

TmoleX features:

- Import and export of coordinates from and to different formats like xyz, cosmo, sdf, ml2, car, arc
- Build your own molecule from scratch or modify and merge it from prefabricated fragments.
- Graphical visualization of molecular structure, including movies of gradients and vibrational frequencies
- Choose from all basis sets of the TURBOMOLE library
- Generation of molecular orbitals and automatic occupation
- Supported methods: Hartree-Fock, DFT, MP2, TDDFT, DFT+D, SCS-MP2, and CC2
- The RI approximation can be used for DFT, DFT+D, MP2, SCS-MP2, and CC2 calculations with automatic assignment of auxiliary basis sets
- Ground and excited state single-point calculations and geometry optimizations
- Run vibrational frequency, NMR shielding, and UV/VIS spectra calculations
- Constraint geometry optimizations, including the option to scan along a fixed internal coordinate
- Job templates as a shortcut to generate default input and job types

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Cover picture: a visualization of molecular orbitals

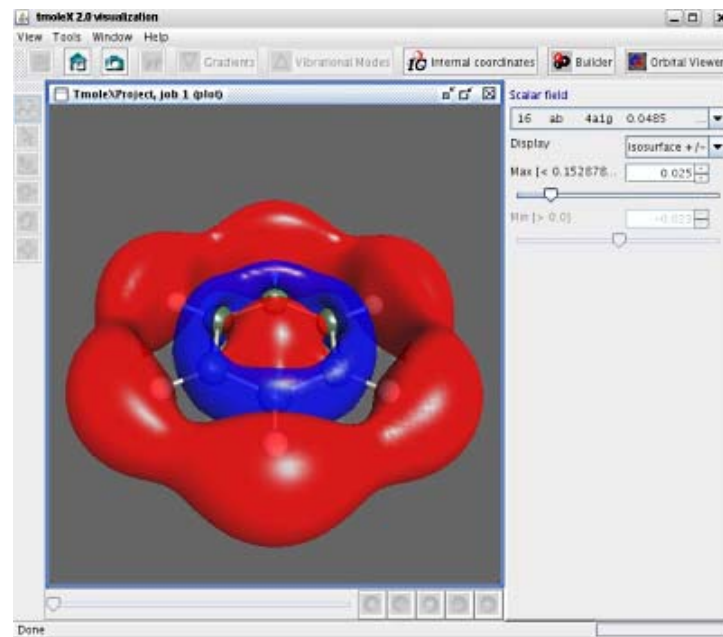
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TmoleX

A Graphical User Interface
for TURBOMOLE



Get the free client version at:
<http://www.cosmologic.de/tmolex-client>

TmoleX is a graphical frontend for the quantum chemical program package TURBOMOLE. It allows you to execute the complete workflow of a quantum chemical investigation, from the initial building of a structure to the visualization of the results, in a user-friendly GUI.

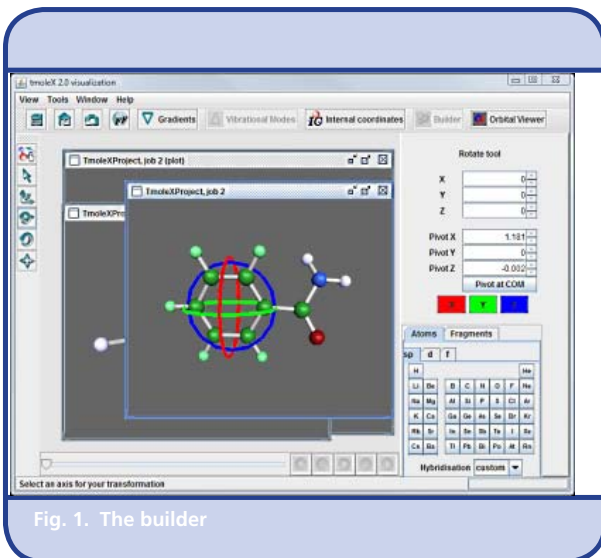


Fig. 1. The builder

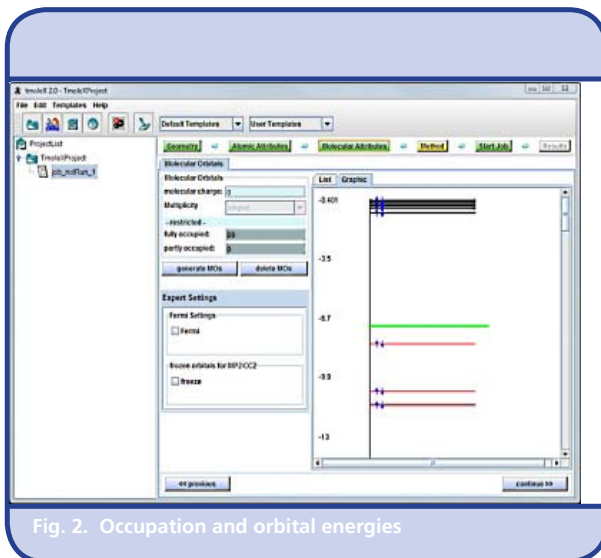


Fig. 2. Occupation and orbital energies

3D Molecule Builder

Use the on-board builder to create input structures from scratch or to modify imported structures. A library of fragments can be used to add chemical relevant groups to the compound. You can also create your own fragment data base.

