Simulated NMR Spectrum using Jmol

Spoken Tutorial Project
https://spoken-tutorial.org
National Mission on Education through ICT

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Learning Objectives

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▶ **Predict the 1H NMR and 13C NMR spectra for organic molecules using JSpecView**

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▶ **Change the display parameters of the plot**

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▶ **Integrate the peaks in the 1H NMR spectrum**

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► **Stack two or more spectra**

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- **Stack two or more spectra**
- **Combine two spectra**

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▶ **Save the spectrum in jdx format**

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▶ **Stack two or more spectra**

▶ **Combine two spectra**

▶ **Save the spectrum in jdx format**

▶ **Export the spectrum in various image file formats**

System Requirements

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- **Working internet connection**

Pre-requisites

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- **Jmol Spoken Tutorials link: https://spoken-tutorial.org**

Code Files

▶ **The input files required for this tutorial are available in the Code files link**

▶ **Please download and extract the files**

▶ **Make a copy of all the files and then use them for practising**

- **JSpecView** is a graphical viewer for spectral data in the JCAMP-DX format
- **https://jspecview.sourceforge.net**
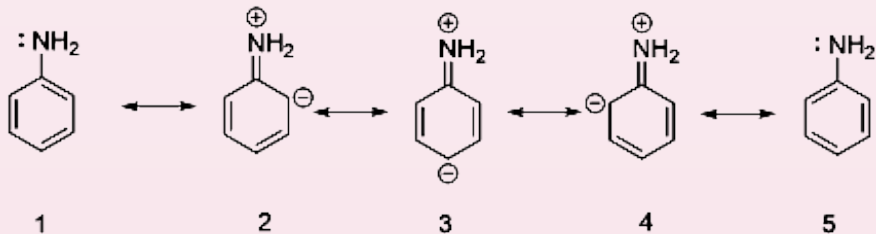
- **JSpecView** has been integrated into the Jmol distribution
- The Simulated 1H NMR and 13C NMR tools have been added in Jmol in the **Tools** menu

Resonance Structures of Aniline

Summary

- Predicted the 1H NMR and 13C NMR spectra for organic molecules using **JSpecView**
- Changed the display parameters of the plot
- Integrated the peaks in the 1H NMR spectrum

Summary

- ▶ **Stacked two or more spectra on the panel**
- ▶ **Combined two spectra**
- ▶ **Saved the spectrum in jdx format**
- ▶ **Exported the spectrum in pdf format**

Assignment

- ▶ **Simulate the 1H and 13C NMR spectra for molecules of your choice**

- ▶ **Explore more features of the JSpecView interface**

About the Spoken Tutorial Project

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Answers for THIS Spoken Tutorial

- ▶ **Questions in THIS Spoken Tutorial?**

- ▶ **Visit**
  https://forums.spoken-tutorial.org

- ▶ **Choose the minute and second where you have the question**

- ▶ **Explain your question briefly**

- ▶ **The Spoken Tutorial project will ensure an answer**

You will have to register to ask questions

Acknowledgements

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