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 2023, this toolbox has significant new features and enhancements that enable:

1. Searching the scientific literature for new journal articles and preprints without leaving Maple.
2. Exploring algorithms and computations for quantum computers with the new QuantumComputing subpackage.
3. Flying through a molecule or an orbital in 3-D with new fly-though molecular animations.
4. Importing molecular geometries and skeletal structures for nearly 100 million chemical structures using SMILES formulas.
5. Customizing your own Hamiltonian in variational calculations of the 2-RDM.
6. Teaching with a new lesson on Fermi's Golden Rule, in addition to the other 30 builtin lessons for classroom learning and self-study, in undergraduate-to-graduate courses in chemistry and physics.
7. Additional enhancements throughout the package.

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

Literature Search

In Quantum Chemistry Toolbox 2023 a new command, *LiteratureSearch,* has been added that searches the scientific literature for you without ever leaving Maple. Just add some keywords to define your search and let Maple do the rest. By default QCT searches a collection of more than 40 million science articles and preprints from the EuropePMC database including the complete PubMed and PubMed Central collections. But QCT can also search the more than 2.2 million preprints on the arXiv server including the latest in physics from quantum physics to biophysics. Before we begin we load the *QuantumChemistry* package,

```
> with(QuantumChemistry);
```

```
[AOLabels, ActiveSpaceCI, ActiveSpaceSCF, AtomicData, BondAngles, BondDistances, Charges,
  ChargesPlot, ContractedSchrodinger, CorrelationEnergy, CoupledCluster, DensityFunctional,
  DensityPlot3D, Dipole, DipolePlot, Energy, ExcitationEnergies, ExcitationSpectra,
  ExcitationSpectraPlot, ExcitedStateEnergies, ExcitedStateSpins, ExcitonDensityPlot,
```

ExcitonPopulations, *ExcitonPopulationsPlot*, *FullCI*, *GeometryOptimization*, *HartreeFock*, *Interactive*, *Isotopes*, *LiteratureSearch*, *MOCoefficients*, *MODiagram*, *MOEnergies*, *MOIntegrals*, *MOOccupations*, *MOOccupationsPlot*, *MOSymmetries*, *MP2*, *MolecularData*, *MolecularDictionary*, *MolecularGeometry*, *NuclearEnergy*, *NuclearGradient*, *OscillatorStrengths*, *Parametric2RDM*, *PlotMolecule*, *Populations*, *Purify2RDM*, *QuantumComputing*, *RDM1*, *RDM2*, *RTM1*, *ReadXYZ*, *Restore*, *Save*, *SaveXYZ*, *SearchBasisSets*, *SearchFunctionals*, *SkeletalStructure*, *SolventDatabase*, *Thermodynamics*, *TransitionDipolePlot*, *TransitionDipoles*, *TransitionOrbitalPlot*, *TransitionOrbitals*, *Variational2RDM*, *VibrationalModeAnimation*, *VibrationalModes*, *Video*]

Find articles on the methylation of RNA.

```
> LiteratureSearch(["RNA", "methylation"], pagesize = 2);
```

"Total Number of Articles Available = 171858"

"Page = 1"

"Title: RNA N6-methyladenosine methylation and skin diseases."

"Author: Yu Y, Lu S, Jin H, Zhu H, Wei X, Zhou T, Zhao M."

"Abstract: Skin diseases are global health issues caused by multiple pathogenic factors, in which epigenetics plays an invaluable role. Post-transcriptional RNA modifications are important epigenetic mechanism that regulate gene expression at the genome-wide level. N6-methyladenosine (m6A) is the most prevalent modification that occurs in the messenger RNAs (mRNA) of most eukaryotes, which is installed by methyltransferases called "writers", removed by demethylases called "erasers", and recognised by RNA-binding proteins called "readers". To date, m6A is emerging to play essential part in both physiological processes and pathological progression, including skin diseases. However, a systematic summary of m6A in skin disease has not yet been reported. This review starts by illustrating each m6A-related modifier specifically and their roles in RNA processing, and then focus on the existing research advances of m6A in immune homeostasis and skin diseases."

