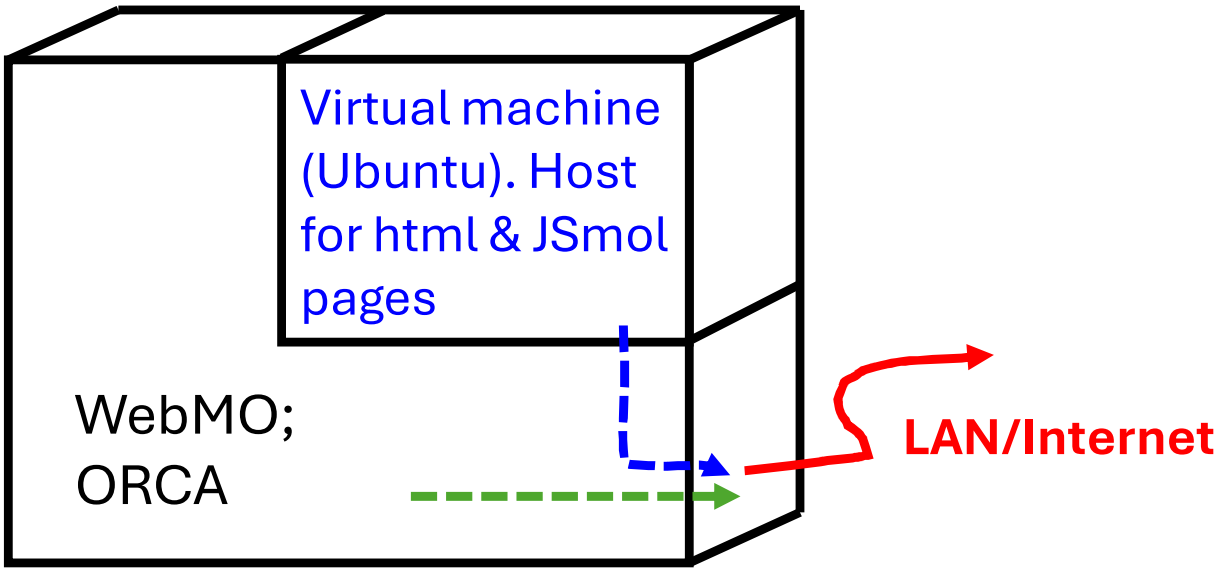
JSmol webpages

JSmol is a web-enabled version of Jmol where the Jmol commands are contained in script sections within the html page. A typical JSmol page contains a 2-column table with a molecular display area and, in the second column, programmable buttons.

