ORCA Input Library - Vibrational Frequencies & Thermochemistry Vibrational Frequencies & Thermochemistry Harmonic vibrational frequencies can be calculated in ORCA either numerically or analytically. For reliable frequencies you should converge the SCF tig

ORCA Input Library - Geometry optimizations Geometry optimizations Geometry optimizations are usually performed at the DFT level as DFT has a very favorable cost-accuracy ratio and because analytical gradients are available for most functionals. It's typically

ORCA Input Library - General Input General Input ORCA both has a Simple keyword syntax as well as a Block syntax. The Simple input is often the only inputline needed (as well as the coordinates block) while some specific settings are only available using the Bl

ORCA Input Library - RI and auxiliary basis sets RI and auxiliary basis sets ORCA includes a number of approximations that are designed to speed up calculations significantly while introducing a very small error (usually smaller than basis set errors and much sma

ORCA Input Library - SCF Convergence Issues SCF Convergence Issues Converging the SCF is a somewhat awkward aspect of computational chemistry. Closed-shell organic molecules tend to be easy to converge with modern SCF algorithms (requiring only oc

ORCA Input Library - Restarting calculations Restarting calculations Restarting geometry optimizations To restart a geometry optimization job that crashed unexpectedly or ran out of iterations, it is easiest to simply take the last set of coordinates and start a new ca

ORCA Input Library - Semiempirical methods Semiempirical methods Semiempirical methods are usually simplified versions of the Hartree-Fock method where certain integrals have been skipped or approximated and empirical parameters introduced. Semiempiri

ORCA Input Library - ORCA-ASE ORCA-ASE ORCA-ASE interface A n ASE interface has been written that is now part of ASE. See ASE for details ORCA-ASE examples Some example ASE inputfiles that use the interface: Geometry optimization with ORCA and

ORCA Input Library - Useful scripts and commands for ORCA Input/Output Useful scripts and commands for ORCA Input/Output The ORCA community has through the years created various shell-scripts or Python scripts to aid ORCA input generation or analysis

ORCA Input Library - DMRG DMRG Todo... Google Sites Report abuse Page details Page updated Google Sites Report abuse This site uses cookies from Google to deliver its services and to analyze traffic. Information about your use of this site is shared with Go

ORCA Input Library - ORCA & Chemshell ORCA & Chemshell ORCA can be used as a QM code in either QM or QM/MM geometry optimizations or molecular dynamics simulations in Chemshell . The current ORCA interface in Chemshell is documented on: http:/

ORCA Input Library - Interfaces and QM/MM Interfaces and QM/MM ORCA can be interfaced to various other programs (geometry optimizers, MD programs, QM/MM programs). These programs then communicate with ORCA via the automatic creation of inputfile

ORCA Input Library - Basis sets Basis sets The use of a basis set in quantum chemical calculations is an approximation which introduces a basis set error. Learning how to control and minimize the basis set error is an important part of doing reliable computational

ORCA Input Library - Minimum energy path calculations Minimum energy path calculations The Geometry Optimizations page and the Saddlepoint optimization tutorial already shows how simple saddle-points can be located via the combination of relaxed surface s

ORCA Input Library - Tutorial: Saddlepoint ("TS") optimization via relaxed scan Tutorial: Saddlepoint ("TS") optimization via relaxed scan - The very cheap (and not very accurate) semi-empirical method PM3 is used here (all these calculations can be run in second

ORCA Input Library - Frozen core calculations Frozen core calculations F rozen core settings in ORCA In post-HF calculations only the valence electrons are typically correlated. The other electrons are kept frozen and define a frozen core. Frozen cores differ betw

ORCA Input Library - MP2 & MP3 MP2 & MP3 ORCA includes different MP2 variants and different approximations to speed up MP2 calculations. MP3 is also available. This page demonstrates the use of all these methods. See this recent paper for a study on the

ORCA Input Library - TDDFT TDDFT Time-dependent DFT is a nice black-box approach to computing excited states in general. UV-VIS, and CD spectra are straightforwardly computed using the %tddft block. TDDFT can also be used for core-level spectroscopy.

ORCA Input Library - Effective Core Potentials Effective Core Potentials Note: ECPs are used automatically for the core electrons of heavy elements when specifying certain basis sets such as the Ahlrichs def2-XVP basis sets (that were intended for use with an E

ORCA Input Library - Double-hybrid DFT Double-hybrid DFT Double hybrid DFT calculations are probably the most accurate way of computing reliable energies of maingroup and organic systems at the DFT/MP2 level as found in the GMTKN30 database study by

ORCA Input Library - Tutorial: Resonance Raman Tutorial: Resonance Raman Work in progress Resonance Raman (rR) Calculations Google Sites Report abuse Page details Page updated Google Sites Report abuse This site uses cookies from Google to deliver

ORCA Input Library - Molecular dynamics Molecular dynamics Molecular dynamics (MD) requires in principle only energies and gradients from the electronic structure calculation, so it is possible to have any flexible external MD program call ORCA and request an

