

A Practical Introduction to Web-based Visualization Using JSMol

David Keffer

Department of Materials Science & Engineering

University of Tennessee, Knoxville

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I. Purpose of Document

The purpose of this document is to provide a complete and unambiguous demonstration of visualizing a molecular object, either locally or via the internet, using the Java Script package, JSMol.

II. JSMol

II.A. What is JSMol?

- JSMol is a free package of JavaScript libraries that allows users to view and interact with atomic and molecular structures using no additional software other than their internet browser.
- JSMol is a JavaScript implementation of an earlier Java package, JMol. Modern browsers will run JavaScript but not Java.
- There is a JSMol wiki at the following URL: <http://wiki.jmol.org/index.php/JSmol>
- There is a history of JSMol at the following URL: <http://jmol.sourceforge.net/history/>. [Prof Robert M. Hanson](#) from the Department of Chemistry at St. Olaf College in Northfield Minnesota has been a longtime champion of JSMol.

II.B. Download JSMol

- JSMol can be downloaded from the following URL: <http://wiki.jmol.org/index.php/JSmol>
- A smaller set (about 12 MB) of core files from JSMol has been uploaded to the “course materials” section of the MSE 614 website.

II.C. Install JSMol

- No installation of JSMol is required.
- For local use—that is viewing files on one’s hard drive—one simply needs to extract the JSMol directory from the downloaded zip file and place it in a working directory.
- For remote use—that is allowing structures to be accessed over the internet—one simply needs to extract the JSMol directory from the downloaded zip file and place it on the web server.

III. Using JSMol

III.A. The Input File

For this example, let us assume that we want to view the structure of Hebelomic Acid A, which contains 106 C, O and H atoms. The input file is provided in standard xyz format in Appendix A. Hebelomic Acid A is suspected to be the offending agent in *Hebeloma crustuliniforme*, a toxic mushroom. See Figure 1.

III.B. The HTML File

The JSMol script can be called through an ordinary HTML file. An example file is given in Appendix B. HTML files can be edited using, for example, Notepad++, which we used to modify the LAMMPS input file in a previous lecture module.

The HTML file contains two sections, a <head> section and a <body> section. In the <head> section we provide a name for the page and the information regarding the type of library, JSMol. This doesn't need to be changed unless you change the location (src) of the JSMol files. In the <head> section, we also specify the details of the particular file to view, including the file name, HebelomicAcidA.xyz, and a variety of commands to control how the structure initially appears on the website.

In the <body> section, we call the script.

III.C. The Local Viewing

If one places the jsmol directory extracted from the downloaded zip, the input file and the HTML file in the same directory, then one should be able to view the file simply by opening the HTML file.

Some browsers do not allow local execution of scripts by default. Chrome, which as of December, 2015 was used to access 68.0 % of webpages, as reported by http://www.w3schools.com/browsers/browsers_stats.asp, is one such browser. In this case, one must run Chrome with a command line option, such as

```
"C:\Program Files (x86)\Google\Chrome\Application\chrome.exe" --allow-file-access-from-files  
This option can be implemented simply by creating a short cut and adding the  
--allow-file-access-from-files
```



Figure 1. *Hebeloma crustuliniforme*, a toxic mushroom, also known as Poison Pie. source:
https://en.wikipedia.org/wiki/Hebeloma_crustuliniforme

option to the “target” field. See Figure 2 for a screenshot of this process. Then the file can be opened simply by dragging the HTML file onto this shortcut.

Note that all other Chrome windows must be closed in order to open the program with this command option.

III.D. The JSMol Manual

JSMol has a tremendous breadth of visualization options. One site for finding a list of JSMol commands that can be entered in the <head> section of the HTML file is located at the following URL:

<http://chemapps.stolaf.edu/jmol/docs/>.

Another page exists in the JSMol wiki at the following URL:

<http://wiki.jmol.org/index.php/Scripting>.

A snapshot of the structure is shown in Figure 3.

