
Abstract

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TorAD: Torsional Angle Driver System for HyperChem/Excel is a package of several Excel spreadsheets and macro programs to be used with HyperChem to obtain and plot information, such as total energy, for the conformations that result from a 360-degree rotation about a torsional-angle system in a molecule. The TorAD system also includes several HyperChem scripts to facilitate its use.

TorAD was developed for use in the undergraduate organic chemistry laboratory. The results obtained with TorAD could be obtained manually with HyperChem, but it would take considerable time and would not be instructive to the students. Use of the TorAD system allows students to spend their time on the more important aspect of conformational analysis—interpretation of results.

The Excel spreadsheet/macro programs in TorAD include:

- TOR_XL_A and TOR_XL obtain and plot the total energy at five-degree torsional-angle intervals. The calculation method, the torsional-angle restraint, and the structure to be used at each angle can be set by the user. The advanced version, TOR_XL_A, which requires HyperChem 4.5 or later, also allows each torsional-angle structure to be saved for later recall as individual structures or, using a HyperChem script, in a movie format. It also provides a rapid scan of the 360-degree rotation where only single-point calculations, rather than geometry optimizations, are performed. The TOR_XL system will perform routine tasks in a manner suitable for most instructional settings.
- TOR_COMP performs molecular mechanics optimizations at five-degree intervals and obtains and plots four energy parameters: total, torsional, nonbonded, and bond (bend plus stretch) energy as a function of torsional angle. The calculation method and the restraint can be specified.
- TORDIPOL produces a plot of the total energy and the calculated dipole moment at five-degree steps of the torsional angle. The default calculation is the semi-empirical AM1 method, but other methods can be used. The calculation method and the restraint can be specified.
- TOR2_180 and TOR2_360 rotate two torsional angles to provide a 3D-plot of the resulting total energy surface. TOR2_180 performs a 0 to 180 degree rotation, in 10-degree steps, on each of the two torsional angle systems (tor1 and tor2) selected. TOR2_360 will do a –180 to +180 (360 total) degree rotation of the two torsional angles in 20-degree steps. Both TOR2_180 and TOR2_360 provide an X, Y, Z plot (X = angle 1, Y = angle 2, Z = energy) and a topo plot (X = angle 1, Y = angle 2, Z = topo lines and color coding). The molecular mechanics method and the restraint can be specified.

Instructor Notes

The TorAD system requires some familiarity with HyperChem and Excel. An effort has been made to make instructions as complete as possible to allow those

students with little or no experience with HyperChem or Excel to complete the exercises. Beginning students should work the Student Exercises in the order they are presented and refer to the User Directions as needed.

Specific information about the operation of each macro in the TorAD system is included in the BKG.PDF file on the program disk. Adobe Acrobat Reader is required to view the file. You can download a free copy of Acrobat Reader from Adobe at <http://www.adobe.com>.

TorAD and Network Installation

If you wish to use the TorAD system on a networked computer, both the HyperChem and Excel programs can be normal networked applications. The TorAD Excel spreadsheets and HyperChem script files are designed to be stored in the c:\hc_excel\ directory. In addition, some of the Excel macros write to the c:\hc_excel\data directory. If you wish to use all of the capabilities of the TorAD system in an unmodified form, your local computer must have the directory c:\hc_excel\data that is *not* read-only. You must be able to write in that directory.

If your computers cannot read and write to c:\hc_excel and c:\hc_excel\data, the Excel spreadsheets (macro files) can easily be modified to specify the network drive of your choice. In general in each TorAD Excel macro (.XLM) file, replace c:\hc_excel and c:\hc_excel\data with the network drive you wish to use. For example, if you have an E: drive that is not read-only, change the directories to **E:\hc_excel** and **E:\hc_excel\data**. You can use the **Replace...** option from the Edit menu to do this in a single step.

The Excel files and the HyperChem script (.scr) files should all be stored in the new drive directory location. If you wish to use the HyperChem script (.scr) files you will also have to modify the directory paths in these files. Use the same new drive and directory for all revised files.

