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1. How do I transfer my license to a new machine?

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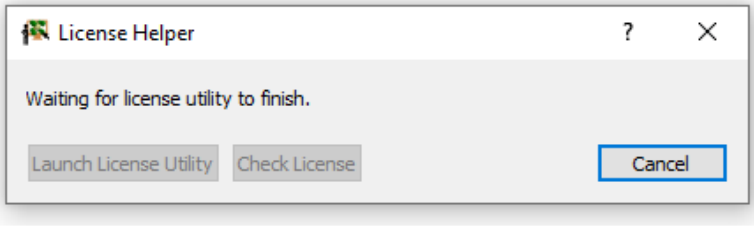
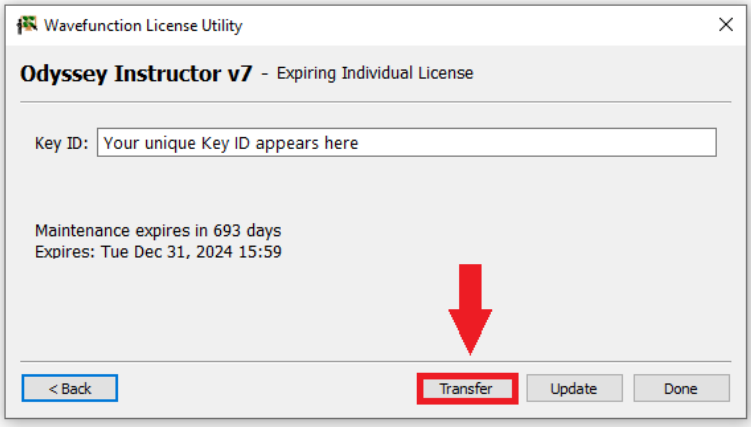
While the following screen captures are from Windows, the directions are platform agnostic.

On the computer running an existing license of ***ODYSSEY***, go to the **Help** menu and click on **License Utility…** This will launch the license helper dialog and prompt for administrator permission; allow the license utility to launch:



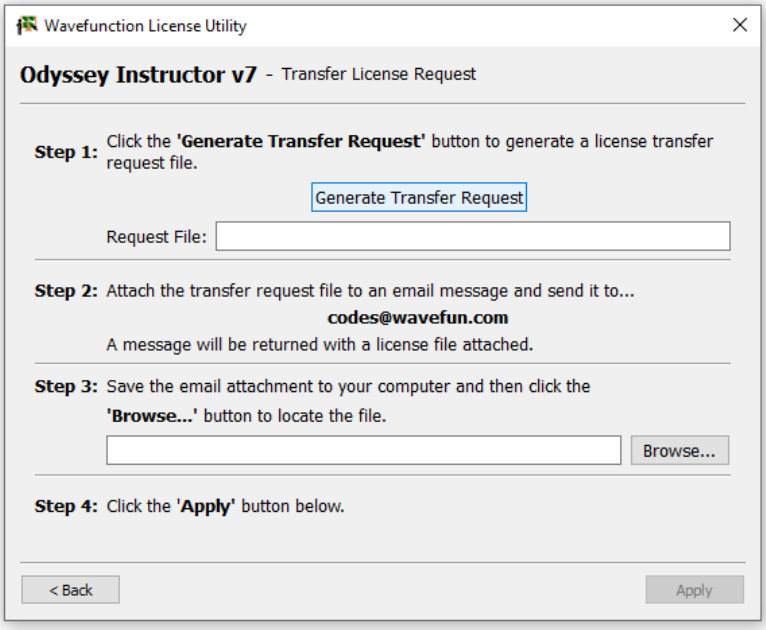
Note: macOS will require **admin** login.

On your OLD (!) machine: In the License Utility dialog, click on the **Transfer** button:



In the ensuing dialog, follow *Steps 1* and *2*:

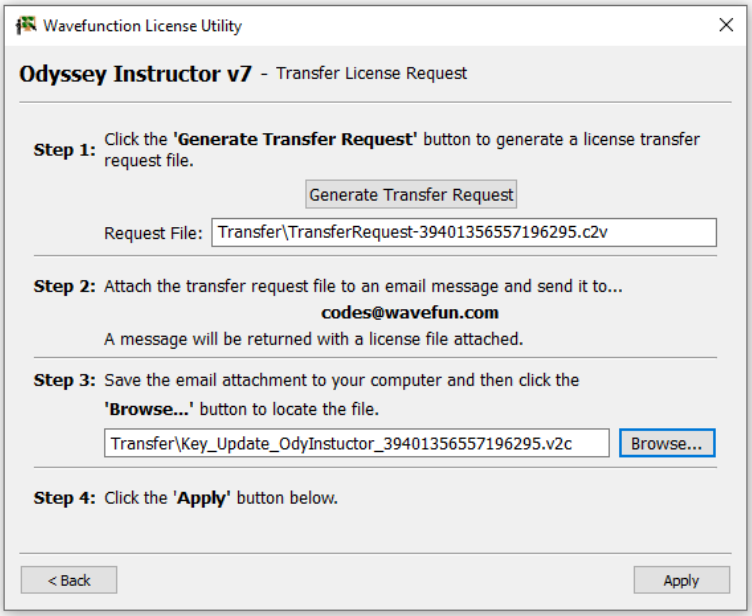
- Click on **Generate Transfer Request**.
- Save the **Transfer Request** (.C2V) file and email it to *codes@wavefun.com*.



Note: This is a manual email response, please allow 24-48 hours for response.

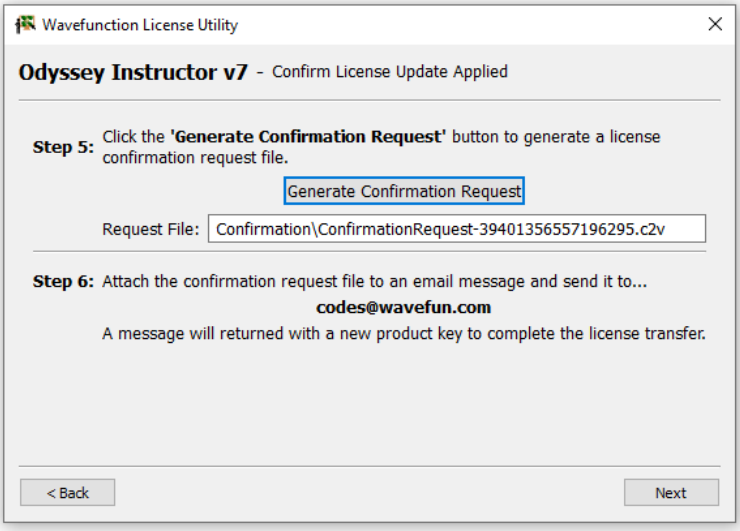
Save the received **Key Update** (.V2C) file to your OLD (!) machine and follow *Steps 3* and *4*:

- Click **Browse…** to locate and open the saved **Key Update** (.V2C) file.
- Click the **Apply** button to apply the received Key Update (.V2C) file to your old machine.



Now follow *Steps 5* and *6*:

- Click on **Generate Confirmation Request**.
- Save the **ConfirmationRequest** (.C2V) file and email this to *codes@wavefun.com*.



Once the **ConfirmationRequest** file has been received and verified, you will receive a new (license) in the form of a new 32-hexadecimal **Product Key** (.V2C) file for the NEW (!) machine.

Note that this is a manual step and may take up to 24-48 hours.

If you encounter any difficulties, contact us at *codes@wavefun.com* or at the general *support@wavefun.com* address. One of our support team will follow up with you to resolve any issues.

2. How do I update my license?

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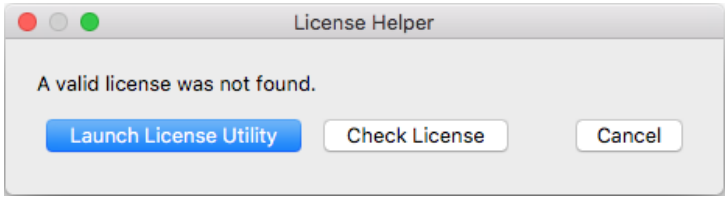
Most of the following screen captures are from Windows, but the directions are platform agnostic.

On the computer running an existing license of ***ODYSSEY***, download the latest ***ODYSSEY*** installer (.exe for Windows) or disk image (.dmg for macOS): **Wavefunction Downloads**.

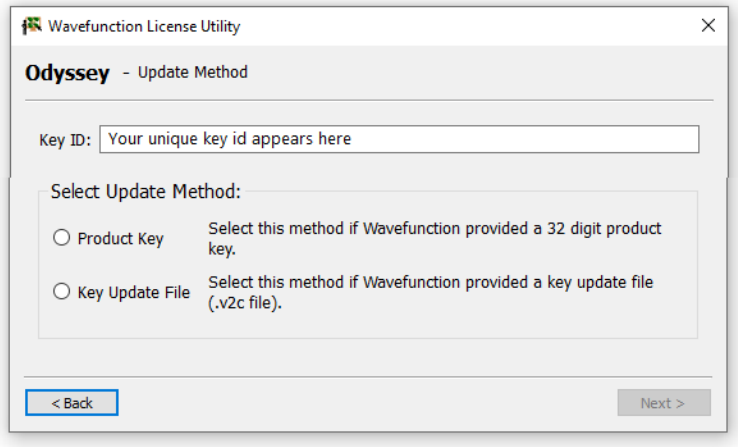
- *Windows:* Double-click on the installer (.exe) and follow the prompts to complete installation.
- *Macintosh:* Open the disk image (.dmg) and drag the program to the computer's **Applications** folder (typically via its Alias). Upon initially opening the application you may be prompted to launch the License Utility:



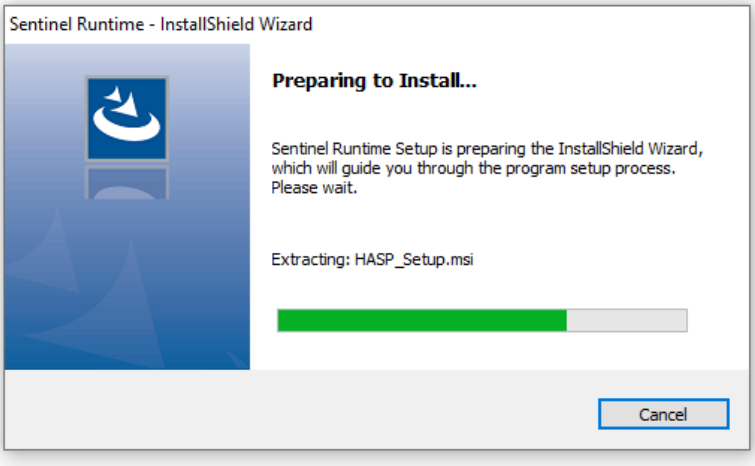
(If you don't get prompted, *manually* launch the License Utility from the **Help** menu).

