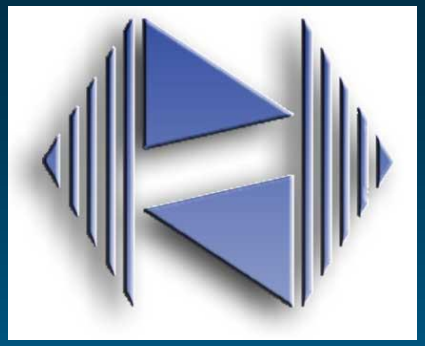


Universidade de São Paulo
Instituto de Física de São Carlos - IFSC

7600142 Introdução a Espectroscopia Física

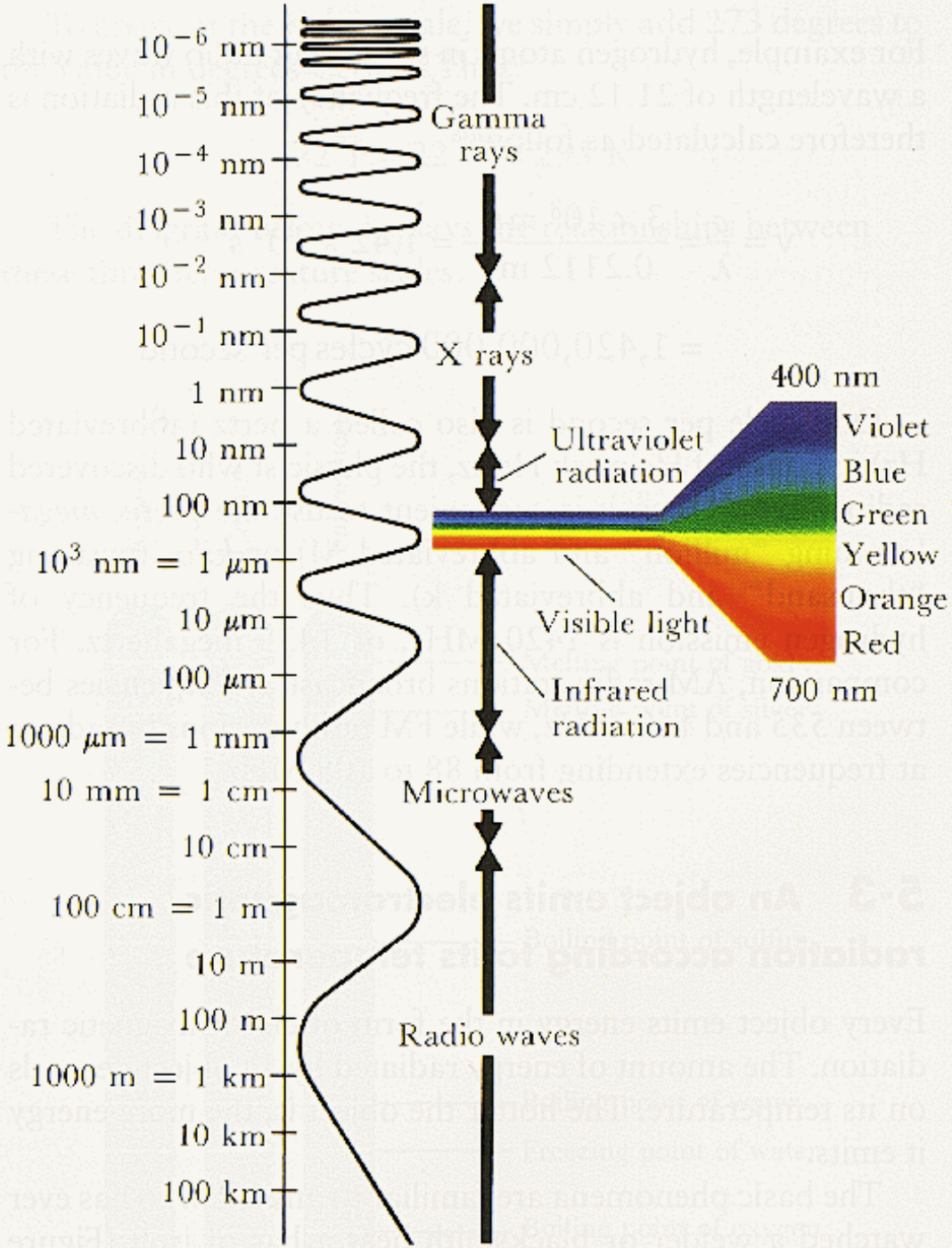
Programa

Prof. Dr. José Pedro Donoso

Introdução: Historia da Espectroscopia

W. Herschel: rad. infravermelha (1800)

Felix Bloch, NMR (1952)



Espectro Eletromagnético

Regiões espectrais:

-**radiofrequência** (RF): RMN

-**microondas**: rotações moleculares; RPE

-**Infravermelho distânte** (FIR)

