

ECCE 6.x RELEASE NOTES

Version 6.0—April 29, 2009
Version 5.1—March 10, 2009
Version 5.0.1—January 19, 2009
Version 5.0—December 12, 2008

The intent of this page is to provide information specific to the 6.x versions of ECCE. Version 6.0 extends ECCE into the field of reaction kinetics, specifically the prediction of rate constants and equilibrium constants, often including error estimates for rate constants. Since version 6.0 is so closely tied to the recent 5.x versions, the release notes for these versions are also included here. Version 5.0 completes the migration of all ECCE applications to the cross platform open source user interface toolkit, wxWidgets. The user interface for the Calculation Viewer has been completely redesigned and integrated with the Builder to create a single combined visualization capability. Version 5.0.1 primarily adds a small number of new Builder/Viewer features. Version 5.1 uses virtual operating system technology to support ECCE running on Microsoft Windows based PCs along with adding a small number of other features. Version 6.0 notes, the most recent, have titles highlighted in **green text**.

RELEASE NOTES FOR PREVIOUS VERSIONS

[Version 4.x Release Notes – December 27, 2007](#)

[Version 3.2.x Release Notes – April 5, 2006](#)

WHAT'S NEW

Reaction Rate Constant Prediction

(6.0) The NWChem DirDyVTST module has been integrated with the POLYRATE code (see <http://comp.chem.umn.edu/polyrate>) into the ECCE user environment yielding a powerful capability to predict gas phase chemical reaction rate constants. This is done through two new ECCE applications, the NWChem DirDyVTST (Direct Dynamics Variational Transition State Theory) Editor and the POLYRATE Editor, as well as extensions to several other ECCE applications including the Organizer, Builder, Basis Set Tool, and Viewer. This work was sponsored by the U. S. Department of Defense, Air Force Office of Scientific Research under a Small Business Technology Transfer effort (contract number: FA9550-07-C-0008) led by Spectral Sciences, Inc., Burlington, MA. Support from the ECCE team as well as documentation for this new capability is limited to the work done during the contract period. These release notes and a new online movie that demonstrates a simple reaction rate calculation make up the full documentation that is available for the initial release.

Organizer

Figure 1 is a screen capture of the ECCE Organizer application showing a reaction study named “ethaneBondRotation”. The reaction rate prediction capability uses the same workflow paradigm as molecular dynamics for chaining together the output of discrete calculations or tasks as the input to subsequent tasks. The Organizer “File” menu now contains an item to create a “New Reaction Study...” as well as the previous “New MD Study...” menu item. Reaction studies contain DirDyVTST and POLYRATE sub-tasks along with the different electronic structure calculations on the transition state, reactant, and product components of the chemical reaction. In Figure 1, the DirDyVTST calculation of the reaction has been selected in the left-hand pane, which displays the ECCE applications available for working on that sub-task in the right-hand pane. Like MD studies, by selecting the reaction study parent task in the left-hand pane, a workflow view showing the flow of data between all sub-tasks is displayed in the right-hand pane.

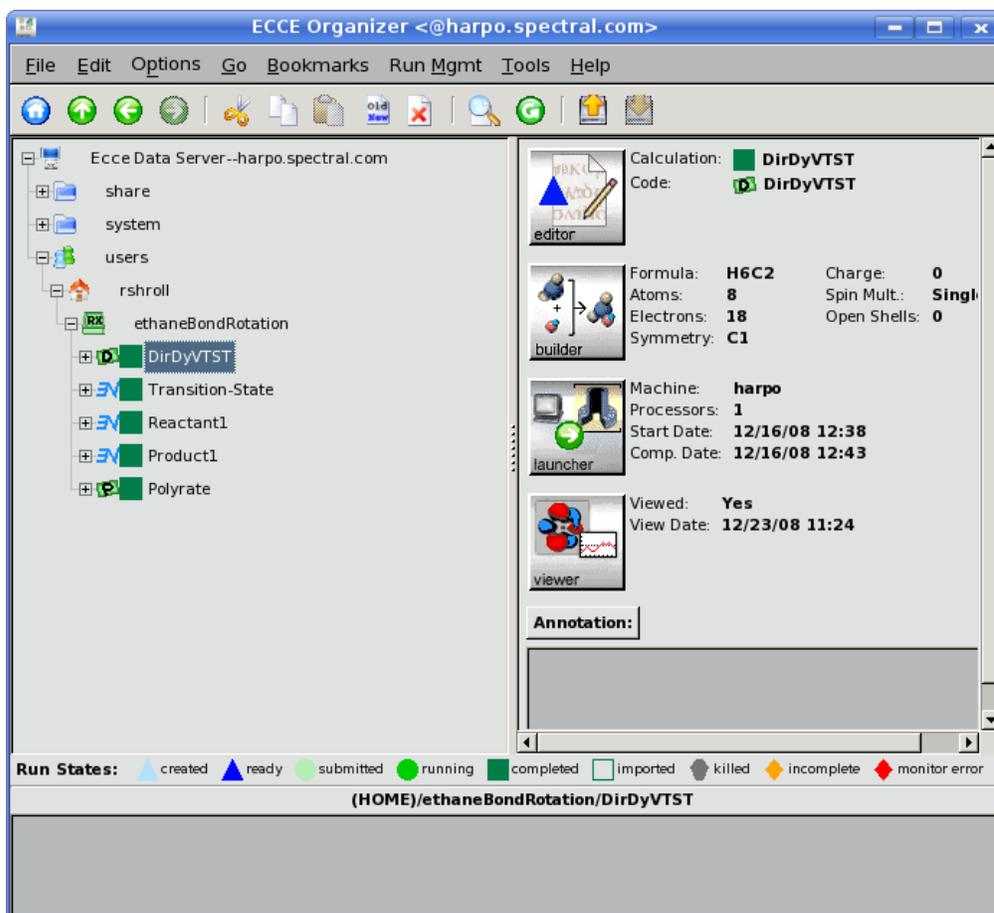


Figure 1. ECCE Organizer in the context of a reaction study

DirDyVTST Editor

The DirDyVTST Editor controls NWChem’s DirDyVTST module, which calculates molecular properties over the reaction path necessary for the transition state calculations.

This routine provides the key to interfacing the NWChem quantum chemistry calculations with the POLYRATE transition state theory rate constant predictions and is thus central to the ECCE reaction rate constant prediction capability. The enhancements made allow the user access to a broad range of quantum chemistry theory types for this purpose. Figure 2 shows the main window of the DirDyVTST Editor. The editor helps the user organize and run up to five separate electronic structure calculations for the reactants, products, and the transition state. Note that thumbnail visualizations of each of the reaction component chemical systems are displayed on the main DirDyVTST Editor window. This allows at-a-glance feedback on the chemical systems that are part of the computation without bringing up the Builder application on each component. The example shown is for internal rotation about the C-C bond of ethane. This is a unimolecular process and thus “Reactant 2” and “Product 2” are unused.

