

UniChem 5.0

S G I , I B M , C r a y , F u j i t s u

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Overview

Release 5.0 of the UniChem molecular modeling package became available from Oxford Molecular, Ltd. in April 2000. It is sent automatically to all UniChem customers who have a current maintenance contract. We anticipate that all customers will eventually upgrade to this version.

This latest release of the UniChem software introduces significant new functionality and differs from release 4.1 in a number of important ways. These release notes call attention to these changes and provide pointers for installing this new version.

The complete UniChem 5.0 package includes:

- UniChem 5.0 Release Notes;
- UniChem 5.0 hard-copy documentation
 - UniChem 5.0 User Guide*
 - UniChem 5.0 Guide to DGauss*
 - UniChem 5.0 Guide to MNDO97*
 - UniChem 5.0 Installation and Administration Guide*
 - UniChem 5.0 CD-ROM booklet with a Quick Install Guide*

- UniChem 5.0 software and online Help, provided either on a CD-ROM or electronically via FTP.

To install the software, follow the instructions provided in the Quick Install Guide in the *UniChem 5.0 CD-ROM booklet* or the more detailed instructions provided in the *UniChem 5.0 Installation and Administration Guide*.

After installing UniChem 5.0, you should contact Oxford Molecular support to obtain new license files. For information on contacting Oxford Molecular, refer to section 8 of these release notes.

Supported platforms

The UniChem 5.0 user interface client software runs on the following platforms:

SGI MIPS	IRIX 5.3
IBM RS/6000	AIX 4.2

The UniChem 5.0 chemistry application server software runs on the following platforms:

SGI R4400, R5000	IRIX 5.3
SGI R10000, R12000	IRIX 6.2
IBM RS/6000	AIX 4.2
Cray Y-MP, J90, SV1	UNICOS 9.0
Cray C90, T90	UNICOS 10.0
Cray T90 IEEE	UNICOS 10.0
Cray T3E	UNICOS/mk 2.0
Fujitsu VPP	UXP/V 4.0

UniChem software should also run on the same hardware with higher levels of the operating systems.

New licenses

As it is a major new release, all users must obtain a new license from Oxford Molecular to run UniChem 5.0 even if they currently have a valid UniChem 4.1 license.

DEMO license keys, which are set to expire June 1, 2000, are installed automatically along with the UniChem 5.0 software. Assuming you install the software before this expiration date, the DEMO licenses will allow you to start using the software immediately. They also serve as place-holders for the new licenses you will receive from Oxford Molecular support.

In previous releases, UniChem used FLEXlm from GLOBETrotter Software, Inc. to license both its client and server software. FLEXlm is not available on all of the server platforms supported by UniChem 5.0. Therefore, in order to simplify its licensing requirements, UniChem 5.0 no longer uses FLEXlm with its server software. Instead, a node-locked licensing scheme developed by Oxford Molecular is used. UniChem 5.0 continues to use FLEXlm with its client user interface software. In this case, FLEXlm's support for floating licenses was essential to maintain.

In line with this change in licensing, UniChem 5.0 uses separate license files for the client and server software. The default names for these files are `gui.license` and `server.license`. In previous releases, the default name of the license file was `UniChem.license.dat`.

If you wish to run an earlier version of the UniChem user interface along with the 5.0 version, you should combine the license files from the separate releases into one file before starting the FLEXlm license manager daemons.

For further details regarding UniChem 5.0 licensing, see the *UniChem 5.0 Installation and Administration Guide* or contact Oxford Molecular support.

Online Help

The UniChem 5.0 online Help requires a separate installation of an HTML browser. By default, UniChem expects to use Netscape. You can download Netscape from:

<http://home.netscape.com/download/index.html>

UniChem invokes the HTML browser using the shell script `<unichem_root>/bin/ucdoc`. You may edit this script if necessary.

In addition to an HTML browser, you must also install the Adobe Acrobat Reader in order to view or print the PDF documents that are a part of the UniChem 5.0 online documentation. You can download Acrobat Reader from:

<http://www.adobe.com/products/acrobat/readstep.html>

New features

This section lists the changes between releases 5.0 and 4.1 in the various UniChem system components.