-**Infravermelho:** vibrações moleculares

-**Visível**: transições eletrônicas

-**Ultravioleta**

-**Raios X**: transições eletrônicas

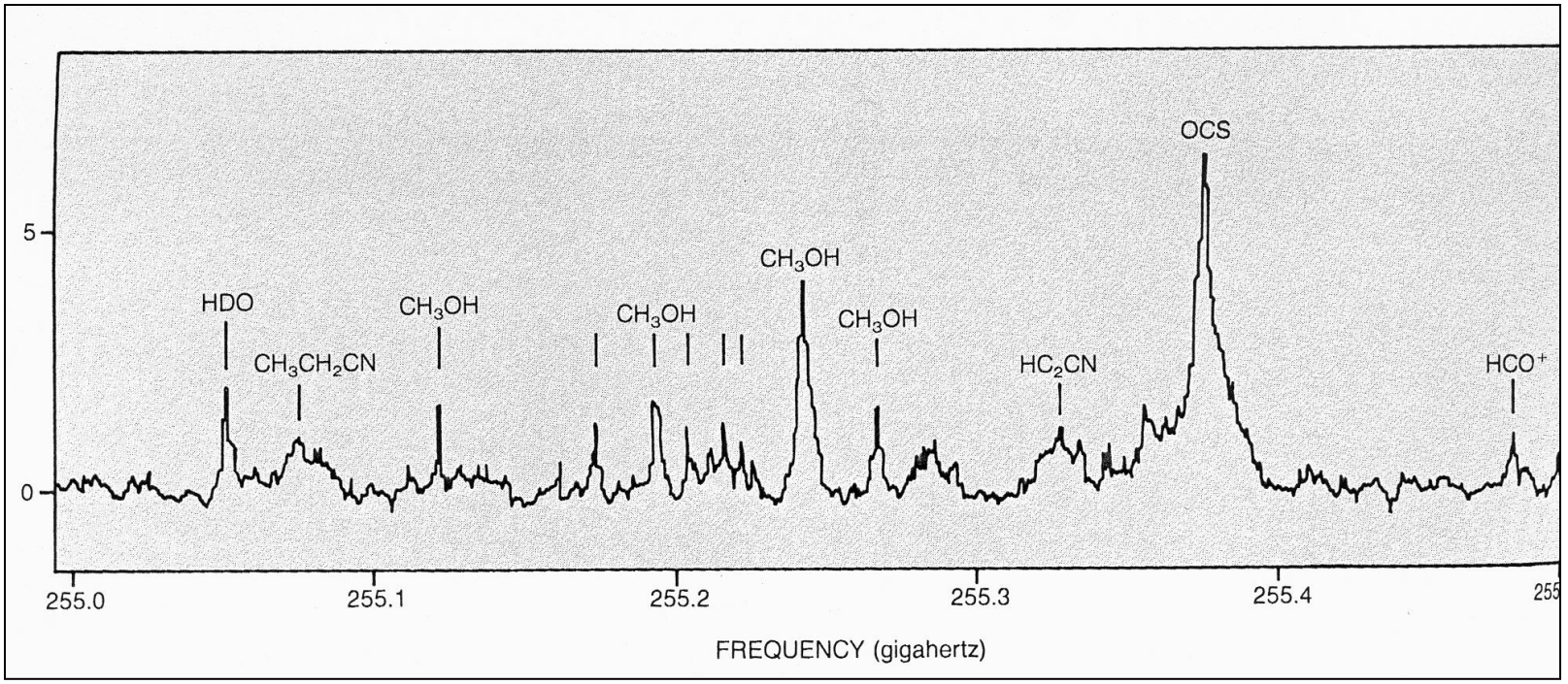
2 - Espectroscopia de Microondas

Espectros rotacionais.

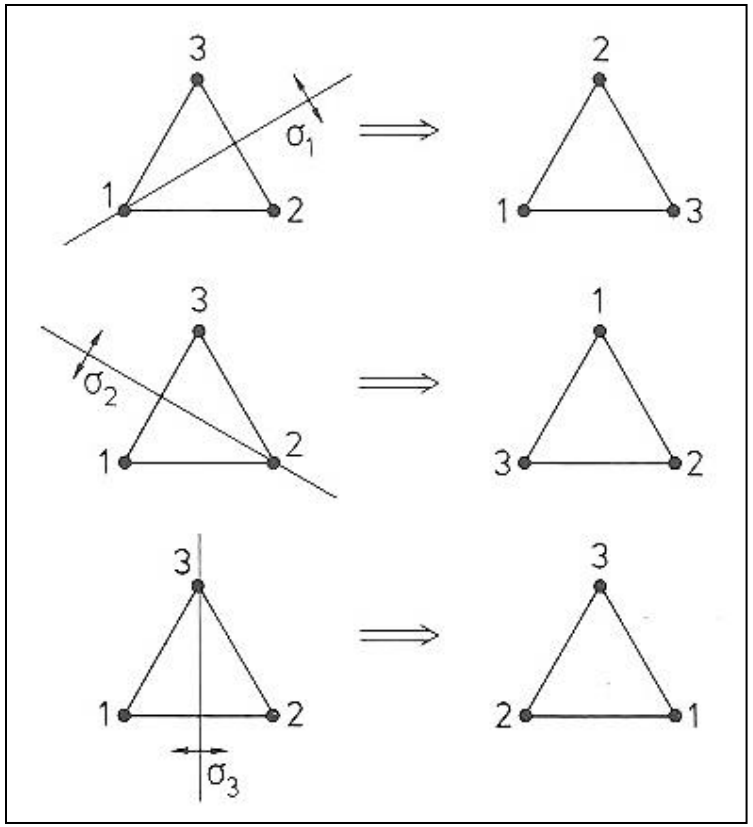
Determinação de momentos dipolares (efeito Stark)

