantum computing subpackage, and (7) Experiencing additional enhancements and improvements throughout the Toolbox.

Note that the Maple Quantum Chemistry Toolbox (QCT) is required in order to execute the examples in this worksheet.

## Talking about Molecular Science with an AI-powered Chat Command

In QCT 2024 we introduced the new command *Chat* to provide the first electronic structure package with builtin AI capabilities. With that command you could ask AI to define a molecule, drug, or compound or to explain a scientific concept, terminology, or method. Now in QC2025 you can do all of that and much more. The *Chat* command has been extended to support entire conversations about molecular science. (Note that before using *Chat*, you need to review and agree to the AI Terms of Use.)

First, we load the QuantumChemistry package

> *with(QuantumChemistry);*

[*AOIntegrals, AOLabels, ActiveSpaceCI, ActiveSpaceSCF, AtomicData, BondAngles, BondDistances, Charges, ChargesPlot, Chat, ContractedSchrodinger, CorrelationEnergy, CoupledCluster, DensityFunctional, DensityPlot3D, Dipole, DipolePlot, Energy, ExcitationEnergies, ExcitationSpectra, ExcitationSpectraPlot, ExcitedStateEnergies, ExcitedStateSpins, ExcitonDensityPlot, ExcitonPopulations, ExcitonPopulationsPlot, FullCI, GeometryOptimization, HartreeFock, Interactive, Isotopes, LiteratureSearch, LocalOrbitals, MOCoefficients, MODiagram, MOEnergies, MOIntegrals, MOOccupations, MOOccupationsPlot, MOSymmetries, MP2, MolecularData, MolecularDictionary,* **(1.1)**

*MolecularGeometry, NuclearEnergy, NuclearGradient, OscillatorStrengths, Parametric2RDM, PlotMolecule, Populations, Purify2RDM, QuantumComputing, RDM1, RDM2, RDMFunctional, RTM1, ReadXYZ, Restore, Save, SaveXYZ, SearchBasisSets, SearchFunctionals, SkeletalStructure, SolventDatabase, Thermodynamics, TransitionDipolePlot, TransitionDipoles, TransitionOrbitalPlot, TransitionOrbitals, Variational2RDM, VibrationalModeAnimation, VibrationalModes, Video]*

For example, we can ask *Chat* for information about a molecule such as hydroxyurea

> *Chat*("Can you tell me about the molecule hydroxyurea?");

"Hydroxyurea is a medication primarily used in the treatment of several conditions, including certain types of cancer and sickle cell disease. It is an oral medication that works by interfering with the synthesis of DNA, thus affecting rapidly dividing cells. Here are some key points about hydroxyurea: **(1.2)**

#### 1. **Chemical Structure and Properties:**

- Its chemical formula is  $\text{CH}_2\text{N}_2\text{O}$ , and it is characterized by the presence of hydroxyl (OH) and urea (NHCO) groups.
  - It is a small molecule that is relatively simple in structure.

#### 2. **Mechanism of Action:**

- Hydroxyurea inhibits the enzyme ribonucleotide reductase, which is essential for DNA synthesis. By doing so, it impedes the replication of cells.
- It is particularly effective against rapidly dividing cells, making it useful for treating certain types of cancer.

#### 3. **Medical Uses:**

- **Cancer Treatment:** It is used in the treatment of chronic myelogenous leukemia (CML), melanoma, and certain head and neck cancers.
- **Sickle Cell Disease:** Hydroxyurea is used to reduce the frequency of painful crises and the need for blood transfusions in sickle cell anemia patients. It increases fetal hemoglobin (HbF) levels, which helps reduce sickling of red blood cells.
- It may also be used in the management of certain myeloproliferative disorders and some forms of anemia.

#### 4. **\*\*Side Effects:\*\***

- Common side effects include bone marrow suppression (leading to low blood counts), gastrointestinal symptoms (nausea, vomiting, diarrhea), and potential skin reactions.
  - Long-term use can increase the risk of secondary cancers due to its mutagenic potential.
  - Regular blood monitoring is necessary to manage and mitigate these risks.