GUI changes

The UniChem 5.0 user interface has been changed in order to support the new functionality in the DGauss 5.0 and MNDO97 chemistry applications and to generalize support for batch jobs.

DGauss changes

The most important changes between DGauss releases 4.1 and 5.0 include:

New exchange-correlation functionals

DGauss 5.0 introduces support for the recently developed HCTH and FT97 functionals. These functionals are a new formulation of the generalized gradient approximation (GGA) and are based on the following papers:

F.A. Hamprecht, A.J. Cohen, D.J. Tozer and N.C. Handy, “*Development and assessment of new exchange-correlation functionals*”, J. Chem. Phys. **109**, 6264 (1998)

M. Filatov and W. Thiel, “*A new gradient-corrected exchange-correlation functional*”, Mol. Phys. **91**, 847 (1997)

Both HCTH and FT97 significantly improve DGauss’ accuracy while retaining its computational efficiency.

Support for Gaussian-based effective core potentials

DGauss 5.0 introduces support for Gaussian-based effective core potentials (ECPs), including the analytic computation of vibrational frequencies. The standard Hay-Wadt, Christiansen-Ermiler, Stuttgart and Stevens-Basch-Krauss ECPs are fully supported for the following elements: Rb-Xe and Cs-At (not including the lanthanides).

The DGauss BASIS file also includes several standard valence orbital basis sets commonly used with these ECPs. Most of these basis sets do not include polarization functions, which may be required to accurately predict molecular properties. Users have at least two options by which they can add these functions.

First, users can edit the BASIS file and add polarization functions to any valence orbital basis already listed in the file. By redefining a basis in this way, users can automatically submit DGauss jobs from the UniChem without any additional editing of the DGauss job script. Second, users can add an additional set of valence orbital bases that include polarization functions to the BASIS file. For further information regarding how to add polarization functions to the valence orbital basis sets, see the “*Effective core potential*” section of the *DGauss 5.0 Reference* manual.

DGsol's SM5.42R solvation model

DGauss 5.0 will also introduce DGsol, an extra-cost add-on to the standard version of DGauss, which significantly enhances its capability to model solvent effects. DGsol uses the SM5.42R solvation model, developed by the research groups of Professors Truhlar and Cramer at the University of Minnesota, to accurately compute solvation free energies for a variety of solutes in various solvents. The SM5.42R solvation model is described in the following paper:

T. Zhu, J. Li, G.D. Hawkins, C.J. Cramer, and D.G. Truhlar, "Density Functional Solvation Model Based on CM2 Atomic Charges", *J. Chem. Phys.* **109**, 9117 (1998).

The SM5.42R model was designed to accurately predict solvation free energies using gas phase optimized geometries. It cannot be used to optimize a solute's geometry in the presence of a solvent.

As implemented in DGauss 5.0, the SM5.42R model is parametrized for the following elements, orbital bases, and exchange-correlation energy functionals:

H, C, N, O, F, P, S, Cl, Br and I

DZVP, 6-31G(d) and MIDI!(6D)

B88-PW91

UniChem 5.0 will not allow users to apply the SM5.42R model to any molecular systems or level of theory outside these limits.

In order to use the SM5.42R model with DGauss, the DGsol module must be purchased in addition to the standard version of DGauss 5.0.

Support for more basis sets

DGauss 5.0 includes a number of new orbital and charge fitting bases. Several of these are required to support some of the new functionality in this release.

In particular, the highly accurate charge fitting bases developed by Ahlrichs were important to include for DGauss' new ECP calculations. For elements H through Kr, these charge fitting bases were developed for use in all electron calculations with Ahlrichs' SVP and TZVP orbital bases. For elements Rb through At (not including the lanthanides), they were developed for use with the ECPs and the valence orbital bases (as modified by Ahlrichs) from the Stuttgart group. We have verified that these charge fitting bases can be reliably used with other orbital bases and ECPs.