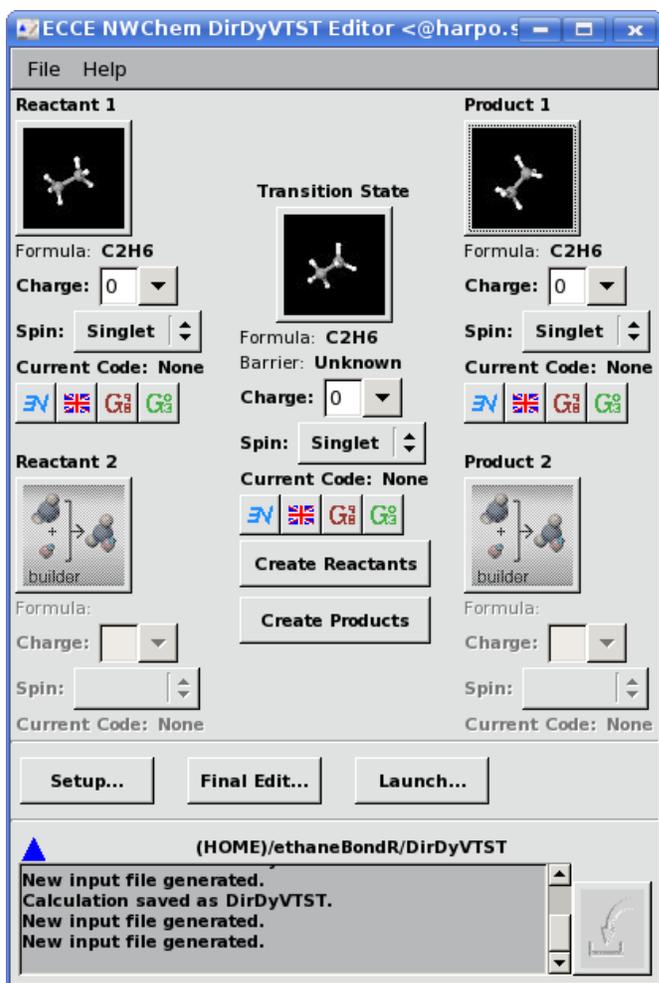


Figure 2. The DirDyVTST Editor is used to initialize quantum chemistry calculations for each molecule and the DirDyVTST routine. Thumbnail images show the reactants, products, and transition state for an example reaction

The organization of the DirDyVTST Editor represents the reaction as proceeding from reactants to products from left to right. On the left, there are two areas for each of the two reactants, where Reactant 2 is optional depending on the reaction being studied. Each area has a title like "Reactant 1" and buttons for launching the ECCE Builder and the electronic structure calculation editors. The Builder is launched by clicking on the thumbnail image, which prior to any input is the generic Builder icon shown under Reactant 2 and Product 2 in Figure 2. The user inputs and saves a molecular structure and its image is displayed as a thumbnail with the chemical formula underneath. The system charge and spin multiplicity are also selected through this interface. This is done for the reaction as a whole and not separately for each molecule, since there are restrictions that must be applied over the entire reaction path. One such restriction is charge conservation, where the total charge of the reactants must be the same as the total charge of the products. Displayed in this single interface, the user can see the charge and spin multiplicity of the entire reaction at once. ECCE will enforce these restrictions, so for instance, if the total system charge for a bimolecular reaction is -1 and the user changes the charge on Reactant 1 from -1 to 0 then ECCE will update the charge on Reactant 2 from 0 to -1. ECCE will thus maintain a viable calculation. When the change is performed, the display is updated and the user is shown that their change has altered the calculation for Reactant 2. Underneath the spin selection, there are four buttons for launching calculation editors for the four supported electronic structure codes. These editors provide similarly structured interfaces to the different codes simplifying their use. The transition state area has two additional buttons for creating the reactants and products. When the DirDyVTST Editor is first launched, the user is guided towards inputting the transition state (Builder access will be disabled for the reactants and products until a transition state is defined). Once this is done, the reactants and products are generated from the transition state. For instance, atoms composing one of the reactants are selected and Create Reactants is chosen. ECCE then generates one reactant from the selected atoms and one reactant from the remaining (unselected) atoms. ECCE fills in the Reactant entry fields and sets up default values for the system charge and spin.

Through the DirDyVTST Editor Setup window (available from the main window), the full range of registered NWChem theory types for the DirDyVTST calculation is supported for both a "General" and "Single Point" calculation. Figure 3 shows the DirDyVTST Editor Setup window. The single point calculation ability is critical to accurate rate constant prediction because a much more accurate and computationally demanding theory may be used to correct the faster theories necessary to follow the reaction path.

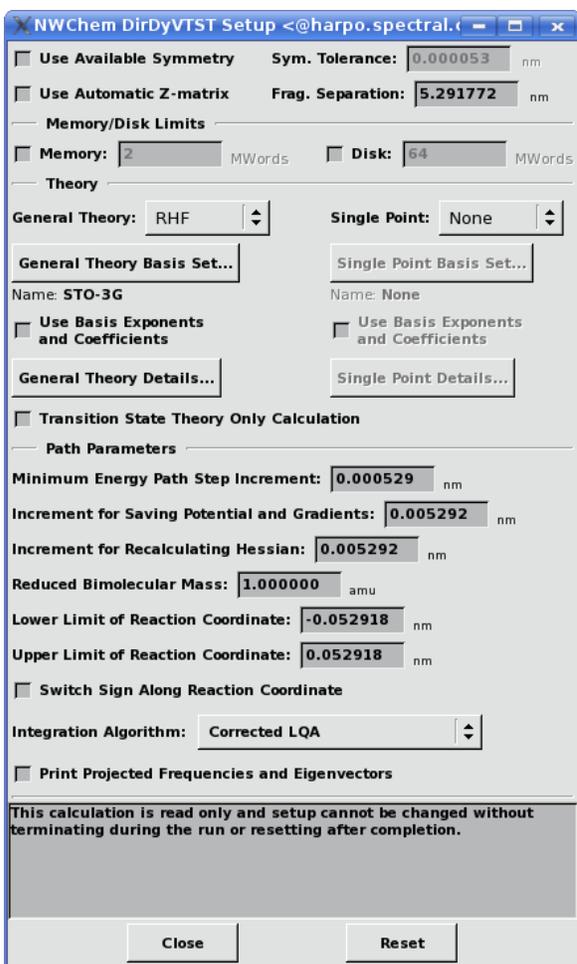


Figure 3. The DirDyVTST Editor Setup window is used to configure the DirDyVTST calculation

The DirDyVTST calculation follows the reaction just before and just after the transition state. It performs many quantum chemistry calculations and is computationally the most expensive step in the entire rate constant calculation process. It does this to locate the free energy maximum, which may be offset from the energy maximum located at the transition state. All of the controls for this calculation are present in the DirDyVTST interface. Upon its initial launch, the input fields are all filled with default values applicable to most cases. Alterations to the defaults may be made to better represent specific systems. This is primarily done through the Theory and Path Parameters sections. In the Theory section the general and single point theories are selected. The general theory is the theory used to perform the path calculation and single point is an optional higher level theory that may be used to correct the lower level theory used by the general calculation. Both calculations require selecting electronic structure methods, basis sets, and basic computational parameters such as self consistent field (SCF) convergence criteria. At the bottom of the Theory section is a toggle labeled “Transition State Theory Only Calculation”. This is the most basic type of calculation and does not require location of the free energy maximum via calculation over the reaction path near the transition state. If this is selected, the Path Parameters section is grayed out.

Otherwise, the path calculation is performed. The Path Parameters section allows the user to change the path calculation characteristics such as number of points calculated, the distance between the points, and the integration algorithm used.

The “General Theory Details” and “Single Point Details” dialogs available from the DirDyVTST Editor Setup window allow the user to specify options such as SCF convergence criteria and theory specific algorithms to use for the general and single point calculations, respectively. Figure 4 shows a Theory Details dialog for the RDFT (restricted density functional theory) level of theory. A small number of fields on the electronic structure NWChem Theory Details dialog are excluded when the dialog is invoked in the context of a DirDyVTST calculation. The symmetry and memory limit fields are among these as the DirDyVTST Setup window includes these fields instead of the lower level NWChem Theory Details dialog.