#### 5. **\*\*Dosage and Administration:\*\***

- Dosage varies based on the condition being treated, patient response, and other individual factors.
  - It is usually administered orally in capsule form.

#### 6. **\*\*Precautions and Considerations:\*\***

- Patients on hydroxyurea require regular monitoring of blood cell counts and renal and hepatic function.
- It is important to discuss with healthcare providers any other medications being taken, as there can be interactions.
- Pregnant or breastfeeding women should use hydroxyurea with caution, as it can potentially harm the fetus or infant.

Hydroxyurea is a potent drug that must be used under strict medical supervision, balancing its therapeutic benefits against potential adverse effects."

Not only do we obtain a much more detailed explanation in QCT2025, but also we can continue the conversation

> *Chat*("Can you tell me more about how it treats sickle-cell anemia?");

"Hydroxyurea is an important treatment option for sickle cell anemia, a genetic disorder characterized by the production of abnormal hemoglobin, known as hemoglobin S (HbS), which causes red blood cells to adopt a rigid, sickle-like shape. These sickle-shaped cells can obstruct blood flow in small vessels, leading to painful episodes known as vaso-occlusive crises, as well as organ damage and other complications.

**(1.3)**

#### **\*\*Mechanism of Action in Sickle Cell Anemia:\*\***

##### 1. **\*\*Induction of Fetal Hemoglobin (HbF):\*\***

- The primary therapeutic effect of hydroxyurea in sickle cell anemia is its ability to increase the

production of fetal hemoglobin (HbF). HbF is a form of hemoglobin that is present in fetuses and infants. It has a higher affinity for oxygen and inhibits the polymerization of deoxygenated sickle hemoglobin (HbS), preventing the sickling of red blood cells.

- By increasing HbF levels, hydroxyurea reduces the proportion of sickle hemoglobin within red blood cells, thereby decreasing sickling and ameliorating disease symptoms.

## 2. **Improvement of Red Blood Cell Hydration:**

- Hydroxyurea may also lead to improved red blood cell hydration, which reduces the tendency of cells to assume a sickle shape under low oxygen conditions.

## 3. **Reduction of White Blood Cell Counts:**

- High white blood cell counts have been associated with an increased risk of complications in sickle cell anemia. Hydroxyurea can reduce the number of circulating white blood cells, which may help decrease inflammation and related complications in small blood vessels.

## 4. **Decreasing Adhesion Molecules:**

- Hydroxyurea has been shown to decrease the expression of adhesion molecules on blood cells and endothelial cells, reducing the tendency for these cells to stick together and block blood vessels.

## **Clinical Benefits:**

- **Reduction in Crisis Frequency and Severity:** By preventing sickling and improving red blood cell function, hydroxyurea decreases the frequency and severity of vaso-occlusive crises.
- **Lower Transfusion Needs:** Patients often require fewer blood transfusions while on hydroxyurea, which reduces the risk of transfusion-related complications.
- **Improved Quality of Life:** With fewer pain episodes and hospitalizations, patients generally experience a better overall quality of life.
- **Decreased Risk of Organ Damage:** Long-term use of hydroxyurea has been associated with a reduction in damage to organs such as the spleen and kidneys.

## **Usage Considerations:**

- Hydroxyurea is typically started in children or adults with sickle cell anemia who have frequent

pain episodes, recurrent acute chest syndrome, or other complications.

- Regular blood tests are required to monitor blood counts and adjust dosages as necessary.
- Not all patients are suitable candidates for hydroxyurea therapy, and decisions are made based on individual patient assessments.

Overall, hydroxyurea has become a cornerstone of managing sickle cell anemia due to its capacity to alleviate symptoms and improve long-term outcomes. However, it requires careful monitoring and adherence to prescribed regimens to maximize its benefits while minimizing potential side effects."