Your previous licensing will be recognized and you will be presented with the *Update Method* panel:

- Choose either **Product Key** or **Key Update** file (if **Key Update** file, make sure the Key ID in the license utility matches the Key ID in the name of the **Key Update** file).
- Click the **Next** button.

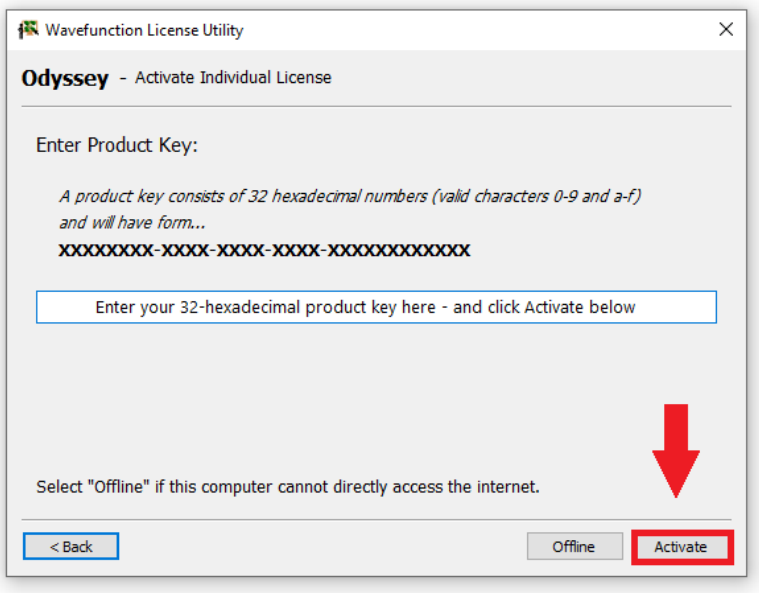


Follow the prompts to complete the license update. *Note:* If your license manager (*Sentinel Runtime Environment* by Thales) needs updating, the installer or license utility may present you with the Sentinel Runtime InstallShield Wizard:

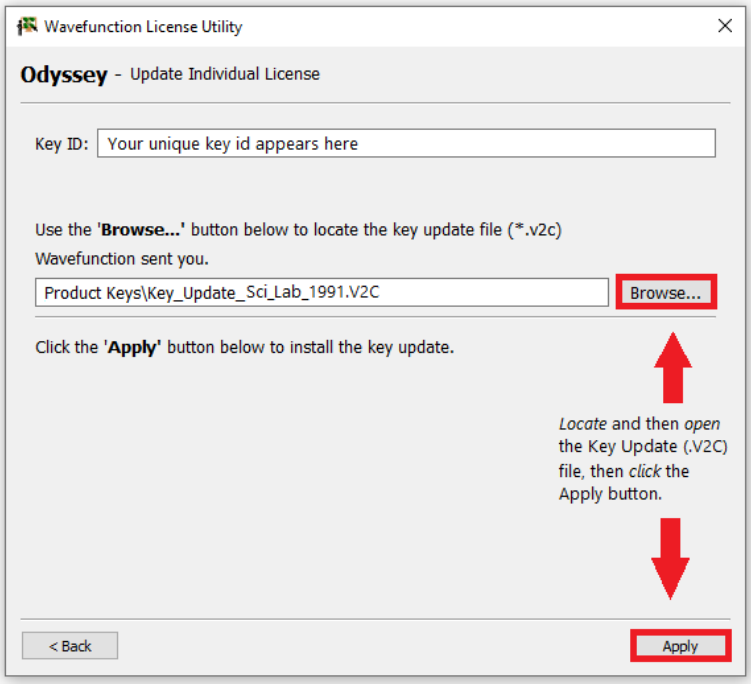


If this happens, follow the prompts to install the latest license manager software as well.

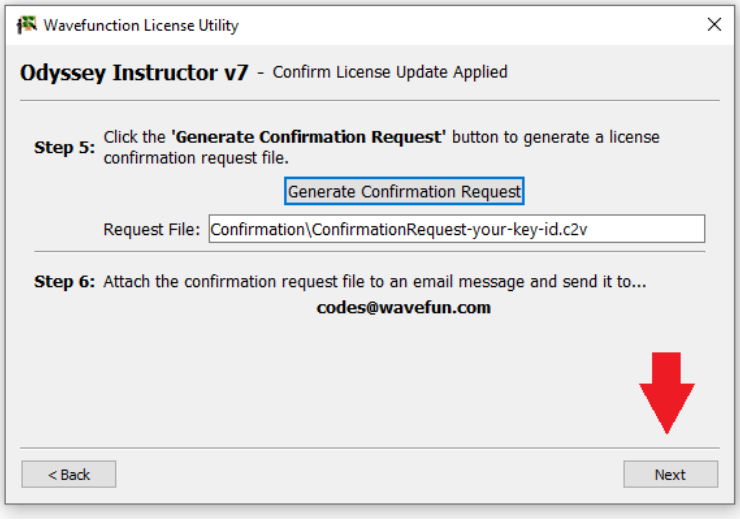
Upon completion, in the case of a **Product Key** update, please *copy/paste* your **Product Key** into the provided field and click the **Activate** button:



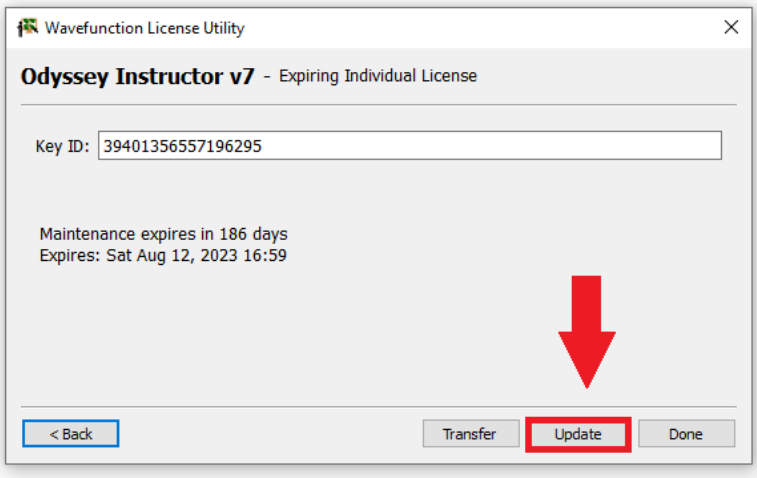
In the case of the **Key Update**, click the **Browse…** button:



Use the resulting browser window to locate and open your **Key Update** (.V2C) file. Once opened, click the **Apply** button. Upon successful application, you will be prompted with **Generate Confirmation Request**. Email the resulting file to Wavefunction via *codes@wavefun.com*. Click the **Next** button to complete the update:



Note: To update the licensing without installing a new version of the application, open the **License Utility…** and click the **Update** button:



Then follow all steps listed in the above description.

Once updated (with either method), click the **Done** button. Contact *support@wavefun.com* with any issues or questions.

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3. The license utility shows a maintenance expiration date for my license. What does this mean?

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New ***ODYSSEY*** licenses include one year of maintenance (excludes student-purchased activation-code licenses). Maintenance provides:

- All minor and major version updates
- Priority technical support
- Any necessary license transfers
- *Applicable to network licensing:* The ability to run in a virtual environment.

The inclusion of maintenance necessitates an initial expiration date for maintenance and the license (at one year from purchase). Wavefunction contacts customers approximately 90, 60, and 30 days prior to expiration with the option to renew maintenance. Customers are not obligated to renew.

- If maintenance is renewed, an updated license is provided valid through the new maintenance date and the benefits of maintenance are extended through this term.
- If maintenance is not renewed, customers are provided with a permanent license (non-expiring key, without maintenance) for the latest version of ***ODYSSEY*** at the time their maintenance expired (future upgrades or transfers are subject to standard upgrade or transfer fees for unsupported versions).

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4. Can I run *ODYSSEY* in a virtual environment?

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New ***ODYSSEY*** licenses include one year of maintenance. Among the benefits is the ability to enable network licensing for virtual environments. This allows for the network license server and/or the client machines to run Wavefunction software in a virtual environment. This means that rather than validating the machine fingerprint based on hardware identifiers, the fully qualified domain name (FQDN) is used to identify/validate licensing (as there are no unique identifiers on virtual machines).

