

Semiempirical NDDO Guide

Schrödinger Suite 2012 Update 2

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Document Conventions

In addition to the use of italics for names of documents, the font conventions that are used in this document are summarized in the table below.

Font	Example	Use
Sans serif	Project Table	Names of GUI features, such as panels, menus, menu items, buttons, and labels
Monospace	<code>\$SCHRODINGER/maestro</code>	File names, directory names, commands, environment variables, command input and output
Italic	<i>filename</i>	Text that the user must replace with a value
Sans serif uppercase	CTRL+H	Keyboard keys

Links to other locations in the current document or to other PDF documents are colored like this: [Document Conventions](#).

In descriptions of command syntax, the following UNIX conventions are used: braces { } enclose a choice of required items, square brackets [] enclose optional items, and the bar symbol | separates items in a list from which one item must be chosen. Lines of command syntax that wrap should be interpreted as a single command.

File name, path, and environment variable syntax is generally given with the UNIX conventions. To obtain the Windows conventions, replace the forward slash / with the backslash \ in path or directory names, and replace the \$ at the beginning of an environment variable with a % at each end. For example, `$SCHRODINGER/maestro` becomes `%SCHRODINGER%\maestro`.

Keyboard references are given in the Windows convention by default, with Mac equivalents in parentheses, for example CTRL+H (⌘H). Where Mac equivalents are not given, COMMAND should be read in place of CTRL. The convention CTRL-H is not used.

In this document, to *type* text means to type the required text in the specified location, and to *enter* text means to type the required text, then press the ENTER key.

References to literature sources are given in square brackets, like this: [10].

The Semiempirical NDDO Module

Schrödinger Suite 2012 provides access to basic semiempirical NDDO capabilities through a library installed with mmshare. The semiempirical NDDO module is based on the public domain version of MOPAC 7.1 available at www.openmopac.net. The module may be used to calculate semiempirical heats of formation, optimized geometries, force constants, and a selection of properties as indicated below. The semiempirical NDDO module can be run from Maestro or from the command line.

Although this module is based on the public domain version of MOPAC 7.1, we have changed some of its behavior. The use of some keywords has been explicitly blocked because the feature does not actually work correctly. Any additional limitations that are discovered will be reported on the Known Issues page on our web site. The supported keywords are listed in this manual. Input files for commercial releases of MOPAC may not work with this module.

1 The Semiempirical NDDO Module Panel

Semiempirical NDDO jobs can be set up and run from Maestro by using the Semiempirical NDDO Module panel. To open this panel, choose Applications > Semiempirical in the main window.

The input structures can come from a file, from the Project Table, or from the Workspace. You can choose the structure source from the Use structures from option menu. If the input structure source is a file, enter the file name in the Input file text box, or click the Browse button and navigate to the input file. The structure file can be in Maestro, SD, or MOL2 format.

You can choose the method to use from the Method option menu. The available methods are RM1, AM1, PM3, MNDO and MNDO/d. If you want to optimize the geometry, select Optimize geometry; to run a single point calculation, deselect this option.

If you want to calculate properties, select the appropriate options in the Molecular and atomic properties section. These options correspond to keywords given in [Section 3.2](#): the SAR properties option corresponds to the **SUPER** keyword. Likewise, if you want to generate grids for the display of surfaces in Maestro, select the appropriate options in the Plot properties section. These options correspond to keywords given in [Section 3.3](#).

To specify other options, you can enter keywords in the Keywords text box. The keywords you can use are described in [Section 3](#).

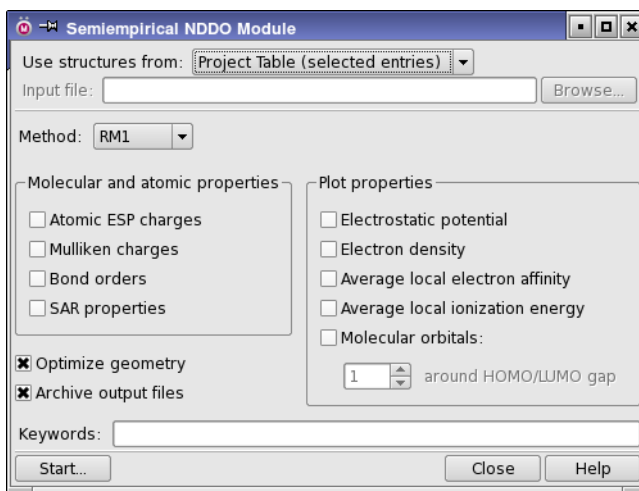


Figure 1. The Semiempirical NDDO Module panel.

