Investigating Crystal Violet Reactivity and Color with Quantum Theory and Interactive Webpages

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Notes for Instructors

I. Directions for interactive webpages

II. WebMO and compute server specifications

III. Alternative implementations

I. Directions for interactive webpages

Interactive molecule website: https://antec12.cns.uaf.edu/cv-expt/index-orca.html

At UAF these pages are located on the same Linux computer that hosts the WebMO site. Conveniently, the web program httpd (or Apache2 on Ubuntu systems) and an SSL certificate should be already installed.

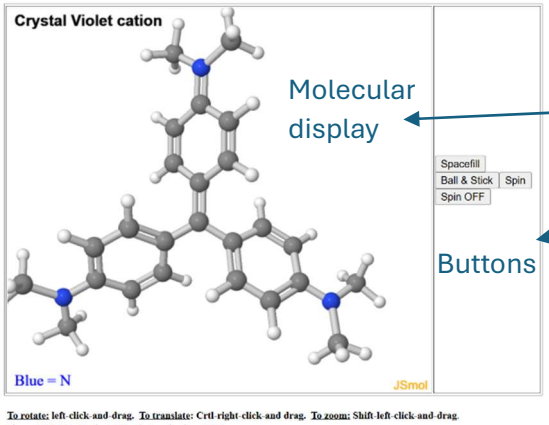
Actually, the JSmol program and interactive webpages can be installed on any webserver readable by students. However, JSmol may not be compatible with content management systems (CMS) such as Blackboard.

JSmol is a web-enabled version of Jmol where the Jmol commands are contained in script sections within the html page. The rather simple JSmol webpages used here contain a 2-column table with a molecular display area and programmable buttons in the second column.

Use Notepad++ to edit 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-orc.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;  set measurementunits angstroms;
    rotate z -12; rotate y 0; rotate x 0; zoom 110; set echo top left; font echo 20
    sansserif bold; color echo black; echo Crystal Violet cation; set echo bottom left;
    font echo 20 serif plain; color echo blue; echo Blue = N;"
    }

$("#mydiv").html(Jmol.getAppletHtml("jmolApplet0",Info))
$("#btns").html( Jmol.jmolButton(jmolApplet0,  " spacefill 75% ","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;
}
.auto-style2 {
    text-decoration: underline;
}
</style>
</head>
```

Visible web page cv.htm



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

The JSmol program files must be present on the server and the JSmol page must reference this location. In the html file shown on the previous page, the src= parameter in line 7 indicates that it is two levels up: **"../../JSmol.min.js"**) The file structure for the interactive webpages in this article looks like this:

/var/www/html

index-orca.html
UAFLogo_A_webblue.gif
/jsmol-16.1.63
JSmol.min.js } Download and expand Jmol and JSmol
/j2s
/org
/cv-orca
cv.htm
cv-orca.mol
oh-4wat.htm
oh-4wat-orc.mol
etc.

Obtain Jmol and JSmol from https://sourceforge.net/projects/jmol/.

II. WebMO and compute server specifications

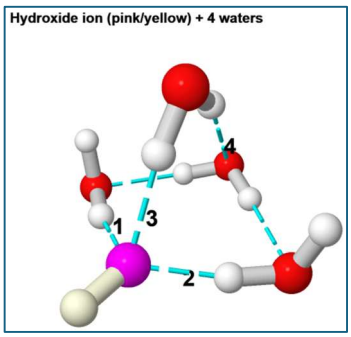
Server*‡	OS	Memory (GB)	Cores/ threads	Programs	CPU
1	Rocky Linux 8.10	64	24/24	WebMO 23, Gaussian 16, ORCA 6,	AMD Threadripper 2970WX
2	Ubuntu 22.04	64	24/32	Gaussian 16, ORCA 6	Intel Core i9 13900K
3	Rocky Linux 9.2	128	24/48	Gaussian 16, ORCA 6	AMD Threadripper 3960X

*This is the server priority order in the WebMO job queue. Servers 2 and 3 were installed on the Remote Server Manager page of WebMO Enterprise. ‡Each computer also contains a 1-TB NVME SSD.

III. Alternative implementations

One need not install a website for display of CV JSmol webpages if you can access https://antec12.cns.uaf.edu/cv-expt/index-orca.html, which is currently world-readable. If this site goes off-line, or if you wish to customize the pages, then you would need to create your own website per the above directions.

Even without access to a website to display the molecules, one could still do most of this exercise by making the .mol files available for download from a learning management system such as Blackboard or Canvas. The density, electrostatic potential and "electrophilic reactivity" surfaces referenced in Part A of the worksheet can be plotted directly in WebMO from the molecular orbitals tab in the View Job page of an ORCA molecular energy calculation. Note that "electrophilic reactivity" term used here refers to WebMO's "Nucleophilic (LUMO) frontier density" plot. The hydrogen bond analysis in Part B can be incorporated by copying the graphics from this article or the UAF website such as the following:



WebMO and ORCA can be installed on a Windows computer using the Windows Subsystem for Linux.

UAF uses the Enterprise version of WebMO that has an external authentication function that allows students to log on with their university username and password. This exercise can instead be done with WebMO Pro, which uses only assigned usernames and passwords. The free version of WebMO is too limited in various ways.

The JSmol webpages, WebMO, and ORCA can all be installed on Google Cloud instances or Amazon Web Services. However, a Google Cloud instance that could match the computational speed of on-premises computers such as those described here would probably be very expensive. If this approach is necessary, perhaps costs can be minimized by activating the cloud instance only for the duration of the scheduled lab.