Support for virtual machines and running in a virtual environment is only available

- for annual site licensing,
- for enterprise licensing, or
- to customers with network licensing and current maintenance.

Note that the request for virtual machine enabled licensing should be made *in advance* of license generation as additional configuration is necessary to support this type of licensing.

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5. With what types of classes can *ODYSSEY* be used?

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ODYSSEY's main usage is in first-year college chemistry (general chemistry) and high school chemistry (including honors chemistry and AP®/IB chemistry). The program can be used as an in-class demonstration tool as well as a student-use learning tool (in a laboratory setting and in take-home assignments). Note ***ODYSSEY***'s powerful molecular visualization is also used by high school Physical Science teachers and even some middle school teachers.

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6. Does using *ODYSSEY* amount to adopting a specific curriculum?

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ODYSSEY does not provide a specific curriculum that the instructor has to buy into. What is offered is a large selection of self-contained topics at different levels of difficulty that the instructor can pick from. Browse through the "New Users" tutorials and the list of "Labs" and you will invariably find applications relevant to your teaching.

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7. Does the program replace conventional textbooks?

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ODYSSEY provides instructors with a firmly science-based tool to acquaint students with the molecular concepts of chemistry. For the most part, this is accomplished through visualization exercises and laboratory-style experiments. If a textbook is used, then ***ODYSSEY*** provides a complement rather than a replacement. The program also complements other teaching software where the emphasis is on repetitive problem drills.

8. What is the difference between *ODYSSEY* and molecular visualizers?

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Unlike molecular visualizers (JSmol, MolView, and others), ***ODYSSEY*** is a full-fledged simulation and teaching tool:

- An open-ended model kit allows students and teachers to build almost any chemical structure imaginable.
- Bulk phase systems (solids, liquids, and gases) are treated on an equal footing with individual molecules.
- Molecular motion can be studied with real-time, open-ended simulations.
- Physical manipulations can be carried out that truly change the nature of a given system.
- Systems of a huge diversity can be studied (from the hydrogen atom to DNA and from liquid water to complex crystals).
- Rich teaching content is integrated into the program.
- The quality of the three-dimensional visualization is unparalleled in a teaching tool.

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9. What is the difference between *ODYSSEY* and other chemistry simulation software?

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- The models used by ***ODYSSEY*** are always fully three-dimensional. (More often than not, the models of other programs are either two-dimensional or do not represent any molecular entities at all.)
- By and large, ***ODYSSEY*** uses models that are realistic representations of molecular matter, not necessarily at the level of the most advanced research software, but of sufficient quality for teaching applications. (In almost all cases, the models of other educational software are highly abstract and cartoonish.)
- ***ODYSSEY*** is an *open-ended*, general purpose tool that can be used for many types of queries. (Simulations using other technologies are typically focused on a single message at a time and not really open-ended.)
- Like a giant microscope, ***ODYSSEY*** provides a computer-based laboratory for exploring the molecular world. (Much other chemistry education software show molecular animations via a mediaplayer, essentially offering animated analogs of textbook illustrations.)

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10. Is *ODYSSEY* available in different versions?

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ODYSSEY doesn't target one narrow set of users—the program rather contains a large amount of content from which the user can pick anything ranging from very simple visualization exercises (for complete novices) to advanced activities that draw on concepts from upper-level chemistry courses.

Similar to introductory textbooks, the program is available in Student and Instructor's Editions. Only the Instructor's Edition includes an Answer Key for the worksheets, the ability to customize labs, and lists of misconceptions. For high school users, the Instructor's Edition provides alignments with the AP® Chemistry curriculum and other science content standards.

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11. Under what operating systems will *ODYSSEY* run?

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ODYSSEY is available for Windows 8.1 and up (including Win 10 and Win 11) and macOS 10.12 Sierra and up (including 10.13 High Sierra, 10.14 Mojave, 10.15 Catalina, 11 Big Sur, 12 Monterey, and 13 Ventura). ***ODYSSEY*** is not available for Chrome OS.

12. Will *ODYSSEY* work on a 64-bit computer?

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Yes, ***ODYSSEY*** can be run with either 32-bit or 64-bit operating systems.

13. Is *ODYSSEY* available for Chromebooks?

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No, ***ODYSSEY*** is not compatible with the operating system of Chromebooks.

14. Is *ODYSSEY* available for Linux?

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No, ***ODYSSEY*** is not available for Linux.

15. Is *ODYSSEY* offered for languages other than English?

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Yes, a large number of learning units in **Japanese**, **Spanish**, and **German** are included with the program—just select the corresponding language buttons on the initial selection page.

In each case, the instructions are provided so as to include explicit pointers to the English language menus and commands.

16. Will the program run under any Windows operating system?

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ODYSSEY requires Windows 8.1, 10, or 11. Older operating systems are not supported.

17. Will the program run on any Macintosh?

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ODYSSEY requires macOS 10.12 Sierra, 10.13 High Sierra, 10.14 Mojave, 10.15 Catalina, 11 Big Sur, 12 Monterey, or 13 Ventura. Older operating systems are not supported.

18. Does *ODYSSEY* require an expensive computer to run on?

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No, ***ODYSSEY*** will successfully run on essentially any modern laptop or desktop computer that runs under Windows or macOS. This includes any computer with a chip from the Intel Core line (i3, i5, i7, Core, Core 2) or with an equivalent chip from AMD. For older computers, the minimum requirement is a clock speed of ~2 GHz (Pentium 4, Celeron) or ~1 GHz (Pentium M, various AMD chips).

19. Will *ODYSSEY* run on machines below the minimum requirements, albeit a little bit more slowly?

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On computers that don't meet the minimum requirements, ***ODYSSEY***'s dynamic simulations—central to the power of the program—will run very slowly, making such simulations impractical.

20. Does the program require online connectivity?

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ODYSSEY is a locally running application that does not access the Internet during the vast majority of operations. The only exceptions are the following:

- During a one-time activation step after purchase, the Wavefunction license server is momentarily accessed to activate the license.
- The **Check for Updates...** utility in the **Help** menu (new in ***ODYSSEY*** 7.1) checks if a newer version of ***ODYSSEY*** is available.

- If the license makes use of an external license manager ("Sentinel Runtime Environment" by Thales), then any updates of that license manager access the internet.
- Hyperlinks to Google Form in the upper right corner of the labs (Instructor's Edition only) allow the user to create personal copies of corresponding Google master forms for many ***ODYSSEY*** labs.
- Hyperlinks to videos link to a dedicated website with ***ODYSSEY*** chemistry content and teaching tips.
- Hyperlinks to WIKIPEDIA provide access to selected chemistry topics at the Wikipedia website.

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21. Doesn't the fact that the program uses a web browser mean that it is an online application?

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No, ***ODYSSEY*** is a locally running application. The program's web browser is only used to navigate among the content (except for embedded hyperlinks to Google Forms, videos, and Wikipedia).

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22. Does *ODYSSEY* run on the iPad?

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The program in its entirety will not run on the iPad, but 15 selected learning units exist as individual apps: ***ODYSSEY* for the iPad**

Note that the apps are for all practical purposes verbatim copies of the corresponding learning units in the full program. Please go to the Apple *App Store* for purchasing the apps.

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23. Will the *ODYSSEY* iPad apps run on the iPhone?

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No, the ***ODYSSEY*** iPad apps will not run on the iPhone.

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24. Does *ODYSSEY* run on Android tablets?

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No, ***ODYSSEY*** is not compatible with Android tablets.

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25. Does *ODYSSEY* run on Windows tablets?

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ODYSSEY runs on Windows tablet computers if the operating system is either Windows 8.1, 10, or 11.

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26. What are the graphics card requirements?

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There are no specific requirements. When visualizing large models (particularly in the "Space Filling" and "Ball and Spoke" styles), dedicated high quality graphics cards will show better performance than computers with integrated (system-on-chip) graphics. The visualization of small models, however, will be little affected. On Windows machines, you can use the **Reduced Graphics for Slower Machines** option in **Tools → Preferences** if the graphics performance seems unsatisfactory.

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27. What do I do if my online activation attempts with a dashed, 21-digit activation code are failing?

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Use the offline activation procedure described below.

28. How do I install with a dashed, 21-digit activation code if I don't have Internet access?

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If you purchased ***ODYSSEY*** with a Wavefunction activation code (a dashed, 21-digit number) and your computer does not have Internet access (or if you have a particularly strong Firewall that foiled your activation attempts), you need to activate offline. The following steps describe the required steps for **Windows**—the procedure for the Macintosh is analogous:

- Choose **Software Key** during the installation process and follow the prompts to complete program installation.
- When you reach the activation dialog, click on the **Offline** button. Click on **Write Request File**—you will be prompted to specify a location to write a "Request.txt" file. Email this file to *codes@wavefun.com*.
- You will receive a response file (normally within 24-48 hours) that is named "Request_code.txt"—save this to your Desktop.
- Open ***ODYSSEY***—when prompted for activation, enter the original dashed, 21-digit activation code (again).
- Click on the **Offline** button, and this time choose **Activate From File**—in the resulting dialog point to the "Request_code.txt" file on your desktop.
- This will complete the activation process—once your software is activated you may delete the "Request.txt" and "Request_code.txt" files.

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29. Can the Windows version be installed using a silent install?

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Yes. Just run the installer executable from a command prompt using "/S" as the modifier. To avoid a confirmation dialog, be sure that the command prompt window is running with Administrator privileges (create the window by searching for "cmd," *right-click* on cmd.exe, and select "Run as administrator").

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30. What do I do if the Windows program crashes immediately after installation?

