

Embedding spectra and structures in your web pages

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Since we dealt with the embedding of spectra and chemical structures in web pages back in 1996 and 1997 there have been a lot of developments—not least in the plug-ins which we described.^{1,2} Nowadays, it is a lot easier to implement a spectra-enabled web page than in the past. The interesting links between infrared spectra and structure displays of their vibrational modes on a single web page can now be generated without the need to edit the original IUPAC/JCAMP-DX files.

With several recent questions coming through to us on how to bind spectra into web pages we decided it was time for a refresher course! Clearly if you have enough software licenses for everyone wishing to view spectra you can deploy the spectroscopy software onto every machine that will be accessing your web-pages and link the data files on your website so that they are downloaded in these external programs. Such programs are often called Helper Applications where the content is viewed outside the browser. It is more convenient and far easier to support viewing the scientific content inside the browser window itself.

In commercial software packages such as electronic laboratory notebooks, analytical workflow management systems and scientific data archiving the capability to view and review spectroscopic data is what can really bring added value for the end-users.

This column does not pretend to meet the demands of professional programmers but it should give the raw amateur some basic starting points from which

they can go on and develop their own applications.

Chemical MIME

Ever wondered how web browsers know how to display different file formats served up to them from web pages? This is achieved for a wide range of formats by relying on standardised file extensions such as Macromedia Flash Player, RealPlayer, Adobe Acrobat, Windows Media Player, QuickTime Movie etc.

In the Mozilla/Netscape world this enhanced capability is delivered through plug-ins, in the Microsoft world they have decided on the terminology Add-Ons although the functionality—“to extend the capability of the web browser” as Microsoft puts it, is essentially the same.

Downloading and installing the MDL Chime plug-in

This couldn't really be simpler. The plug-in is available from the MDL website under <http://www.mdl.com/products/framework/chime>

During the installation process the first option is for the installer to locate your browsers via the registry (Figure 1).



Figure 1

If this option is taken it is possible that not all your installed browsers are located by the installer. In this case you should not bother taking the search all local drives for web browser(s) option as this took a long time on my machine and only delivered the same results with Internet Explorer as had the registry option. I tried the “Specify the Location” option which also failed to accept my Netscape or Mozilla Firefox browsers existed in their directories. (MDL have not fully tested CHIME with all browsers and now recommend IE.)

I managed a work-around by allowing the installer to install the plug-in files to the Internet Explorer plug-ins directory (C:\Program Files\Internet Explorer\PLUGINS) and then copying them into the equivalent directories in my Netscape installation (C:\Program Files\Netscape\Netscape Browser\plugins) and my Firefox installation (C:\Program Files\Mozilla Firefox\plugins). Although not all the files are required by the various browsers I simply copied over everything with CHIME in the name.

Most of the information in the older articles is fundamentally correct and it would be pointless to repeat the content here as they are available from http://www.spectroscopyeurope.com/td_col.html should you not be aware of our archive!

Checking the installation

Your browser can tell you which plug-ins are currently known. How to see this is browser-specific.

For Internet Explorer use the Tools: Manage Add-Ons drop-down menu (Figure 2).

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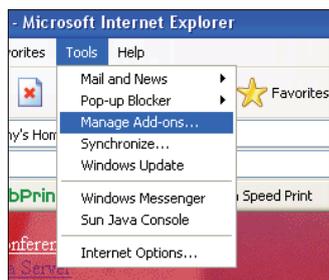


Figure 2

For those with Mozilla Firefox typing about:plugins in the URL address area will bring up a local web page with extensive information about your installed plug-ins (Figure 3).

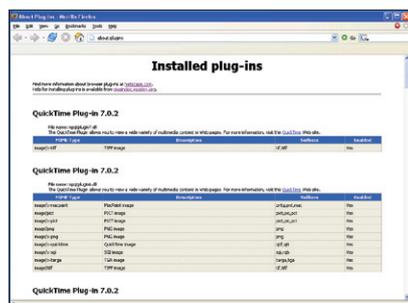


Figure 3

In Netscape you get a somewhat poorly formatted display with the same command about:plugins but you also have the capability to manage which file extensions are active. It is a bit more complicated using the Tools: Options:

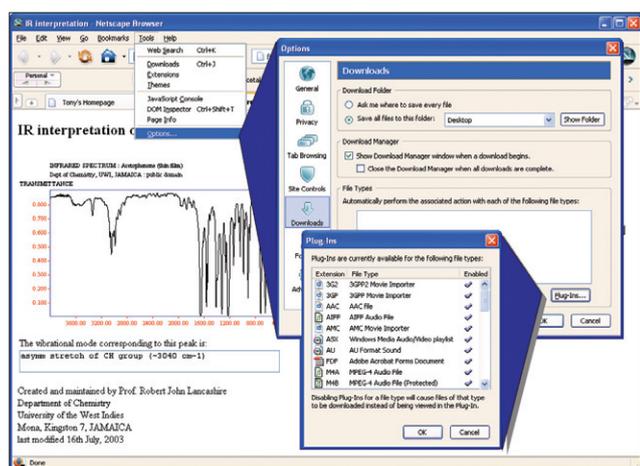


Figure 4

Download: Plug-ins menus to arrive at a somewhat different display (Figure 4).