In DGauss 5.0, Ahlrichs' charge fitting bases are labeled J-SVP and J-TZVP. J-SVP bases are available for elements H through At for the following types of calculations:

H - Kr	all-electron
Rb - Cd	semi-core ECP
In - Xe	full core ECP
Cs - Hg	semi-core ECP (lanthanides not included)
Tl - At	full core ECP

A charge fitting basis developed for use with a semi-core ECP may also be used with a full core ECP since the semi-core ECP calculations involve all of the electrons treated explicitly in the full core ECP calculation plus some inner shell electrons. The converse is not reasonable.

J-TZVP bases are available for elements H through F.

In their most accurate form, Ahlrichs charge fitting bases include up through *g* functions. Ahlrichs also suggests that their fitting bases without the *f* and/or *g* functions are sufficiently accurate for many purposes. In DGauss 5.0, the J-SVP and J-TZVP labels specifically refer to Ahlrichs fitting bases including only up through *d* functions, while the J-SVP(*f*) and J-TZVP(*f*) labels include up through *f* functions. When DGauss is able to handle *g* functions, the J-SVP(*fg*) and J-TZVP(*fg*) labels will include the complete set of functions published by Ahlrichs.

Geometry optimization

The DGauss geometry optimizer performs a series of micro-iterations to determine the optimal length of the step to take along the direction of the displacement vector. If it cannot find a point on this line at which the energy is lower, the optimizer will fail and DGauss will terminate. Users have reported problems with DGauss 4.1 geometry optimizations failing the micro iteration test at the end of line search. This test is disabled by default in DGauss 5.0. This will allow DGauss to proceed and, hopefully, to complete the optimization.

To enable the micro-iteration test in DGauss 5.0, add the following line to the DGauss input deck:

```
OPT_TYPE MICROTTEST
```

DGauss-DFT pseudopotential bug fix

DGauss-DFT pseudopotential calculations for some of the elements in the fifth row of the periodic table (e.g., W) do not agree between releases 4.1 and 5.0. This difference is due to a bug in the DGauss

4.1 atomic SCF code that has been fixed. If you encounter differences between releases 4.1 and 5.0 and you are not sure that they are related to this bug, please report them to Oxford Molecular support.

MNDO97 changes

UniChem 5.0 introduces support for the MNDO97 semiempirical from Professor Walter Thiel at the Max-Planck-Institut in Muelheim, Germany. MNDO97 offers many new features and enhancements over the previous version of Thiel's program (MNDO94), including:

More MNDO/d parameters

Elements supported for the first time with MNDO97 include: Hf, Ni, Pd, Ag, Ga, In and Tl.

New semiempirical OM1 & OM2 methods

MNDO97 introduces support for the OM1 and OM2 semiempirical methods. These recently developed methods provide greater accuracy than the established MNDO, AM1 and PM3 methods. They go beyond the MNDO model by employing explicit orthogonalization corrections. OM1 parameters are available for H, C, N, O, and F and OM2 parameters for H, C, N, and O.

Added support for the COSMO solvation model

MNDO97 will use the COSMO solvation method to model solvent effects on molecular properties. The van der Waals radii used by default in MNDO97 COSMO calculations are not the same as the values in MOPAC. The values used by default by MNDO97 are those published by Bondi (J. Phys. Chem. **68**, 441 (1964)). To use the MOPAC values in MNDO97 COSMO calculations, users should edit their MNDO97 input deck and change "ICOSMO=1" to "ICOSMO=3" and add "NVDW=-2". With these keywords, MNDO97 results should closely reproduce MOPAC calculations.

New semiempirical predictions of NMR chemical shifts

MNDO97 provides a special MNDO parametrization to compute H, C, N, and O NMR chemical shifts accurately at relatively low computational cost.

New methods to compute semiempirical electrostatic potentials

MNDO97 efficiently computes electrostatic potentials using special MNDO and AM1 parametrizations for C, H, N, and O.