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Try to lower the "Graphics Hardware Acceleration" if ***ODYSSEY*** crashes immediately after installation:

- Go to **Control Panel → Display → Settings → Advanced → Troubleshoot**.
- Set the "Hardware Acceleration Slider" to the highest setting that still allows the program to run properly

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31. How do I uninstall the Windows version?

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To uninstall the **Windows** version of ***ODYSSEY***:

- Use the **Uninstall** shortcut in the ***ODYSSEY*** program group that is found in **Start → All Programs**.

If the **Uninstall** shortcut in the ***ODYSSEY*** program group is not available:

- Use the **Start Menu → Control Panel → Add or Remove Programs** dialog.

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32. Can I change the size of the text, properties, and plot areas?

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The user can control the screen layout by changing the size of the window tiles.

Vertical separators (between Build/Cell/Plots area, Sample area, and Text area):

- Position cursor on boundary between tiles, click, and drag

Horizontal separator (between Sample area and Properties area):

- Position cursor on the line just below the "Start/Stop" button, click, and drag

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33. How do I change the size of the text?

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The text size can be altered independent of the screen resolution.

- From the **View** menu, select **Zoom Text → Zoom In** (or **Zoom Out**).

ODYSSEY will remember the new setting the next time you start the program.

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34. Can I change the fonts?

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The fonts of the main text panel as well as of other text strings in the program cannot be changed.

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35. Can I use an icon toolbar similar to the one seen in *SPARTAN*?

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To display a toolbar with icons for *Build*, *Minimize*, *Evaluate*, *Name*, and more:

- From the **View** menu, select **Toolbar**.

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36. Does clicking on the Refresh/Reload icon only affect the currently displayed sample?

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No, clicking on the refresh icon refreshes the HTML of the currently shown page as well as *all* samples associated with the current page. (Experiments in other tabs are unaffected by a refresh.)

A **Reload** option is also available in the shortcut (right-click) menu when the cursor is within the text area. Unlike the general reload, the effect of this particular reload is limited: It only refreshes the HTML of the current page, i.e., it does not refresh the associated sample(s).

---

37. Can I suppress the text panels of open pages?

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The text panel can be temporarily hidden (the toolbar must be displayed):

- Click on the "Hide Text" icon  .

---

38. Can I put the program into true Full Screen Mode, similar to PowerPoint?

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ODYSSEY can be put into presentation-style full screen mode:

- From the **View** menu, select **Full Screen**

To exit full screen mode:

- In the **View** menu, deselect **Full Screen**

---

39. What do the colors in the Periodic Table stand for?

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The **Periodic Table**  (also in the **Tools** menu) can be displayed with the following color overlays:

- *Default:* Coloration by ***ODYSSEY*** atom colors
- Coloration by standard state (gas, liquid, or solid)
- Coloration by metallic character (metallic, semimetallic, or nonmetallic)
- Coloration by valence electron configuration (s/p/d/f blocks; noble gases)

---

40. Where do I declare the charge when I build an ion with the 3D Model Kit?

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Click on **Set Charges...** in either the **Entry-Level** or **Advanced** builder, then use the up/down arrows to set the charge (labeled "molecular" charge for the sake of generality). In build mode, the charge is displayed for all charged species.

---

41. How do I change the chirality of a stereocenter while building?

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Tetrahedral stereocenters of chiral molecules can be inverted by *double-clicking* (or, where applicable, double-tapping) on the stereocenter while holding down the CTRL key (Windows) or the ⌘ key (Macintosh).

You can also invert stereocenters via the shortcut menu (right-click; *touchscreen:* long press; *Macintosh trackpad:* CTRL + Click). Choose **Invert Molecule Chirality** (will invert all stereocenters simultaneously) or **Invert Atom Chirality** (will invert just the selected stereocenter).

---

42. How do I add labels to a model?

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Labels (as many as desired) can be attached to all samples:

- Select **Build→New Label**, then *double-click* (or double-tap) on the background. Add any text.
- To edit an existing label, select the label from its shortcut menu (right-click; *touchscreen:* long press; *Macintosh trackpad:* CTRL + Click) and select **Edit Label**.
- To move an existing label, select the label and use the same method that you use otherwise for translating individual molecules.
- To delete a label, select the label from its shortcut menu (right-click; *touchscreen:* long press; *Macintosh trackpad:* CTRL + Click) and select **Delete Label**.

---

43. How do I build a two-component liquid model with a "straight interface"?

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The program does not include a building tool exclusively dedicated to the building of interfaces. However, you can use the ability do temporarily introduce "artificial gravity" (= gravity that is many orders of magnitude larger than the actual gravity at the surface of Earth) in order to create models with a more or less straight interface. The following is a description of how to build a model with an "Pentane-Water Interface" that is basically the same as that included with the program. The procedure can be generalized to other systems of two liquids.

You start by using the build panel in order to build a bulk simulation cell for the denser component (water in this case) at only *half* the density of the corresponding bulk liquid (i.e., for water declare the density as 0.5 g/cm^3 rather than the true 1.0 g/cm^3):

- Start a **New Sample**  . Use the **Build**  → **Entry-Level** build panel to *insert a single water molecule* (**Oxygen with two single bonds**).

- Go to the **Build** → **Simulation Cell** panel and select the **Liquid** tab. Set the "Density" to **0.5**, the "Number of Molecules" to **95**, and the "Periodic Boundary Conditions" to **XY** (note that this is *not* the default).
- Click **Apply** and wait for cell to be finished. Quit the build panel.
- Go to **Tools** → **Expert Keywords**. Add the following line: **EXTERNAL_FIELD=GRAVITY_CELL**.
- Also add the following line: **FIELD_STRENGTH=0.05**, then click **OK**.
- Rotate the cell just a tiny bit (this causes the new conditions to be recognized by the program).
- Run the simulation: the water phase will accumulate at the bottom of the cell. (Note that the type of gravity used in this situation is *independent* of the lab frame, i.e., if you "turn the cell around", you will see the accumulation at the top. In other words, the gravity acts strictly within the cell, independent of its orientation in space. This is the best choice for a system with only partial periodic boundary conditions.)
- Stop the simulation, then go back to **Tools** → **Expert Keywords** and *remove* the two extra lines added earlier.
- Use the **Build** → **Entry-Level** build panel to *insert a single molecule of pentane* (a chain of 5 tetrahedral carbons) in the upper "empty space."
- Go to the **Build** → **Simulation Cell** panel and switch to **Set Volume and Number of Molecules** in the drop-down menu at the top.
- Adjust the number of pentanes from "1" to **15**, then click **Apply**.
- Quit the build panel, then "manually move" (CTRL + right button + drag; *Macintosh trackpad:* CTRL + command key + drag) the few pentanes that ended up in the water phase to "holes" in the pentane phase at the top. This should only be necessary for a few molecules; most of the pentanes should have ended up at the top of the cell even without any extra manipulation.
- Start the simulation and wait for things to adjust themselves. If you want to make the interface "cleaner" (for example, move some water molecules that were pulled into the pentane phase back into the aqueous phase), you can do this via additional "manual moves" (Maxwell's Demon!).

---

44. I built the same system as found in the Stockroom, but it doesn't behave the same. Why?

Return to Top

When building molecules and bulk phase samples from scratch, ***ODYSSEY*** draws on a set of all-purpose rules and parameters (since the structure space of chemistry is huge and the computer obviously doesn't exactly know what you are after). Models in the Stockroom, on the other hand, are sometimes defined with custom settings that help with improving the general quality of the model.

As a consequence, self-built models will occasionally not "behave as well" as the pre-built models. However, it is rare for a self-built model to behave completely differently.

---

45. Are my students prevented from building "nonsense" molecules?

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No, just as is the case for plastic model kits, students are not prevented from building chemical nonsense structures. *However*, the "Validity" function provides feedback regarding the chemical reasonableness of any user-built or pre-built structure:

- From the **Build** menu, select **Validity** .

Working with this functionality allows students to assimilate chemical rules in an open-ended, highly interactive manner. Note that this approach is distinctly different from that of "drilling software" where the chemical intelligence has been programmed into a sequence of dialogs that leave the student with essentially nothing but the memorization of rules.

46. How do I avoid that datapoints are covered up by a plot's caption?

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To move the caption of plots (e.g., in order to expose datapoints "hidden" behind the caption):

- Position the cursor on the caption, click, and drag

47. What types of histograms can be generated?

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Three kinds of histograms can be generated:

- *Speed Distribution*: A histogram showing the probability of encountering speed values.
- *Translational Kinetic Energy Distribution*: A histogram showing the probability of encountering translational kinetic energy values.
- *Dipole Distribution*: A histogram showing the probability of encountering dipole moment values.

To generate a histogram:

- Select **Plots**  (also in the **View** menu).
- From the list of "Plots" (upper left corner of the Plots panel), select either **Speed Distribution**, **Translat. Kinetic Energy Distribution**, or **Dipole Distribution**.

The appearance of a histogram can be customized:

- Make the histogram "active" by selecting it.
- Bring up the "Plot Edit" panel by selecting the pencil icon at the top of the plots panel.
- Items available for customization include:
  - The histogram *Title*.
  - The histogram *Style*: **Bar** or **Line**.
  - The *Samples* setting: The default is **Single**. If set to **Multiple**, histograms for multiple samples (then automatically forced to be in the *Line* style) can be shown in the same plot.
  - *Labels* for the X and Y Axis.
  - The histogram range for the X Axis.
  - The number of tickmarks for the X Axis.
  - The number of histogram *Bins* within the range.

48. How do I print snapshots of molecular samples?

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- From the **File** menu, select **Print Sample Image...**.

49. How do I print a plot?

Return to Top

- Select the plot.
- From the **File** menu, select **Print Active Plot...**.