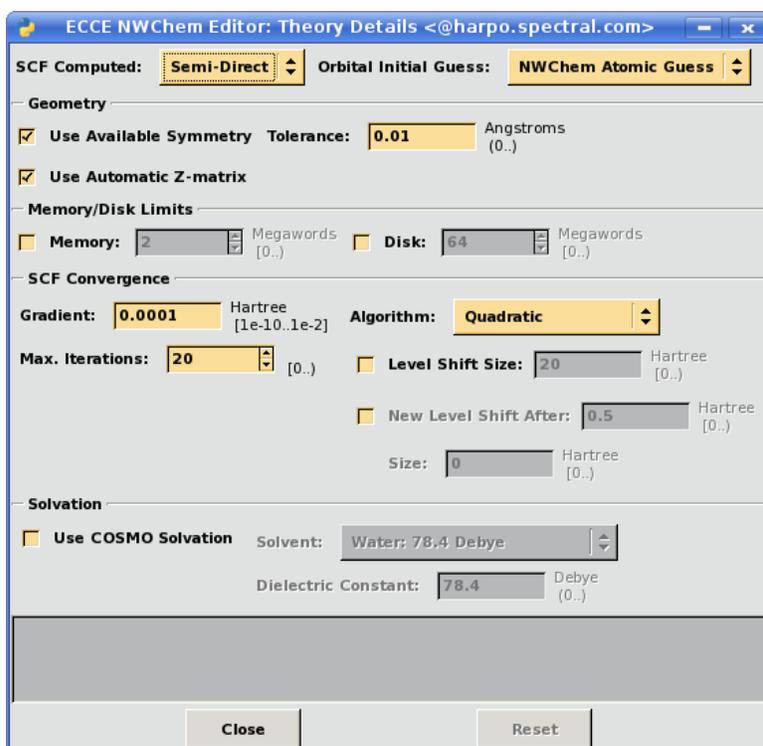


Figure 4. The DirDyVTST Editor Theory Details dialog is where the chosen quantum chemistry method is configured

Electronic structure geometry optimizations can be run on reaction components (transition state, reactants, products) prior to invoking the DirDyVTST calculation using NWChem, Gaussian 03, Gaussian 98, or GAMESS-UK. This option to run calculations on the reaction components is accessed via icons representing each code, shown below each of the chemical system thumbnail visualizations on the DirDyVTST Editor main window.

The DirDyVTST Editor enforces consistency between the transition state chemical system number of electrons, overall charge, spin multiplicity, and level of theory. Based

on the number of electrons and charge set by the user, the spin multiplicity and theory choices are restricted to maintain the integrity of the overall calculation. This consistency encompasses the reaction component calculations and the follow-on POLYRATE calculation, described next. This kind of guaranteed consistency is a primary reason ECCE is so valuable in setting up these complex, detail oriented, and multi-step calculations.

POLYRATE Editor

Figure 5 shows two screen captures of the POLYRATE Editor used to create the input file for the POLYRATE code.

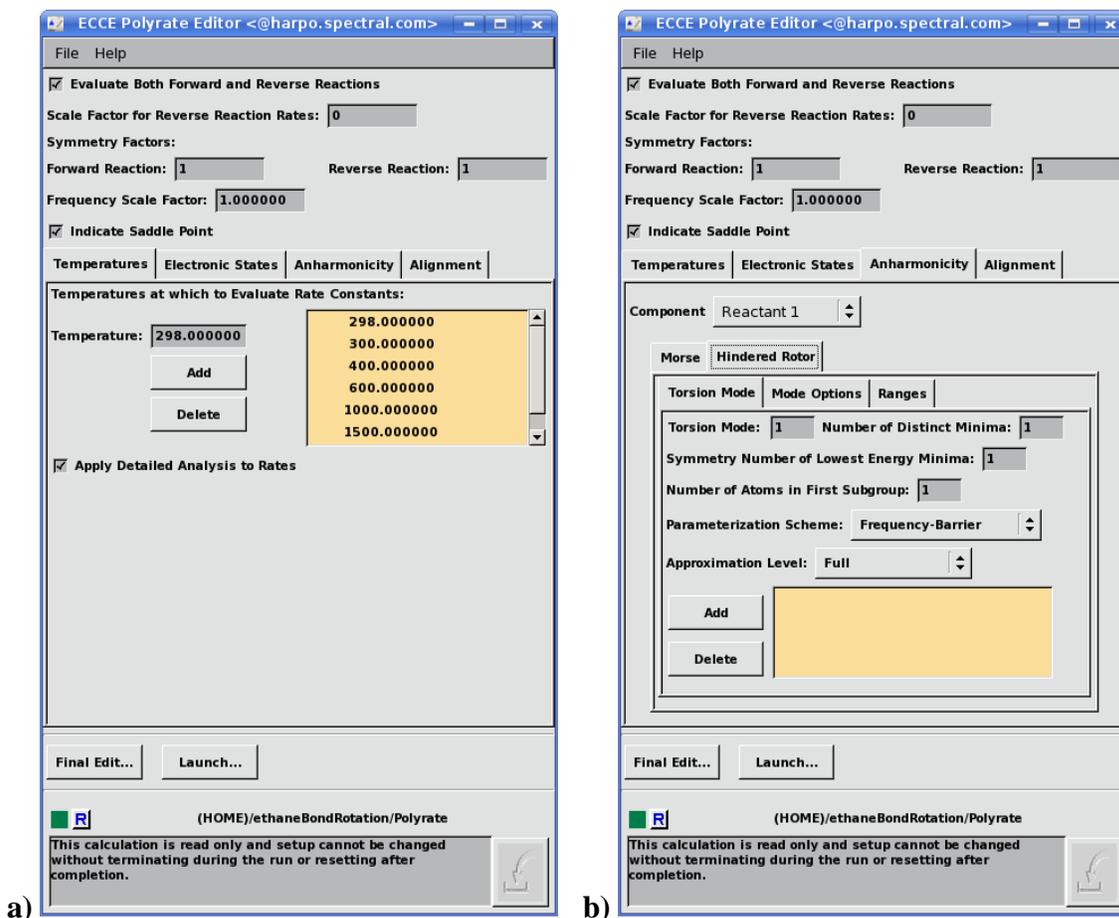


Figure 1. The POLYRATE Editor is used to enter parameters for the transition state theory rate constant calculation. Four tabs are available with input fields associated with Temperatures, Electronic States, Anharmonicity, and Alignment. The editor is shown with a) the Temperature tab selected on the left and b) the Anharmonicity tab selected on the right

The POLYRATE Editor is composed of three main areas. The top area is where basic information relevant to all rate constant calculations may be entered, such as calculating both forward and reverse rate constants and the use of symmetry factors. The middle is where more complex parameters may be entered. The interface is structured

for the user to enter parameters for their system via four tabs. The parameters under each tab have default values assuming a broad range of temperatures, one electronic ground state, and no anharmonicity. Starting with these values, a user may make alterations based on their specific system. The bottom of the interface has an option for making a “Final Edit”, where users may edit the POLYRATE input file just prior to running the calculation. This provides the more advanced user with access to any feature of POLYRATE that is not directly supported by the editor.

Support for running POLYRATE calculations through ECCE is accomplished by generating the POLYRATE “fu5” primary input file and copying the “fu30” file from the NWChem DirDyVTST calculation to the directory where POLYRATE will run on the compute resource selected through the ECCE Launcher. This final step gives ECCE the ability to run an entire kinetics calculation from basic electronic structure calculations to the final transition state theory rate constant prediction.

Viewer

The results for a POLYRATE reaction rate constant calculation are presented by the Viewer in Figure 6. The Viewer displays the transition state and the option to view calculation output in tables and plots inside panels on the left. Figure 6 shows three expanded plots for the equilibrium constant, rate constant, and a comparison between transition state theory and variational transition state rate constants. The plots and tables may be detached from the Viewer, as shown in Figure 7, and expanded.