In addition to a Maestro file, the output from the job includes output files (.out) for each structure. You can collect these files into a zip file by selecting Archive output files (the default).

To start the job, click Start, make settings in the Start dialog box, then click Start. You can choose not to incorporate the results into the Maestro project, or to append new entries to the project. The output properties include the semiempirical energy as an entry property, and the atomic partial charges as atom-level properties.

2 Running a Semiempirical NDDO Job from the Command Line

To run a semiempirical NDDO job from the command line, use the following syntax:

```
$SCHRODINGER/run semi_emp.py [options] [job-options] structure-file
```

The input structure file can contain multiple structures, which will all be processed in the job. The file can be in Maestro, SD, or MOL2 format. The command options are given in [Table 1](#).

As an example, if you have a multi-structure Maestro file called myfile.mae that contains three ligands whose geometries you would like to optimize with the PM3 method, and you also want to print out the final bond order matrix, and the sigma-pi bond order matrix, you would use this command:

```
$SCHRODINGER/run semi_emp.py -method pm3 -keywords "bonds pi" myfile.mae
```

Table 1. Options for the `semi_emp.py` command

Option	Description
<code>-v[ersion]</code>	Show the program version and exit.
<code>-h[elp]</code>	Show usage message and exit.
<code>-geopt</code>	Run a geometry optimization. This is the default.
<code>-nogeopt</code>	Don't run a geometry optimization.
<code>-method <i>method</i></code>	Specify the method to be used. Choices are AM1, MNDO, MNDO-d, PM3, RM1. Default: RM1.
<code>-keywords <i>options</i></code>	Specify a string that contains additional keywords.
<code>-j[obname] <i>jobname</i></code>	Specify a jobname for <code>.log</code> and <code>.out</code> files. Can only be used with single input files.
<code>-no_out</code>	Don't save the <code>.out</code> files, leaving only the output structures.
<code>-zip_out</code>	Create a <code>.zip</code> file with all <code>.out</code> files
<i>Job Control Options:</i>	
<code>-HOST <i>host</i></code>	Run job remotely on the indicated host entry.
<code>-WAIT</code>	Do not return control to the shell until the job finishes.
<code>-DEBUG</code>	Show details of Job Control operation.
<code>-SAVE</code>	Return zip archive of job directory at job completion.
<code>-NOJOBID</code>	Run the job directly, without Job Control.

This job produces files named `myfile_1.out`, `myfile_2.out`, and `myfile_3.out`, which contain the output, together with an output structure file called `myfile_out.mae`, which contains the final geometries, the method used, the semi-empirical energy, and the atomic charges (which are calculated by default). This structure file may be manually imported into Maestro. Atoms may be labeled with their partial charges by selecting Atomic Charge from the list of available labels in the Atom Labels panel. These charges may also be used in docking calculations with Glide. In addition, a log file is produced, which includes information about the job options used.

3 Supported Keywords

The keywords that are supported for use with the `-keywords` command option are given in this section. Keywords are not case-sensitive. The keywords listed below are the only keywords that are supported. Any other keywords that exist in the original code might work, but you use them at your own risk, as they might not give the results you expect.

3.1 General Keywords

RM1, AM1, PM3, MNDO, MNDOD

These keywords select the method used to calculate the semi-empirical heat of formation. RM1 is the default, and is recommended. It is a reparameterization for some of the elements covered by AM1. The module automatically uses AM1 parameters for elements covered by AM1 that are not covered by RM1. The elements covered by the methods (as they were implemented in the source MOPAC 7.1 code) are given in [Table 2](#).

Table 2. List of elements covered by semiempirical methods.