Espectros de inversão (NH_3)

Espectros de estrelas e do espaço interlestelar



3 - Simetria e Teoria de Grupos aplicada a espectroscopia



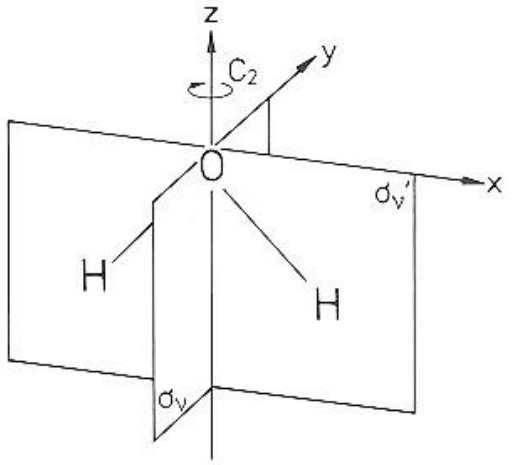


Table 6.14. Character table for C_{2v}

C_{2v}	E	C_2	σ_v	σ_v'		
A_1	1	1	1	1	z	x^2, y^2, z
A_2	1	1	−1	−1	R_z	xy
B_1	1	−1	1	−1	x, R_y	xz
B_2	1	−1	−1	1	y, R_x	yz

4 - Espectroscopia Vibracional : Infravermelho e Raman

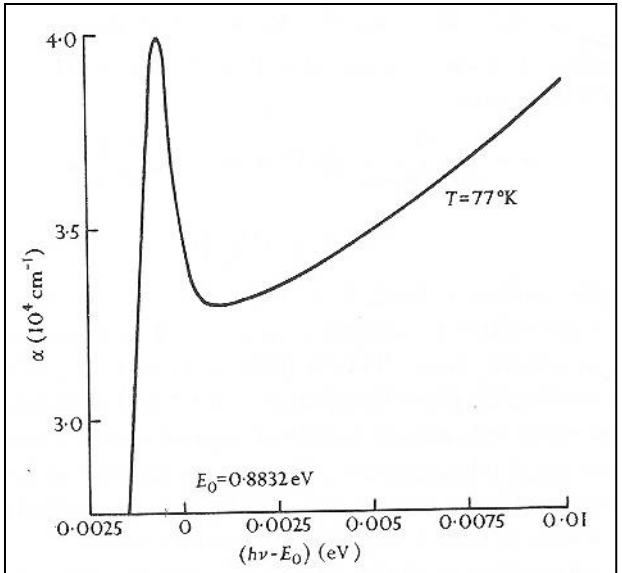
Espectrômetro infravermelho Kore

Espectroscopia vibracional de moleculas.

Espectroscopia Infravermelha de sólidos.

Excitons.

Semicondutores: gap de energia.



Direct exciton line in germanium (after McFarlane, McLean, ton, and Roberts).