"Journal: Autoimmunity 56, 2167983 (2023)"

"First Publication Date: 2023-12-01"

"URL: https://doi.org/10.1080/08916934.2023.2167983"

"Title: The chromatin signatures of enhancers and their dynamic regulation."

"Author: Barral A, Déjardin J."

"Abstract: Enhancers are cis-regulatory elements that can stimulate gene expression from distance, and drive precise spatiotemporal gene expression profiles during development. Functional enhancers display specific features including an open chromatin conformation, Histone H3 lysine 27 acetylation, Histone H3 lysine 4 mono-methylation enrichment, and enhancer RNAs production. These features are modified upon developmental cues which impacts their activity. In this review, we describe the current state of knowledge about enhancer functions and the diverse chromatin signatures found on

enhancers. We also discuss the dynamic changes of enhancer chromatin signatures, and their impact on lineage specific gene expression profiles, during development or cellular differentiation."

"Journal: Nucleus 14, 2160551 (2023)"

"First Publication Date: 2023-12-01"

"URL: https://doi.org/10.1080/19491034.2022.2160551"

By default, the page size is ten entries per page. Here we selected two entries per page to facilitate the demonstration. Upon executing the command again, the Quantum Chemistry Toolbox automatically gives you the next page of entries. The command can be reset to the first page of entries with the keyword *resetpage*. Search results can be simultaneously printed to the screen and a file with the *filename* keyword. We can search by keyword, author, and journal separately or all at once. Next, search the arXiv for the most recently posted preprints on quantum tunneling in molecules.

```
> LiteratureSearch(["quantum tunneling", "molecules"], pagesize = 2, database = "arXiv");
```

"Total Number of Articles Available = 117"

"Page = 2"

"Title: Radical Addition and H Abstraction Reactions in C2H2, C2H4 and C2H6: A Gateway for Ethyl and Vinyl Bearing Molecules in the Interstellar Medium"

"Author: German Molpeceres and Victor M. Rivilla"

"Summary: Recent interstellar detections include a significant number of moleculescontaining vinyl (C2H3) and ethyl (C2H5) groups in their structure. For severalof these molecules, there is not a clear experimental or theoretical evidencethat support their formation from simpler precursors. We carried out asystematic search of viable reactions starting from closed shell hydrocarbonscontaining two carbon atoms (ethane, C2H6; ethylene, C2H4; and acetylene, C2H2)with the goal of determining viable chemical routes for the formation of vinyland ethyl molecules on top of interstellar dust grains. Our results show thatboth H and OH radicals are key in converting acetylene and ethylene into morecomplex radicals that are susceptible to continue reacting and forminginterstellar complex organic molecules. The relevant reactions, for example OHadditions, present rate constants above 10^{1} s^{-1} that are likelycompetitive with OH diffusion on grains. Similarly, H atom addition toacetylene and ethylene is a very fast process with rate constants above10^{4} s^{-1} in all cases, and greatly enhanced by quantum tunneling.Hydrogen abstraction reactions are less relevant, but may play a role inspecific cases involving the OH radical. Reactions with other radicals NH2, CH3are likely to have a much lesser impact in the chemistry of ethyl and vinylbearing molecules."

"ID: http://arxiv.org/abs/2206.00350v1"

"Published arXiv: 2022-06-01T09:34:15Z"

"Updated arXiv: 2022-06-01T09:34:15Z"

"Journal: A&A 665, A27 (2022)"

"Title: Quantum tunnelling driven H$_2$ formation on graphene"

"Author: Erxun Han, Wei Fang, Michail Stamatakis, Jeremy O. Richardson, and Ji Chen"