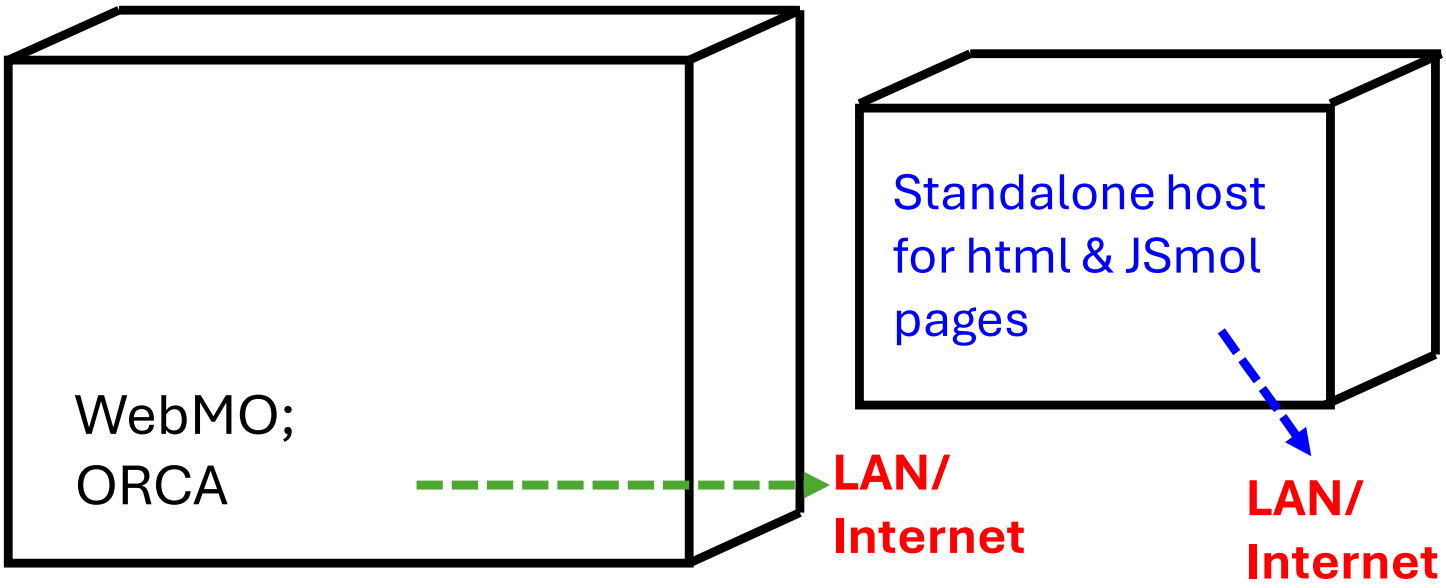
All common browser programs automatically display JSmol molcules.

Presenting JSmol pages for students requires a server computer connected to the Internet and running Apache or Microsoft IIS. This could be a dedicated web server if one is available. If not, a virtual machine (VM) running another instance of Linux and the Apache web host program can be installed on the WebMO hosting machine.

The webpages shown here are hosted on a VirtualBox VM with 2 CPUs, 4 GB memory, and 20 GB of disk space (a minor inconvenience on a modern multi-core server). This is enough for JSmol and webpages for several chemistry courses. VirtualBox for Linux, Windows, or Mac computers is free.



A virtual machine is installed on WebMO server with the two Linux OS's sharing a network interface. In my experience, the Linux/Apache instance running WebMO cannot also host a normal html websites.



Alternatively, a separate server can host Jsmol webpages.

Setting up a VirtualBox VM on a Linux host

Install VirtualBox

- Download VirtualBox for Linux (VirtualBox-7.0-7.0.18_162988_el8-1.x86_64.rpm)
- As root:
  $ dnf install gcc make SDL qt5 kernel-headers* -y
  $ dnf localinstall [path_to_rpm_file]

Install Ubuntu and configure as web server

- Download ubuntu-24.04-desktop-amd64.iso
- Start VB
- Machine, New
- Select the above iso file in its download location.
- Check “skip unattended”
- Choose username, password, hostname, and domain name. (These are VB’s reference to the guest machine. The actual Linux OS username, password hostname and domain are set inside Ubuntu)
- Memory and processors (8 Gb and 2 procs are plenty).
- Hard disk (recommend about 50 GB). Check pre-allocate. Should be plenty of room if your host system as a 1- or 2-TB SSD or NVME drive.
- Finish

- Ubuntu Install dialog starts. Check download updates. Choose username and password. Ubuntu automatically partitions the disk.
- Log in
- Activate the root user.
  $ sudo –i
  $ (your password)
  $ passwd
  $ (enter root password)
  $ (retype root password)
- As root: $ apt install apache2 openssh-server

- Turn on the firewall and open it to ssh and html connections:
  $ ufw enable
  $ ufw allow ssh
  $ ufw allow http
  $ ufw allow https
  $ ufw status
- Create webmasters group and add the ubuntu user to the group:
  $ groupadd –g 499 webmasters
  $ usermod –aG webmasters <ubuntu user>
- Restart VM:
  $ reboot now
- log back in as ubuntu user, then
  $ su
- Adjust permissions on website directory /var/www/html per https://gist.github.com/stefanbc/9956ed211cd32571e73f
- Log off

SSL certificate. If your WebMO server has an SSL certificate installed, then use the same procedure to obtain and install SSL and the SSL certificate on the VM.