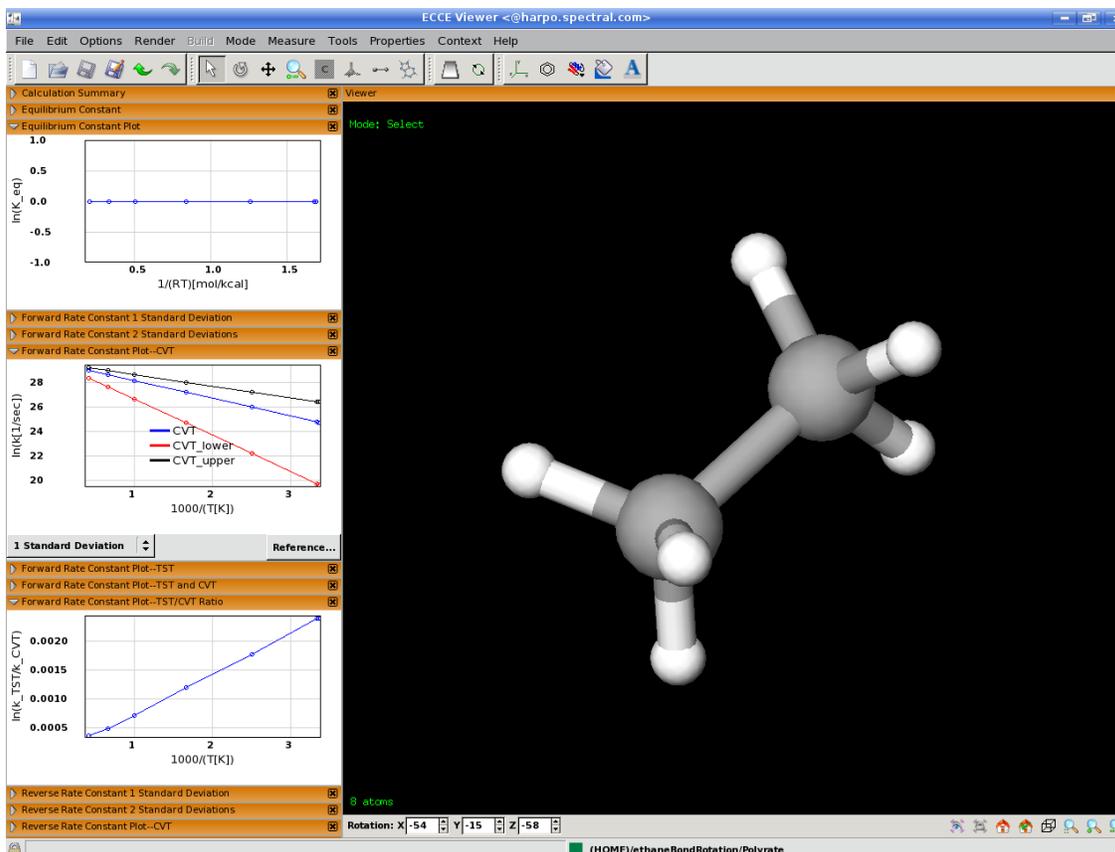


Figure 6. The ECCE Viewer displaying the results of a POLYRATE calculation. The transition state is displayed on the right along with the options to view tables and plots of calculation output on the left. The plots for the equilibrium constant, rate constants, estimated error, and a comparison between rate constants are shown

Forward Rate Constant 1 Standard Deviation <@harpo.spectral.com>

T	1000/T	ln(k_TST)	ln(k_TST-lower)	ln(k_TST-upper)	ln(k_CVT)	ln(k_CVT-lower)	ln(k_CVT-upper)	ln(k_TST/k_CVT)
298.000000	3.355705	24.726609	19.660630	26.415269	24.724215	19.658236	26.412875	0.002394
300.000000	3.333333	24.759416	19.727210	26.436818	24.757028	19.724822	26.434431	0.002388
400.000000	2.500000	25.980761	22.206607	27.238813	25.978989	22.204834	27.237040	0.001772
600.000000	1.666667	27.196369	24.680266	28.035070	27.195179	24.679076	28.033880	0.001190
1000.000000	1.000000	28.157051	26.647389	28.660271	28.156341	26.646679	28.659562	0.000709
1500.000000	0.666667	28.631322	27.624881	28.966802	28.630844	27.624403	28.966324	0.000478
2400.000000	0.416667	28.983991	28.354966	29.193667	28.983629	28.354604	29.193305	0.000362

Figure 7. A table of rate constants and predicted errors detached or “floated” from the main Viewer window

Error Estimates

Error estimates will be displayed and plotted for predicted reaction rate constants for specific combinations of level of theory and basis set. Currently only two basis sets are supported: 6-31++G** and aug-cc-pVTZ. For the 6-31++G** basis, the level of theory must be either MP or DFT, the latter with an exchange-correlation functional of “Modified Perdew-Wang 1K”, “B3LYP”, or “BB1K”. For the aug-cc-pVTZ basis, the level of theory must be CC. The use of any other combination of basis sets and levels of theory will produce predicted reaction rates without error estimates. It is important to note that the same basis set and level of theory should be applied to any reaction component geometry optimizations as well as the DirDyVTST calculation in order to be confident in the integrity of the results and specifically the error estimates. An example of plotted error estimates is shown in Figure 8. The detached Viewer plot shows the predicted rate constant (CVT, blue line) and the errors estimated for one sigma (CVT_lower, CVT_upper, red and black lines). The plot allows the user to change the value of sigma via the menu on the bottom-left. There is also access to a reference citing where the error estimates were derived on the bottom-right.

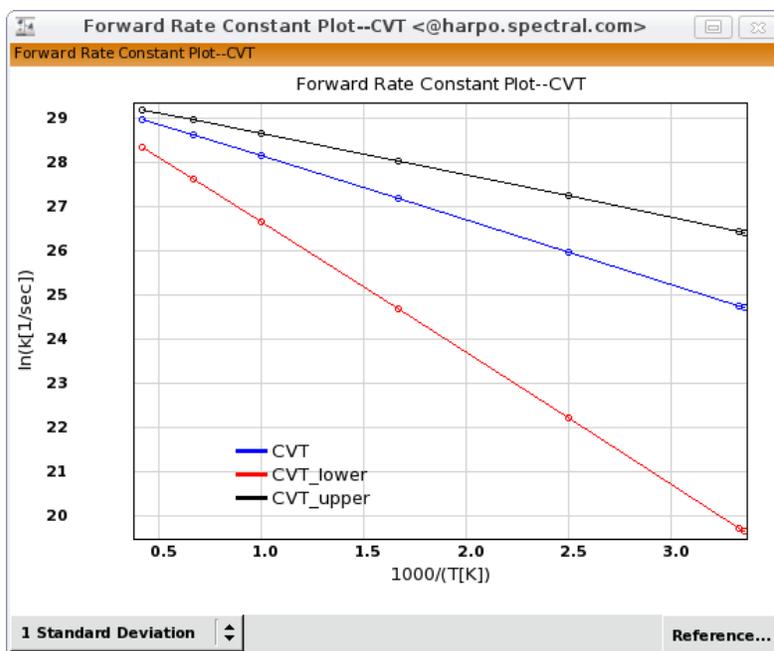


Figure 8. A plot of the Variational Transition State Theory rate constant (CVT), shown with estimated errors (CVT_lower and CVT_upper)

ECCE Rate Constant Prediction Demonstration Walkthrough

This section provides an end-to-end description of a demonstration of the reaction rate constant prediction capability, the same demonstration as the online movie. The steps assume a basic familiarity of the underlying ECCE software.