New calculations of polarizabilities & hyperpolarizabilities

MNDO97 predicts static polarizabilities as well as first and second hyperpolarizabilities using a finite-field algorithm.

Expanded analytic derivatives

MNDO97 will provide analytic derivatives for all of the standard MNDO, AM1, PM3 and MNDO/d methods and for the following types of wavefunctions:

- 1st & 2nd derivatives for closed-shell RHF
- 1st & 2nd derivatives open-shell UHF
- 1st derivatives for open-shell half-electron ROHF
- 1st derivatives for small CI expansions

Improved transition state search algorithm

MNDO97 now optionally uses an eigenvector following algorithm to more effectively locate transition states.

Generalized support for batch jobs

UniChem 5.0 offers more general support for batch jobs. This includes extending support for NQS to include not only Cray UNICOS systems, but now also SGI IRIX and Fujitsu VPP platforms. In addition to supporting NQS on various platforms, UniChem 5.0 also supports the LSF workload management system by Platform Computing, Inc. SGI has adopted LSF as its preferred solution for workload management on its IRIX platforms.

Platform specific issues

There are a number of issues that are specific to a particular platform that are covered in this section.

Cray-specific issues

UniChem 5.0 will be the last release that is supported under UNICOS 9.x on any of the Cray platforms. The next release will only be supported under UNICOS 10.x.

The Cray T3E version of DGAUSS allocates a fixed amount of memory for the quadrature algorithm in the SCF, gradient and second derivative calculations. The default value is 5MW. You can enter the following keyword in a DGAUSS input deck to set the size of this fixed amount of memory:

```
FIXMEM <# of Words>
```

SGI-specific issues

UniChem 5.0 will be the last release that is supported under IRIX 5.3 or IRIX 6.2 on any of the SGI platforms. The next release will only be supported under IRIX 6.5 or higher.

IBM-specific issues

UniChem 5.0 will be the last release that is supported under AIX 4.2 on the IBM RS/6000 platforms. The next release will only be supported under AIX 4.3 or higher.

Under AIX, executable binaries can by default access no more than 32 Mwords (256 Mbytes). If users need to run jobs requiring more than 32 Mwords, they can modify the executable binary using the `dd` command.

For instance, users can use the following command to enable the DGauss binary so that it can access up to 128 Mwords (1 Gbyte) of memory.

```
% /usr/bin/echo '\0100\0\0\0' | dd of=dgauss bs=4 \
count=1 seek=19 conv=notrunc
```

Contacting Oxford Molecular

For support and further information about other products available from Oxford Molecular Ltd., please contact your local Oxford Molecular office. Telephone and e-mail information is listed below.

We welcome comments from our customers on the software and its documentation. Suggested changes are entered into our Quality Database and reviewed during the planning of upgrades to the programs and manuals.

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UK

e-mail: support@oxmol.co.uk

If you choose to fax us, you can use the form on the last page to submit your comments. If you phone or send e-mail, please be sure to include the following information:

- Your name and organization
- How to get in touch with you (fax, phone and/or email)

- The hardware and operating systems for the machines running the GUI and server applications
- A description of the problem
 - If with the GUI, provide the steps needed to reproduce the problem
 - If with one of the server applications, provide an input and output file that demonstrate the problem

By providing this information, you will greatly facilitate the support process and can expect a faster resolution to the problems you report.

UniChem 5.0 Software Problem Report

Fax to:
Oxford Molecular
+1-503-533-5099

Name: _____ e-mail: _____
Organization: _____ Phone: _____
_____ Fax: _____

Client (GUI) Information _____

Hardware type: _____

Operating system: _____

Number of CPUs: _____

hostname: _____

host id: _____

Server Information

Hardware type: _____

Operating system: _____

Number of CPUs _____

hostname: _____

host id: _____

The problem is with (circle as appropriate)

GUI MND097

DGauss CADPAC

Gaussian interface

Documentation

Licensing

Please describe the problem. If this is a bug in the GUI, include the steps to reproduce the problem. If this is a bug in a server application, please attach an input deck which reproduces the problem.

