

## DEPARTAMENTO DE QUÍMICA INORGÁNICA

### Tutorial sobre *Inorganic Chemistry Spectroscopy Tutorial*

Una web interactiva sobre **espectroscopía** UV-Vis, IR y de RMN, realizado por el Dr. J. Cooke, de la Universidad de Alberta.

<https://sites.google.com/ualberta.ca/inorganic-chemistry-labs/online-resources/spectroscopy-tutorial>

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El Inorganic Chemistry Spectroscopy Tutorial es una página web interactiva muy fácil e intuitiva de manejar. En la primera página a la izquierda nos muestra un índice desplegable con el contenido, con una introducción de cómo utilizarla, y después los apartados de las diferentes espectroscopías: UV-Vis, IR y RMN. La web proporciona además muchos ejemplos y preguntas interactivas. Y finalmente hay un índice con los tópicos abordados ordenados alfabéticamente, bibliografía sobre los contenidos y otro índice de los compuestos estudiados también ordenados alfabéticamente.

La página funciona como una presentación de PowerPoint, en la que se pueden pasar las diapositivas (pantallas) con la ayuda de los botones **PREV** y **NEXT**. La página inicial contiene un índice desplegable a la izquierda:

The screenshot shows a web browser displaying the 'Inorganic Chemistry Spectroscopy Tutorial' page. On the left is a 'Menu' sidebar with a tree view containing: Title, Help, Introduction, UV-Visible Spectroscopy, Infrared Spectroscopy, Nuclear Magnetic Resonance Spectroscopy, Index, and Chemical Compound Index. The main content area features a green background with the title 'Inorganic Chemistry Spectroscopy Tutorial' and subtitle 'Theoretical Principles and Applications'. Below the title are three plots: a UV-Vis absorption spectrum showing absorbance vs wavelength (400-700 nm) with a peak at 610 nm; an IR transmittance spectrum showing % Transmittance vs Wavenumber (2500-500 cm<sup>-1</sup>) with a peak at 2000 cm<sup>-1</sup>; and an NMR spectrum showing chemical shift (δ in ppm) with peaks at 93.5 and 85.3 ppm, each with a 1.8 Hz scale bar. At the bottom, it lists authors: Jason Cooke, Enrico Fok, June Ng, and Greg Nilsson (Department of Chemistry); Komalpreet Nandra and Tij Sachdeva (Technologies in Education, University of Alberta). It also includes Creative Commons icons, a version number (2.02, 2021/03), and a 'NEXT >' button.

Página de ayuda con los comandos para utilizar el tutorial (**Button Descriptions**):

www.chem.ualberta.ca/~inorglab/spectut2/story\_html5.html

Inorganic Chemistry Spectroscopy Tutorial

## Button Descriptions

- Back** Click to move backwards or forwards through frames *within a page*.
- More** Click to find out the answer to a question.
- Answer** Click to find out the answer to a question.
- PLAY** Click to start and stop animations.
- STOP** Click to start and stop animations.
- Reset** Click to reset an interactive exercise.
- Command** Performs the stated command when clicked.
- Yes** Click the circle to make a selection.
- No** Click the circle to make a selection.
- References** Click to view specific references for the page you are on.
- Close** Click to close the active pop-up dialogue box.

◀ PREV    NEXT ▶

Página con los principios básicos de la espectroscopia:

www.chem.ualberta.ca/~inorglab/spectut2/story\_html5.html

Inorganic Chemistry Spectroscopy Tutorial

## Introduction

### Spectroscopy

Spectroscopy is the study of the interaction of electromagnetic radiation with matter. In a chemical context, spectroscopy is used to study energy transitions in atoms and molecules. The transitions that are observed are interpreted and can serve to identify the molecule or give clues about the molecular structure. Spectroscopy is a powerful tool for inorganic chemists and is used frequently in the inorganic chemistry laboratory.

When a molecule interacts with electromagnetic radiation, energy is absorbed and the molecule is promoted, or is said to undergo a transition, to a higher energy state (excited state). In order for absorption to occur, the energy of the radiation must match the energy difference between the **quantized** energy levels of the molecule.

