Molcas 7: A program package for quantum chemists and code developers

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Methods

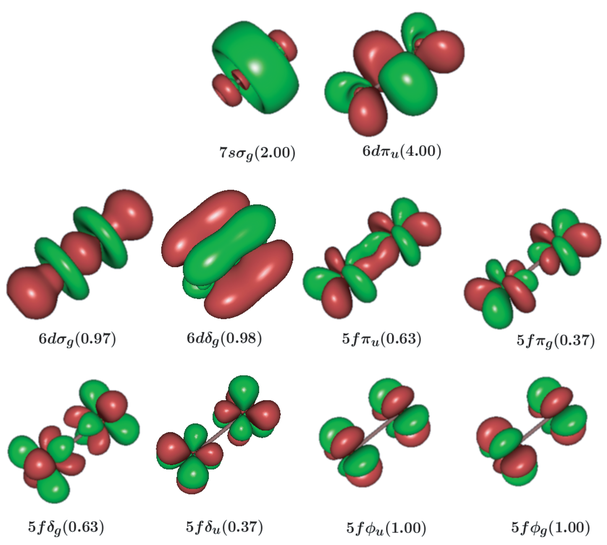
The program system MOLCAS is a package for calculations of electronic and structural properties of molecular systems in gas, liquid, or solid phase.

MOLCAS contains a number of modern quantum chemical methods for studies of the electronic structure in ground and exited electronic states, including Hartree-Fock, Density Functional Theory, Coupled-Cluster, multiconfigurational SCF (RASSCF) with dynamical electron correlation treated with multi-reference CI or second order perturbation theory (MS-CASPT2). MOLCAS gives possibility to treat molecules in solutions (PCM model), and in solid state (cluster embedding), and as a part of QM/MM system.

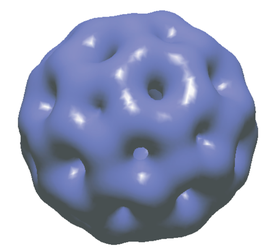
MOLCAS has the aim to provide methods for calculations on molecules containing atoms from the entire periodic system. It provides basis sets that are especially designed for multiconfigurational and relativistic calculations. MOLCAS can be used to compute molecular structures, bond energies, energy barriers for chemical reactions, excitation energies (including spin-orbit coupling), vibration spectra.

Applications

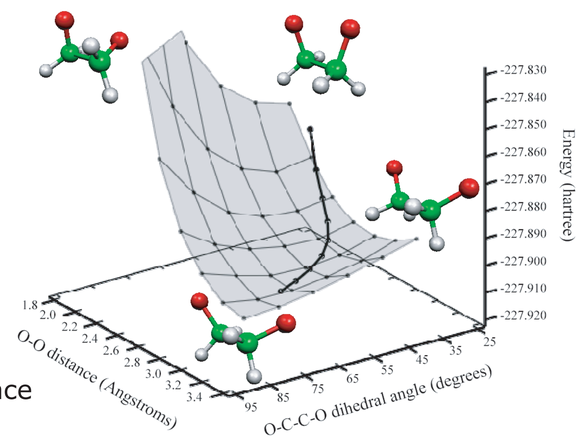
The typical applications for MOLCAS are: accurate potential energy curves, molecular spectroscopy, photochemistry, reaction mechanisms, heavy element chemistry, biochemistry



CASSCF/CASPT2/RASSI-SO calculations on the uranium dimer gives a quintuple bond with a bond distance of 2.43Å and $^7 11_{14}$($^7 O_{14}$) ground state. The binding energy was estimated to be 30 kcal/mol (40 kcal/mol without spin-orbit coupling)
L.Gagliardi and B.O.Roos, Nature, 433, 848 (2005).
The picture shows the bonding orbitals.



Geometry of charged (n=0,-1..-6) C_{60}^n molecules has been optimized in CASSCF and CASPT2 level. The calculations of electronic structure of C_{60}^n-C_{60}^m molecules is in a progress.



The potential energy surface of triplet 1,2-dioxetane as a function of the O-O bond distance and the O-C-C-O dihedral angle. The shaded surface was obtained by imposing constraints on the two coordinates, and relaxing all the rest. The black line represents a steepest descent path over the same surface
L. De Vico, M. Olivucci and R. Lindh, submitted to "Journal of Chemical Theory and Computation"

Availability

MOLCAS runs on almost all UNIX-like platforms and also on MS Windows and Mac OS X. It has a straightforward installation from a source code and a set of configuration files for different platforms and compilers.
For Linux operating system MOLCAS could be compiled by GCC/G77, Intel, PGI, NAG, PathScale, Absoft.
It runs on 32- and 64- bit architectures, on SMP, on clusters and on grid. A complete list of tested platforms and compilers, as well as benchmark results, is available on MOLCAS homepage.

Development

MOLCAS is not only a program suite for quantum chemistry calculations, but also a toolkit for development of new software. Basic ideas of programming for MOLCAS include:
- using standard libraries for solving of common computational problems,
- using wrappers for low-level routines,
- a single source code (FORTRAN 77 and C) with C preprocessor instructions.

MOLCAS programming environment includes:
- Application Programming Interface (API) calls to solve typical quantum chemical problems, and to get access to the data, produced by MOLCAS codes.
- Self explained documentation for main API calls
- Patch system for independent (via web-interface) development
- Verification suite for an automatic check of the code
- Set of scripts for maintaining and debugging the code

MOLCAS environment allows developers to concentrate on the scientific part of the code. Several external developer's groups already made interface of their codes to MOLCAS, or use it as a platform for development.

Licenses

MOLCAS has major releases approximately every 3 year, with free updates within this period.
No limitations for the number of CPUs or architecture. There are three types of licenses - academic group, computer center/university, and commercial.

More info...

MOLCAS has a comprehensive set of manuals containing information about the code and its use. It includes User's Guide, Tutorials and Examples, Installation Guide, and Programming's Guide. Manuals are available on-line. Also MOLCAS provides text mode help system with information about modules and keywords.

MOLCAS workshops are arranged every year.

MOLCAS Homepage: http://www.teokem.lu.se/molcas