We can ask about recommendations for electronic structure methods to treat hydroxyurea

> *Chat*("What methods in the Maple Quantum Chemistry Toolbox do you recommend for treating hydroxyurea?");

"The Maple Quantum Chemistry Toolbox is designed to interface with powerful quantum chemistry engines to perform a variety of electronic structure calculations. While the specific capabilities of the toolbox would depend on the version and the quantum chemistry software it integrates with, here are some general recommendations on methods for studying hydroxyurea using Maple Quantum Chemistry Toolbox: (1.4)

#### 1. **Geometry Optimization:**

- Start with optimizing the molecular geometry of hydroxyurea to find its lowest energy conformation. This is often a prerequisite for many quantum chemistry calculations.
- Density Functional Theory (DFT) is a suitable method for geometry optimization due to its balance of accuracy and computational cost.

#### 2. **Electronic Properties:**

- Use DFT to calculate electronic properties such as molecular orbitals, electron density distributions, and partial charges.
- DFT can provide insights into the nature of bonds and the electronic structure of the molecule.

#### 3. **Vibrational Analysis:**

- Perform vibrational frequency calculations to understand the normal modes of vibration. This helps in comparing with experimental IR spectra and confirming the geometry is a true minimum.

#### 4. **Reaction Pathways and Energetics:**

- Utilize DFT or post-Hartree-Fock methods like Møller-Plesset perturbation theory (MP2) to study potential energy surfaces and reaction pathways, particularly if investigating hydroxyurea's interactions or breakdown mechanisms.

#### 5. **UV-Vis Spectra:**

- Employ Time-Dependent Density Functional Theory (TDDFT) for calculating excited states and simulating UV-Vis spectra.

#### 6. **Electron Correlation Effects:**

- If more precision is needed, consider employing post-Hartree-Fock methods such as MP2 or CCSD(T) to capture correlation effects more accurately.

#### 7. **Solvent Effects:**

- If you are interested in hydroxyurea in an aqueous environment or other solvents, look into utilizing continuum solvation models available in the software, such as the Polarizable Continuum Model (PCM).

The choice of method largely depends on the specific properties and phenomena you are interested in studying about hydroxyurea. Using the Maple Quantum Chemistry Toolbox in combination with these methods, you can gain deep insights into the molecule's physicochemical properties and behavior, aiding in both theoretical studies and practical applications."

We can also ask for a starting molecular geometry

> *Chat*("Can you give me a molecular geometry using a format that can be read into the Toolbox, i.e. with ReadXYZ?");

"Certainly! When using the Maple Quantum Chemistry Toolbox, and specifically the `'ReadXYZ'` **(1.5)** function, you would need to provide the molecular geometry in an XYZ format. This format includes the number of atoms, an optional comment line, and then lines listing each atom with its element type and Cartesian coordinates.

Here is an example of how you might represent hydroxyurea in a format suitable for the `'ReadXYZ'` function:

```

``plaintext
7
Hydroxyurea
C 1.2074 -0.0905 0.0000
O 0.0000 -0.6092 0.0000
N -1.1627 0.2784 0.0001
N 2.0979 0.9964 0.0000
H -1.9945 -0.2528 0.0002
H 2.1818 1.6012 0.8936
H 2.1818 1.6012 -0.8936
``

```

### ### Explanation:

- **The first line (7)** indicates the total number of atoms in the molecule.
- **The second line (Hydroxyurea)** is a comment or a label for the molecule, which is optional but helps in identifying the molecule.
- **Subsequent lines** specify each atom with its type (C, N, O, H) followed by its Cartesian coordinates (x, y, z).

### ### Instructions for Using the XYZ File:

1. Save the content above into a text file with an `.xyz` extension, for example, `hydroxyurea.xyz`.
2. Use the `ReadXYZ` function within the Maple Quantum Chemistry Toolbox to import this geometry. The function typically requires the file path as an argument, like so:

```

``maple
molecule := ReadXYZ("path/to/hydroxyurea.xyz");
``

```

### ### Additional Tips:

- Ensure that your software environment is properly set up to access file paths and read files as needed.
- Depending on the subsequent calculations, ensure that any necessary parameters (like the charge and multiplicity) are set correctly in your quantum chemistry setup.
- If accurate geometrical parameters are required, use experimental data or optimize the structure with a quantum chemistry calculation as a preliminary step."

