GEISA-PC DEMO

Tutorial

2016

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1 GEISA-PC Demo

This document helps you deploy and use GEISA-PC Demo software. The software package has been developed using Embarcadero RAD Studio.

The Demo works with a portion of GEISA-2015 spectroscopic database that includes over 1,000,000 lines of H_2O, CO_2, and O_3 molecules within the 0 - 25000 cm^{-1} spectral range.

With this Demo, you can perform the following tasks:

- Plot the “stick” spectra of selected molecules
- Plot the diagrams of energies of the lower transition levels
- Zoom in on charts to view detailed images
- Scroll the charts
- Save the charts to the bitmap files

1.1 Getting Started

1.1.1 GEISA Demo Files

After unzipping the downloaded Zip archive, in your work directory, you find the following files:

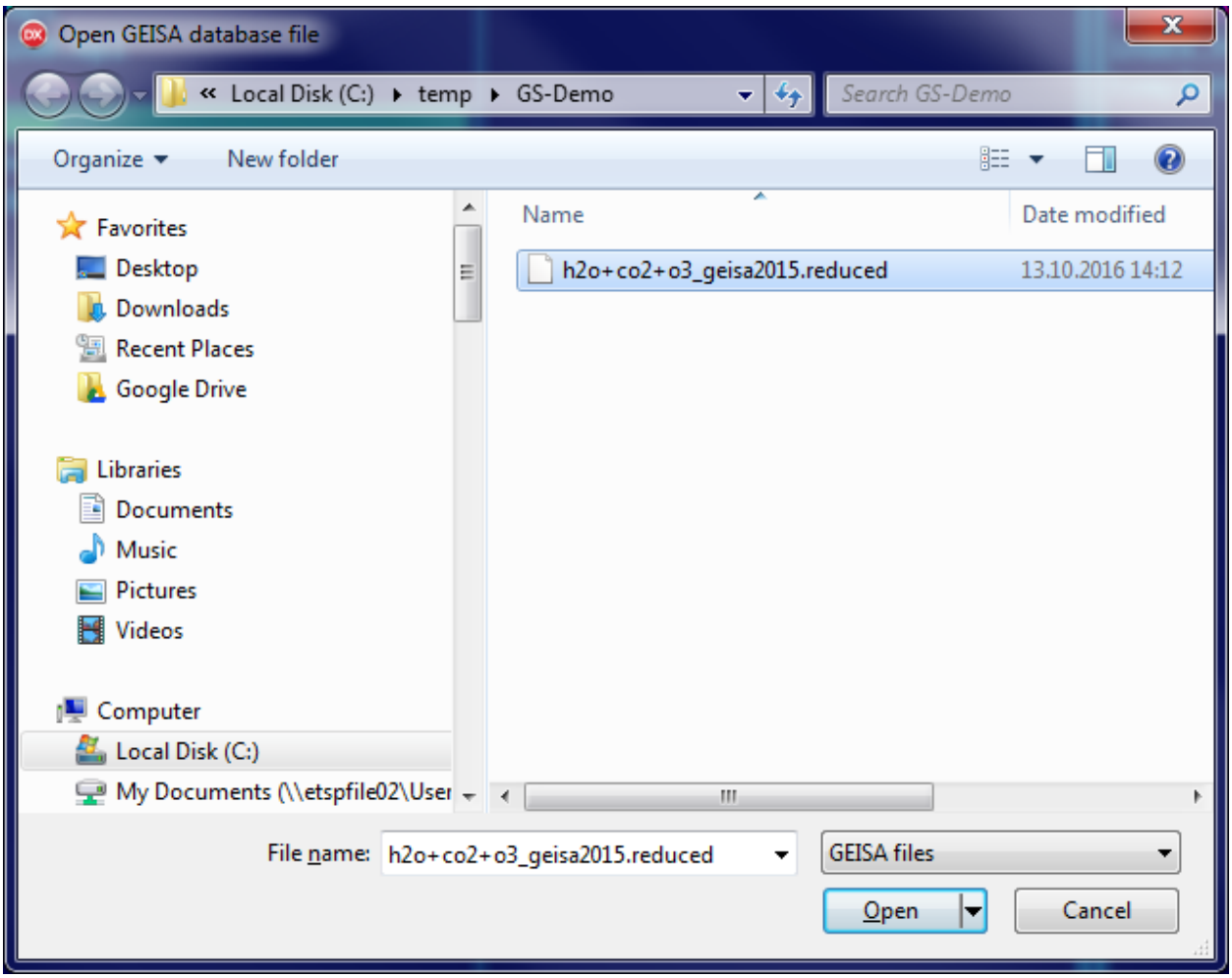
File name	**Description**
ReadMe.pdf	This documentation file.
gs2015.exe	GEISA Demo executable file (**64-bit version**). Run it to start working with this Demo (for 64-bit machines only).
gs2015_32bit.exe	GEISA Demo executable file (**32-bit version**). Run it to start working with this Demo if you have a 32-bit machine.
h2o+co2+o3_geisa2015.reduced	GEISA database file for this Demo. **NOTE:** Please do not edit or modify this file!
fmx240.bpl	A binary file used by this Demo.
FMXTee9240.bpl	A binary file used by this Demo.
openDB.png	A binary file used by this Demo.
rtl240.bpl	A binary file used by this Demo.