50. How do I print the text panel?

Return to Top

- From the **File** menu, select **Print Text...**.

51. How do I print the properties table?

Return to Top

Use the computer's screen-capture facility (many machines have a special "Print Screen" key):

- Paste the screen shot into any picture editing program.
- Using the editing features of the picture editing program, *crop* the screenshot around the Table of Properties.
- Print the cropped picture directly from the picture editing program.

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52. How do I print the entire screen?

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- Use the screen-capture facility of your computer—many machines have a special "Print Screen" key.
- Paste the screen shot into any picture editing program.
- Print directly from the picture editing program.

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53. Can *ODYSSEY* be used with interactive whiteboards?

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Yes, ***ODYSSEY*** is well suited for classrooms that are equipped with Smartboards or other interactive whiteboards.

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54. Can I use the program with PowerPoint?

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ODYSSEY can be seamlessly hyperlinked into PowerPoint. You have the choice among the following possibilities:

- Hyperlinking individual samples (no accompanying text included)
- Hyperlinking labs (Instructor's Edition only)
- Hyperlinking ***ODYSSEY***'s initial page

In each case all features of the ***ODYSSEY*** interface (simulation control icons, etc.) are fully available after following the hyperlink in your PowerPoint presentation. See the following items for detailed instructions on how to create hyperlinks.

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55. How do I hyperlink an individual molecular sample?

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- Save the sample that you want to hyperlink as an `.xodydata` file in a folder of your choice. Note that "surface data" such as electron densities, potentials, and orbitals will be lost (→ link through the initial page to access such samples).
- **`Windows`**: Before you can hyperlink the file into your PowerPoint presentation, you must "register" the `.xodydata` file extension with the Windows operating system (only this way PowerPoint will know that it needs to start ***ODYSSEY*** on encountering your hyperlink):
  1. Try to directly open the `.xodydata` file by double clicking on its icon. If ***ODYSSEY*** starts up and the sample displays, you don't need to do anything else. Move on to item 3).
  2. If ***ODYSSEY*** doesn't start up, right-click on the `.xodydata` file and select **Open With...**. In the ensuing dialog, navigate to the ***ODYSSEY*** folder and select "OdysseyStudent.exe" (Student Edition) or "OdysseyInstructor.exe" (Instructor's Edition). In most cases, you will find the ***ODYSSEY*** folder in the "Program Files → Wavefunction" folder of "Local Disk (C:)"
  3. Check off the "Always Open With This Program" option (this creates a registry entry).
  4. Open the file, then close ***ODYSSEY***.

- Creating the hyperlinks in PowerPoint:
  - **Windows**: Use the "Hyperlink" attribute and navigate to the location of your saved `.xodydata` file.
  - **Macintosh**: Use the "Action Settings" attribute (i.e., do *not* use the "Hyperlink" attribute). In the drop-down menu for "Hyperlink to", select "Other File..." and navigate to the location of your saved `.xodydata` file.

---

56. How do I hyperlink a lab?

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Entire labs from the program's **Labs** section can be hyperlinked in the Instructor's Edition (not in the Student Edition):

- Switch for the lab that you want to hyperlink from **Normal** to **Text Edit** (at the bottom of the text section).
- Click on **Save Lab** (in the lower right corner). In the subsequent dialog, click on either **Save as Teacher Lab** (includes comments and answers to questions if any are present) or **Save as Student Lab** (excludes comments and answers). Pick a location of your choice for the `.odylab` file that is about to be saved.
- In PowerPoint, create a hyperlink to the saved `.odylab` file—***ODYSSEY*** will open automatically when clicking on the hyperlink in the PowerPoint presentation.

---

57. How do I hyperlink the program's initial page?

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If you link to ***ODYSSEY***'s initial page, you can access any lab and/or sample via that hyperlink:

- In your PowerPoint slide, select the object that you wish to hyperlink.
- Right-click and select **Action Settings**.
- Select **Run Program** and browse for the name of the ***ODYSSEY*** executable:
  - **Windows:** The executable in the ***ODYSSEY*** folder is either "OdysseyStudent.exe" (Student Edition) or "OdysseyInstructor.exe" (Instructor's Edition) or an equivalent name for other versions of the program. In most cases, you will find the ***ODYSSEY*** folder in the "Program Files → Wavefunction" folder.
  - **Macintosh:** The executable is either "Odyssey Student [Release Number].app" (Student Edition) or "Odyssey Instructor [Release Number].app" (Instructor's Edition) or an equivalent name for other versions of the program. In most cases, you will find the file in the "Applications" folder.

Clicking on the object in the PowerPoint slide (when in presentation mode) will now always take you to the initial page of ***ODYSSEY***. You can go wherever you wish from there.

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58. How do I incorporate animations (sequences of frames) into my classwork?

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To incorporate ***ODYSSEY*** animations (dynamic sequences of frames) into lectures, PowerPoint presentations, laboratory experiments, and homework assignments:

- Save the corresponding molecular sample (normally as an `.xodydata` file) to the needed location.
- Run the corresponding simulation live, with full access to all visualization and system manipulation features of the ***ODYSSEY*** interface.

Since ***ODYSSEY*** is organized around the paradigm of live, interactive simulations, corresponding "movies" cannot be saved.

59. How can I assess student work carried out with *ODYSSEY*?

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ODYSSEY includes questions with many of the labs. Assessment can be carried out in several ways:

- Use the `Google Form` hyperlinks in the upper right corner of the labs (available in the ***ODYSSEY*** Instructor's Edition only) to create assignments where all student responses will be conveniently collated into a single spreadsheet.
  - Clicking at the top of the lab on `Google Form` allows you to create a **copy** of the supplied form.
  - Once you have the form in your own Google Drive, you can edit it (or you can use it as is). The answer options will be shuffled unless the feature is removed.
  - Share the form (for example, via a Google Classroom assigment).

  By opening the form in a web browser that is running in parallel with ***ODYSSEY***, students will be able to answer the questions. The collated student responses are downloadable as a spreadsheet (`.csv`) in the usual way (see the plentiful online documentation if you need to familiarize yourself with Google Forms).
- Students fill out the answer fields that follow the questions and then print out the answer sheet. If desired, snapshots of the molecular samples, or even galleries of snapshots, can be included.
- Alternatively, students can save the completed answer sheet to the computer for subsequent forwarding (for example by e-mail) for grading by the instructor.
- In a fourth scenario, the instructor prints out paper copies of the worksheets to be manually filled out by the students.
- Finally, if an online homework system is available, the teacher can enter questions and assignments into that system. Students work with ***ODYSSEY*** while entering their answers into the online homework system.

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60. In the Instructor's Edition, how do I print out the worksheets with the answers included?

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The following is only applicable to the Instructor's Edition, not the Student Edition:

- At the top of the Lab, select **Answers** such that the answers are shown below in the corresponding fields.
- From the **File** menu, select **Print Text...**.

---

61. How does *ODYSSEY* visualize dynamic phenomena?

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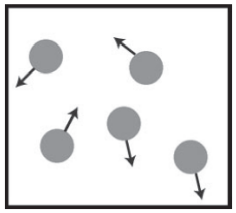
ODYSSEY's simulations are very different from the simulations of many other science media products. The motion of the molecules does *not* arise because a human designer used a software tool to create an animation. Instead, ***ODYSSEY*** uses the basic laws of nature in order to represent molecular matter and specifically molecular motion. Hence the dynamic behavior is an outcome of applying these laws, very much like the forces of gravity determine the motion of the planets in the solar system. In short, there are no “movie” files in ***ODYSSEY***.

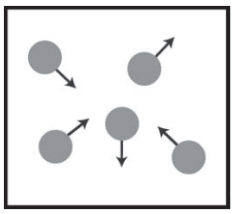
Suppose you want to simulate liquid water. When you load an ***ODYSSEY*** page with liquid water as the sample, you retrieve a file that contains the positions and velocities of a set of water molecules in a simulation cell at an arbitrary moment in time. The following picture symbolizes the “start configuration”—for simplicity we represent water molecules as single spheres:



In order to perform a simulation, ***ODYSSEY*** must do several things:

1. Calculate the forces acting between the molecules—this is done using a set of rules that were developed by chemists and other scientists in years of laborious research. While partly empirical, the rules are based on a strict physical analysis of the forces that act between atoms.

   The arrows in the following picture represent the computer's knowledge of the forces acting on the molecules:

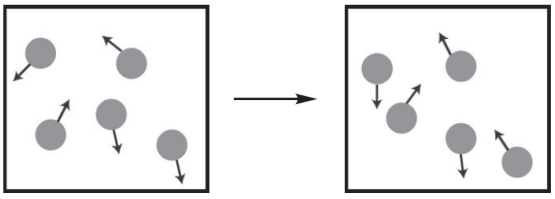


2. Next, ***ODYSSEY*** applies a formula that has been known since 1686. Newton's Second Law states that the force acting on an object and the object's acceleration are proportional:

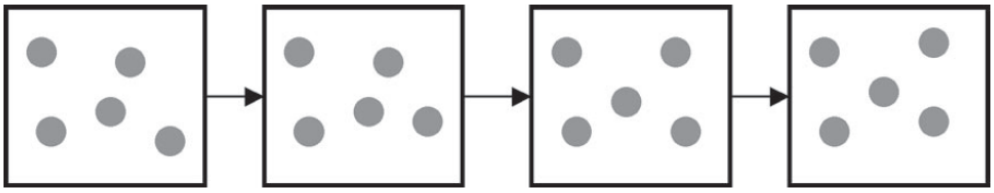
   $F = m \bullet a$

   Since we already know the force acting on a given water molecule (see above) and since the mass of a water molecule is well-known, we can now calculate the molecule's acceleration. Knowing the molecule's acceleration, however, amounts to being able to predict where it will move to and what its new velocity will be! More formally, this is called solving the "equations of motion," and it is really no different than predicting the trajectory and velocity of a satellite that is fired off into space (all we need to know are the "initial conditions").