As the example shows, the command *Chat* allow you to connect to the power of AI without leaving either Maple or the Quantum Chemistry package.

## Treating Strong Correlation from a Faster Generalization of DFT

A well-known limitation of density functional theory (DFT) is its difficulty in predicting the energies and properties of molecules with static correlation. Static correlation is important to the accurate prediction of charges, van der Waals forces, barrier heights, and bi- and multiradicals. In the previous release (QCT 2024) we introduced a generalization of DFT that can treat static correlation. The command *RDMFunctional* adds a universal correction, based on the 1-electron reduced density matrix (1-RDM) rather than the density alone, to any DFT functional. In QCT2025 we *increase the speed* of the algorithm behind *RDMFunctional* such that it approaches that of DFT.

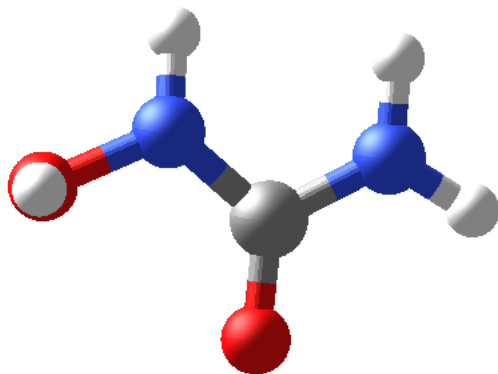
As an example, let us compute the ground-state energy and properties of hydroxyurea. While we could use the geometry above, we can also immediately import its geometry with the command *MolecularGeometry*

```
> mol := MolecularGeometry("hydroxyurea");  
mol := [ ["O", 1.88790000, -0.00950000, -0.00270000], ["O", -0.48550000, -1.30440000, (2.1)  
        -0.00030000], ["N", 0.67610000, 0.69460000, 0.00260000], ["N", -1.61350000,  
        0.69390000, -0.00290000], ["C", -0.46490000, -0.07450000, 0.00330000], ["H",  
        0.71730000, 1.68970000, 0.18780000], ["H", -1.57330000, 1.70750000, -0.00260000],  
        ["H", -2.53340000, 0.26600000, -0.00670000], ["H", 2.08350000, -0.00760000,  
        -0.95500000]]
```

With the command *PlotMolecule* we can quickly visualize the molecule before computing its electronic structure

```
> PlotMolecule(mol);
```





Then we can use the command *RDMFunctional* to compute its energy and properties

```
> data := RDMFunctional(mol);
```

$$\text{data} := \text{table} \left( \begin{array}{l} \text{mo\_occ} = \begin{bmatrix} 2.00000000 \\ 2.00000000 \\ 2.00000000 \\ 2.00000000 \\ 2.00000000 \\ 2.00000000 \\ 2.00000000 \\ 2.00000000 \end{bmatrix}, \text{rdm1} \end{array} \right) \quad (2.2)$$

29 element Vector[column]

=



$$\begin{bmatrix} 0.99355621 & 0.00004003 & 0.00066955 & 9.97775454 \times \dots \\ 0.02853681 & -0.00005174 & -0.00429399 & -0.000042 \dots \\ -0.00193456 & 0.00003567 & 0.00343684 & 0.0000551 \dots \\ 0.00161188 & -0.00007442 & -0.00194889 & 0.0000451 \dots \\ -0.00375631 & -6.85861577 \times 10^{-6} & -0.00042158 & -4.49541935 : \dots \\ -0.00003412 & 0.99351853 & -0.00004526 & -0.000058 \dots \\ -0.00004450 & 0.02943306 & 0.00028377 & 0.0003828 \dots \\ -0.00001590 & 0.00010095 & 0.00047321 & -0.000505 \dots \end{bmatrix},$$

$$\begin{bmatrix} 29 \times 29 \text{ Matrix} \end{bmatrix}, \text{charges} = \begin{bmatrix} -0.17911056 \\ -0.26781736 \\ -0.25775527 \\ -0.41587414 \\ 0.30097117 \\ 0.20063225 \\ 0.19174759 \end{bmatrix}, \text{dipole} = \begin{bmatrix} -0.59544168 \\ 3.57654760 \\ -1.05024342 \end{bmatrix}, \text{group}$$