ORCA Input Library - Tutorial: Setting up the orbitals for a CAS calculation Tutorial: Setting up the orbitals for a CAS calculation This tutorial will describe how to set up the orbitals for a CASSCF calculation, with optional NEVPT2 or MRCI steps to follow. Note that

ORCA Input Library - DFT calculations DFT calculations See also Geometry optimization section. General recommendations about molecular DFT calculations (Ragnar Bjornsson) For GGA calculations (functionals like PBE, BP86, TPSS), use of the RI-J approxim

ORCA Input Library - Geometry input Geometry input The geometry is given to ORCA either in the form of Cartesian coordinates (x,y,z) or internal coordinates (bonds, angles, dihedrals). The coordinates can be in the inputfile or in a separate xyz file. Important: nu

ORCA Input Library - Broken-symmetry DFT Broken-symmetry DFT Converging to a broken-symmetry state (single-point calculation) There are two main ways to converge to a broken-symmetry state in ORCA. Fe(III)-Fe(III) example: Here a high-spin S=5/2 Fe(III

ORCA Input Library - orbs orbs ch3-eprii.eldens.cube ch3-eprii.mo0a.cube ch3-eprii.mo1a.cube ch3-eprii.mo3a.cube ch3-eprii.mo4a.cube ch3-eprii.mo5a.cube ch3-eprii.spindens.cube Google Sites Report abuse Page details Page updated Google Sites Report ab

ORCA Input Library - Continuum solvation (CPCM,COSMO, SMD) Continuum solvation (CPCM, SMD) The conductor-like polarizable continuum model, CPCM, is implemented in ORCA and is an efficient, albeit crude, way of accounting for solvent effects in quant

ORCA Input Library - Excited state calculations Excited state calculations Excited state calculations in ORCA can be carried out in multiple ways in ORCA. ?SCF calculations and orbital rotations It is sometimes possible to guide SCF calculations (HF or DFT) to an

ORCA Input Library - Numerical precision Numerical precision T he user is always responsible for the numerical precision you get from whatever quantum chemistry code you use. Below are some helpful keywords and recommendations to deal with numerical pre

ORCA Input Library - Relativistic approximations Relativistic approximations Using scalar relativistic methods in DFT calculations with ORCA is made easy if the recommended basis sets are used. The Ahlrichs def2 basis set family has been recontracted for use ir

ORCA Input Library - Tutorial: Intrinsic Reaction Coordinate (IRC) Tutorial: Intrinsic Reaction Coordinate (IRC) The Intrinsic Reaction Coordinate (IRC) method is useful to confirm that a located saddlepoint lies on the minimum energy path between 2 assumed min

ORCA Input Library - Coupled cluster Coupled cluster Coupled cluster theory is the most robust way of introducing dynamic electron correlation into the wavefunction and the CCSD(T) method (coupled cluster singles doubles perturbative triples) is often referred to

ORCA Input Library - FOD analysis FOD analysis Stefan Grimme and coworkers have come up a static electron correlation diagnostic that is easy to use and reveals the nature of the static electron correlation as well. The diagnostic is based on fractional occupati

ORCA Input Library - Tutorial: NEB calculations Tutorial: NEB calculations This page is under construction... The Nudged Elastic Band method is tool both for finding the minimum energy path and the saddlepoint connecting two minima. While very popular in the s

ORCA Input Library - ORCA Common Errors and Problems ORCA Common Errors and Problems This page lists common errors and problems encountered when running calculations with ORCA. For problems with installing or setting up ORCA see Setting up OR

ORCA Input Library - Molecular properties Molecular properties Calculations of molecular properties in ORCA are performed using either the %elprop or the %eprnmr block if computed with an SCF-type method (HF, DFT) or MP2. Most electric properties are perfo

ORCA Input Library - Extrapolation methods Extrapolation methods Automatic extrapolation of correlated methods to the complete basis set limit, CBS, (for both HF energies and correlation energies). See manual for more details and more options. Extrapolation o

ORCA Input Library - X-Ray Spectroscopy (XAS, XES, ROCIS) X-Ray Spectroscopy (XAS, XES, ROCIS) Computational core-level (or X-ray ) spectroscopy has been implemented in ORCA in various ways. Currently, X-ray absorption and emission calculations ca

ORCA Input Library - Orbital and density analysis Orbital and density analysis See Visualization page for information on ways to plot the different families of orbitals and electron/spin densities discussed here. Mulliken/Löwdin/Hirshfeld charge and spin population a

ORCA Input Library - Localized orbital centroid analysis Localized orbital centroid analysis How to do localised orbital centroid analysis of a molecule as in the paper by Vidossich and Lledos : Scripts: orblocfind.py (Python3 script that finds localized orbitals in local

ORCA Input Library - CASSCF calculations CASSCF calculations The complete active space self-consistent field (CASSCF) method requires some chemical insight of the problem under investigation. The setup of the calculation requires a careful design of the act

ORCA Input Library - Visualization and printing Visualization and printing single Visualization programs Various GUI programs that can visualize results from ORCA output and/or create coordinates/inputfiles are available: Chemcraft: Good molecular builder. Can c