A. Finding the Transition State

1. Create a new Reaction Study in the ECCE Organizer
2. Launch the NWChem DirDyVTST Editor (right mouse button popup over the task or main menubar Tools menu) after selecting on the DirDyVTST task in the right-hand side Organizer workflow view of the Reaction Study
3. Launch the ECCE Builder for the transition state in the DirDyVTST Editor
4. Build ethane, CH₃-CH₃
5. Edit a torsion to generate eclipsed ethane--i.e. ethane with D_{3h} symmetry or if you look down the C-C bond you only see 3 hydrogen atoms (eclipsed) instead of 6 (staggered). This can be done by selecting H-C-C-H, in that order and changing the torsional angle from 60 to 0. Clear the torsion measure and selection
6. Optional: Use symmetry toolkit to find (verify) D_{3h} symmetry (no need for symmetry clean operation)
7. Save and exit Builder
8. Open the NWChem Electronic Structure Editor by hitting the NWChem code icon button in the DirDyVTST Editor under "Current Code" label for the transition state

9. Select the STO-3G basis set from the Quick Basis Menu in the NWChem Editor
10. Select Theory RHF and Runtime GeoVib
11. Open the Runtime Details window and set the "Find" field to "Minimum". Typically, we would search for a transition state. For this case, symmetry restrictions will cause the Minimum to be located at the transition state.
12. Hit "Launch..." button, select appropriate machine from the Launcher and launch the job
13. The transition state is located (calculation completes) in just a few seconds
14. Launch the Viewer for the Transition-State task (right mouse button popup over the Transition-State icon in the Organizer workflow view) and verify that you have one negative frequency. Animate the negative frequency to verify that it is the ethane bond rotation frequency that is of interest

B. Finding the Reactants and Products

1. Launch Viewer for the completed transition state calculation from the DirDyVTST Editor by hitting the transition state thumbnail
2. Select All (Ctrl-A) in the Viewer
3. Hit "Create Reactants" button in the DirDyVTST Editor
4. Hit "Create Products" button in the DirDyVTST Editor
5. Close the Viewer for the transition state calculation
6. Open Builder for the reactant by hitting the reactant thumbnail in the DirDyVTST Editor
7. Select 4 atoms H-C-C-H (in that order), whose torsion angle is 0 in the transition state structure
8. Set torsion angle to -60
9. Find (verify) symmetry as D3d
10. Save and exit Builder
11. Repeat steps 6-10 for the product, setting the torsion angle to 60 this time

C. The DirDyVTST Calculation

1. From the DirDyVTST Editor open the Setup window
2. Divide the symmetry tolerance by 10 (making it 0.0001 Bohr or 0.00000529 nm depending upon the units selected)
3. Set the general theory to RHF (leave single point theory as None)
4. Click on "General Basis Set..."
5. Double-click to select STO-3G, save and exit the Basis Set Tool
6. Set the following Path Parameters in the DirDyVTST Editor Setup window:
 - a. Minimum Energy Path Step Increment 0.002 nm (0.0378 Bohr)

- b. Increment for Saving 0.002 nm (0.0378 Bohr)
 - c. Increment for Recalculating Hessian 0.004 nm (0.0756 Bohr)
 - d. Lower Limit -0.01 nm (-0.189 Bohr)
 - e. Upper Limit 0.01 nm (0.189 Bohr)
7. Set the Integration Algorithm to “Corrected LQA”
 8. Optional: Click on Final Edit in the DirDyVTST Editor to show the NWChem input file ECCE has created via the GUI
 9. Launch the DirDyVTST calculation via the Launcher. Note: NWChem DirDyVTST requires a special patch to run on more than a single processor. As of NWChem release 5.1.1, this patch had not been incorporated into the standard NWChem release.
 10. As the calculation is running, open the Viewer and look at the Reaction Trace property where the geometry can be animated over the dividing surface. Depending on machine, the job will take a few minutes to complete

D. The POLYRATE Calculation

1. In the Organizer, create a POLYRATE task under the Reaction Study
2. Open the POLYRATE Editor on this newly created task
3. Select Final Edit (no changes needed) to view the ECCE generated input file
4. Hit “Launch...” button, select appropriate machine from the Launcher and launch the job. Job completes almost immediately
5. Open Viewer and look at reaction rate and equilibrium constant tables and plots
6. If desired, hit "Shell in Calculation Run Directory..." from the Organizer and look at regular POLYRATE output files

Builder Lasso Selection

(6.0) The capability to select multiple atoms and bonds at once in the Builder or Viewer by surrounding them with a rectangular “lasso” has been restored. This feature was temporarily lost when direct atom dragging was added in ECCE 5.0.1. Both of these features use the left mouse button in select mode and thus the user must choose their preferred behavior from the menu item labeled “Select Mode Action” under the “Options” menu. The default behavior is “Atom Drag” although if “Lasso Select” is specified instead, ECCE will remember this setting as a preference and restore it in subsequent Builder invocations.

Higher Order Spin Multiplicities

(6.0) The electronic structure Calculation Editor now supports spin multiplicities beyond “nontet” (eight open shells). The entry field for multiplicity has been changed from a non-editable choice box to an editable drop-down combo box. The same set of values (“singlet”, “triplet”, etc. for an even number of total electrons and “doublet”, “quartet”, etc. for an odd number of total electrons) will be displayed when clicking on the drop-down menu button next to the entry field. But, it is also possible to type directly into the

text field and enter a value without selecting from the drop-down menu items. For values above “nontet”, an integral number must be entered (9=“nontet”). For “nontet” and values below, either an integral number can be entered (e.g. 1 for “singlet”) or the full name can also be entered (lower-case, upper-case, or the first letter capitalized). If an inappropriate value is entered (less than 1, greater than the total number of electrons, invalid based on whether the total number of electrons is even or odd, or just a typo in the spin multiplicity name), a feedback area message will be issued and the value will be reset to maintain a consistent calculation. This capability was primarily added in anticipation of an upcoming ECCE release that adds support for building periodic (lattice) systems and running NWChem Planewave module calculations, where chemistry on higher spin state systems is common.

Windows PC Support

(5.1) A special distribution of ECCE has been created for users wishing to run ECCE on a Windows based PC. The freely available VMware Player virtual operating system software is required for using this distribution to run the Linux release of ECCE on a Windows host. The distribution includes a pre-installed version of the ECCE application and server software under the CentOS 4 (<http://www.centos.org/>) Linux operating system. These components are bundled as a virtual machine that is directly installed within VMware Player, which must be downloaded from the VMware website (<http://www.vmware.com/products/player>) and installed separately. A web browser viewable movie has also been created that documents the installation of VMware Player, the ECCE CentOS virtual machine, running ECCE in this environment, and common VMware Player configuration changes.

Once the virtual machine is installed and running, three icons for accessing ECCE are shown on the desktop. One provides access to ECCE with a local ECCE data and messaging server suitable for those running off the network or when there is only a single user at a site. In this case the local ECCE server is started automatically as needed when the ECCE application software is invoked with the “ecce” command. Thus there is normally no need to run the start_ecce_server script explicitly as there is with a regular ECCE Linux install. The remote ECCE server icon is used to run against a shared ECCE server on another (typically native Linux) workstation. By default the remote server is configured as eccetera.emsl.pnl.gov, the production ECCE server maintained for EMSL users (not accessible outside the PNNL firewall). But, a script named config_remote_server in the \$ECCE_HOME/siteconfig/RemoteServer directory can be run to setup access to any desired ECCE server. The VMware ECCE installation supports users who start the application software with a remote server in some instances and a local server in others (such as a laptop that is taken off the network for travel). The third desktop icon is used to start just the ECCE Builder/Viewer application without the rest of the ECCE application software (nor need for an ECCE server).