IMPORTANT For GEISA Demo to work properly, please do not modify or move these files. All files should be placed into *a directory* on your PC.

1.1.2 Running Demo and Selecting a Database

This section explains how to run Demo and select a database file to work with.

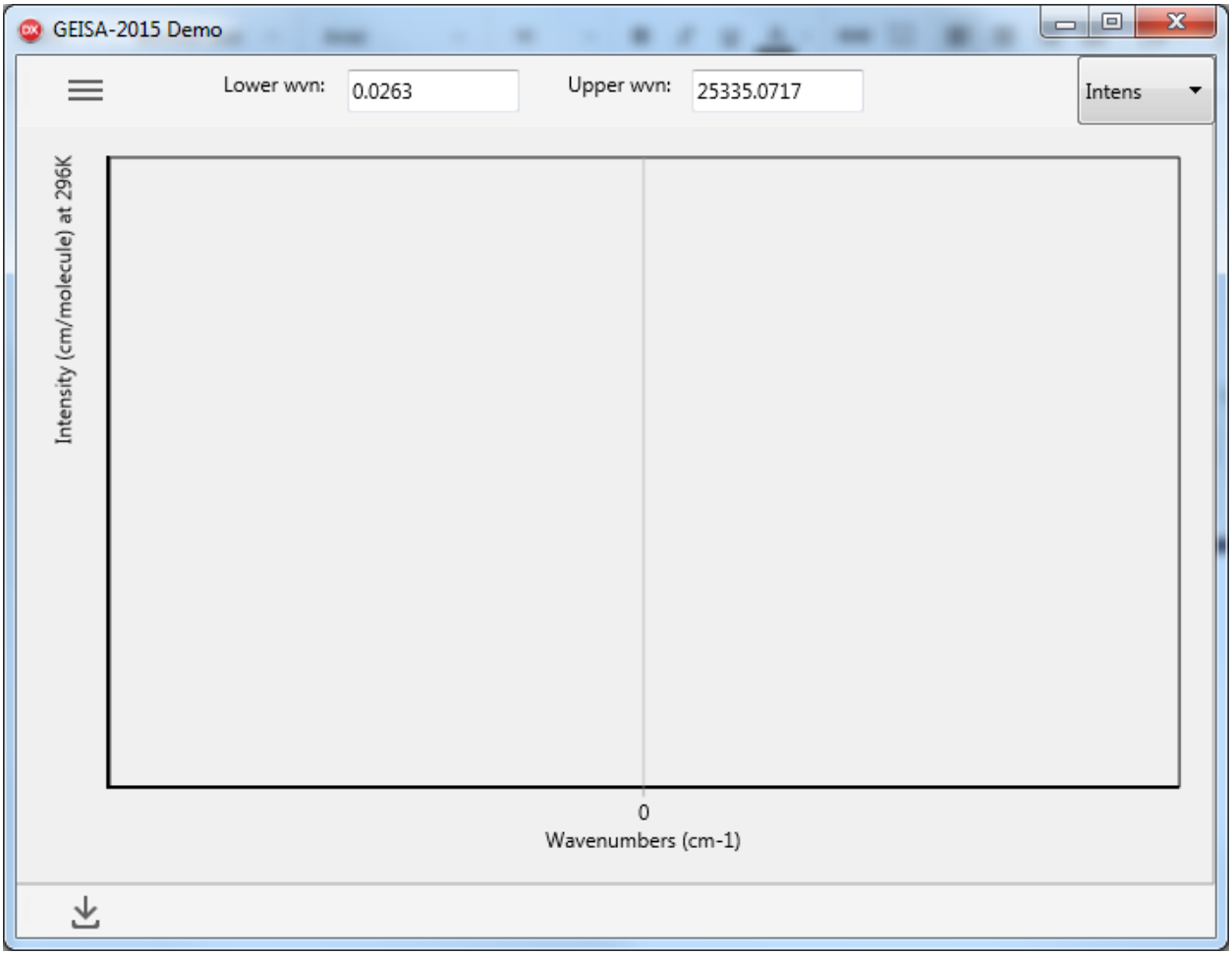
- To start GEISA Demo, run **gs2015.exe** (for 64-bit machines) or **gs2015_32bit.exe** (for 32-bit machines).
- At startup, GEISA Demo prompts you to select a database file.
  NOTE: In this Demo, you can use the only file **h2o+co2+o3_geisa2015.reduced**.