9 element Vector[column]

$$= \text{"C1"}, \text{aolabels} = \begin{bmatrix} \text{"0 O 1s"} \\ \text{"0 O 2s"} \\ \text{"0 O 2px"} \\ \text{"0 O 2py"} \\ \text{"0 O 2pz"} \\ \text{"1 O 1s"} \\ \text{"1 O 2s"} \end{bmatrix}, \text{mo\_symmetry} = \begin{bmatrix} \text{"A"} \\ \text{"A"} \\ \text{"A"} \\ \text{"A"} \\ \text{"A"} \\ \text{"A"} \\ \text{"A"} \end{bmatrix}, \text{populations}$$

29 element Vector[column]                      29 element Vector[column]

$$= \begin{bmatrix} 1.99774080 \\ 1.87422281 \\ 1.26456656 \\ 1.73639812 \\ 1.30618226 \\ 1.99788371 \\ 1.88588239 \end{bmatrix}, e_{tot} = -296.32380068$$

29 element Vector[column]

Note that we can easily examine all entries of the output data through Maple's scrollable Vectors, Matrices, and Arrays.

## Computing with Newly Added Basis Sets

The Quantum Chemistry Toolbox (QCT) now includes pc0 through pc4 and a comprehensive set of effective core potential (ECP) basis sets related to the cc-pVXZ and aug-cc-pVXZ families, including regular, heavy-element (he), and region-specific (reg) variations.

The pc-n (Polarization Consistent) basis sets, including pc0 through pc4, systematically improve density functional theory (DFT) calculations by providing a consistent treatment of polarization effects. Here's a brief overview of pc0 to pc4:

pc0 – A minimal polarization-consistent basis set, designed for fast, low-cost DFT calculations. It offers a balanced description of electronic structure but with minimal polarization functions.

pc1 – A double-zeta level basis set that includes more polarization functions than pc0, improving accuracy while still keeping computational cost manageable.

pc2 – A triple-zeta level basis set, further improving accuracy, particularly for polarizability and dispersion interactions.

pc3 – A quadruple-zeta level basis set, offering even more flexibility in polarization functions for highly accurate DFT response properties.

pc4 – The highest-level pc basis set, reaching quintuple-zeta quality. It is intended for

high-accuracy DFT calculations, particularly when aiming for convergence with respect to basis set size.

For example, let's try a DFT calculation of hydroxyurea with one these basis sets

> `data_dft := DensityFunctional(mol, basis = "pc0");`

$$\text{data\_dft} := \text{table} \left( \begin{array}{l} e\_tot = -299.51657846, \\ converged = 1, \\ mo\_energy \end{array} \right) \quad (3.1)$$

$$= \left[ \begin{array}{c} -19.20999285 \\ -19.12489535 \\ -14.42465624 \\ -14.37190504 \\ -10.34840114 \\ -1.11029466 \\ -1.03790974 \end{array} \right], rdm1$$

53 element Vector[column]



=

$$\begin{bmatrix} 0.26864488 & 0.00056951 & 0.00001728 & -6.16704704 \times 10^{-6} \\ 0.78215497 & 0.00190941 & 0.00058206 & -0.00006179 \dots \\ 0.03127625 & -0.00199411 & -0.00264678 & 0.00089930 \dots \\ -0.00057528 & 0.00015185 & -0.00003685 & -0.00044903 \dots \\ 0.00043101 & 0.00012748 & 3.66788792 \times 10^{-6} & -0.00012124 \dots \\ -0.00099971 & 0.00006447 & 0.00011136 & 0.00008377 \dots \\ -0.00423177 & 0.00124757 & 0.00415897 & 0.00071916 \dots \end{bmatrix},$$

$$\begin{bmatrix} 53 \times 53 \text{ Matrix} \end{bmatrix}, \text{dipole} = \begin{bmatrix} -0.84172452 \\ 5.13995139 \\ -1.53058729 \end{bmatrix}, \text{mo\_occ} = \begin{bmatrix} 2.00000000 \\ 2.00000000 \\ 2.00000000 \\ 2.00000000 \\ 2.00000000 \\ 2.00000000 \\ 2.00000000 \end{bmatrix}, \text{charges}$$