4 - Espectroscopia Vibracional : Infravermelho e Raman

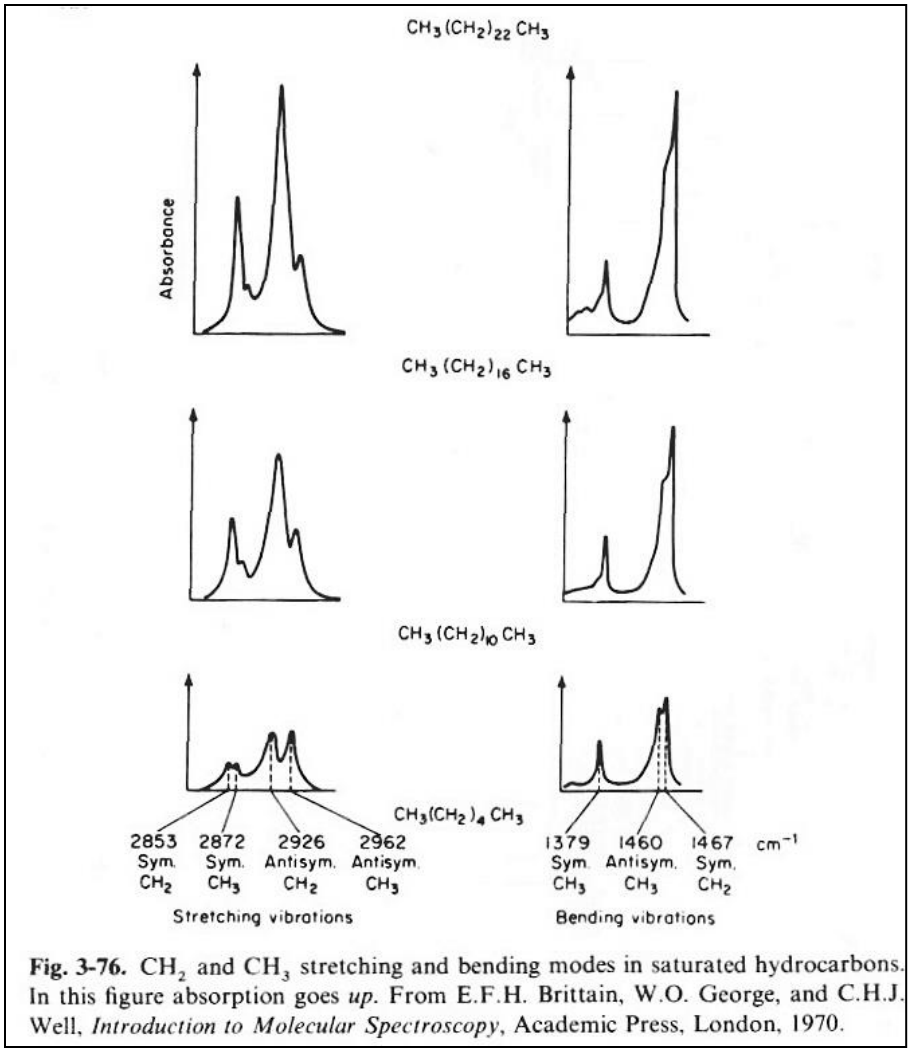
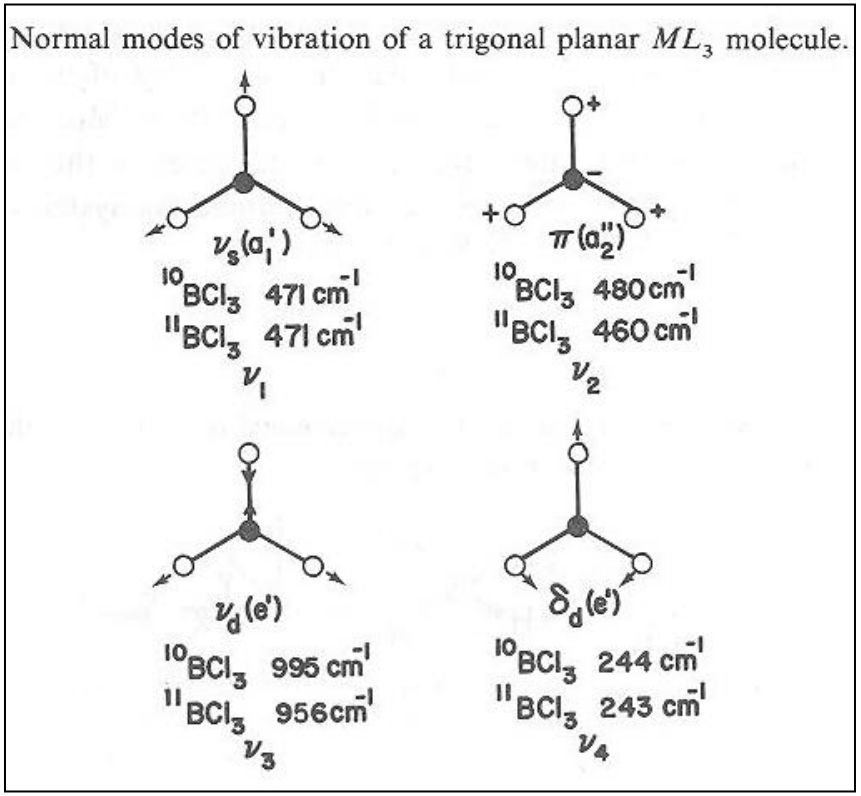


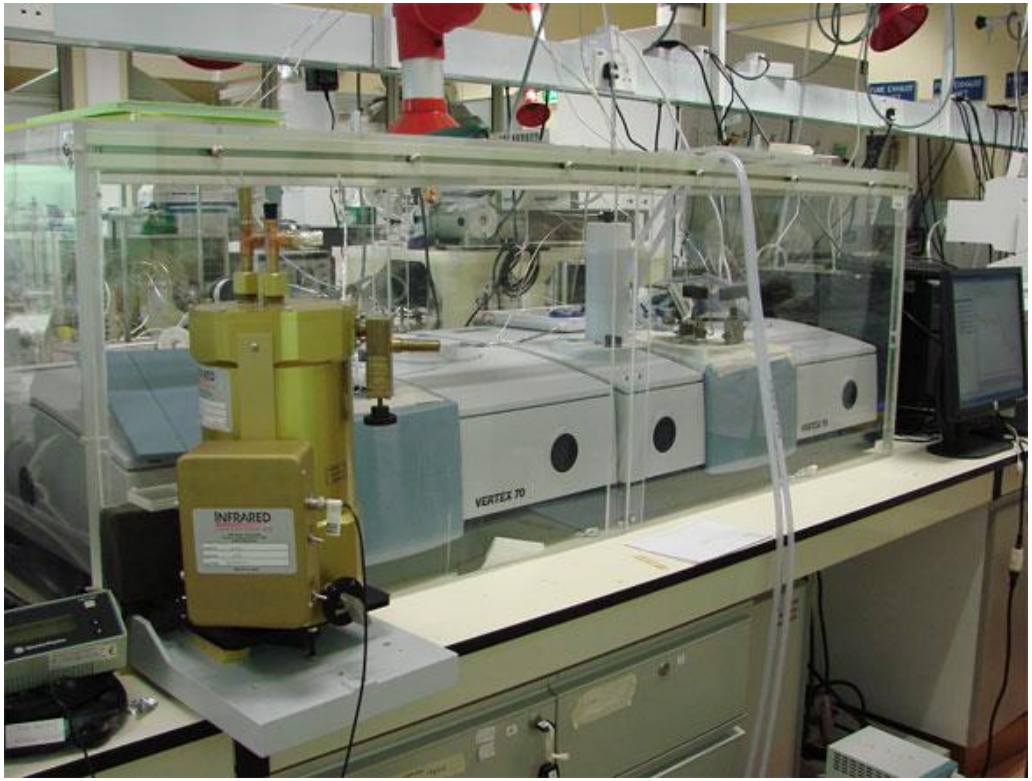
Fig. 3-76. CH_2 and CH_3 stretching and bending modes in saturated hydrocarbons. In this figure absorption goes *up*. From E.F.H. Brittain, W.O. George, and C.H.J. Well, *Introduction to Molecular Spectroscopy*, Academic Press, London, 1970.