"Summary: It is commonly believed that it is unfavourable for adsorbed H atoms oncarbonaceous surfaces to form H$_2$ without the help of incident H atoms. Usingring-polymer instanton theory to describe multidimensional tunnelling effects,combined with ab initio electronic structure calculations, we find that thesequantum-mechanical simulations reveal a qualitatively different picture.Recombination of adsorbed H atoms, which was believed to be irrelevant at lowtemperature due to high barriers, is enabled by deep tunnelling, with reactionrates enhanced by tens of orders of magnitude. Furthermore, we identify a newpath for H recombination that proceeds via multidimensional tunnelling, butwould have been predicted to be unfeasible by a simple one-dimensionaldescription of the reaction. The results suggest that hydrogen moleculeformation at low temperatures are rather fast processes that should not beignored in experimental settings and natural environments with graphene,graphite and other planar carbon segments."

"ID: http://arxiv.org/abs/2204.00808v1"

"Published arXiv: 2022-04-02T08:30:39Z"

"Updated arXiv: 2022-04-02T08:30:39Z"

Quantum Computing

Use Quantum Chemistry Toolbox 2023 to explore quantum computing with the power of computer algebra. Perform simulations of a quantum computer in Maple. Unlike most simulators, Maple can compute with both exact arithmetic (i.e. rational and irrational numbers) and symbolic variables. The wave function is printed using an easy-to-understand Dirac-like notation. First, load the new *QuantumComputing* subpackage

```
> with(QuantumComputing);
```

$$[ConvertDirac, Gate, InitialState, MeasureState, PrepareState, QubitPopulations, QubitPopulationsPlot]$$

Maple knows the standard 1- and 2-qubit gates. For example, Pauli Z gate

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

$$Uz := \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

or the Pauli X and Y gates

```
> Uz, Uy := Gate("X"), Gate("Y");
```

$$Uz, Uy := \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \begin{bmatrix} 0 & -I \\ I & 0 \end{bmatrix}$$

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);
```

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

or a 2-qubit gate like the CNOT gate.

```
> Ucnot := Gate("CNOT");
```

$$Ucnot := \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}$$

We can initialize a state of 4 qubits on our simulated quantum computer with the *InitialState* command

```
> state0 := InitialState(4);
```

$$state0 := \Psi_{0,0,0,0}$$

The initial wave function has each of its 4 qubits in the lower state of the qubit, denoted by 0. To illustrate preparing a state on the quantum computer, use a product of gates (unitary transformations), known as a circuit, to prepare a Schrodinger cat state in which the state of all qubits down becomes entangled with the state of all qubits up. In the Quantum Chemistry Toolbox, the circuit is readily assembled as a Maple list of equations. The left side of an equation indicates the qubit or qubits on which the gate acts and the right side provides the gate itself.

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

$$circuit := \left[1 = \begin{bmatrix} \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \\ \frac{\sqrt{2}}{2} & -\frac{\sqrt{2}}{2} \end{bmatrix}, [1,2] = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}, [2,3] = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}, [3,4] = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}\right]$$

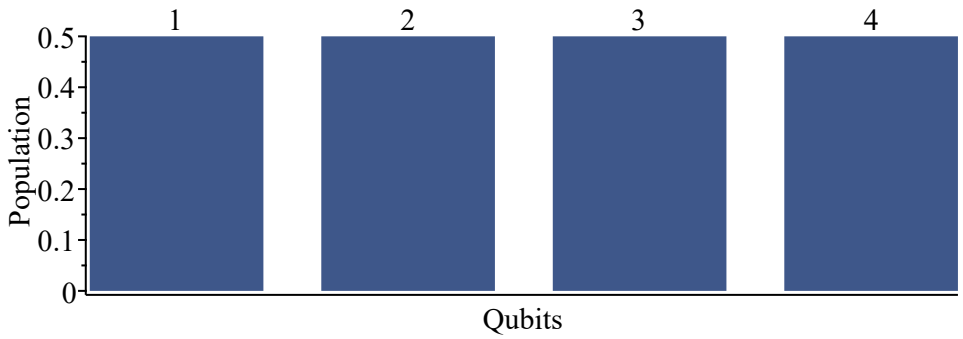
To prepare the new state, we act on the initial state *state0* with our circuit.