53 element Vector[column]

$$\begin{aligned}
&= \begin{bmatrix} -0.31232505 \\ -0.33780810 \\ -0.39074942 \\ -0.63939044 \\ 0.48523260 \\ 0.29357554 \\ 0.27448486 \end{bmatrix}, \text{group} = \text{"C1"}, \text{populations} = \begin{bmatrix} 0.46183298 \\ 1.52823663 \\ 1.76152625 \\ 0.59731770 \\ 0.78902715 \\ 0.67648224 \\ 0.73315722 \end{bmatrix}, \text{mo\_symmetry} \\
&\qquad\qquad\qquad 9 \text{ element Vector[column]} \qquad\qquad\qquad 53 \text{ element Vector[column]} \\
&= \begin{bmatrix} \text{"A"} \\ \text{"A"} \\ \text{"A"} \\ \text{"A"} \\ \text{"A"} \\ \text{"A"} \\ \text{"A"} \end{bmatrix}, \text{aolabels} = \begin{bmatrix} \text{"0 O 1s"} \\ \text{"0 O 2s"} \\ \text{"0 O 3s"} \\ \text{"0 O 2px"} \\ \text{"0 O 2py"} \\ \text{"0 O 2pz"} \\ \text{"0 O 3px"} \end{bmatrix} \\
&\qquad\qquad\qquad 53 \text{ element Vector[column]} \qquad\qquad\qquad 53 \text{ element Vector[column]}
\end{aligned}$$

## Localizing Molecular Orbitals to Analyze Chemical Bonding

In QCT2025 the new command *LocalOrbitals* computes the local molecular orbitals of a molecule from the canonical molecular orbitals. Local orbitals offer an alternative, spatially localized rotation of the canonical molecular orbitals, which can be particularly useful for visualizing chemical bonding, improving the convergence and cost of correlated methods, and enhancing the wave function's representation of the molecule (e.g., selecting active spaces in active-space methods like CI-CASSCF (*ActiveSpaceCI* or *ActiveSpaceSCF*) and V2RDM-CASSCF (*Variational2RDM*)). Such orbitals can be generated in QCT2025 through three different localization methods: Boys, Pipek-Mezey (PM), and Edmiston-Ruedenberg (ER). Users can specify the localization method using the keyword *localization*, with options "Boys", "PM", or "ER". Boys Localization ("Boys") creates the most compact orbitals by keeping electron density as close together as possible in space; Pipek-Mezey Localization ("PM") emphasizes orbitals that are strongly associated with



individual atoms, enhancing their atomic identity, and Edmiston-Ruedenberg Localization ("ER") arranges orbitals to minimize electron repulsion, resulting in orbitals that closely resemble natural bonding patterns.

Here we use the result from the DFT calculation in the previous section to compute the localized orbitals using the "ER" option

```
> local_mo_coeff := LocalOrbitals(mol, data_dft[mo_coeff], basis = "pc0", localization = "ER");
local_mo_coeff := (4.1)
```

-0.56480286	0.00104541	0.00272087	-0.00022450	( ...
1.39420535	-0.00292330	-0.00770843	0.00063425	- ...
-0.28732276	0.02183982	0.03304309	-0.00800503	( ...
-0.02857645	-0.00195185	-0.00087873	0.00437822	- ...
0.02196706	-0.00092847	0.00060004	0.00126226	- ...
-0.02649656	-0.00113270	-0.00250554	-0.00086129	- ...
0.06438430	-0.01309718	-0.04633740	-0.00814050	- ...
-0.04805276	0.01196992	0.01752692	-0.00815487	( ...