Espectroscopia vibracional de moleculas.



Espectroscopia Vibracional

Infravermelho distânte (FIR)



Bruker

Aplicações:

-determinação do gap de supercondutores

-determinação da *attempt frequency* de condutores iônicos

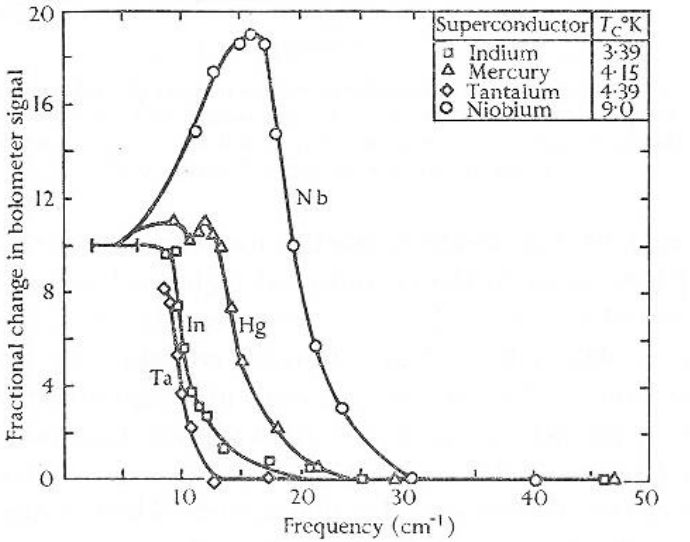


FIG. 7.15. Low-temperature absorption curves for four pure superconductors as measured by Richards and Tinkham.

Espectroscopia Vibracional

Espectroscopia Raman.

Horiba Jobin-Yvon

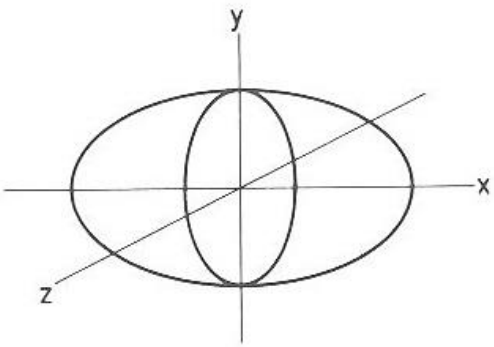


Figure 5.14 The polarizability ellipsoid.

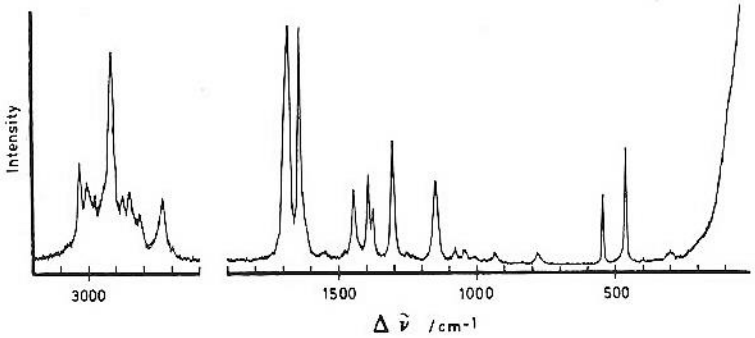
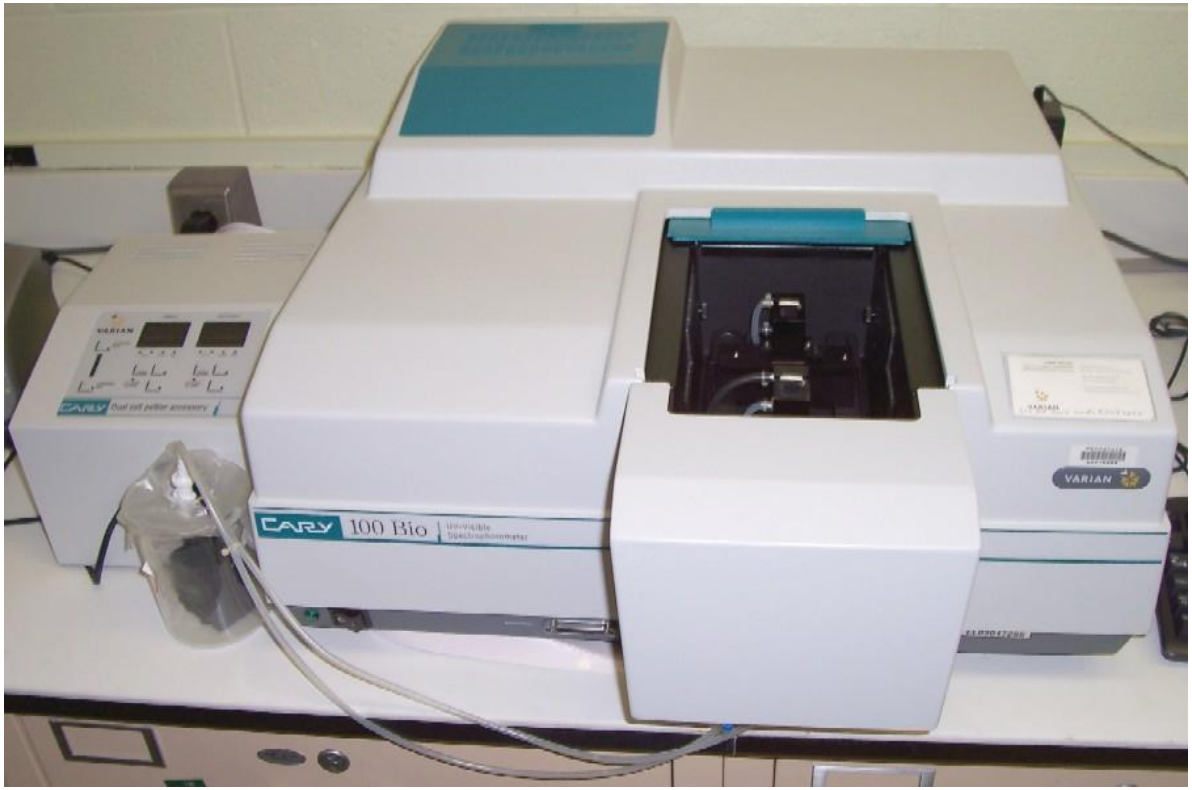