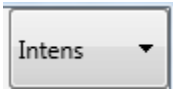
Please, select **h2o+co2+o3_geisa2015.reduced** in the **Open GEISA database file** dialog box (it opens automatically) and click **Open** to proceed with Demo.

1.1.3 GEISA Demo Control Panel

After selecting the database file, the Demo displays the control panel similar to the following screen:



The control panel defines the following control elements:

Element	Description	Remarks
	Opens a pane with the molecules lists.	Click this button to select molecules.
	Selects a work mode: • **Intens** (default): plots the stick spectrum • **Energ**: plots the energy levels diagram • **HW (air)**: plots the airbroadening pressure halfwidth (not available in this Demo)	Use this element to specify the work mode.

	Selects the work database.	This option is not available in this Demo.
Lower wvn **Upper wvn**	These text boxes specify the work spectral range (in cm^{-1}) for your charts.	At startup: • **Lower wvn** = minimum wavenumber in the GEISA database file • **Upper wvn** = maximum wavenumber in the GEISA database file

NOTE: The control panel has additional elements that are hidden at startup and will be displayed when necessary.

1.2 Using GEISA Demo

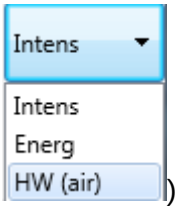
This section describes some typical use cases of GEISA Demo. The following scenarios are covered:

- Plotting the stick spectra
- Zooming in and scrolling the charts
- Displaying and hiding spectra of selected molecules
- Saving charts to bitmap files