53 × 53 Matrix

To visualize one of the 20<sup>th</sup> local orbital, we replace the canonical MO coefficients in *data\_dft* with the local MOs

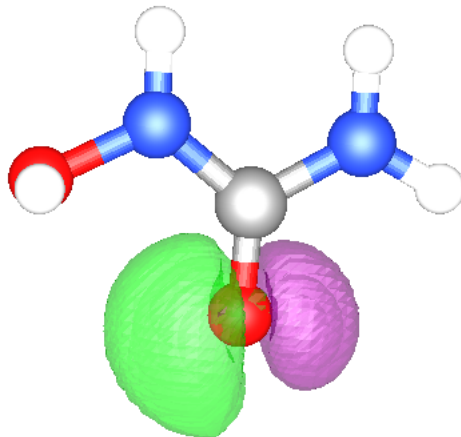
```
> data_dft[mo_coeff] := local_mo_coeff;
data_dft_local_{mo_coeff} := (4.2)
```

-0.56480286	0.00104541	0.00272087	-0.00022450	( ...
1.39420535	-0.00292330	-0.00770843	0.00063425	- ...
-0.28732276	0.02183982	0.03304309	-0.00800503	( ...
-0.02857645	-0.00195185	-0.00087873	0.00437822	- ...
0.02196706	-0.00092847	0.00060004	0.00126226	- ...
-0.02649656	-0.00113270	-0.00250554	-0.00086129	- ...
0.06438430	-0.01309718	-0.04633740	-0.00814050	- ...

53 × 53 Matrix

And then we use the *DensityPlot3D* command

```
> DensityPlot3D(mol, data_dft, basis = "pc0", orbitalindex = 20);
```



Note that the localized orbital is a  $p$  orbital on the oxygen atom connected to the central carbon atom.

## Obtaining Atomic Orbital Integrals for Energies and Properties

In QCT2025 the Toolbox has been extended to compute atomic orbital (AO) integrals using the *AOIntegrals* command, enabling direct evaluation of key one- and two-electron integrals. Supported integrals include overlap (measuring orbital interactions), kinetic energy (describing electron motion), nuclear attraction (electron-nucleus interactions), electron repulsion (Coulomb interactions between electrons), electron-nuclear coupling, and multipole moment integrals (dipole, quadrupole). This extension provides greater flexibility for custom applications in quantum chemistry.

For example, we can compute the overlap integrals for hydroxyurea

```
> overlap_ints := AOIntegrals(mol, integral_type = "overlap");
```

```
overlap_ints :=
```

**(5.1)**

$$\begin{bmatrix}
 1.00000000 & 0.23670394 & 0. & 0. \\
 0.23670394 & 1.00000000 & 0. & 0. \\
 0. & 0. & 1.00000000 & 0. \\
 0. & 0. & 0. & 1.00000000 \\
 0. & 0. & 0. & 0. \\
 0. & 0.00001104 & -0.00003264 & -0.00001781 \\
 0.00001104 & 0.00366491 & -0.00603795 & -0.00329423 \\
 0.00003264 & 0.00603795 & -0.00908775 & -0.00564395
 \end{bmatrix}$$

29 × 29 Matrix

or the electronic dipole integrals

> *dipole\_ints* := *AOIntegrals*(*mol*, *integral\_type*="dipole");

*dipole\_ints* :=

(5.2)

$$\begin{bmatrix}
 3.56761395 & 0.84446827 & 0.05079193 & 0. & 0. \dots \\
 -0.01795240 & -0.00424940 & -0. & 0.05079193 & -0. \dots \\
 -0.00510226 & -0.00120773 & -0. & -0. & 0.05079 \dots
 \end{bmatrix}$$

slice of 3 × 29 × 29 Array

where the first index of the output 3 × 29 × 29 Array selects from the x-, y-, or z-components of the dipole integrals.