Figure 6.17 The laser Raman vibrational spectrum of liquid crotonaldehyde. (Reproduced, with permission, from Durig, J. R., Brown, S. C., Kalasinsky, V. F., and George, W. O., *Spectrochim. Acta*, **32A**, 807, 1976. Copyright (1976) Pergamon Press.)

5 - Espectroscopia Eletrônica

Espectros eletrônicos moleculares. Regras de seleção



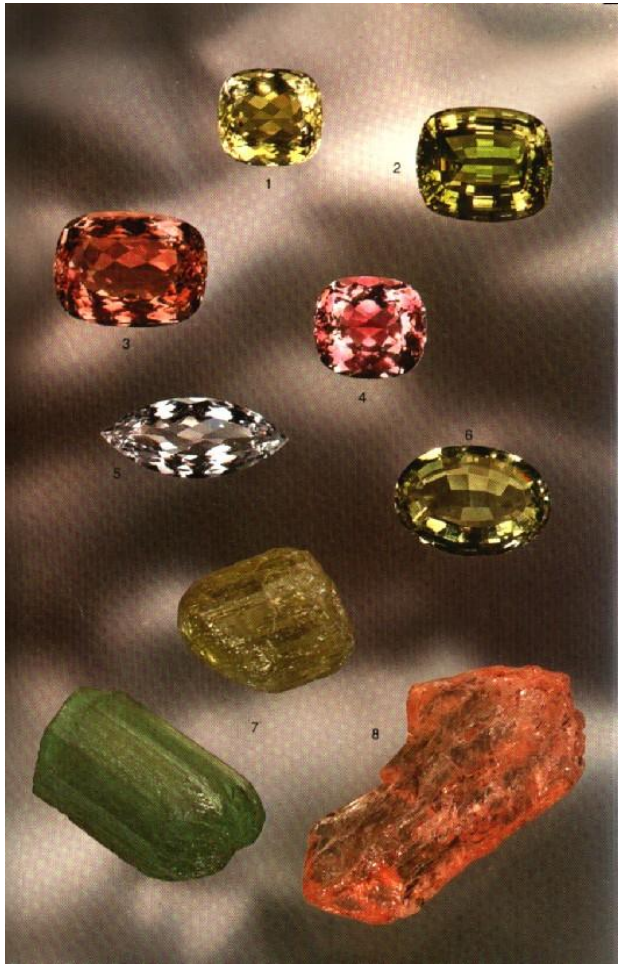
Espectrofotômetro UV-Vis Cary

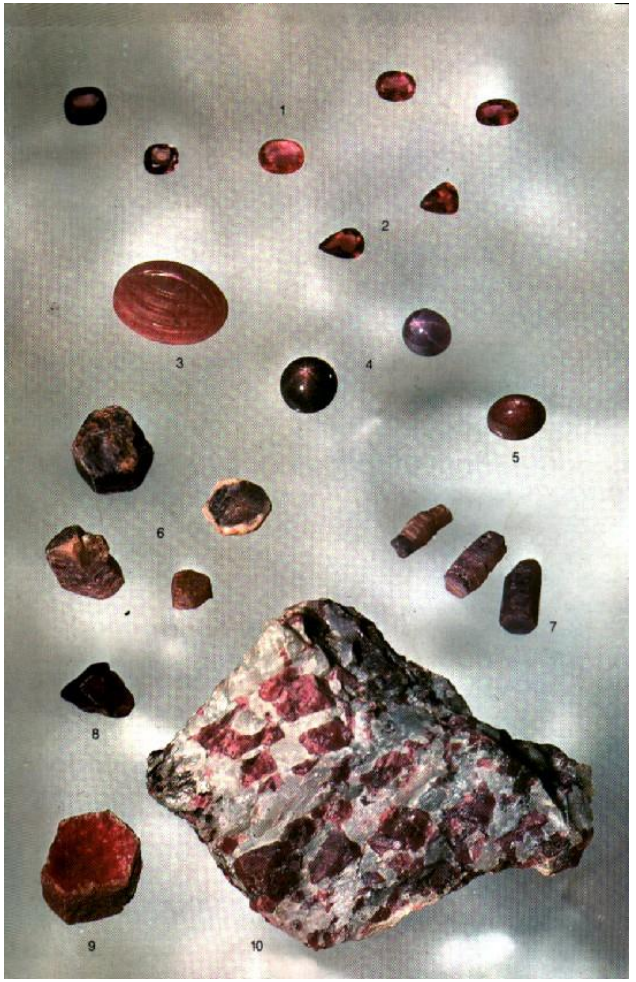
5 - Espectroscopia Eletrônica

Espectros de complexos de metais de transição.

Campo cristalino

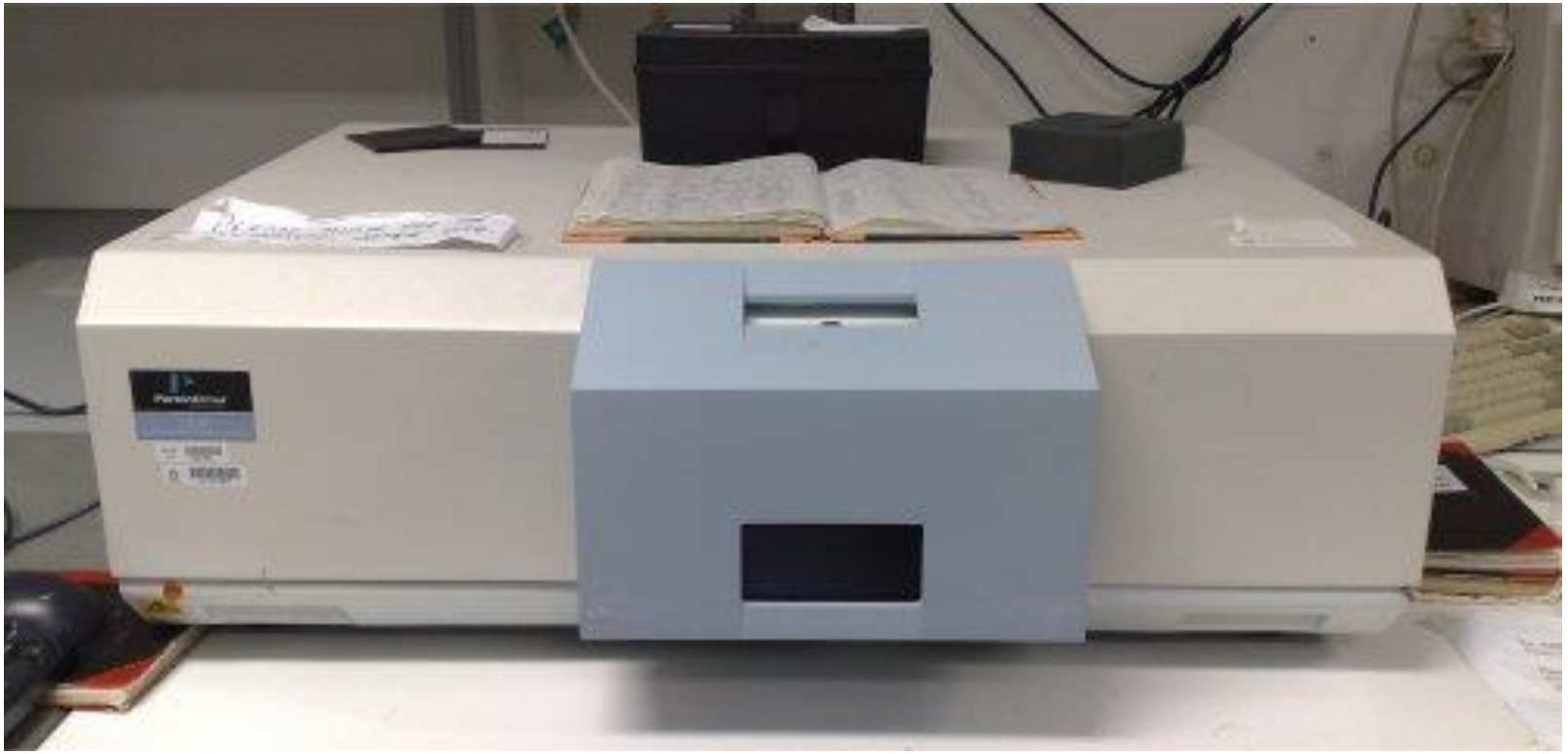
Bronzes. Centros de cor.