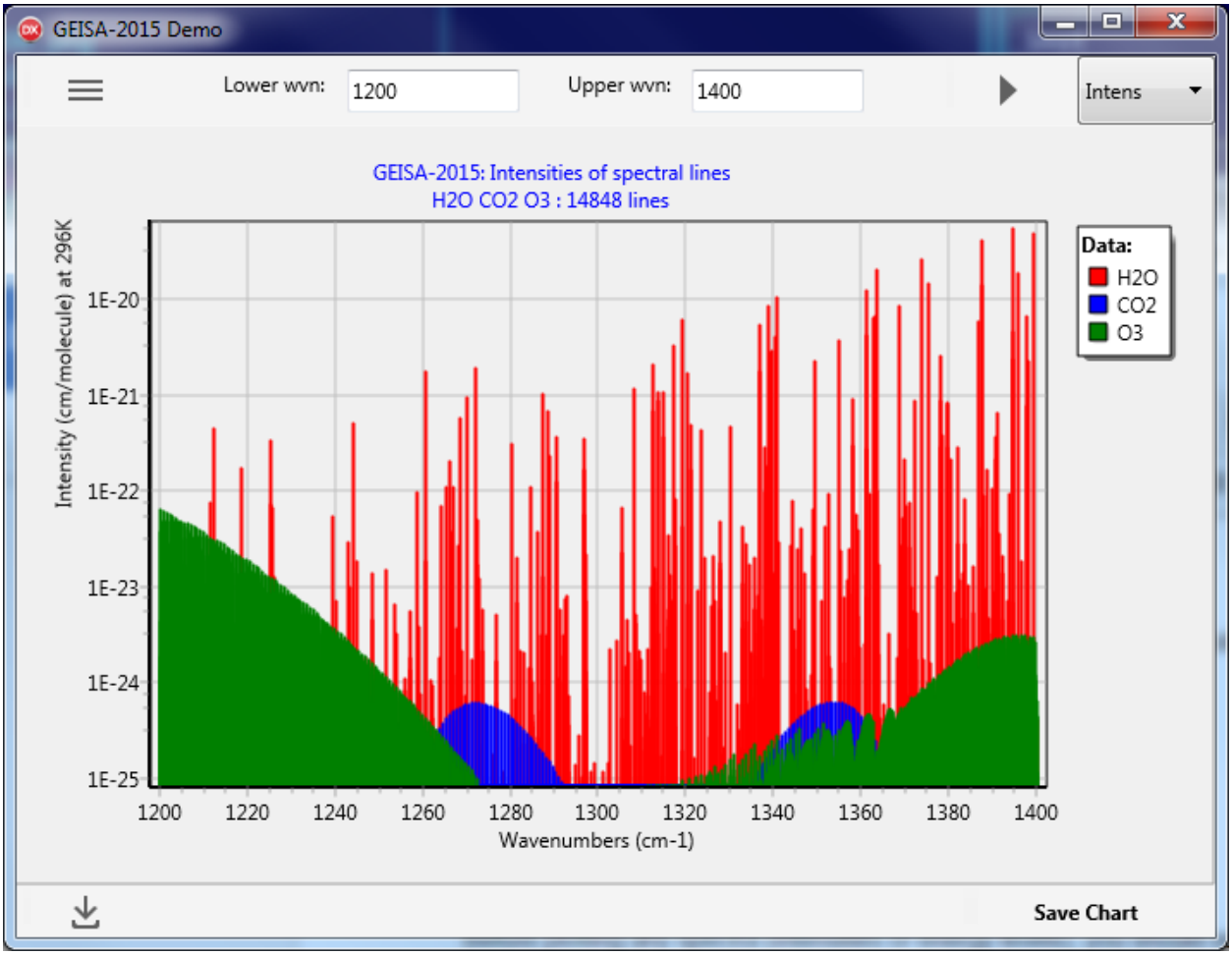
1.2.1 Plot Spectra

Before plotting any spectra (intensities or energy levels), select the molecules and specify the spectral range. After this, click  to start plotting the selected molecules spectra.

To plot spectra

1. Click  and select the molecules of interest.
2. In the **Lower wvn** and **Upper wvn** text boxes, specify the spectral range (in cm^{-1}).
3. Specify the plot mode (use the mode selector ).
4. Click  to start.

The following screen displays the stick spectra of CO_2, H_2O, and O_3 molecules within the 1200 - 1400 cm^{-1} spectral range:



The following sections help you manipulate with plotted spectra and chart.