The Mozilla Firefox entry for the current CHIME version is shown in Figure 5 and you can see that your browser can now recognise and display a multitude of chemical structure formats including protein database format PDB and JCAMP-DX files.

Embedding science content

In order to have your scientific content displayed on your web pages you must add certain commands into the web pages' HTML. How this should be achieved is somewhat different from our previous advice.

The simple <embed> command still functions. This means that for our test reference mass spectrum file from the International Spectroscopic Data Bank of 1-ethoxy-2,6-dimethyl-4-nitrobenzene, with the file name 438-D1099.jdx, we would use a line in the HTML file such as

```
<embed src="438-D1099.jdx" width="500"
height="300" jcamp_revplot="true"
name="MSDisplay">
```

and for the reference chemical structure

```
<embed src="438-D1100.mol"
display3d="wireframe" bgcolor="white"
width="300" height="300"
name="MOLDisplay" startspin="true">
```

A test HTML file called "simple spectra display - no scripts.htm" with these data sets can be found on the IS-DB archive (<http://www.is-db.org>).

However, this type of embedding requires you to edit a new HTML page for every new file you wish to display.

A somewhat more modern approach makes use of scripts within the HTML page which allows you to reference out to a .js file where you can store the various filenames and other web content.

The variables in the stored .js file are loaded into the HTML through the addition of two entries in the HTML head area. In our example they would be

```
<script language="JavaScript"
src="dispdata.js" type="text/javascript">
</script>
```

which reads the "dispdata.js" file.

If we take the same simple example as above, then the scripts to be added to the HTML page making use of the variables defined in the dispdata.js to access the same content would look like Code 1.

Both the original HTML-based web page and the Javascript-based web page look the same within the browser window although the different browsers do slightly change the way the page is displayed (Figure 6).

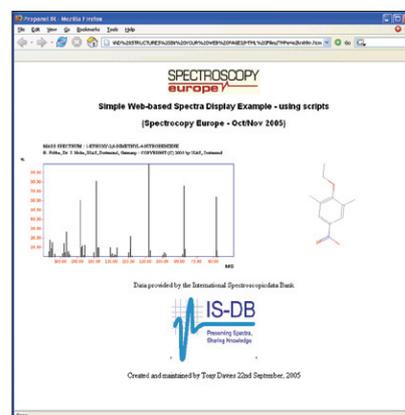


Figure 6

MDL® Chime 2.6 SP6

MIME Type	Description	Suffixes	Enabled
chemical/x-mdl-molfile	MDL MOL	mol	Yes
chemical/x-mdl-zmfile	MDL RMN	rmn	Yes
chemical/x-pdb	Brookhaven PDB	pdb,emb,mbdl	Yes
chemical/x-cv2	3DMol CV2	cv2	Yes
chemical/x-gaussian-input	Gaussian input	gau	Yes
chemical/x-mopac-input	MOPAC Input	mcp	Yes
application/x-sct	RAMMol Script	sct	Yes
chemical/x-csml	CSML	csml,csml	Yes
chemical/x-jcamp-dx	JCAMP-DX	jdx,jdx	Yes
application/x-rasnm	RASNMol Script	scr	Yes
chemical/x-mdl-sgff	MDL SSEARCH	sgf,skc	Yes
chemical/x-gaussian-cube	Gaussian Cube	cube,cube	Yes

Figure 5

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```
<SCRIPT language="javascript" type="text/javascript">
  document.writeln('<table width=99%><tr><td>');
  document.writeln("&<embed src="+MSfileName+" width='500' height='300'
  jcamp_revplot='true' bgcolor='white' name='MSdisplay' ></embed>");
  document.writeln('<br>');
  document.writeln('</td><td>');
</SCRIPT>
<SCRIPT language="JavaScript" type="text/javascript">
  document.writeln("&<embed src="+MolfileName+" display3d='wireframe' bgcolor='white'
  width='300' height='300' name='MOLdisplay' startspin=true frank=false>
  </embed>");
  document.writeln('</td> </table>');
</SCRIPT>
```

Code 1

```
//edit the following lines
var IRInfo = new Array();
function IRLinks(x,y,w,script,desc) {
  var n=IRInfo.length;
  IRInfo[n] = new Array();
  IRInfo[n].xpos=x;
  IRInfo[n].ypos=y;
  IRInfo[n].width=w;
  IRInfo[n].script=script;
  IRInfo[n].desc=desc;
}
//you should not need to edit the html files.
```

Code 2

```
//edit the following lines
var IRfileName= "acetoph.jdx";
var MolfileName= "acetoph.mol";