Method	Elements covered
RM1	H, C, N, O, F, P, S, Cl, Br, I
AM1	H, B, C, N, O, F, Al, Si, P, S, Cl, Zn, Ge, As, Se, Br, Sb, Te, I, La, Ce, Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu, Hg
PM3	H, Li, Be, C, N, O, F, Na, Mg, Al, Si, P, S, Cl, Zn, Ga, Ge, As, Se, Br, Cd, In, Sn, Te, I, Hg, Tl, Pb, Bi
MNDO	H, Li, Be, B, C, N, O, F, Na, Al, Si, P, S, Cl, K, Zn, Ge, Br, Sn, I, Hg, Pb
MNDOD	Na, Mg, Al, Si, P, S, Cl, Zn, Br, Cd, I, Hg

The literature citations for the sources of parameters for these elements is printed by the program when the parameters are used, so please consult the output file for this information.

CHARGE=*n*

For charged molecules, CHARGE must be set to the overall molecular charge.

DOUBLET

The default spin multiplicity is singlet, but spin doublets may be modeled by including the DOUBLET keyword. The doublet wave function is spin-restricted.

MMOK, NOMM

One of these two keywords must be set whenever a calculation is performed on a molecule containing a peptide bond. For the convenience of batch processing large numbers of structures, MMOK is set by default, and is ignored for molecules that do not contain a peptide bond. With MMOK set, a correction factor (derived from molecular mechanics) is applied to the rotational barrier around each peptide bond. This is to compensate for the fact that all of the NDDO methods in the module underestimate this rotational barrier. To prevent this correction from being applied, set NOMM.

FORCE, THERMO(*nnn,mmm,lll*)

The **FORCE** keyword requests calculation of the vibrational frequencies for the input molecule. The **THERMO** keyword, without any of the optional arguments in parentheses, requests calculation of the thermodynamic properties such as internal energy, enthalpy, and entropy, plus the vibrational, rotational, translational partition functions. By default, the thermodynamic functions are calculated at 298K and at 10K increments from 200K to 400K. A different starting temperature, final temperature, and increment can be specified using the (*nnn,mmm,lll*) options. For example, use **THERMO (273 , 293 , 20)** to print thermodynamic properties at 298K (which is always done) and at 273K and 293K.

3.2 Molecular Properties

MULLIK

By default, atomic charges are calculated by summing up the density matrix elements for each atom's basis functions. To take into account the overlap of basis functions between atoms, use this keyword to perform a Mulliken analysis.

ESP

Print the atomic charges that best reproduce the molecular electrostatic potential.

BONDS

Print the bond orders for all pairs of atoms.

PI

Print bond orders broken down into sigma and pi components.

SUPER

Several atomic properties which have proven useful in developing structure-activity relationships can be calculated with the keyword **SUPER**. These include the HOMO and LUMO energies, the molecular hardness and electronegativity, which are added as structure-level properties. For each atom, the electrophilic and nucleophilic frontier electron density, the electrophilic, nucleophilic, and radical superdelocalizability, and the atom self-polarizability are calculated as atom-level properties; these are summed to give a total value, added as a structure-level property. The atomic properties are calculated according to the equations given in Ref 1. For applications, see the review article, Ref 2, and citations therein.

VECTORS

Print the coefficients, energies, and symmetries for the molecular orbitals near the HOMO and LUMO.

3.3 Plot Keywords

These keywords are used to generate a 3-dimensional grid of electronic properties that can be used in Maestro to display surfaces. For ESP, ALIE, and ALEA surfaces, an analysis of the values of the property on the isodensity surface is included in the output and recorded as Maestro properties in the output structure file. See [Appendix 5.3.7.7](#) of the *Jaguar User Manual* for a fuller description of the analysis (as applied to ESP surfaces).

PLOTDEN

Evaluate the electron density on a grid and write the data to the file *jobname_density.vis*.

PLOTESP

Evaluate the molecular electrostatic potential on a grid and write the data to the file *jobname_potential.vis*. Since the ESP is usually visualized as a color-coded mapping onto an isosurface of the electron density, the electron density is also evaluated on the same grid, as if PLOTDEN had been set.