```
> state2 := PrepareState(circuit, state0);
```

$$state2 := \frac{\sqrt{2}\,\Psi_{0,0,0,0}}{2} + \frac{\sqrt{2}\,\Psi_{1,1,1,1}}{2}$$

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. The probability of being "up" in each qubit 1/2 as we can see from the *QubitPopulationsPlot* command

> *QubitPopulationsPlot*(*state2*);

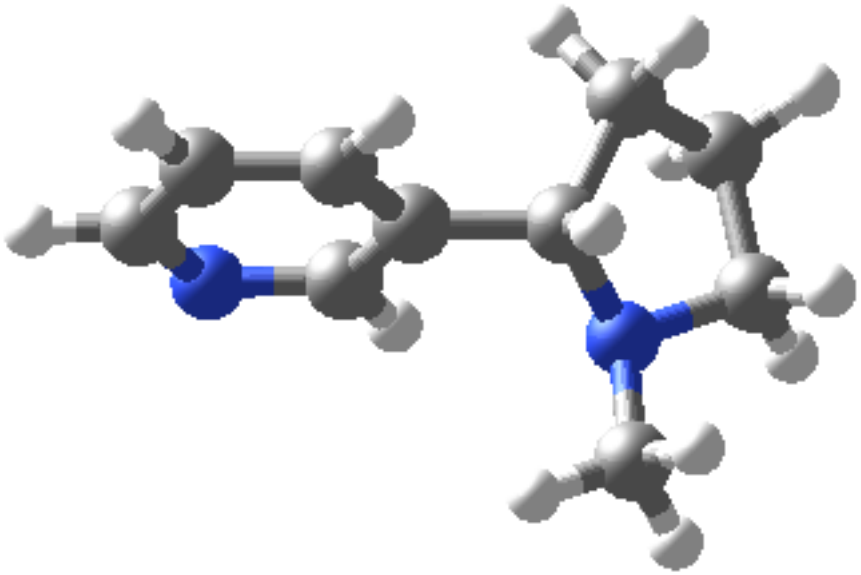


SMILES

Entering a molecule's geometry can be tedious. That is why in the Quantum Chemistry Toolbox there are unconventional ways to import geometries, such as retrieving them by chemical name from a database of nearly 100 million molecules. Now in Quantum Chemistry Toolbox 2023 you can also import molecular geometries and skeletal structures by their SMILES (Simplified Molecular-Input Line-Entry System) formula. Import some molecular geometries with SMILES and make some molecular plots

> *mol* := *MolecularGeometry*("smiles=CN1CCC[C@H]1c2cccnc2");
PlotMolecule(*mol*);

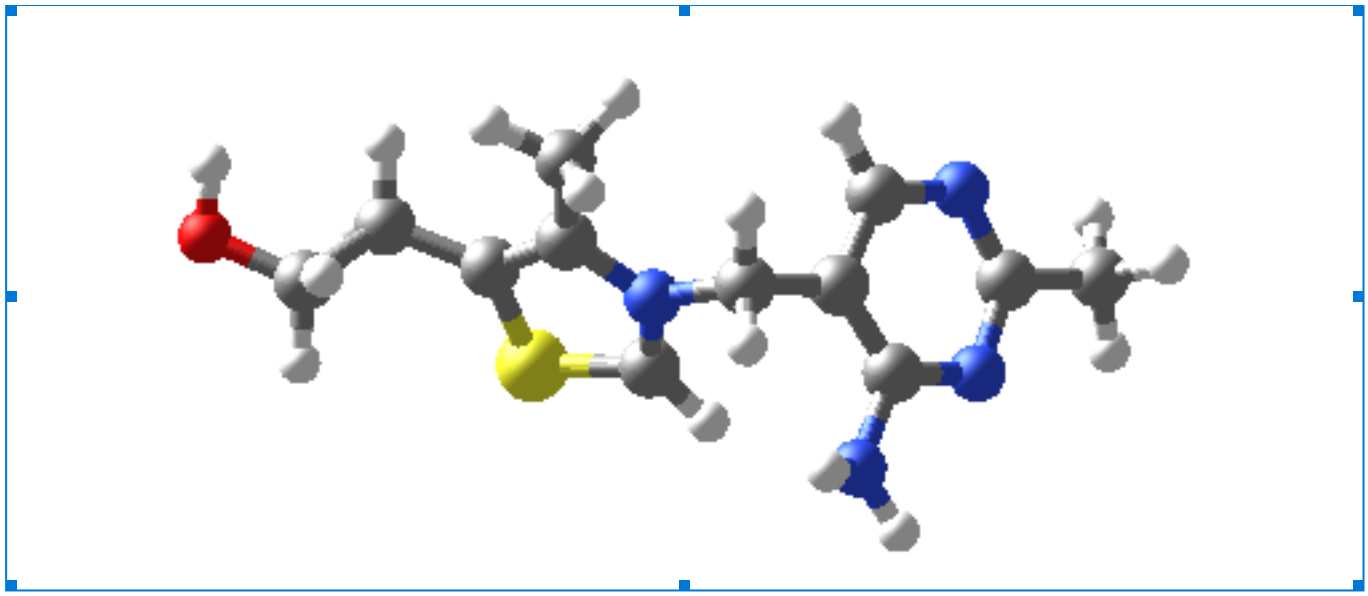
mol := [["N", −1.70230000, −0.79620000, −0.03390000], ["N", 2.29680000, −0.70910000, 1.21710000], ["C", −0.88460000, 0.30950000, −0.57130000], ["C", −1.49550000, 1.58240000, 0.04360000], ["C", −2.68570000, 1.09840000, 0.85960000], ["C", −3.02810000, −0.23820000, 0.23290000], ["C", 0.58720000, 0.15440000, −0.25130000], ["C", −1.76180000, −1.95030000, −0.92170000], ["C", 1.55690000, 0.70250000, −1.07910000], ["C", 1.00080000, −0.53570000, 0.87380000], ["C", 2.90090000, 0.54510000, −0.75930000], ["C", 3.21560000, −0.16270000, 0.38950000], ["H", −1.00840000, 0.36650000, −1.66240000], ["H", −1.84540000, 2.24560000, −0.75710000], ["H", −0.80180000, 2.15280000, 0.67090000], ["H", −2.38960000, 0.96500000, 1.90760000], ["H", −3.52200000, 1.80290000, 0.82930000], ["H", −3.60940000, −0.86620000, 0.91510000], ["H", −3.60210000, −0.08800000, −0.69030000], ["H", −2.36430000, −2.74600000, −0.46980000], ["H", −0.76270000, −2.36680000, −1.08850000], ["H", −2.19750000, −1.70360000, −1.89650000], ["H", 1.27980000, 1.25440000, −1.97280000], ["H", 0.30270000, −0.97780000, 1.57700000], ["H", 3.67750000, 0.96380000, −1.38900000], ["H", 4.24910000, −0.31340000, 0.68330000]]



and