   If we apply this procedure to all water molecules in the simulation cell (in fact, it is applied to all molecules at once), we get the next snapshot of our system, or the next "time step":



   In order to sustain a full-fledged simulation, all that is required is to repeat the same steps, again...and again…and again:



When you watch a simulation of liquid water in ***ODYSSEY***, the computer is calculating “time steps” (the program actually makes several steps between screen updates—a technical detail). The steps are separated by approximately 10^{-15} sec of physical time—a very short time indeed! Typically, the computer calculates several thousand time steps during a simulation (up to hundreds of thousands of steps for some systems).

In the start configuration as well as at any time thereafter, each molecule has not only a position, but also a certain velocity. In fact, where the molecule will move to in the next step is affected by both the force acting on the molecule and its velocity. The molecule’s velocity is updated step after step, just like its position.

---

62. How do I simulate a sample whose dynamics button is faded out?

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Some of the samples in ***ODYSSEY*** are "static", i.e., the toggle below the sample for initiating a room temperature simulation is faded out. Samples are shown in this manner for one of the following reasons:

- The selected sample has precalculated electronic surfaces (such as molecular orbitals or a polarity map) that would be "lost" as soon as the system changes its geometry. Note that updating the quantum mechanics-based data while the simulation is running (→ solving the time-dependent Schrödinger equation) is simply not feasible with an off-the-shelf computer.
- The selected system is a case where the classical potential function is unable to keep the system "stable" when a molecular dynamics simulation is initiated.
- The selected system is a single atom in vacuum—the concept of "dynamics" wouldn't make much sense.

If desired, even static samples can be animated:

- From the **File** menu, select **Save Sample**.
- In the ensuing dialog, click on **Save**, i.e., save the sample using the shown default file name and file type (it doesn't even matter where you save the sample—you won't need to access it again).
- The operation makes the program switch to a new tab where a *copy* of the original sample is shown (minus any electronic surfaces if such were available before) and where the dynamics button is not faded out. Click on the button to start a room temperature simulation.

---

63. Can I depict lone pairs?

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To display a schematic representation of lone pairs (where applicable):

- From the **Style** menu, select **Lone Pairs**.

Note: For samples with "electronic surfaces," the visualization of lone pairs may not always be available.

---

64. Why can't I highlight the collisions of the sample of gas that I built?

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The "Collisions" attribute (in the **Style** menu) is only available for samples whose density is not too high (this protects the computer from being overwhelmed by collision counting in higher density samples). A rule of thumb is that letting the pressure drop to less than ~10 atm (use **Build**  → **Simulation Cell → Gas**) will make the "Collisions" attribute available.

---

65. Can I highlight the sequence of residues in proteins and nucleic acids?

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Proteins and nucleic acids that contain explicit residue information (this includes samples that have been built with ***ODYSSEY***'s Peptide or Nucleotide builder as well as PDB files from the Protein Data Bank) can be displayed as "Ribbon" models with a visual indicator for the sequence of residues:

- From the **Style** menu, select **Ribbons** (if the entry does not appear in the menu, then the underlying file does not contain the necessary residue information), and in the following submenu, select **By Residue**.

---

66. Why do molecules of liquids and solids sometimes "disappear"?

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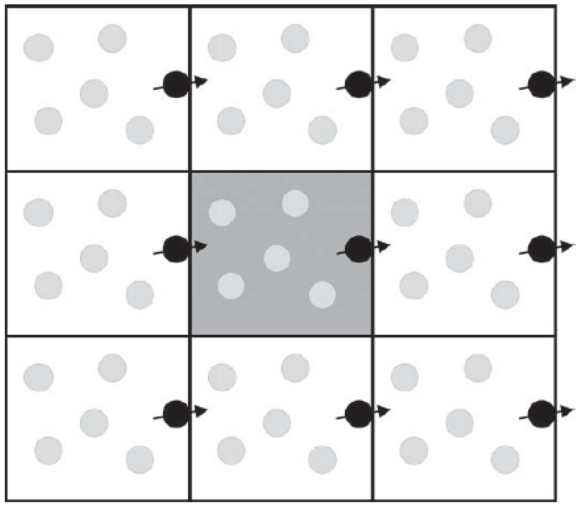
In simulations of liquids or solids, you may notice that some molecules or atoms seem to *leave* the simulation cell, i.e., when close to one of the boundaries they often seem to be gone a few moments later. If you look carefully, however, you will also notice the opposite, namely "new" molecules (or atoms) that seem to enter the simulation cell.

What is going on? The explanation is that there really aren't any boundaries when ***ODYSSEY*** simulates a liquid or solid despite the obvious presence of a simulation cell. What the program really uses is called "Periodic Boundary Conditions"—essentially, the simulation cell wraps around in each of the three dimensions:



If, for example, a molecule leaves the simulation cell towards the right, the same molecule re-enters from the left! In effect, we have allowed the molecule to cross the system boundary while not losing anything—the system density remains perfectly constant.

The huge advantage of this approach is that there are no walls in the system that can interfere with the calculated bulk properties. Just think of a glass of water: The vast majority of the ~10^{23} molecules are *not* close to any of the container walls. Periodic boundary conditions allow us to accomplish the same in a simulation. In effect, the cell boundaries become a device for organizing the simulation rather than a representation of an actual container.

---

67. Why do some molecules at the simulation cell boundaries look "clipped"?

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ODYSSEY generally employs "Periodic Boundary Conditions" when simulating liquids and solids (see FAQ "Why do molecules of liquids and solids sometimes disappear?"). By default, the visualization is such that molecules always leave and re-enter the simulation cell as “complete” entities, i.e., all atoms of a given molecule are drawn *either* on one side *or* on other side of the simulation cell.

Alternatively, a visualization mode is available where any molecules that fall right on the boundaries are shown with some of their atoms still on one side, while the molecule's other atoms are already shown re-entering on the other side. This will make all surfaces of the simulation cell look “smooth” (not corrugated). At the same time, it will also make some molecules look “clipped”, i.e., some atoms seem to be missing (in fact, they can be seen on the other side of the simulation cell). To select this type of visualization:

- From the **Tools** menu (Windows) or from the **Odyssey** menu (Macintosh), select **Preferences...**
- Check (select) **Alternate Visualization of Periodic Boundaries**.

Note that the clipping preference only affects the *visualization* of molecular systems—the underlying simulations are completely unaffected by the preference setting. Also note that some systems (such as liquid sulfur) have a fixed setting for the periodic boundary clipping that is not overridden by the preference setting.

---

68. Can I show two samples at the same time?

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Yes, select **Compare**  → **Side-by-Side** (also in the **View** menu) to add a second sample to the one originally shown.

---

69. What can I do if the graphics performance is poor when using the "Space Filling" style?

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On **Windows** computers, you can try the following:

- In the **Tools** menu, select **Preferences**.
- Check off **Reduced Graphics for Slower Machines**. Click **OK**.

---

70. What can I do about unsatisfactory graphics performance when running on battery?

Return to Top

On **Windows** computers, you can try the following:

- In the **Tools** menu, select **Preferences**.
- Check off **Reduced Graphics for Slower Machines**. Click **OK**.

---

71. How do I measure physical properties?

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To query the numerical values of physical properties:

- Select **Properties**  (also in the **View** menu).
- From the **Add Property** menu in the lower left corner, select the desired property, such as **Atom** → **Electronegativity**
- If a *selection* is required, then this is indicated in the column to the right of the properties list; e.g., adding **Mole Fraction** to the list necessitates a **Select Group** action.

---

72. How do I change the physical units?

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To change the default settings:

- From the **Tools** menu (**Windows**) or from the **Odyssey** menu (**Macintosh**), select **Preferences...**
- Adjust the radio buttons within **Units** to reflect your desired settings.

73. Can I overwrite the "slider" limits in the property table?

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Built-in limits for temperature, volume, and composition sliders can be overwritten by entering the property value as a numerical value:

- Click the *numerical value* field for the property in the "Table of Properties" and enter your desired value (excluding units).

Note: The limits of the corresponding slider are immediately updated to include the newly requested value.

---

74. How do I minimize the energy of a sample?

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To minimize the energy of a sample:

- Select **Minimize** (also in the **Build** menu).

Note: Systems with a container boundary (typically gases) or systems under periodic boundary conditions (liquids and solids) are minimized at constant volume.

For some samples, particularly those with electronic (wavefunction-based) data, the energy minimizer and the dynamics option are deliberately disabled. If you really must minimize the energy of such a system, you can still do so after saving the sample as a new file.

---

75. How are the (classical) energies calculated?

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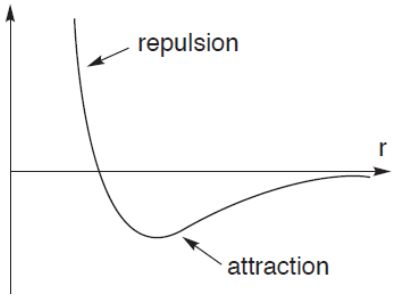
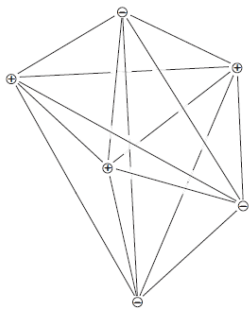
For each molecular sample, ***ODYSSEY*** calculates the energy of interaction between the atoms that are present, regardless of whether the sample is an isolated molecule or a bulk phase with many molecules. The "potential function" is very complicated—there are many hundreds of parameters for all the elements and valence states encountered in chemical compounds. At least conceptually, however, the potential function can be thought of containing the following main terms:

- Intermolecular *repulsive* energy and intermolecular *attractive* energy: the former is a steeply varying term for steric interactions at short distance (makes a close "overlap" of non-bonded atom unlikely); the latter represents Van der Waals forces (dispersion forces) between non-bonded atoms.