To connect the VM to the network, in VirtualBox Manager, select the VM, click Settings; Network, Attached to…Bridged Adapter. Name..choose the name of the working ethernet adapter on the host machine, most commonly, eno1.

- Lastly create and test Jsmol and other html pages on your local machine, then upload to the VM:
- Download and install XAMPP for windows.
- The c:/XAMPP/htdocs folder is analogous to /var/www/html on the webserver. Save html files within the file structure in xampp, then upload same folders and files using Filezilla or WinSCP.

John Keller University of Alaska Fairbanks 2024

JSmol webpages

JSmol is a web-enabled version of Jmol where the Jmol commands are contained in script sections within the html page. A typical JSmol webpage contains a 2-column table with a molecular display area and programmable buttons in the second column.

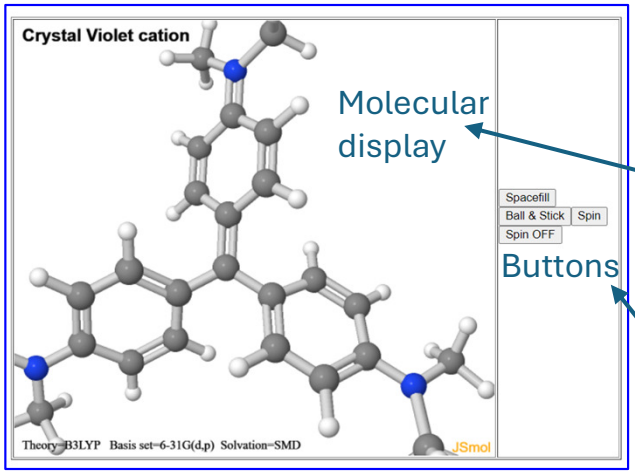
Typically, the subject .mol file is placed in the same directory as the .html file.

Also, the JSmol program files must be present on the server and the JSmol page must reference its location. Here it is 2 levels up: `"../../JSmol.min.js"`)

```
/var/www/html
    /jsmol-16.1.63
        JSmol.min.js
        /j2s
        /org
            /cv-orca
                cv.mol
                cv.htm
                oh-4wat.htm
                oh-4wat-orc.mol
                etc
```

Download and expand Jmol and JSmol

Visible web page



Html code for crystal violet web page

```
<!DOCTYPE html>
<html>

<head>
<title>Crystal violet cation</title>
<meta charset="utf-8">
<script type="text/javascript" src="../../JSmol.min.js"></script>
<script type="text/javascript">

$(document).ready(function(){

Info = {
    width: 550,
    height: 500,
    debug: false,
    j2sPath: "../../j2s",
    disableJ2SLoadMonitor: true,
    disableInitialConsole: true,
    addSelectionOptions: false,
    use: "HTML5",
    readyFunction: null,
    script: "load cv.mol; background white; set antialiasdisplay on; wireframe 0.15;
    spacefill 22%; set cameradepth 0.4; select *; set multiplebondradiusfactor 0.75;
    set multiplebondspacing -0.5; color bond gainsboro; rotate z -12; zoom 100; set
    echo top left; font echo 20 sansserif bold; color echo black; echo Crystal Violet
    cation; set echo bottom left; font echo 14 serif plain; echo Theory=B3LYP   Basis
    set=6-31G(d,p)  Solvation=SMD;"
      }

$("#mydiv").html(Jmol.getAppletHtml("jmolApplet0",Info))
$("#btns").html( Jmol.jmolButton(jmolApplet0,  " spacefill 90% ","Spacefill")
  +Jmol.jmolButton(jmolApplet0, " isosurface off; wireframe 0.15; spacefill 22%; set
  cameradepth 0.4; set multiplebondradiusfactor 0.75; set multiplebondspacing -0.5; "
  ,"Ball & Stick")
  +Jmol.jmolButton(jmolApplet0, "spin y 30","Spin")
  +Jmol.jmolButton(jmolApplet0, "spin off","Spin OFF")
)
});

</script>
<style type="text/css">
.auto-style1 {
    font-size: small;
}
</style>
</head>
```