Below is listing of the modifications that need to be made if you are using a networked computer that is unable to read and write to a local hard drive c:\hc_excel.

Excel Macro (.xlm) Files

These files are written in Excel 4.0 Macro language and can be edited using Excel 4.0 or later. The exception to this is the set of macro commands that are in the TorAD.XLS file, which is written in Visual BASIC. The files are saved in the read-only setting; so after the directory modifications are made the revised files should be saved using the **Save As...** item in the File menu to the new directory and the read-only setting applied. Use the same new drive directory for all revised files.

TOR_XL.XLM

If this TorAD component is used in the **initial** structure setting, the original HyperChem structure is stored as c:\hc_excel\tor_xl.hin. Change every **c:\hc_excel** to the directory you wish to use (such as **E:\hc_excel**). Select **Save As...** from the File menu to save **TOR_XL.XLM** in your new directory.

TOR_XL_A.XLM

The macro commands are on the two worksheets of TOR_XL_A.XLM named TOR_XL and MACROS. To gain easy access to these two worksheets, make the worksheet tabs visible. From the Tools menu select **Options...**, then click the **View** tab and click the box in front of **Sheet tabs**.

In both the TOR_XL and the Macros worksheets, change every **c:\hc_excel** to the directory of choice (such as **E:\hc_excel**). Turn off the **Sheet tabs** and use **Save As...** from the File menu to save **TOR_XL_A.XLM** in your new directory.

TOR_COMP.XLM

All of the commands that need to be changed are in the TOR_COMP.XLM main worksheet. Change every **c:\hc_excel** to the directory you wish to use (such as **E:\hc_excel**). Use **Save As...** from the File menu to save **TOR_COMP.XLM** in your new directory.

TORDIPOL.XLM

All of the commands that need to be changed are in the TORDIPOL.XLM main worksheet. Change every **c:\hc_excel** to the directory you wish to use (such as **E:\hc_excel**). Use **Save As...** from the File menu to save **TORDIPOL.XLM** in your new directory.

TOR2_180.XLM and TOR2_360.XLM

All of the commands that need to be changed are on the TOR2_180.XLM and TOR2_360.XLM main worksheets. Change every **c:\hc_excel** to the directory you wish to use (such as **E:\hc_excel**). Use **Save As...** from the File menu to save the files under their old filenames, but in your new directory.

TORAD.XLS

The macro within this menu spreadsheet is written in Visual BASIC.

The macro can be edited directly from Excel 5.0. Make the sheet tabs visible (see instructions above) and go to the **Module 1** worksheet. Edit this sheet to replace **c:\hc_excel** with the destination of your choice (such as **E:\hc_excel**). Return to the **Menu** sheet, turn off the sheet tab display, and use **Save As...** from the File menu to save the file as **TorAD.XLS** in the new directory.

If you have an Excel version later than 5.0 (such as Excel 97), click the right mouse button on any macro button, such as the **Tor_xl** button. All of the macro commands can be edited from any button. Select **Assign Macro** from the pop-up menu and then click the **Edit** button in the dialog. Change every **c:\hc_excel** to the directory you wish to use (such as **E:\hc_excel**). After making these changes go back to the Excel sheet by selecting **Close and Return to Microsoft Excel** from the File menu. Use **Save As...** from the File menu to save the edited spreadsheet as **TorAD.XLS** in the new directory.

HyperChem Script (.scr) Files

These files were written in HyperChem Script language. They can be edited using any text editor, such as Windows Notepad or the HyperChem Script Editor (a part of ChemPlus: Modular Extensions to HyperChem, not included with standard HyperChem). For each HyperChem script file included in the TorAD disk, change every **c:\hc_excel** to the network drive and directory you wish to use. For example, change to **E:\hc_excel**. Most of these script files will only require changing the lines that specify the file path. Save the modified script files as unformatted text files (this is the default file format for Script Editor and Notepad) under the old filename but to the new directory. All script files should be in the same directory. The network drive should also have a data directory (an empty folder named data), such as **E:\hc_excel\data**.

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HyperChem is a product of HyperCube, Inc.

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