*Spectroscopy is a problem-solving tool for chemists.*

◀ PREV    NEXT ▶

Veamos, por ejemplo, una página con una pregunta interactiva. La página 5 de la introducción ([intropg5](#)) es de este tipo.

www.chem.ualberta.ca/~inorglab/spectut2/story\_html5.html

**Inorganic Chemistry Spectroscopy Tutorial**

## Introduction Page 5

Real molecules have more than one excited state, and absorption spectra frequently show more than one peak. In this example,  $E_2$ ,  $E_3$ ,  $E_4$  are the first three excited states. How many absorption peaks should appear in this spectrum?

**Answer**

← PREV    NEXT →

El texto de la página enuncia una pregunta, cuya respuesta puede verse haciendo clic en **Answer**. En la nueva dispositivo se muestra la respuesta de la pregunta de la página anterior. Podemos volver a la presentación presionando en **Back**.

www.chem.ualberta.ca/~inorglab/spectut2/story\_html5.html

**Inorganic Chemistry Spectroscopy Tutorial**

## Introduction Page 5

Three absorption peaks are detected, corresponding to the three **transitions**. It takes higher energy radiation to promote the molecule to higher excited states.

**← Back**

← PREV    NEXT →

Veamos otro ejemplo de preguntas para responder en el tutorial. Dentro de los contenidos de **UV-Visible Spectroscopy**, la dispositiva 8 (**UVpg8**) es la siguiente:

www.chem.ualberta.ca/~inorglab/spectut2/story\_html5.html

Inorganic Chemistry Spectroscopy Tutorial

## UV-Visible Spectroscopy Page 8

### Multi-Electron Systems

Systems with more than one d electron have additional complexities. In multi-d electron systems, the interactions between electrons must also be considered. Electron-electron interactions produce a number of possible **spin states** between which electronic transitions can occur. Obtaining a full understanding of the UV-visible spectra of most multi-d electron transition metal complexes is beyond the scope of this tutorial. However, it is still possible to interpret spectra if the foundation is provided. For example, the electrons in an octahedral  $d^2$  complex can be arranged into four different **spin states**.

Term symbols:  ${}^3T_{1g}(F)$   ${}^3T_{2g}$   ${}^3T_{1g}(P)$   ${}^3A_{2g}$

How many spin-allowed electronic transitions are expected for a  $d^2$  octahedral complex? **Answer**

Why do the energies of the  ${}^3T_{2g}$  and  ${}^3T_{1g}(P)$  states differ? **Answer**

◀ PREV    NEXT ▶

Obsérvese como el menú de la izquierda está desplegado el contenido de la espectroscopia UV-Visible.

Si nos vamos al inicio de la espectroscopía IR, se observa en el desplegable de la izquierda el contenido de la espectroscopia infrarroja

www.chem.ualberta.ca/~inorglab/spectut2/story\_html5.html

Inorganic Chemistry Spectroscopy Tutorial

## Infrared (IR) Spectroscopy

### Theory

Absorption of energy in the infrared region ( $\bar{\nu} = 4000 - 200 \text{ cm}^{-1}$ ) arises from changes in the vibrational energy of the molecules. There are two types of vibrations that give rise to transitions in an IR spectrum: **stretching** and **bending**. *Stretching* involves rhythmical displacement along the bond axis such that the interatomic distance alternately increases and decreases. *Bending* involves a change in bond angles between two bonds and an atom common to both.

Stretching      Bending

◀ PREV    NEXT ▶

Y si nos vamos el inicio de la espectroscopía de RMN, en la página se observa en el desplegable de la izquierda el contenido de la espectroscopia de resonancia magnética nuclear.

Algunas páginas contienen ejercicios. Por ejemplo, en la página [RMRpg18](#) se propone un ejercicio de espectroscopia de RMN

A la solución correcta se llega tras cuatro pantallas interactivas es las que se tiene que medir las integrales en mm (con la regla azul), reducir los valores a la relación más sencilla de números enteros y asignar los picos con ayuda de un menú desplegable.