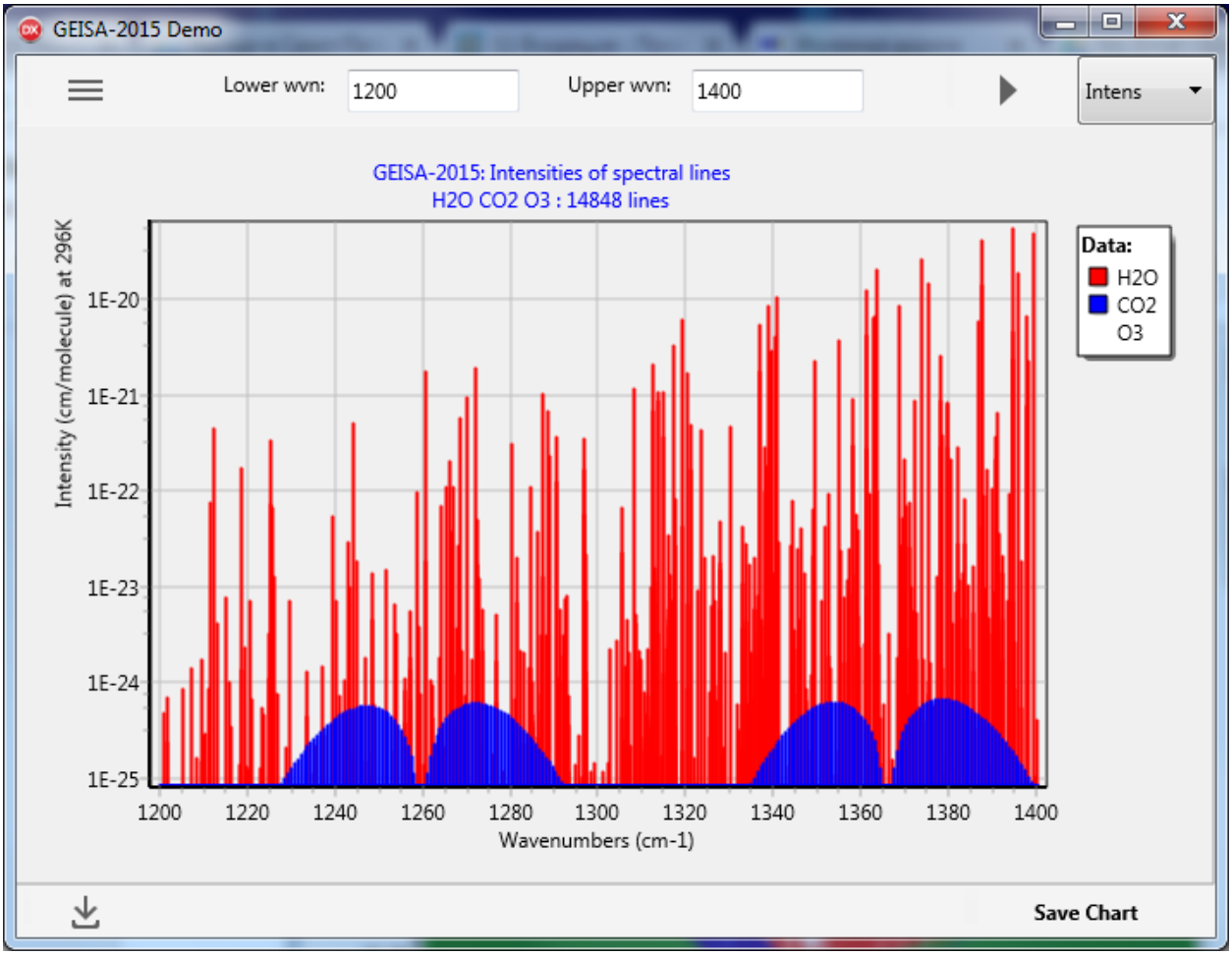
1.2.2 Display or Hide Spectra for Certain Molecules

Consider a scenario: you have plotted the stick spectra of three molecules (water, carbon dioxide, and ozone) as shown in the previous screenshot. Optionally, you can hide or display a spectrum of any molecule.

To hide or display a spectrum of a molecule

- Click the molecule name in the chart legend.
  This operation displays/hide the molecule spectrum.

To clarify, consider the following scenario: you want to hide the ozone spectrum (green sticks in the previous screenshot) to view only the water and carbon dioxide spectra. In this case, you should click the **O3** name in the chart legend. After this, GEISA Demo displays the following chart:



In this figure, the ozone spectrum is hidden. To display the ozone spectrum, click **O3** again.