IRLinks(3101, 1, 20, "mode3199_359.xyz","symm stretch of aromatic CH group (~3100 cm-1)");
IRLinks(3086, 1, 15, "mode3191_028.xyz","asymm stretch of aromatic CH group (~3085 cm-1)");
IRLinks(3062, 1, 15, "mode3184_096.xyz","asymm stretch of CH group (~3060 cm-1)");
IRLinks(3038, 1, 10, "mode3179_944.xyz","asymm stretch of CH group (~3040 cm-1)");
IRLinks(3029, 1, 10, "mode3168_859.xyz","asymm bend of CH3 group (~3030 cm-1)");
IRLinks(3005, 1, 20, "mode3154_485.xyz","symm stretch of methyl group (~3005 cm-1)");
IRLinks(2969, 1, 30, "mode3064_505.xyz","asymm stretch of methyl group (~2970 cm-1)");
IRLinks(2921, 1, 30, "mode3062_601.xyz","symm stretch of CH group (~2920 cm-1)");
IRLinks(1684, 1, 30, "mode2038_519.xyz","Carbonyl stretching band (~1685 cm-1)");
IRLinks(1599, 1, 30, "mode1628_422.xyz","C-C of aromatic group (~1600 cm-1)");
IRLinks(1449, 1, 20, "mode1461_934.xyz","symm stretch of CH3 group (~1450 cm-1)");
IRLinks(1359, 1, 30, "mode1385_552.xyz","C-H twist of methyl group (~1360 cm-1)");
IRLinks(1265, 1, 20, "mode1242_431.xyz","scissors of aromatic C-H groups (~1265 cm-1)");
IRLinks(1180, 1, 40, "mode1198_093.xyz","scissors of CH group (~1180 cm-1)");
IRLinks(1078, 1, 30, "mode1081_536.xyz","symm stretch of CH3 group (~1080 cm-1)");
IRLinks(1025, 1, 20, "mode1066_982.xyz","symm stretch of CH group (~1025 cm-1)");
IRLinks(1001, 1, 20, "mode1055_054.xyz","asymm bend of CH3 group (~1000 cm-1)");
IRLinks(956, 1, 20, "mode1011_181.xyz","aromatic ring perturbation mode (~955 cm-1)");
IRLinks(760, 1, 20, "mode0891_705.xyz","aromatic ring perturbation mode (~760 cm-1)");
IRLinks(691, 1, 20, "mode0808_075.xyz","aromatic ring perturbation mode (~690 cm-1)");
IRLinks(588, 1, 20, "mode0581_953.xyz","concerted rocking mode of CH groups (~590 cm-1)");

var ShowDesc= "T";

var title= "acetophenone";
var author= "Prof. Robert John Lancashire modified for Spectroscopy Europe Article by Tony Davies";
var address1= "Department of Chemistry";
var address2= "University of the West Indies";
var address3= "Mona, Kingston 7, JAMAICA";
var lastMod= "original file date 9th August 2005 - modified 23 September 2005";

//you should not need to edit the html files.
```

Code 3

Adding complexity

Once you have mastered the simpler display of spectra and structures you can progress to the more complicated interactive displays such as on the University

of the West Indies, Jamaica web site at <http://wwwchem.uwimona.edu.jm/spectra/index.html> where a number of worked examples of the integration of chemistry and spectroscopy are available.

With scripts, the linking of chemistry display to spectroscopic features becomes possible through the use of the .js file rather than editing the JCAMP-DX file. This is a significantly more elegant way to generate the excellent educational web pages.

An example of the more complicated .js file usage is as follows. Two .js files are used, one to declare the variables and one in which, for this example, the infrared mode information is stored.

The first file declaring the arrays looks like Code 2, and the second containing the data required by the active webpage itself like Code 3. Here you can see the array IRLinks stores all the information required for the active display. The wave-number position and width of the various vibrational bands assigned as well as the XYZ file containing the molecular motion to be displayed corresponding to the respective IR peak. In this particularly informative version an additional variable in the array contains explanations of the vibrational modes and through the use of the scripts automatically loads and displays when one of the peaks is selected. By placing all the sample specific information in the .js files it is possible to use the HTML file as a template. Each new demonstration then only requires minor editing of the HTML file telling it to load the new .js file.

Summary

I hope this short starter leaves you with some idea of how it is possible to generate web pages with active spectra/structure displays using the current MDL Chime plug-in. It is far easier to learn-by-doing so we have deposited the examples shown here on the International Spectroscopic Data Bank for you to access and play with. They are deposited under the IS-DB id 441.

References

1. A.N. Davies, "Internet Chemical MIME", *Spectroscopy Europe* **8(1)**, 42–43 (1996).
2. A.N. Davies and R.J. Lancashire, "Setting up a chemically active internet/intranet site", *Spectroscopy Europe* **9(1)**, 30–32 (1997).
3. <http://plugindoc.mozdev.org/winmime.html>