The Windows VMware Player version of ECCE is distributed as a compressed archive of files in “zip” format. The movie documenting the install process is also distributed as a “zip” archive file separately from the VMware Player ECCE distribution. This same movie is also available online from the ECCE public website under

http://ecce.pnl.gov/support/movie_index.shtml, although performance when viewing it online can be agonizingly slow depending upon a number of factors. Thus, we recommend downloading and viewing the movie locally. These “zip” format archive files first need to be uncompressed and extracted. Windows XP and Vista allow users to double click on these files as a “compressed zip folder” to display the contents and then drag and drop them to a regular file folder to extract them. There are also a number of separately available Windows applications that can be downloaded and installed to efficiently extract these archives. The 7-zip utility (<http://www.7-zip.org>) is freely available and therefore recommended. WinZip (http://www.winzip.com/prod_down.htm) is also widely used, but is a licensed commercial product with a 45-day free trial period. We highly recommend users watch the movie before attempting to install the VMware Player ECCE distribution as VMware Player provides several options for installing including hardware configuration and networking. To watch the movie after extracting the files from the “zip” archive, open the file “Installing_ECCE_VM.html” in the extracted folder from a web browser such as Internet Explorer (may require the Macromedia Flash plug-in to be installed).

Macintosh Support

(5.1) The VMware ECCE distribution can also be run on the Intel processor based (not supported on PowerPC processors) Mac OS X platform. However, rather than requiring VMware Player, VMware Fusion must be used as the virtual machine technology. VMware Fusion is not freely available like VMware Player, but the cost is reasonable after a free 30-day trial has expired. Since the movie documenting the installation procedure is targeted for Windows users, a README_ECCE.txt file is included in the folder that is extracted with the VMware ECCE distribution that describes the small number of extra steps specific to running on a Mac. Besides Windows and Mac support, this distribution also runs on 32- and 64-bit Linux hosts with freely available VMware Player. As with Macintosh, the README_ECCE.txt file describes Linux installation specifics.

Software Based OpenGL Support

(5.1) Because OpenGL support as needed for the ECCE Builder/Viewer is the single most common problem experienced by ECCE users, software based OpenGL libraries are now provided with the ECCE distribution as backup if hardware graphics card OpenGL support is not available or cannot be made to work. Given the differences between hardware platforms, graphics cards, and operating systems along with the limited support the ECCE team can provide for this variation, there are some circumstances where there is no practical alternative to using the software OpenGL libraries even when a hardware graphics card supporting OpenGL along with driver software has been installed. For instance, ECCE currently runs as 32-bit applications meaning that on 64-bit systems there must be 32-bit compatibility libraries installed including for OpenGL. Additionally, if the GLIBC version supported by the local /lib/libc.so.6 system library is significantly different from that which ECCE was built with, this can also lead to incompatibility with the hardware OpenGL driver. By default ECCE will attempt to use locally installed (hardware based) OpenGL libraries. However, by setting the \$ECCE_MESA_OPENGL (Mesa, <http://www.mesa3d.org>, is the implementation that is bundled) variable before

starting ECCE, the software OpenGL libraries bundled with ECCE will be used instead. This variable can be set in a login environment setup script (.cshrc, .bashrc) for individual users or it can be set as a site-level default in the \$ECCE_HOME/siteconfig/site_runtime file (not recommended if there are multiple machines that will use the ECCE installation at a site). Unfortunately, rendering performance when using software OpenGL will be significantly slower than when a hardware graphics card with OpenGL driver is used. However, for electronic structure “small molecule” chemistry ECCE is typically used for, it likely won’t be objectionable. Only with molecular dynamics (such as interactively manipulating PDB file based structures) or viewing trajectory files is the amount of information being rendered large enough to make hardware OpenGL graphics much more desirable.

NWChem 5.1.1 Bundled

(5.1) Newly released NWChem version 5.1.1 has been bundled with ECCE 5.1. This is the version that will be used when calculations are run on the host where the ECCE application software is installed. No specific changes to support new NWChem 5.1.1 features have been made to ECCE. ECCE bundles NWChem as a matter of convenience for those evaluating either ECCE or NWChem with the intent that users running the software for actual research will install NWChem separately. For less demanding computational applications on low-end hardware, it may be feasible though to continue using the ECCE bundled NWChem distribution.

Gaussian Cube File Visualization

(5.0.1) Restoring a pre-ECCE 5.0 feature for visualizing Gaussian Cube format files, the 5.0.1 Viewer handles both cube files that are part of the output from a calculation run from within ECCE and standalone cube files. Any cube files produced by an ECCE run calculation can be displayed using the new “Cube File” property panel in the Viewer similar to other properties for the calculation. To display a standalone cube file that is on the local machine where the Viewer is being run, use the “Open in new context...” menu item under the File menu after opening the Viewer from either the Gateway toolbar or the command line with the “ebuilder” command. Alternatively, the name of the cube file can be passed as a command line argument to the “ebuilder” command (the “ebuilder” command is used to bring up the integrated Builder/Viewer application whether it is to be used for building molecules or viewing calculated properties). Select the surface to display from the list on the left side of the “Cube File” property panel. Note that the property panel allows linear combinations of two different surfaces to be calculated and displayed by left mouse button clicking on the name of the first surface, right mouse button clicking on the name of the second surface, and then entering the coefficients for the linear combination into the “A” and “B” numeric entry fields on the property panel.

MO Panel Energy Graph

(5.0.1) Another pre-ECCE 5.0 feature, this time for displaying molecular orbital occupation energies graphically, has been restored. From the Viewer “MOs” property panel select “Graph” or “Graph by Symmetries” from the dropdown option menu near the right hand side of the panel title bar. The color of each orbital on the graph denotes its occupation number as indicated by the graph legend. Note that the orbital occupation

energies graphed are integrated with the MO visualization by left mouse button selecting an orbital from within the graph and hitting the “Compute” button below the graph.

Builder Atom Dragging

(5.0.1) Atoms and groups of atoms selected in the Builder can be moved (translated) in space by dragging (left mouse button selection and holding down the mouse button during the operation) over any one of the selected atoms in space. This is a quick and imprecise, although often very useful, alternative to using the other Builder manipulator tools or entering atom coordinates directly in the Atom Table. Note that any atom translations made in this way can be undone with the undo (ctrl-z) capability from the Edit menu.

Exporting Tabular Data

(5.0.1) Data in the Builder and Calculation Viewer can be exported to a comma-separated values (CSV) file using the right mouse button popup “Export...” menu item. This includes tabular data such as the atom table, residue table, MOs, vibrational frequencies, moments, etc. The Organizer also supports exporting calculation summary fields displayed in the right-hand side project context panel to a CSV file.

Adding Ghost Atoms

(5.0.1) The Builder allows ghost atoms (normally used in the Symmetry panel) to be added arbitrarily as atom placeholders when building a chemical system or for any other desired purpose. Under the Build panel “More...” button the ghost atom is shown with the symbol “X” in the bottom left corner of the periodic table. Selecting this “X” element allows any number of ghost atoms to be added to the workspace by clicking in free space as with the other periodic table elements. The default bonding hybridization for ghosts is a lone atom although this can be changed in the Build panel to allow bonded ghost atoms.

BqX Atom Behavior

(5.0.1) The Builder Atom Table contains two new dropdown option menu items for setting the behavior to BqX for all currently selected atoms and clearing the behavior field for all atoms, selected or not. Additionally the different types of atom behavior (Point, Quantum, Bq, BqX) can be entered directly (case insensitive) in the behavior field of the table for an atom. BqX atoms are typically used in NWChem QM/MM calculations, although ECCE does not currently offer any additional support for this type of calculation.

Authenticating as a Different Data Server User

(5.0.1) The initial ECCE login window now contains a “Data Server Login” field above the password field. This is used for remapping from a Linux login name (specified by the \$USER environment variable) to a different name on the Apache2 DAV server used by ECCE to store calculation data. The first time a user starts ECCE the “Data Server Login” field will be editable with a default value of the current Linux login name. This allows the user to change the name of the initial data server account that is created on the ECCE server (assuming automatic data server account creation is enabled). Note that if a name is specified that is an existing data server account, the user will need to give the

proper data server password for that account (in a different password dialog that is displayed after the ECCE login window) in order to access that data. This allows multiple users to share the same data server account and home directory either temporarily or longer term. After the initial login to ECCE the “Data Server Login” field will be disabled so a different user name cannot be specified, although the current setting will be displayed. However, it is still possible to set a different name after the initial login by starting ECCE with the command “`ecce -l <DataServerLogin>`” with the new login specified after the “-l” command line option (lower case letter “el”, not the number “one”). Since changing the data server login name is typically seldom needed, disabling the “Data Server Login” field after the initial login was done to keep users from inadvertently changing to a different user resulting in confusion and unintentional creation of new data server accounts.