```
> mol := MolecularGeometry("smiles=OCCc1c(C)[n+](cs1)Cc2cnc(C)nc2N");
  PlotMolecule(mol);
```

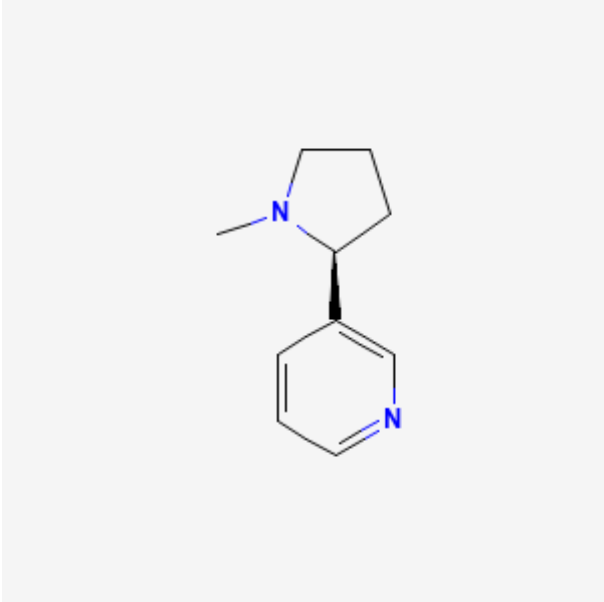
```
mol := [["S", 1.94820000, −1.40310000, 1.19600000], ["O", 6.45600000, 0.09140000, 0.44660000],
    ["N", 0.66470000, −0.10680000, −0.49410000], ["N", −3.72010000, −0.86390000, 0.04040000],
    ["N", −3.34680000, 1.42530000, 0.69440000], ["N", −2.12290000, −2.00110000, −1.29370000],
    ["C", 1.85520000, 0.55790000, −0.41890000], ["C", −0.42200000, 0.31120000, −1.38250000],
    ["C", 2.70540000, −0.03130000, 0.48630000], ["C", 4.07610000, 0.34630000, 0.88360000], ["C",
    −1.72050000, 0.27850000, −0.65990000], ["C", 0.52940000, −1.15310000, 0.27350000], ["C",
    2.06490000, 1.74550000, −1.26000000], ["C", 5.16290000, −0.31970000, 0.02050000], ["C",
    −2.54090000, −0.83010000, −0.61450000], ["C", −2.17910000, 1.38880000, 0.01930000], ["C",
    −4.05660000, 0.28130000, 0.66400000], ["C", −5.35400000, 0.28280000, 1.39900000], ["H",
    −0.40200000, −0.32280000, −2.27510000], ["H", −0.27810000, 1.32830000, −1.75880000],
    ["H", 4.26260000, 0.10170000, 1.93770000], ["H", 4.19890000, 1.43580000, 0.83240000], ["H",
    −0.30950000, −1.81830000, 0.36420000], ["H", 1.90230000, 1.52020000, −2.31890000], ["H",
    1.40560000, 2.56520000, −0.95710000], ["H", 3.09180000, 2.11650000, −1.17670000], ["H",
    5.04610000, −0.05620000, −1.03630000], ["H", 5.11190000, −1.41040000, 0.10210000], ["H",
    −1.60930000, 2.31230000, 0.04930000], ["H", −1.61830000, −1.91060000, −2.16530000], ["H",
    −2.74050000, −2.80040000, −1.21170000], ["H", 6.49690000, 1.05930000, 0.36180000], ["H",
    −5.61620000, −0.72690000, 1.73010000], ["H", −5.29750000, 0.92530000, 2.28330000], ["H",
    −6.14840000, 0.65430000, 0.74510000]]
```



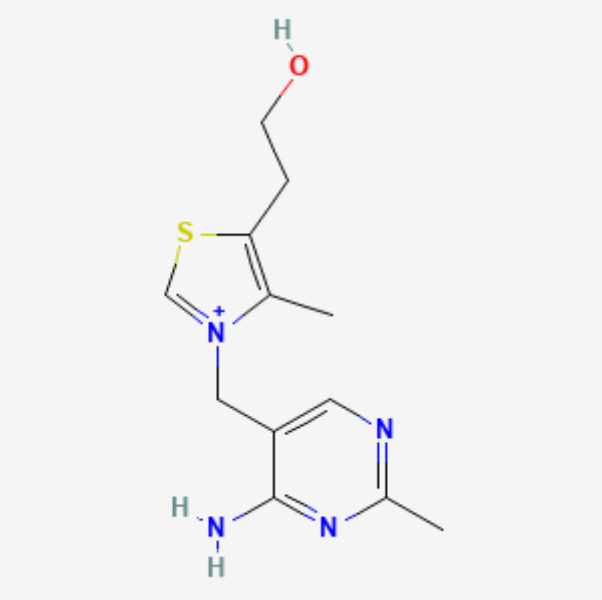
Similarly, we can import the skeletal structures of these molecules from SMILES formulas