**Inorganic Chemistry Spectroscopy Tutorial**

## NMR Spectroscopy Page 18

**Integration Line Measurement**  
You have accurately measured the integration lines.

**More** →

$C_5H_7O_2^- =$

1 H ✓ 15 mm ✓ CH ✓ 3 H ✓ 45 mm ✓ CH3 ✓ 3 H ✓ 45 mm ✓ CH3 ✓

Hide ruler Reset

← PREV NEXT →

Las últimas páginas de la presentación contienen:

1. Un índice de tópicos ordenados alfabéticamente:

www.chem.ualberta.ca/~inorglab/spectut2/story\_html5.html

**Inorganic Chemistry Spectroscopy Tutorial**

## Inorganic Chemistry Spectroscopy Tutorial Index and References

### Subject Index

➡ A-B   ➡ E   ➡ I-L   ➡ R-S

➡ B-C   ➡ F   ➡ M-N   ➡ T-W

➡ D   ➡ G-H   ➡ N-Q   ➡ X-Z

➡ Chemical Compound Index   ➡ General References

▼ Subtopics

← PREV NEXT →

## 2. Un listado de referencias.

The screenshot shows a web browser window with the URL [www.chem.ualberta.ca/~inorglab/spectut2/story\\_html5.html](http://www.chem.ualberta.ca/~inorglab/spectut2/story_html5.html). The page title is "Inorganic Chemistry Spectroscopy Tutorial" and the main heading is "General References". A left-hand menu is visible, with "General References" selected. The main content area lists five references:

- Brisdon, A.K. *Inorganic Spectroscopic Methods*, Oxford University Press: Oxford 1998.
- Iggo, J.A. *NMR Spectroscopy in Inorganic Chemistry*, Oxford University Press: Oxford, 1999, pp. 1 - 21; 31 - 35.
- Harris, D.C.; Bertolucci, M.D. *Symmetry and Spectroscopy*, Dover: New York, 1978.
- Nakamoto, K. *Infrared and Raman Spectra of Inorganic and Coordination Compounds*, Pt. A, 5th ed.; John Wiley & Sons: New York, 1997.
- Silverstein, R. M.; Bassler, G.C.; Morrill, T.C. *Spectrometric Identification of Organic Compounds*; 5th ed.; Wiley: New York, 1991.

Below the list, a note states: "\* Specific reference citations are marked with  on individual pages. Clicking the  icon will open a window with reference details." The word "References" is written below the icon.

Navigation buttons for "PREV" and "NEXT" are located at the bottom right of the page.

## 3. Y un índice de los compuestos estudiados.

The screenshot shows the same web browser window, but the page title is "Inorganic Chemistry Spectroscopy Tutorial" and the main heading is "Chemical Compound Index". The left-hand menu is visible, with "Chemical Compound Index" selected. The main content area displays a list of chemical compounds and their corresponding spectroscopic data:

<b>A</b>	[AgP(C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> (CH <sub>3</sub> )] [OSO <sub>2</sub> CF <sub>3</sub> ], <sup>31</sup> P NMR spectrum	NMRpg39
<b>B</b>	BF <sub>3</sub> , IR spectrum	IRpg10
	BF <sub>3</sub> , vibrational modes	IRpg9
	BH <sub>4</sub> <sup>-</sup> , IR spectrum and vibrational modes	IRpg11
	BH <sub>3</sub> NH(CH <sub>3</sub> ) <sub>2</sub> , IR spectrum	IRpg18
	BH <sub>3</sub> N(C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> , IR spectrum	IRpg17
	B <sub>2</sub> H <sub>6</sub> , IR spectrum and vibrational modes	IRpg12
	B <sub>3</sub> H <sub>6</sub> N <sub>3</sub> , <sup>1</sup> H NMR spectrum	NMRpg12

Navigation buttons for "PREV" and "NEXT" are located at the bottom right of the page.