Closing Remote Shells when Exiting

(5.0.1) A Gateway Preferences dialog toggle labeled “Close Remote Shells on Exit” has been added. Toggling the preference “on” will result in all xterm shells (tail -f on output file, shell in calculation run directory) started in the current ECCE session being closed automatically when the Gateway (session) is exited. The default behavior is still to leave these remote shells up indefinitely even after the ECCE session is gone, allowing users to continue working in them. A word of caution to those who change the default behavior to close remote shells on exit: be careful that you aren’t performing tasks in these remote shell windows where you haven’t saved your work when exiting from ECCE, such as editing a file or running a program. ECCE immediately terminates these remote shells when exiting the Gateway and you may lose work as a result. A related bug was also found and fixed so the “ecmd” process that ECCE creates for each remote xterm shell is now properly cleaned up from the process table when the user exits the shell or the shell is closed when ECCE exits based on the preference setting. Previously these ecmd processes lived indefinitely after the shell and even the ECCE session where it had been created no longer existed.

New Calculation Viewer

(5.0) ECCE 5.0 features a redesigned user interface for the Calculation Viewer. The Viewer is now integrated into a single application with the Builder, itself redesigned for the previous ECCE 4.5 release. A single ECCE visualization application is now used for building chemical systems and viewing calculation/task output. This design ensures that all panels that are applicable to both the Builder and the Viewer, such as the selection panel, are available when needed with reduced maintenance overhead.

The dockable panel user interface paradigm first used for the ECCE 4.5 Builder is now used for the Viewer property panels in addition to the Builder tool panels. The Viewer main window is divided into property panels along the left hand side (as with the pre-5.0 Calculation Viewer), the visualization/work area in the center, and build tools along the right hand side. For build tool panels, the panel layout is completely configurable by the user dragging the panels and docking them in different places within the main window or “floating” them outside the main window as their own windows. These build tool panel locations, including docked or floated, are saved as user preferences and restored with the

next invocation. Viewer property panels are an exception to saving and restoring their layout. Their location can be changed within an invocation, but will not be saved and restored between invocations.

Although the Builder and Viewer are actually the same executable, ECCE still maintains the distinction between the two in the Gateway toolbar and Organizer—each can be invoked separately. For a calculation or task that is being setup and run within ECCE, the run state determines whether it is a “Builder” or “Viewer” type invocation. Any calculation with a run state of Created or Ready will start a “Builder” instance regardless of whether the Builder or Viewer was selected in the Organizer. Likewise, for a calculation with a run state of Submitted, Running, or one of the completion states, a “Viewer” instance will be started regardless of whether the Builder or Viewer was selected in the Organizer. The type of instance, Builder or Viewer, simply determines which panels and operations are available to the user (cannot modify a chemical system for a running calculation for example) and whether the window title indicates a Builder or Viewer.

Like the build tool panels, in order to conserve screen space within property panels, option menus are commonly used to access functionality not on the panel itself. These option menus are displayed by hitting the left mouse button over top of the blue and white window icon near the right hand side of the property panel title bar. If you can't find functionality that was in the old Calculation Viewer in a new Viewer property panel, this is the first place to check.

The dockable panel nature of the Builder/Viewer and fussiness of the wxWidgets implementation for this capability sometimes results in undesirable if not bizarre and unusable panel layouts. In this case the “Reset Defaults Tools/Toolbars” operation in the Options menu can be used to restore sanity. After answering “Yes” to the confirmation dialog, you must exit and restart the Builder/Viewer to restore the default layout.

The Builder/Viewer is the only ECCE application that supports multiple contexts (calculations, chemical system files, trajectory animations, etc.) at the same time in a single instance of the tool. This design should be transparent to traditional ECCE users who bring up the Builder/Viewer in the context of an existing calculation to build a chemical system or visualize results and then close the application when done with their immediate task. But, for those who deviate from this usage, the multiple context design can take a bit of getting used to. Contexts mimic the design of many other visualization tools. A “Context” panel, which shows up with the other right-hand build panels, lists the current contexts and enables quick switching between them. The “File” menu contains three menu items for controlling contexts. “New context” creates an empty context whose name initially starts with “Unnamed”. This empty context can be used, for instance, to build chemical systems from scratch or using the “Import chemical system...” menu item. “Open in new context...” combines the “New context” operation with selecting a file to display in the newly created context. The selected file can be a chemical system, but this is also the way to open and animate the frames of a trajectory file or sequence of batched trajectory files (by selecting any single file in the sequence).

Finally, “Close context” will close the currently displayed context, prompting to save any work if there are unsaved changes.

The “Save as...” operation in the Builder/Viewer is more powerful than in previous releases of ECCE. “Save as...” is used for saving chemical system file formats (xyz, pdb, etc.), saving image snapshots of the visualization area (jpeg, POV-Ray, etc.), and for saving out the current context as a brand new electronic structure calculation (NWChem, etc.). A drop down menu below the file name text entry field is used to specify the type of file to generate. Saving a chemical system as an electronic structure calculation allows users to start the setup process by building their structure and then defining the chemistry code and where they want to put it on the ECCE data server. Further, if a geometry trace or trajectory is being visualized, the “Save as...” operation saves the step that is currently being displayed allowing explicit control for creating structures to serve as the starting point for additional work inside or outside ECCE.

As with previous releases, the “ebuilder” script is used to invoke the standalone version of the Builder from the command line. The “ebuilder” command is also used to open trajectory files (NWChem trj, or generic xyz format) as a “Viewer” instance of the standalone builder. The chemical system or trajectory file to load can be given as a command line argument to ebuilder. Alternatively, the “Open in new context...” (chemical systems or trajectories) or “Import chemical system...” (chemical systems only) File menu operations can be used to load a file after invoking “ebuilder” without command line arguments. Invoking the Builder from the Gateway toolbar is equivalent to an “ebuilder” invocation without any arguments while invoking the Viewer from the Gateway toolbar automatically performs an “Open in new context...” operation from the newly created application—used for opening chemical systems or trajectories. An enhancement from previous ECCE releases, the “ebuilder” script is now fully functional even in a full ECCE install. Previously the “Structure Library”, “DNA Builder”, and “Peptide Builder” would not work from “ebuilder” except when a “standalone builder” distribution of ECCE was downloaded and installed.

Unfortunately, for the initial release there exists no additional documentation on using the ECCE 5.0 Builder/Viewer beyond these release notes. We strived to make it as intuitive and stick with names and conventions established by previous releases of ECCE where feasible. You are encouraged to play with it to see how it can be applied to your work. Finally, please don’t hesitate to ask questions or give us feedback by sending email to ecce-support@emsl.pnl.gov.