To make your own Jsmol page, **save this one** and replace the Jmol commands with your own.
https://chem4.cns.uaf.edu/jsmol-16.1.63/org/cv/cv.htm

Informational webpage

Department of Chemistry & Biochemistry

Crystal Violet and Quantum Theory

5 Models for Study

The following are links to webpages that display 3D models of crystal violet and other molecules involved in the color bleaching reaction. After opening each webpage, download the model to your computer as a .mol file. Right-click on the molecule (Mac, ctrl-click) and use the File, Save, entry on the pop-up menu.

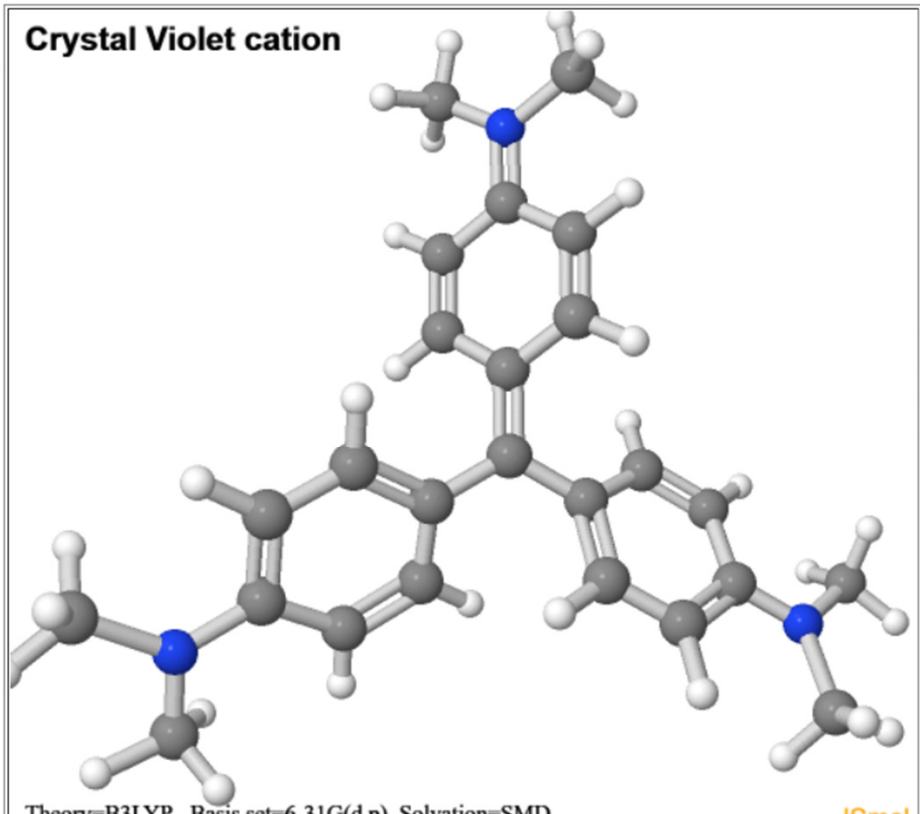
- Crystal violet cation CV
- Crystal violet alcohol CVOH
- OH- ion solvated by 4 waters OH-..4waters
- Crystal violet alcohol solvated by 4 waters CVOH...4waters
- Crystal violet - OH transition state solvated by 4 waters CV..OH...4waters

A 2-min Youtube video showing how to save a .mol file and import the structure into WebMO

- CV cation surfaces

JSmol web page

Crystal Violet cation



Spacefill
Ball & Stick Spin
Spin OFF

Rotate: left-click-and-drag. Translate: Crtl-right-click-and drag. Zoom: Shift-left-click-and-drag.