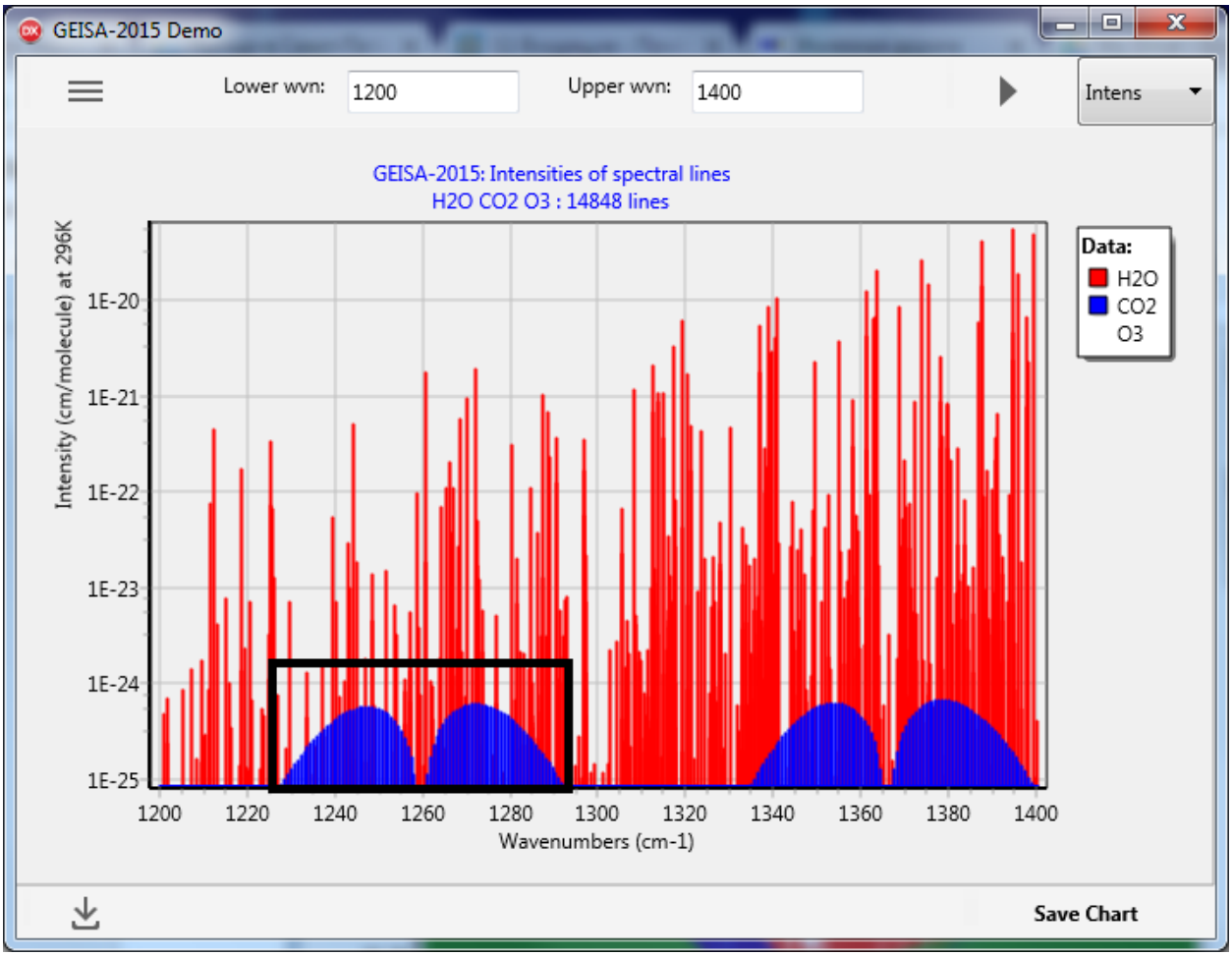
1.2.3 Zoom in and Scroll the Charts

Zoom and Scroll are useful aids for focusing on specific data in a densely populated chart. This section explains how to perform these operations using the mouse.