## Using the Package in the Classroom

The Maple Quantum Chemistry Toolbox includes approximately 30 lessons that can be used in chemistry and physics courses from advanced high school courses through the graduate level. These lessons and associated curricula provide instructors and students with real-time quantum chemistry computations and visualizations that quickly deepen understanding of molecular concepts. Detailed lesson plans and curricula are provided for Introductory (General) Chemistry, Physical Chemistry (Quantum Mechanics and Thermodynamics), Thermodynamics (Physics), Quantum Mechanics (Physics), Computational Chemistry, and Quantum Chemistry as well as Advanced Placement (AP) and International Baccalaureate (IB) chemistry courses. Topics include atomic structure,

chemical bonding, the Maxwell-Boltzmann distribution, heat capacity, enthalpy, entropy, free energy, particle-in-a-box, vibrational normal modes, infrared spectroscopy, as well as advanced electronic structure methods. Additional resources and lessons are available at the [Great Quantum Chemistry Dictionary](#) and in the Maple [Application Center](#). Use of the QCT in the classroom is described in a [recent paper in J. Chem. Ed.](#)

QCT 2025 includes a new lesson entitled "Introduction to Quantum Computing." For example, the following sections provide two short excerpts from the lesson in which we (1) introduce the concept of the quantum bit (qubit) and (2) study the action of a quantum gate on a quantum state symbolically (a significant advantage of the *QuantumComputing* subpackage in QCT2025 is that it supports symbolically parameterized gates and states).

## Quantum Gates

First, we load the *QuantumComputing* subpackage

```
> with(QuantumComputing);
[ConvertDirac, Gate, InitialState, MeasureState, PrepareState, QubitPopulations,
  QubitPopulationsPlot] (6.1.1)
```

In quantum computing unitary operators are known as gates. One such 1-qubit gate is the Pauli-Z gate

```
> Uz := Gate("Z");
```

$$U_z := \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \quad (6.1.2)$$

which has no effect on the 0-qubit state

```
> state := InitialState(1);
```

$$state := \Psi_0 \quad (6.1.3)$$

```
> PrepareState([1 = Uz], state);
```

$$\Psi_0 \quad (6.1.4)$$

or the Pauli Y gate

```
> Uy := Gate("Y");
```

$$U_y := \begin{bmatrix} 0 & -I \\ I & 0 \end{bmatrix} \quad (6.1.5)$$

which flips the qubit while introducing an imaginary phase

> `PrepareState([1 = Uy], state);`

$$I\Psi_1 \tag{6.1.6}$$

or the most general 1-qubit gate, known as the U (universal) gate that depends on 3 angles that we keep symbolic

> `Uu := Gate("U", theta = theta, phi = phi, lambda = lambda);`

$$Uu := \begin{bmatrix} \cos\left(\frac{\theta}{2}\right) & -e^{i\lambda} \sin\left(\frac{\theta}{2}\right) \\ e^{i\phi} \sin\left(\frac{\theta}{2}\right) & e^{i(\phi+\lambda)} \cos\left(\frac{\theta}{2}\right) \end{bmatrix} \tag{6.1.7}$$

which generates the following general rotated state

> `PrepareState([1 = Uu], state);`

$$\cos\left(\frac{\theta}{2}\right) \Psi_0 + e^{i\phi} \sin\left(\frac{\theta}{2}\right) \Psi_1 \tag{6.1.8}$$

## State Preparation

To demonstrate state preparation, we make a Schrodinger cat state in which the state of all qubits down becomes entangled with the state of all qubits up.

First, we prepare our initial state with all qubits in the 0 state.

> `state := InitialState(4);`

$$state := \Psi_{0,0,0,0} \tag{6.2.1}$$

The necessary circuit is an initial application of the Hadamard gate followed by 3 CNOT gates

> `circuit := [1 = Gate("H"), seq([i, i + 1] = Gate("CNOT"), i = 1..3)];`

$$circuit := 1 = \begin{bmatrix} \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \\ \frac{\sqrt{2}}{2} & -\frac{\sqrt{2}}{2} \end{bmatrix}, [1, 2] = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}, [2, 3] \tag{6.2.2}$$

$$= \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}, [3, 4] = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}$$

We prepare the new state by applying the circuit to the initial state

>  $state2 := PrepareState(circuit, state);$

$$state2 := \frac{\sqrt{2} \Psi_{0,0,0,0}}{2} + \frac{\sqrt{2} \Psi_{1,1,1,1}}{2} \quad (6.2.3)$$

The new state entangles a state of 4 "down" qubits with a state of 4 "up" qubits. Like Schrodinger's cat, our state is half up and half down.