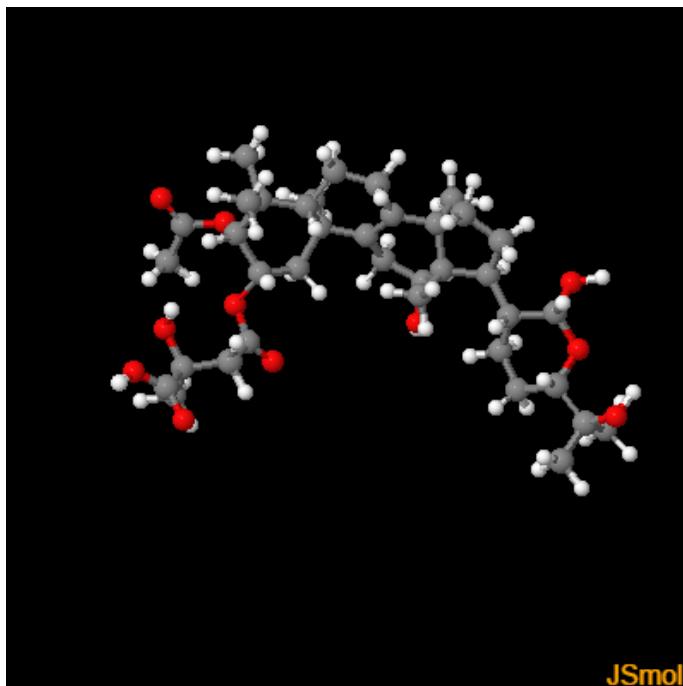


Figure 3. Hebelomic Acid A.

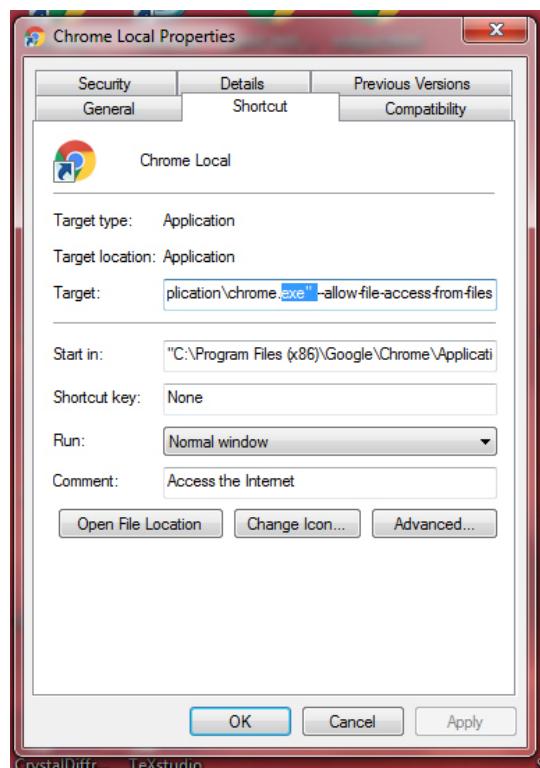


Figure 2. Specifying the command option to allow JSMol to execute in Chrome on local files.

Appendix A. Sample Input File: HebelomicAcidA.xyz

This sample input file is in standard xyz format. The first line indicates the number of atoms. The second line can contain a descriptive comment. The remaining lines contain the atomic symbol and the x, y and z coordinates.

```
106
Hebelomic Acid A
C -0.785000397 -0.521535153 -0.131999385
C 0.509720469 -1.089748855 0.414530843
C 1.711785819 -0.490621845 -0.360672991
C 3.037805835 -1.045761762 0.093803406
O 3.310257614 -2.439521521 -0.002108878
O -1.785462690 -1.322828390 -0.434658148
O -0.928445525 0.779418089 -0.274470961
C 0.598698260 -0.746370519 1.909035260
O 3.900687768 -0.275611186 0.599584047
O 0.500571619 -2.534175014 0.282376437
C 3.905920394 -2.728472114 -1.299012383
C 3.591284312 -4.187990156 -1.676029800
C 5.429473977 -2.448772426 -1.263560281
O 4.180942265 -5.085126002 -0.681811806
C 4.101365968 -4.520900975 -3.132432984
C 6.285655687 -3.163364819 -2.372506697
C 5.326868362 -3.597938373 -3.538182165
C 3.159825428 -5.716715312 0.084611282
C 4.424544361 -6.033471487 -3.269298058
C 2.929597237 -4.239540595 -4.117178889
C 7.067921667 -4.353176450 -1.750521078
C 7.372963395 -2.197047638 -2.910030917
O 2.594611915 -6.755217779 -0.356507467
C 2.788479435 -5.189750614 1.433648605
C 6.128980457 -4.079758114 -4.758650366
C 7.683729396 -2.121514741 -4.244469858
C 6.955911627 -2.922425018 -5.311240712
C 8.768475731 -1.139039017 -4.673014698
C 8.279601984 -1.466255980 -1.897128393
C 8.907977843 -0.111900444 -2.372411015
C 10.142500600 -1.865714855 -4.475177728
C 8.739817432 -0.674565432 -6.132579260
C 8.601697571 0.206491920 -3.878340670
O 8.428823774 0.929842872 -1.494348508
C 7.146747343 0.783735609 -3.994249101
C 9.598216821 1.151565572 -4.649725992
C 9.502104531 0.653108328 -6.125039162
C 9.426636071 2.720245909 -4.609695276
C 10.438486625 3.450006276 -5.569188711
C 9.564866377 3.341331969 -3.209136049
O 10.768204906 4.816125160 -5.162276851
C 9.289612003 4.857280435 -3.224090266
C 9.613966886 5.490005355 -4.595466975
O 11.678581333 2.713304623 -5.650232863
C 9.866094911 7.029540383 -4.553753522
C 11.167133919 7.394657096 -3.805263755
C 8.682390648 7.759967822 -3.896456965
O 9.960497550 7.519118404 -5.915570467
H 1.722837159 0.619307077 -0.244206254
H 1.594243729 -0.701289363 -1.448615232
H -2.659509918 -0.958919932 -0.788348546
H -0.297727262 -1.133313139 2.446915306
H 0.657105649 0.356617097 2.059897288
H 1.498898016 -1.217128024 2.366046475
H 0.477073087 -2.757598838 -0.730001239
H 3.446028960 -2.085764659 -2.091449469
H 2.471601923 -4.265897332 -1.669341846
H 5.817283579 -2.700855328 -0.247956989
H 5.526915588 -1.342781195 -1.368930657
H 2.588406680 -3.181420894 -4.046873850
```