```
> SkeletalStructure("smiles=CN1CCC[C@H]1c2cccnc2");
```

and



> *SkeletalStructure*("smiles=OCCc1c(C)[n+](cs1)Cc2cnc(C)nc2N");



Fly-through Molecular 3-D Animations

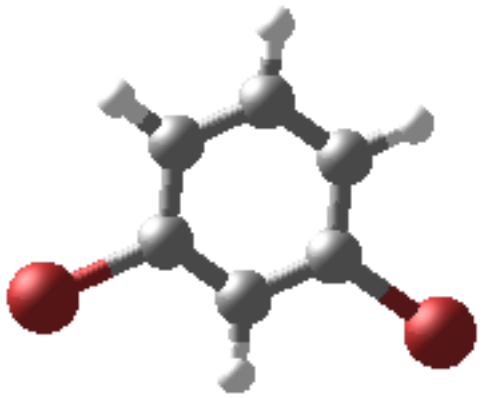
It's a bird ... it's a plane ... it's Superman. Now you can fly through molecules with the new fly-though molecular 3-D animations in QCT 2023. We can make fly-through animations by adding the *viewpoint* keyword in *PlotMolecule*, *DensityPlot3D*, *ChargesPlot*, *DipolePlot*, *TransitionDipolePlot*, and *ExcitonDensityPlot*. The user can choose the strings "flythrough", "flythrough2", "flythrough3", "flythrough4", "circleright", or "circleleft" to obtain six different 3-D fly-through animations. For example, consider the molecule 1,3-dibromobenzene

> *mol* := *MolecularGeometry*("1,3-dibromobenzene");

mol := [["Br", −2.84530000, −1.23120000, 0], ["Br", 2.84540000, −1.23100000, 0], ["C", 0.00010000, −0.98450000, 0.00010000], ["C", −1.20800000, −0.28710000, 0], ["C", 1.20800000, −0.28700000, −0.00010000], ["C", −1.20810000, 1.10770000, −0.00010000], ["C", 1.20790000, 1.10780000, 0.00010000], ["C", −0.00020000, 1.80520000, 0], ["H", 0.00020000, −2.07230000, 0.00010000], ["H", −2.14060000, 1.66640000, −0.00010000], ["H", 2.14030000, 1.66660000, 0.00010000], ["H", −0.00020000, 2.89130000, 0]]

With the *PlotMolecule* command we have