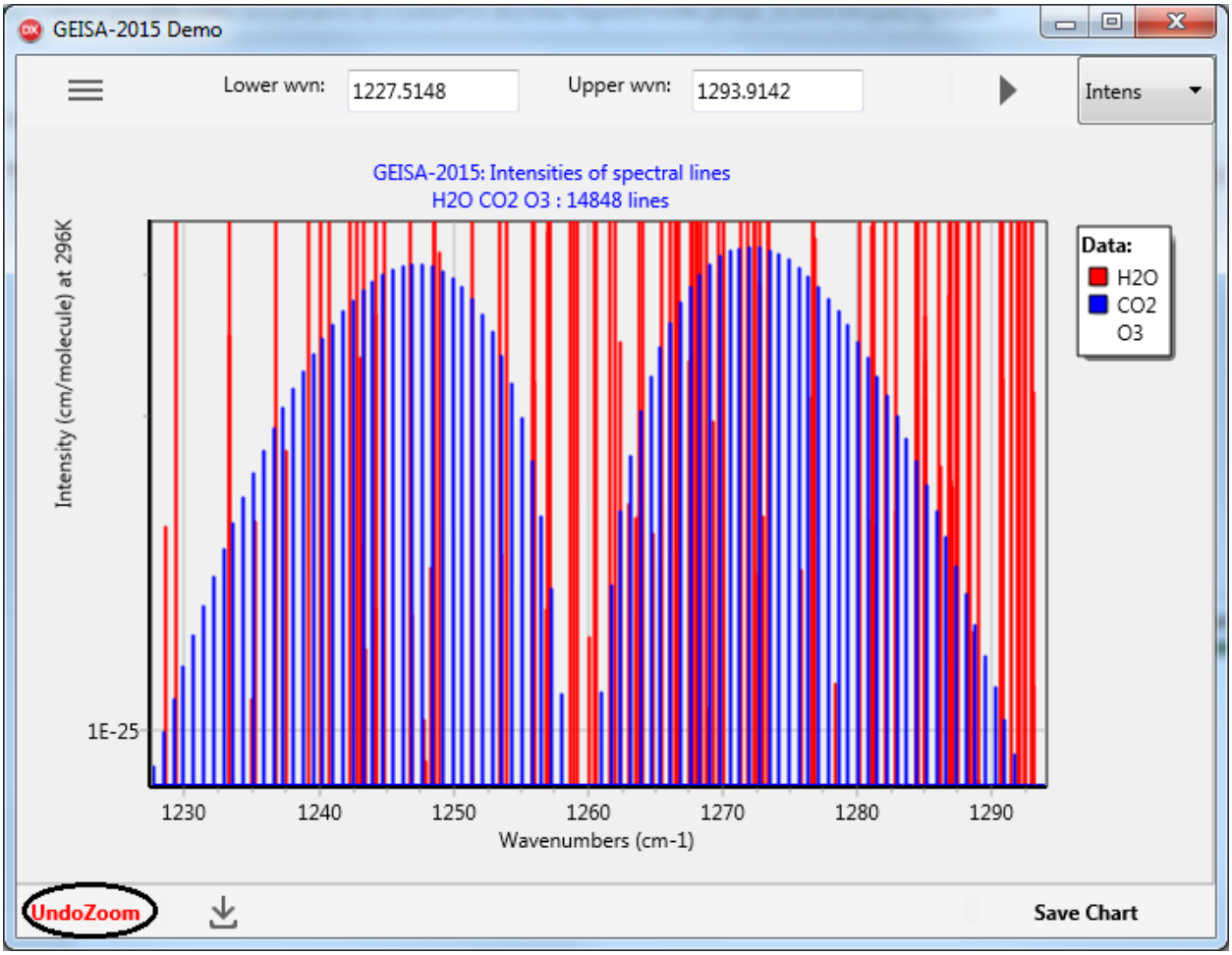
To zoom in

- Press the left mouse button at the top left hand corner of the area you wish to zoom in on and, maintaining the mouse button pressed, drag out the rectangle to the bottom right hand corner of the zoom area.
- Release the mouse button to cause the chart to redraw the area selected.

To clarify, consider the following screenshots:



After releasing the mouse button, GEISA Demo displays the following detailed image:



TIP: To undo zoom, click **UndoZoom** displayed in the left low corner of the chart.

IMPORTANT: The Zoom function is not supported if total number of the displayed lines exceeds 400,000.