H	2.054623788	-4.892648488	-3.890110961
H	3.221849571	-4.435105863	-5.172563679
H	3.569002834	-6.646518965	-2.904434874
H	5.326077050	-6.333070873	-2.701063598
H	4.596247092	-6.316280173	-4.332726573
H	4.863380016	-2.635663321	-3.875037545
H	7.731371442	-3.997752866	-0.929861276
H	7.723488364	-4.852695815	-2.496526170
H	6.423044273	-5.113198341	-1.286564081
H	1.741241260	-4.814303022	1.413650348
H	3.471860346	-4.362768183	1.727781095
H	2.873265882	-6.002979945	2.189028115
H	5.450699216	-4.426025397	-5.569459485
H	6.790760380	-4.935589888	-4.502774956
H	6.273794923	-2.236358185	-5.864420292
H	7.693808345	-3.332713280	-6.038378739
H	9.101092774	-2.159655338	-1.610144552
H	7.698095604	-0.502764773	-6.486458512
H	9.210530015	-1.403802941	-6.834153204
H	10.323987270	-2.207609320	-3.438682966
H	11.008860645	-1.234757618	-4.770845278
H	10.177925775	-2.780554985	-5.111658898
H	7.741932499	-1.297996546	-0.939694878
H	10.017152071	-0.180022595	-2.252939193
H	8.969699285	0.852705272	-0.613577778
H	6.862293453	1.003147178	-5.045938156
H	10.622227145	0.932732714	-4.267328266
H	8.400874555	2.959643329	-4.976826034
H	8.956204130	1.371923540	-6.779970649
H	10.523579303	0.504958208	-6.546650814
H	9.987544834	3.493763690	-6.589943821
H	10.588847655	3.142789244	-2.813401016
H	8.831630524	2.910716102	-2.515129168
H	9.883840372	5.320690788	-2.406977698
H	8.212300367	5.037583461	-2.996265383
H	8.732542036	5.334643289	-5.267706631
H	12.219962372	3.141234564	-6.422568271
H	11.093972535	7.179321047	-2.716607541
H	11.375765010	8.483148079	-3.920654755
H	12.036331003	6.837057701	-4.221509759
H	8.816632265	8.862877879	-3.983871525
H	8.599056794	7.507963203	-2.814751629
H	7.728634173	7.486861735	-4.403756862
H	10.798051725	7.093102134	-6.352770978
H	7.047749077	1.738189742	-3.434438969
H	6.378146373	0.101249002	-3.573340920

Appendix B. Sample HTML File: `jsmol_test.html`

The following file is a sample HTML file, which calls JSMol, in order to view the structure provided in Appendix A.

```
<html>
  <head>
    <!-- <meta content="text/html; charset=ISO-8859-1" http-equiv="content-type"> -->
    <title>JSMol Test</title>
    <script language="JavaScript" type="text/javascript"
src="jsmol/JSmol.min.js"></script>
    <script language="JavaScript">
var figure01 = {
  width: 400,
  height: 400,
  // serverURL: "http://chemapps.stolaf.edu/jmol/jsmol/jsmol.php ",
  use: "HTML5 WEBGL JAVA",
  j2sPath: "jsmol/j2s",
  script: "load HebelomicAcidA.xyz; background [x000000]; rotate x 180; rotate y 20;
rotate z 45; set spin y 15;  spin on; wireframe on; wireframe 0.15; spacefill on;
spacefill 25%",
  // console: "jmolApplet0_infodiv"
}
    </script>
  </head>
  <body>
    <center>
      <script> myJmol = Jmol.getApplet("myJmol", figure01); </script>
    </center>
  </body>
</html>
```