Basis Sets

The TURBOMOLE basis set library is fully accessible. Basis sets can be assigned for all atoms, each element, or individual atoms.

Occupation

By default the multiplicity is determined automatically from an extended Hückel calculation. After the generation of start MOs the occupation can be customised conveniently.

Methods

Choose between different levels of theory. DFT, DFT+D, MP2, and SCS-MP2 as the most frequently used methods for ground state investigations are available. For calculations in electronically excited states TD-DFT and linear response CC2 can be used.

The RI Approximation

The resolution-of-the-identity approximation is nowadays industry standard. It is a very efficient way to reduce the CPU times of calculations as well as memory and disk space demands with only negligible and well-behaved errors. TURBOMOLE makes use of this approximation consistently for fast and robust calculations. In addition to the orbital basis set auxiliary basis are needed. TmoleX assigns them automatically for you.

Job Types

When basis sets and methods are selected, you can choose between the different types of jobs. You can calculate single point energies, vibrational frequencies, NMR shieldings, excitation energies, oscillatory and rotatory strengths (for UV/Vis or CD spectra prediction) or perform geometry optimizations in the ground state as well as in excited states and transition state searches.

Potential Energy Scans

Fix an internal coordinate and set up constraint geometry optimizations for several values of this coordinate. This lets you scan potential energy surfaces.

Start Jobs

Calculations can be started either on your local desktop or you can submit them to remote computers. Also submitting to queuing systems is supported

Job Handling

The project list helps you to keep track of your jobs, whether they were started on local or remote computers.

Vibrational Modes

You can use TmoleX to visualize the modes of vibrational frequencies calculations.

Iso- and Vector Plots

For post-processing plots of several properties can be created, e.g. molecular orbitals, the total and spin densities, the electrostatic potential, electric field gradient, or difference densities of ground and excited states.

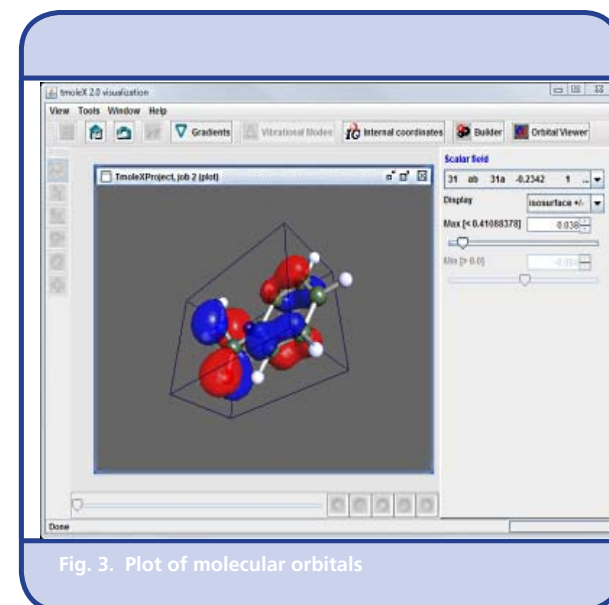


Fig. 3. Plot of molecular orbitals

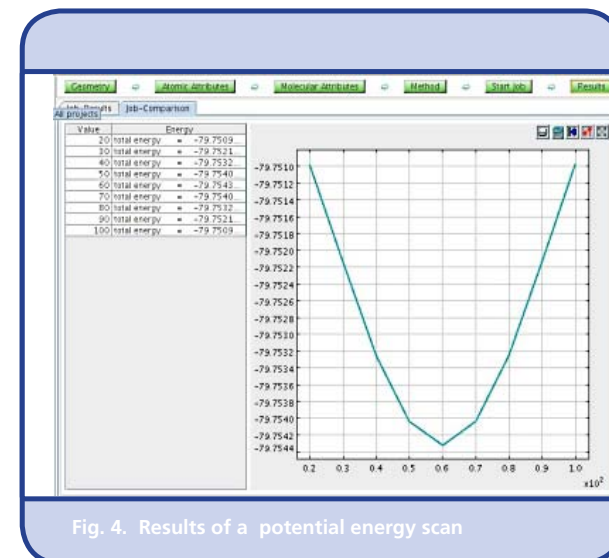


Fig. 4. Results of a potential energy scan

Download a demo version at www.cosmologic.de/turbomole-demo or the free client version at www.cosmologic.de/tmolex-client