PLOTALIE

Evaluate the average local ionization energy on a grid and write the data to the file *jobname_alie.vis*. Since the ALIE is usually visualized as a color-coded mapping onto an isosurface of the electron density, the electron density is also evaluated on the same grid, as if PLOTDEN had been set.

PLOTALEA

Evaluate the average local electron affinity on a grid and write the data to the file *jobname_alea.vis*. Since the ALEA is usually visualized as a color-coded mapping onto an isosurface of the electron density, the electron density is also evaluated on the same grid, as if PLOTDEN had been set.

PLOTMO[=*N*]

If PLOTMO is set by itself, then the HOMO and LUMO are evaluated on a grid and written to files called *jobname_mo_n.vis*, where *n* is the molecular orbital index number corresponding to the HOMO or LUMO. If PLOTMO=*N* is used, where *N* is a positive integer, then the *N* highest occupied orbitals and the *N* lowest unoccupied orbitals are tabulated on the grid. If you want all molecular orbitals to be tabulated, set *N* to a large number such as 999.

GRIDEXT=*N.M*

By default, the grid on which the above properties are evaluated extends 3.5 angstroms beyond the nuclei. This should be adequate to avoid truncating displayed isosurfaces as long as the isovalues are not too small. However, if you find that a displayed isosurface has been truncated,

you can specify a larger grid extension distance by setting GRIDEXT to a value larger than 3.5. Note that increasing GRIDEXT increases the calculation time.

GRIDRES=*N.M*

The default grid resolution is 5.0 points per angstrom along each side of the grid box. This yields reasonably smooth displayed surfaces while keeping calculation times short. If a higher quality surface is desired, set GRIDRES to a number larger than 5.0. Note that increasing GRIDRES increases the calculation time.

4 Limitations

The following limitations should be noted:

- Spin states higher than doublet are not available.
- ESP and SUPER calculations cannot be run with the MNDO/d method.
- UHF (unsupported keyword) cannot be used for ESP, MULLIKEN, or SUPER calculations.

5 Troubleshooting

If you use a Maestro structure file as input, and you experience a problem running the module and want to see the input file that is created from the .mae file, include the -SAVE option on the command line. This option creates a .zip file of the job scratch directory, including the input file, which has the name *jobname*.mop. You might be able to edit this file to work around the problem, and then submit the job using the .mop file as input.

6 Citing the Semiempirical NDDO Module

The use of this module should be acknowledged in publications as:

Schrödinger Suite 2012 Semiempirical NDDO Module, Schrödinger LLC, New York, NY, 2012.

References

1. Gancia, E.; Montana, J. G.; Manallack, D. T. *J. Mol. Graph. Model.* **2001**, *19*, 349.
2. Karelson, M.; Lobanov, V. S.; Katritzky, A. R. *Chem. Rev.* **1996**, *96*, 1027.

Getting Help

Information about Schrödinger software is available in two main places:

- The `docs` folder (directory) of your software installation, which contains HTML and PDF documentation. Index pages are available in this folder.
- The Schrödinger web site, <http://www.schrodinger.com/>, particularly the Support Center, <http://www.schrodinger.com/supportcenter>, and the Knowledge Base, <http://www.schrodinger.com/kb>.

Finding Information in Maestro

Maestro provides access to nearly all the information available on Schrödinger software.

To get information:

- Pause the pointer over a GUI feature (button, menu item, menu, ...). In the main window, information is displayed in the Auto-Help text box, which is located at the foot of the main window, or in a tooltip. In other panels, information is displayed in a tooltip.

If the tooltip does not appear within a second, check that **Show tooltips** is selected under **General → Appearance** in the Preferences panel, which you can open with **CTRL+, (⌘,)**. Not all features have tooltips.

- Click the **Help** button in a panel or press **F1** for information about a panel or the tab that is displayed in a panel. The help topic is displayed in your browser.
- Choose **Help → Online Help** or press **CTRL+H (⌘H)** to open the default help topic in your browser.
- When help is displayed in your browser, use the navigation links or search the help in the side bar.
- Choose **Help → Manuals Index**, to open a PDF file that has links to all the PDF documents. Click a link to open the document.
- Choose **Help → Search Manuals** to search the manuals. The search tab in Adobe Reader opens, and you can search across all the PDF documents. You must have Adobe Reader installed to use this feature.