To scroll a chart

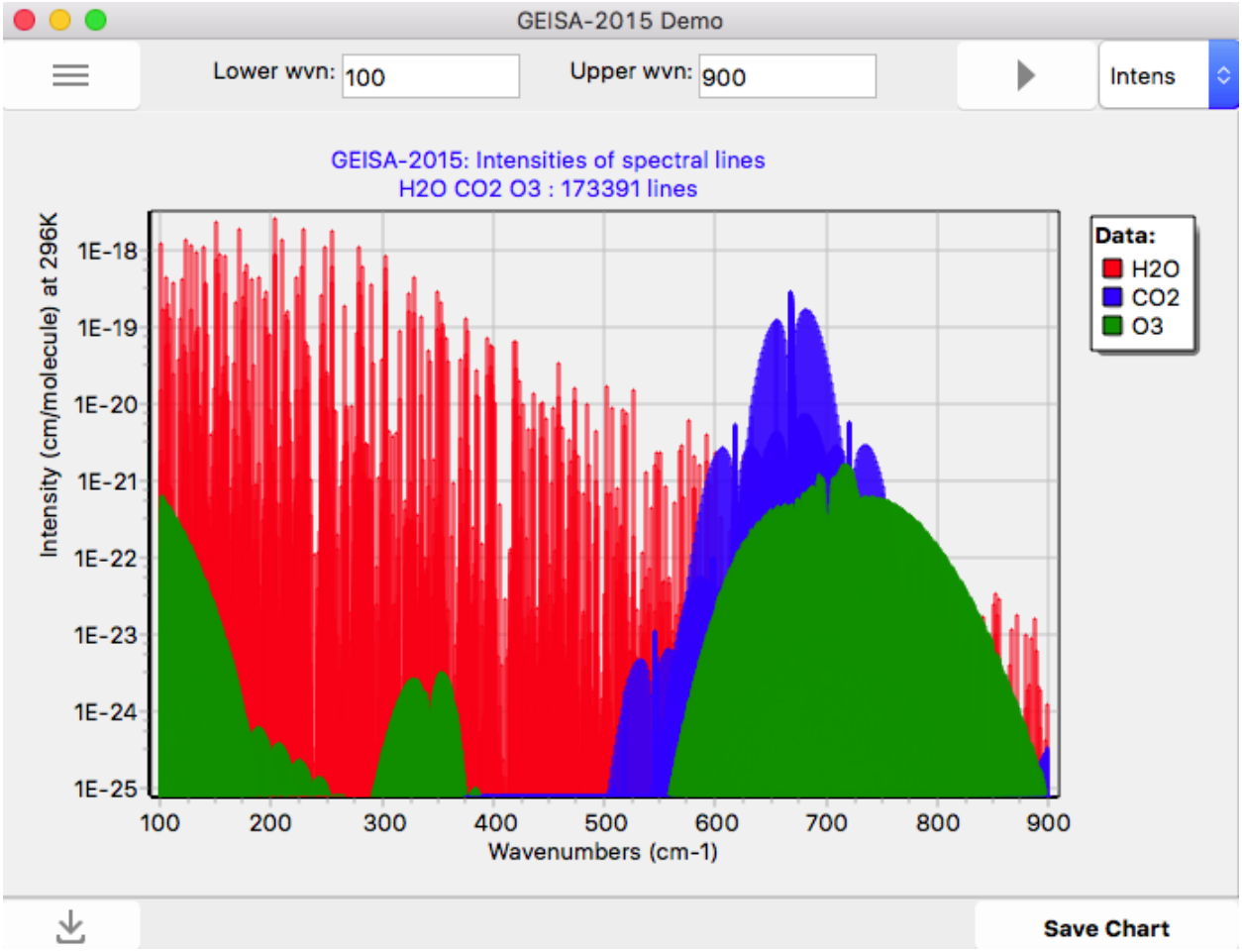
- To scroll a Chart across, press the right mouse button and, maintaining the mouse button pressed, drag the mouse in the direction you wish to scroll the Chart. When you release the mouse button, the Chart will remain at the new location.

1.2.4 Save the Charts to Graphic Files

To save the current chart to a graphic file (in Demo, only BMP format is supported) click **SaveChart** displayed in the right low corner of the chart and then specify the BMP file name.

1.3 GEISA-Demo for Other Platforms

RAD Studio allows us to develop applications for Windows, OS X (mac), Android and iOS target platforms.
This Demo has been also checked on OS X platform. The distribution of iOS and OS X application is regulated by Apple policy. The following is a screenshot of GEISA Demo taken on OS X (mac):



In future, it is possible to develop GEISA clients for OS X, Android, and iOS target platforms.