```
> PlotMolecule(mol, viewpoint = "circleright");
```

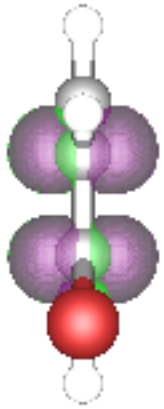


or the *DipolePlot* command

```
> DipolePlot(mol, viewpoint = "flythrough3");
```

or the LUMO from the DensityPlot3D command

```
> data := HartreeFock(mol) :
> DensityPlot3D( mol, data, orbitalindex = round( add(i, i in MOOccupations(mol)) / 2 + 1 ),
      gridspacing = 0.001, maximumpoints = 400000, viewpoint = "flythrough3" );
```



Custom Hamiltonians in Variational2RDM

While the Quantum Chemistry Toolbox allows any molecule to be computed, sometimes it is useful to be able to solve a custom Hamiltonian, i.e. for a spin model. In Quantum Chemistry Toolbox 2023 any custom Hamiltonians can be used with the Variational2RDM method. Additional details and an example are available in the Help pages.

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. Use of the Quantum Chemistry Toolbox in the

classroom is described in a recent paper in J. Chem. Ed. Quantum Chemistry Toolbox 2023 includes a new lesson on Fermi's Golden Rule. The Maple environment allows us to seamlessly combine analytical work with electronic structure calculations and visualizations from the Quantum Chemistry Toolbox .