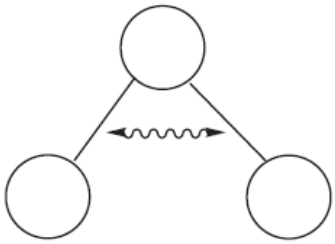


- *Coulomb* energy (both inter- and intramolecular): energy term due to the assignment of "effective charges" to all the atoms of a molecule; at the intermolecular level, this term represents charge-charge, charge-dipole, and dipole-dipole interactions.

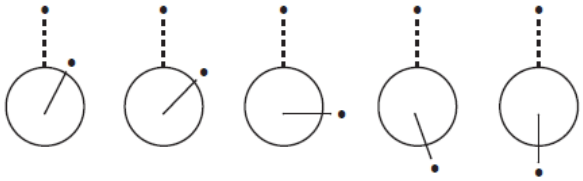


- Intramolecular energy of *bond-stretching*: a spring-like term that represents distortions of a bond from its equilibrium bond distance. This energy term (and sometimes also the following one) is effectively absent in simulations where the molecular geometry is kept rigid.

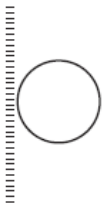
- Intramolecular energy of *angle-bending*: the energy that it takes to distort any three bonded atoms from their preferred bond angle.



- Intramolecular energy of *rotation around dihedral angles*: a periodic function that describes the relative energies of the various "staggered" and "eclipsed" conformations of any four consecutively bonded atoms.



- Repulsive interactions between the molecules of the system and the confining *walls* (if there are any).



There are a few other terms, but essentially it is the sum of these energies that yields the total energy of a given system. Calculation of the derivatives of the total energy with respect to the coordinates of all the atoms yields the intermolecular forces that are at the heart of the algorithm that takes the system from one time step to the next. As the energy depends on the coordinates of all the atoms in the system, the calculation has to be repeated even if only a single atom moves.

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76. Why are the molecules in dynamic simulations often "rigid"?

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If you monitor the intramolecular bond distances during an ***ODYSSEY*** simulation, you may notice that often they do not change. Why? Keeping the molecules partially rigid is a common device for "speeding up" the simulations; it allows for using a larger physical time step than would otherwise be possible.

The rigidity is an excellent approximation of the real physical situation for very stiff *hydrogen*-containing bonds because these bonds are largely in the vibrational ground state (which has its maximum amplitude at the equilibrium bond length). However, the enforced rigidity is of relatively little consequence for the calculated properties also in many other situations.

77. How are the Polarity Maps, Low Density Surfaces, and High Density Surfaces calculated?

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- ***ODYSSEY*** uses the coordinates *as they are defined by the user* (which may include arbitrary distortions of the molecule, arbitrary relative replacements of the molecules in a cluster, etc.). If, and only if, the user has previously hit **Minimize**  , the geometry is the one obtained by optimization with ***ODYSSEY***'s classical mechanics force field. If the user has *not* previously hit **Minimize**, the structure is the one defined by the user. (This corresponds to the "Energy" option in the program ***SPARTAN*** and *not* to the default "Equilibrium Geometry" option.)
- The program then uses semiempirical quantum chemistry (PM3 method) to generate a trial wavefunction.
- The final wavefunction comes from ab initio quantum chemistry using the Hartree-Fock method and the 3-21G basis set. Note that the basis set is small and that correlation energy is not included. This "cheap" type of quantum chemistry is sufficient if the emphasis is on qualitative features and standard structural properties (bond lengths, bond angles). The approach is insufficient for transition states, unusual bonding schemes, and high spin molecules (i.e., transition metals). The quantum mechanics capability in ***ODYSSEY*** is not intended to be a substitute for a *bona fide* quantum chemistry program such as ***SPARTAN***.
- **Polarity Maps** (= Electrostatic Potential Maps in ***SPARTAN***), **Low Density Surfaces** (= Density Surfaces in ***SPARTAN***), and **High Density Surfaces** (= Bond Density Surface in ***SPARTAN***) are calculated from the square of the wavefunction and (when applicable) the electrostatic potential.

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78. What are the isovalues and what is the range of the calculated electronic surfaces?

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The following applies to surfaces calculated with the **Electron Cloud**  option in ***ODYSSEY***. It does not apply to surfaces from `.spartan` that have been read in—such surfaces will frequently have very specific custom settings.

- The isovalue for calculated **Low Density Surfaces** is 0.002 electrons per a.u.^{3}. This is the same as the default setting for "Density" in ***SPARTAN***.
- The isovalue for calculated **High Density Surfaces** is 0.2 electrons per a.u.^{3}. This is larger than the default setting for "Density (Bond)" in ***SPARTAN*** (which is 0.08 electrons per a.u.^{3}).
- The range for calculated **Polarity Maps** is –175 kJ/mol to +175 kJ/mol for uncharged systems and –800 kJ/mol to +800 kJ/mol for charged systems. This is somewhat different from the default range for "Electrostatic Potential Maps" in ***SPARTAN*** (which is –200 kJ/mol to +200 kJ/mol).

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79. Can the isovalues of calculated electronic surfaces and the limits of the range be adjusted?

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In order to keep the program reasonably simple, ***ODYSSEY*** does not provide the ability to set isovalues and range limits in an arbitrary fashion. Use a dedicated quantum chemistry program (such as ***SPARTAN***) for such tasks.

80. What is the number shown as the total energy?

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- For single molecules and well-defined one-component systems, **Energy → Total Energy (Molar)** is available—it is the classical strain energy of the molecule or system (see the FAQ "How are the classical energies calculated?") given ***ODYSSEY***'s force field and some arbitrary zero of energy. Because of the varying zero of energy, this number is unsuitable for comparing molecules or systems that are not closely related.
- For multi-component systems, **Energy → Total Energy** is available as an absolute, tiny number (typically on the order of 10^{-21} J). This approach avoids ambiguities regarding the meaning of "molar" in systems with more than one component.
- After calculating an isosurface with one of the **Electron Cloud** options, **Energy → Energy (from Quantum Theory)** becomes available in the **Properties** table. Note that this quantity that has absolutely nothing to do with the **Total Energy (Molar)** that represents the (classical) strain energy of the molecule. It will typically be a huge number of hundreds of thousands of kJ/mol because of the strong attraction between electrons and nuclei in the system.

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81. How are partial (atomic) charges and the dipole moment calculated?

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- The properties available as **Electrostatics → Partial (Atomic) Charge** and **Electrostatics → Dipole Moment** are by default calculated from ***ODYSSEY***'s classical force field. They are replaced by quantum mechanically calculated values as soon as an isosurface has been requested with one of the **Electron Cloud** options. The partial charges are "electrostatic charges" as familiar from ***SPARTAN***.
- Quantum mechanically calculated values are automatically displayed if a `.spartan` model is opened in ***ODYSSEY*** and that model includes a calculated wavefunction (at whatever level of theory).

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82. How are hydrogen bonds identified?

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ODYSSEY identifies a hydrogen bond if an atom with an attached hydrogen is close to another atom and *all* of the following criteria are satisfied:

- The partnering atoms must involve a *known* hydrogen bond donor and a *known* hydrogen bond acceptor. Oxygen, nitrogen, and fluorine are the most important formers of hydrogen bonds, but not necessarily in all valence states. In liquid water, for example, sp^3 oxygen acts as both a donor and an acceptor of hydrogen bonds. The sp^2 oxygen of carbonyl groups, however, can only act as an acceptor and must pair up with some other donor if it is to form a hydrogen bond.
- The distance between the hydrogen atom and the acceptor atom has to fall within a range of 122-260 pm.
- Overtly bent hydrogen bonds are excluded by requiring that the angle ∠(hydrogen atom-donor atom-acceptor atom) is smaller than a set value. For water and ammonia this angle is 30°, for hydrogen fluoride it is 86°.

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83. How are enthalpies calculated?

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For some substances enthalpies ***ODYSSEY*** calculates enthalpies (equivalent to heats of formation) from empirical formulas that represent best fits of experimental data. Following the usual approach of thermochemistry, the standard enthalpy is taken as zero when dealing with an element in its standard state at 25°C (even though the entropy is of course not zero).

In order to allow for an intuitive interpretation of temperature changes, the program adopts a unique reference state, i.e., the displayed value is always relative to the elements in their standard states at 25°C. Note that this is different from what is implicit in the NIST-JANAF thermochemical tables and similar data collections. If such tables give heats of formation as a function of temperature, the assumed reference state is temperature dependent because the enthalpy of formation of the stable phase of an element is by definition zero for all temperatures. ***ODYSSEY*** refrains from working with varying reference states.

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84. How are entropies calculated?

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ODYSSEY displays standard entropies. The algorithm used depends on the complexity of the given system and involves certain combinations of analytical statistical thermodynamical theory and empirical formulas (with the latter representing best fits of experimental data).

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85. How are free energies calculated?

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For some substances ***ODYSSEY*** calculates free energies from empirical formulas that represent best fits of experimental data. Following the usual approach of thermochemistry, the standard free energy is taken as zero when dealing with an element in its standard state at 25°C (even though the entropy is of course not zero).