Old Builder and Viewer No Longer Distributed

(5.0) The ECCE 5.0 distribution no longer contains the old X Window Motif versions of the Molecule Builder and Calculation Viewer applications. In the ECCE 4.5.x distributions the old Builder was distributed as a backup to the new wxWidgets version. This was done in case users found problems with the new Builder significant enough that they needed to revert to the old version to accomplish their work. Plus, some rarely used components of the old Builder (e.g., the MD Topology Viewer and Force Field Editor) have not been ported to the new wxWidgets version. Since the initial ECCE 4.5 release,

the new Builder, now integrated with the Viewer, has become significantly more robust and reliable and the ECCE team does not anticipate sites needing to use the old versions. This decreases the size of the distribution and installation, especially with third party libraries for only a single GUI toolkit being distributed instead of two GUI toolkits. A not unintentional side effect is that if problems are found with either the new Builder or Viewer, feedback to the ECCE team will be needed, which might not be the case if the old versions were easily available. There are a small number of what the ECCE team considers to be minor features that were not implemented in the new Viewer (conversely, there are a large number of new capabilities not previously available). If you discover a missing feature from the old Builder or Viewer that you found valuable that you would like to see added back, please contact us. We are also still able to provide these old Builder and Viewer versions on request.

Normal Modes Property Renamed

(5.0) For consistency with NWChem and other chemistry codes, the Normal Modes property panel in the Viewer has been renamed to Vibrational Frequencies. Calculations that were run prior to ECCE 5.0 will automatically display what was Normal Mode data in the Vibrational Frequencies panel.

Open Source GUI Migration

(5.0) The redesign of the Viewer porting it to the wxWidgets GUI toolkit completes the migration of all ECCE applications to rely on only freely available open source products. This effort was undertaken in 2005 with one or more applications being ported to wxWidgets (see <http://www.wxwidgets.org>) with each release starting with 4.0, all while continuing to simultaneously add computational chemistry domain functionality. Core ECCE applications use the wxWidgets C++ toolkit, while the code registration dialogs are implemented under wxPython, the wxWidgets binding to the Python scripting language. In addition to being an open source product, wxWidgets is a cross platform toolkit that supports all major operating systems. Eliminated are two proprietary GUI development tools for the UNIX/Linux only X Window System Motif toolkit, which date back to the first production release of ECCE: Aonix TeleUSE and Quest XRT PDS widgets. This milestone opens up several new possibilities for the future of ECCE such as collaborative and contributed code developed outside the ECCE project team (only electronic structure code registration was previously possible) and ports to different operating systems including Microsoft Windows and Macintosh OS X. While the ECCE project team is not currently scoped for completing the ports to operating systems beyond Linux, please contact us if you are interested in doing ECCE development, including porting to another operating system or adding chemistry domain functionality. At this time there is no task to make ECCE source code available for download in a useful form; i.e., able to compile in an autoconf type environment (there are numerous third party packages ECCE relies on that make it more complex to build than lower-level software like NWChem). However, it is feasible that the identification and commitment of an outside group to extend ECCE in a way that benefits a broad base of users could justify this task of creating and documenting a build environment. Finally, of note to those who would like to run ECCE on Microsoft Windows based systems is a task planned for 2009 to make a distribution of ECCE available that runs under virtualization software such as

VMware (see <http://www.vmware.com>) and/or VirtualBox (see <http://www.virtualbox.org>). While not a native operating system port, this will make running ECCE feasible at sites where Linux is not available. For sites with limited access to Linux systems, the use of X Window Server software that supports OpenGL such as Hummingbird Exceed 3D (see <http://connectivity.hummingbird.com/products/nc/exceed>) or Cygwin/X (see <http://x.cygwin.com>) already allow users to run ECCE from a backend Linux workstation displaying on Windows based desktops.

Color Themes

(5.0) ECCE now allows colors for application windows and GUI controls to be changed at the site level and by each user. Colors can either be changed individually by type of control or one of a small number of themes can be selected. The default ECCE colors have been changed in the 5.0 release to conform to the new Pacific Northwest National Laboratory branding although the “Classic” theme can be selected to restore the familiar pre-5.0 look. Colors are specified in a configuration file in the `$ECCE_HOME/siteconfig` directory name `AppColors`. This file also documents what control type colors can be changed, what the theme names are, how to specify a color value, and how users can create their own `MyAppColors` file to override the site level colors. Alternatively, the Gateway toolbar Preferences dialog contains a “Color Theme” choice box that updates the user `MyAppColors` file, but does not allow control of the individual control colors. The ECCE login window has also been changed to match the new branding with PNNL and EMSL logos added. The color of the ECCE wave logo in the background of the login window has also been changed (now PNNL-branded copper) and will not update with changes to the `AppColors` or `MyAppColors` files (same for the animated wave logo in the ECCE Gateway toolbar).

Renamed Applications

(5.0) Several ECCE application names have been shortened or changed for consistency. The Calculation Viewer is now simply Viewer. The Job Launcher is now Launcher. The Calculation Editor is now Electronic Structure Editor in a generic sense or NWChem Editor, etc. when in the context of a chemistry code. This is more consistent with the variety of new ECCE editor applications for different fields of chemistry—molecular dynamics and upcoming support for thermodynamics. Finally, the Molecule Builder is simply Builder as most users refer to it already.

SITE ADMINISTRATOR WHAT’S NEW

Upgrades of ECCE Data and Messaging Servers

(5.0) The Apache2 HTTP server (see <http://httpd.apache.org>) used for the ECCE data server along with the bundled `mod_dav` module has been upgraded from release 2.0.59 to the latest 2.2.10. The ActiveMQ Java Messaging Server (see <http://activemq.apache.org>) used for the ECCE JMS messaging server has also been upgraded from release 4.1.1 to 5.1.0. When installing, we highly recommend upgrading the ECCE server to 5.0 rather than solely the application software. In fact, we have experienced messaging session disconnects with accompanying java stack trace output in the window where the ECCE

application session was started when running ECCE 5.0 application software against an ECCE 4.5.x server. These problems can be attributed to incompatibilities between the ActiveMQ 5.1.0 client side java messaging libraries used by ECCE 5.0 and the ActiveMQ 4.1.1 server distributed with ECCE 4.5.x.

Upgrade of wxWidgets GUI Toolkit

(5.0) The wxWidgets C++ GUI toolkit (see <http://www.wxwidgets.org>) used by ECCE core applications has been upgraded to the latest stable release, 2.8.9. Likewise, the wxPython toolkit (see <http://wxpython.org>) used for code registration theory and runtime details dialogs has also been upgraded to use the same distribution of wxWidgets. For ECCE this wxWidgets release primarily improves on the behavior of the dockable panel capability that is integral to the Builder/Viewer application.

WHAT'S FIXED

SITE ADMINISTRATOR WHAT'S FIXED

Crashes Saving Thumbnails and Image Files from the Builder and Viewer

(5.0.1) Certain operating systems and OpenGL hardware graphics drivers do not support the OpenGL off-screen rendering feature required by ECCE to save image files (JPEG, GIF, TIFF) and the thumbnail visualizations of chemical systems that are shown for the icon to access the Builder for a calculation. Typically the X Window session will completely crash trying to use these ECCE features when off-screen rendering is not supported; returning the user to the Linux login screen. Thumbnail visualizations are created by default when saving a chemical system in the Builder so it will appear as if a “save” operation is causing the crash. The `$ECCE_NO_VIZIMAGES` environment variable has been created to keep ECCE from creating any image files including thumbnail visualizations. Search for “`ECCE_NO_VIZIMAGES`” in the `$ECCE_HOME/siteconfig/site_runtime` file to override the default setting where off-screen rendering is used. Without off-screen rendering the POV-Ray format for capturing images of visualizations can still be used. Since POV-Ray produces publication/presentation high quality graphics and there are utilities to translate POV-Ray files to image formats like JPEG, the lack of off-screen rendering is an inconvenience rather than a loss of functionality.

Machine Registration Queued Machine Support

(5.0.1) Several bugs were fixed with the Machine Registration application's support for registering batch queued machines. Because of the severity of these bugs, it was not previously possible to use the GUI application to register anything other than workstation class machines. Now the Machine Registration application (accessible via “`ecce -admin`” for users with write permission to the `$ECCE_HOME/siteconfig` directory) can be used for registering both workstations and batch queued compute resources to ECCE.

WHAT'S BROKEN