For information on:

- Problems and solutions: choose Help → Knowledge Base or Help → Known Issues → *product*.
- Software updates: choose Maestro → Check for Updates.
- New software features: choose Help → New Features.
- Scripts available for download: choose Scripts → Update.
- Python scripting: choose Help → Python Module Overview.
- Utility programs: choose Help → About Utilities.
- Keyboard shortcuts: choose Help → Keyboard Shortcuts.
- Installation and licensing: see the *Installation Guide*.
- Running and managing jobs: see the *Job Control Guide*.
- Using Maestro: see the *Maestro User Manual*.
- Maestro commands: see the *Maestro Command Reference Manual*.

Contacting Technical Support

If you have questions that are not answered from any of the above sources, contact Schrödinger using the information below.

E-mail: help@schrodinger.com

USPS: Schrödinger, 101 SW Main Street, Suite 1300, Portland, OR 97204

Phone: (503) 299-1150

Fax: (503) 299-4532

WWW: <http://www.schrodinger.com>

FTP: <ftp://ftp.schrodinger.com>

Generally, e-mail correspondence is best because you can send machine output, if necessary. When sending e-mail messages, please include the following information:

- All relevant user input and machine output
- Semiempirical NDDO module purchaser (company, research institution, or individual)
- Primary Semiempirical NDDO module user
- Installation, licensing, and machine information as described below.

Gathering Information for Technical Support

This section describes how to gather the required machine, licensing, and installation information, and any other job-related or failure-related information, to send to technical support.

For general enquiries or problems:

1. Open the Diagnostics panel.
 - **Maestro:** Help → Diagnostics
 - **Windows:** Start → All Programs → Schrodinger-2012 → Diagnostics
 - **Mac:** Applications → Schrodinger2012 → Diagnostics
 - **Command line:** \$SCHRODINGER/diagnostics
2. When the diagnostics have run, click Technical Support.

A dialog box opens, with instructions. You can highlight and copy the name of the file.
3. Attach the file specified in the dialog box to your e-mail message.

If your job failed:

1. Open the Monitor panel in Maestro.

Use Applications → Monitor Jobs or Tasks → Monitor Jobs.
2. Select the failed job in the table, and click Postmortem.

The Postmortem panel opens.
3. If your data is not sensitive and you can send it, select Include structures and deselect Automatically obfuscate path names.
4. Click Create.

An archive file is created in your working directory, and an information dialog box with the name of the file opens. You can highlight and copy the name of the file.
5. Attach the file specified in the dialog box to your e-mail message.
6. Copy and paste any log messages from the window used to start Maestro (or the job) into the email message, or attach them as a file.
 - **Windows:** Right-click in the window and choose Select All, then press ENTER to copy the text.
 - **Mac:** Start the Console application (Applications → Utilities), filter on the application that you used to start the job (Maestro, BioLuminate, Elements), copy the text.

If Maestro failed:

1. Open the Diagnostics panel.

- **Windows:** Start → All Programs → Schrodinger-2012 → Diagnostics
- **Mac:** Applications → Schrodinger2012 → Diagnostics
- **Linux/command line:** \$SCHRODINGER/diagnostics

2. When the diagnostics have run, click Technical Support.

A dialog box opens, with instructions. You can highlight and copy the name of the file.

3. Attach the file specified in the dialog box to your e-mail message.

4. Attach the file `maestro_error.txt` to your e-mail message.

This file should be in the following location:

- **Windows:** %LOCALAPPDATA%\Schrodinger\appcrash
(Choose Start → Run and paste this location into the Open text box.)
- **Mac:** Documents/Schrodinger
- **Linux:** Maestro's working directory specified in the dialog box (the location is given in the terminal window).

5. On Windows, also attach the file `maestro.EXE.dmp`, which is in the same location as `maestro_error.txt`.

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New York, NY 10036

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