In order to allow for an intuitive interpretation of temperature changes, the program adopts a unique reference state, i.e., the displayed value is always relative to the elements in their standard states at 25°C. Note that this is different from what is implicit in the NIST-JANAF thermochemical tables and similar data collections. If such tables give free energies as a function of temperature, the assumed reference state is temperature dependent because the free energy of the stable phase of an element is by definition zero for all temperatures. ODYSSEY refrains from working with varying reference states.

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86. Do the calculated properties reproduce experimental data?

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There is no blanket answer to the question. In many cases, there is qualitative agreement between calculated and experimentally measured properties. Particularly "trends" (such as variation with atomic mass, variation with dipole moment, or variation with temperature) are very often predicted correctly. Predictions that are quantitatively correct are rare as the program employs models that are computationally inexpensive and therefore imperfect.

While not very common, outright failures also occur. However, it should be kept in mind that the presence of failures and limitations is a *defining characteristic* of all models—not only scientific models, but also models anywhere else. The pedagogical value of models derives from their ability to be experimented with, not from being perfect replacements of the "real thing."

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87. Why do the vapor molecules don't seem to move faster than the corresponding liquid molecules?

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In order to facilitate observations of a wide variety of systems, ***ODYSSEY*** *autoscales* the size of the simulation cell to the screen size regardless of the physical state of the substance. As gas phase simulation cells are typically much bigger than condensed phase simulation cells (see the Cell Dimensions displayed above the sample area!), the net motion in the gas phase *is* in fact much faster than the net motion in the liquid phase.

In accordance with temperature, the molecular speeds themselves are also higher in the gas phase than in the liquid phase:

- Select **Properties**  (also in the **View** menu).
- From the **Add Property** menu in the lower left corner, select **Dynamics → Speed**.
- Compare the speed data for the liquid phase (low temperature) and gaseous phase (high temperature) of the same substance.

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88. Does *ODYSSEY* assume ideal gas behavior?

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No, ***ODYSSEY*** never assumes ideal gas behavior. Gas molecules are always modeled as particles of finite volume that exhibit non-negligible interactions (if sufficiently close).

Nevertheless, ideal gas behavior will be *observed* in many situations, namely whenever the physical conditions happen to closely correspond to the assumptions that are implicit in the Ideal Gas Law.

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89. Can I simulate the liquid-vapor transition?

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The liquid-vapor transition can easily be simulated for most liquids:

- Retrieve a sample of liquid from the Stockroom, or build one yourself using the 3D Model Kit (you will need to know the density of the desired liquid).
- Select **Properties**  (also in the **View** menu).
- From the **Add Property** menu in the lower left corner, select first **Thermodynamics → Temperature** and then **Thermodynamics → Volume**.
- Start the simulation.
- Overwrite the **Volume Field** by a number that is at least 100 times bigger than the number shown.
- Resize the simulation cell: **Edit → Resize**.
- Increase the temperature with the slider provided to speed up the process of evaporation.

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90. Will gases condense on cooling?

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Yes, given sufficient simulation time and a sufficiently low temperature, samples of gas will eventually show condensation. However, the condensation will happen via the formation of irregular molecular clusters rather than through the formation of a "neat" horizontal interface. The reason for this is the insignificance of gravitational forces in samples that are as small as those simulated by ***ODYSSEY*** (see FAQ "When I turn a partially filled simulation cell upside down, why doesn't the liquid flow to the bottom?").

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91. When I turn a simulation cell "upside down," why doesn't the liquid flow to the bottom ?

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The reason for this at first glance strange behavior of partially filled simulation cells is that gravitational forces are so weak that they do not make a difference on the time scale of molecular simulations. Phenomena that crucially depend on the effects of gravity, such as the flow of liquids and the formation of "neat" interfaces, are therefore not reproduced by the simulations. There is simply not enough time for these phenomena to become noticeable.

Effectively, the behavior observed in ***ODYSSEY*** simulations is the same as that seen for real-world, macroscopic samples in the absence of gravity (such as on any orbiting spacecraft).

92. If I cool a liquid to below its freezing point, why doesn't it freeze?

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ODYSSEY focuses on real simulations of physical phenomena, rather than on cartoon-style animations. While the freezing transition *can* be simulated, it is very hard to do and requires sample sizes and time scales that lie beyond the scope of ***ODYSSEY***.

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93. If I melt a crystal of ice, why doesn't its density increase?

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For a number of reasons, ***ODYSSEY*** performs its simulations with unit cells of constant volume. The user has to manually adjust the volume in order to represent changes in density:

- Select **Properties**  (also in the **View** menu).
- From the **Add Property** menu in the lower left corner, select first **System** → **Density** and then **Thermodynamics** → **Volume**.
- Adjust the volume with with the provided slider so as to reach the desired density.

Alternatively, the **Build**  → **Simulation Cell** → **Liquid** tab can be used for density adjustments.

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94. When I dissolve a molecule of hydrogen chloride in liquid water, why doesn't it dissociate?

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While ***ODYSSEY*** is capable of representing a large variety of physical and chemical processes, the program cannot directly carry out real-time simulations when one or both of the following apply:

- Covalent bonds are being broken or formed.
- The time scale of the process in question does not fit within the typical picosecond (10^{-12} sec) time range that is accessible to the program.

The dissociation of strong acids falls into the first one of these categories. If desired, models of the dissociated species—such as $(Cl^-)_{aq}$ and $(H_3O^+)_{aq}$, $(H_5O_2^+)_{aq}$, or $(H_7O_3^+)_{aq}$—can be built with ***ODYSSEY***'s 3D Model Kit.

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95. If I have a sodium chloride–water interface, why don't the ions gradually dissolve?

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While ***ODYSSEY*** is capable of representing a large variety of physical and chemical processes, the program cannot directly carry out real-time simulations when one or both of the following apply:

- Covalent bonds are being broken or formed.
- The time scale of the process in question does not fit within the typical picosecond (10^{-12} sec) time range that is accessible to the program.

The process of dissolving an ionic solid falls into the second one of these categories. The issue can still be addressed by building "snapshots" of the system in various stages of the dissolution process. (There is an entire Lab dedicated to this topic.)

96. Can all molecular samples be saved?

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Yes, the currently displayed sample can almost always be saved as an `.xodydata` file into locations outside of the ***ODYSSEY*** folder (the program folder itself is *Read Only* in order to preserve the integrity of the software):

- From the **File** menu, select **Save Sample As...**
- Navigate to the desired location, select a filename, and save the file.
- The saved sample is shown in a new browser tab.

The following restriction applies when saving samples:

- "Surface" information (Orbitals, Electron Density Distributions, Electrostatic Potentials, Polarity Maps) is not saved.

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97. In what format should three-dimensional samples be saved?

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The default file format is "`.xodydata`" which is XML-based and includes a complete record of the model except for wavefunction-based surfaces (the latter can be read by ***ODYSSEY***, but cannot be saved).

The alternate `.spinput` format is needed for exporting files to Wavefunction's program ***SPARTAN***.

You can also make yourself an "Expert" (go to the **Preferences** dialog). You are then able to save samples as SMILES strings—these are understood by many other chemistry programs.

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98. Can I open saved samples with "drag and drop"?

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All ***ODYSSEY*** files (`.xodydata` or `.odyssey`) and also all `.spartan` files can be opened by dragging the file onto the desktop shortcut created by the installer.

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99. Can pictures of the molecular samples be saved?

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Yes, screen shots of molecular samples can be saved in several formats:

- From the **File** menu, select **Save Sample Image As...**
- Choose a file name and one of the following file types:
  - **.jpg** (**Windows** and **Macintosh**)
  - **.png** (**Windows** and **Macintosh**)
  - **.bmp** (**Windows** only)
- Save the image file to the desired location.

Tip: For best resolution, zoom in prior to saving the screenshot. You can furthermore hide the text panel using the corresponding toolbar icon.

The *clipboard* (**Edit → Copy**) can also be used to export pictures.

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100. Can I import files from other modeling programs?

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ODYSSEY reads `.pdb` files (generated by most other modeling programs and also the file format of many databases), `.spartan` files (generated by Wavefunction's program ***SPARTAN***), and SMILES files (`.smi`). Other file formats understood include XYZ (`.xyz`), ChemDraw (`.cdx`), and ISIS/Draw (`.skc`).

Use **File → Open** in order to import an external file.

101. Is *ODYSSEY* compatible with Protein Data Bank files?

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Yes, ***ODYSSEY*** can serve as a high quality viewer for any Protein Data Bank file.

102. Can I annotate the text pages?

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Yes, all ***ODYSSEY*** pages can be annotated:

- Click on the "document" icon (looks like a piece of notebook paper) at the top of the text panel. This opens a *Notes* page that accepts any text that is entered.
- Return to the originating page by clicking on the **Save+Close** link at the bottom of the *Notes* page.

The annotations for a given Experiment or Stockroom entry are retained by the computer and will be shown whenever you return to the corresponding *Notes* page later.

103. Can I add my own content?

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- Yes, the labs in the Instructor's Edition of ***ODYSSEY*** are editable (although this does not always strictly extend to all parts of a given page; some parts can only be deleted, not edited).
- If uploaded to the instructor's own website, the custom content can be made accessible to students by providing hyperlinks (***ODYSSEY*** will automatically open when clicking on a corresponding hyperlink in a webpage).
- In the Instructor's Edition, entirely new labs can also be created after setting the **Enable Authoring of New Labs** flag in the **Preferences** dialog.

Please contact Wavefunction with suggestions for incorporation of new content into future releases of the program.