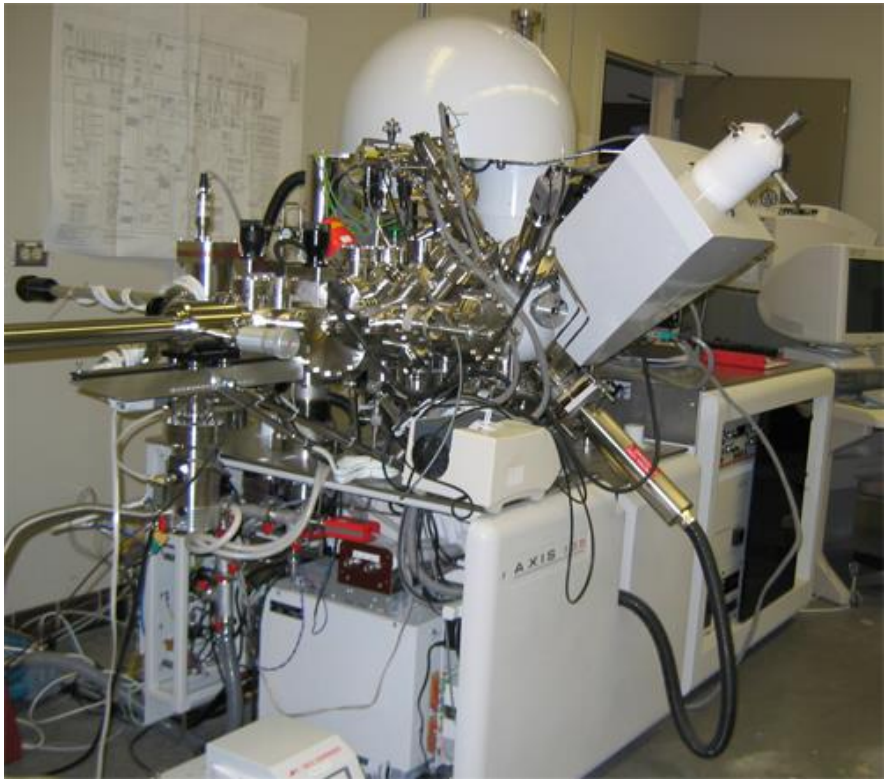
Espectroscopia Eletrônica

Luminescência em cristais



Perkin - Elmer

Espectroscopia Fotoeletrônica



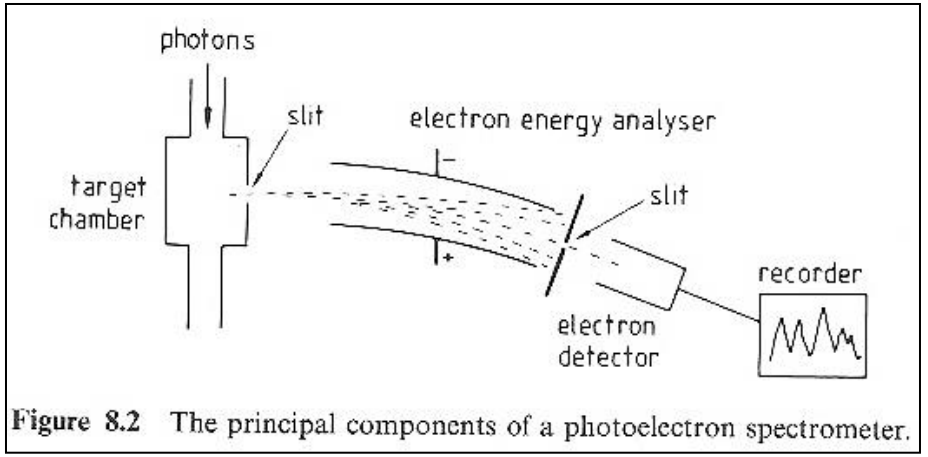
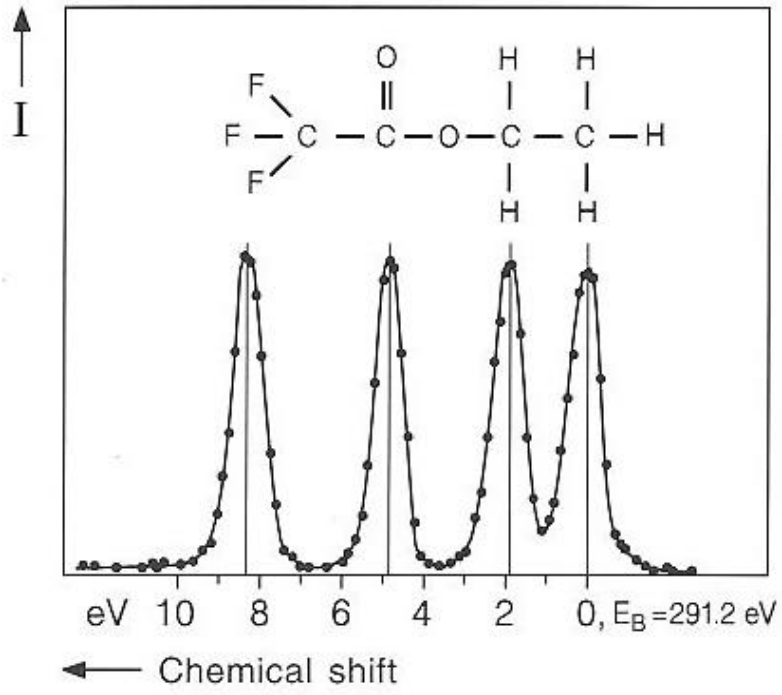


Figure 8.2 The principal components of a photoelectron spectrometer.

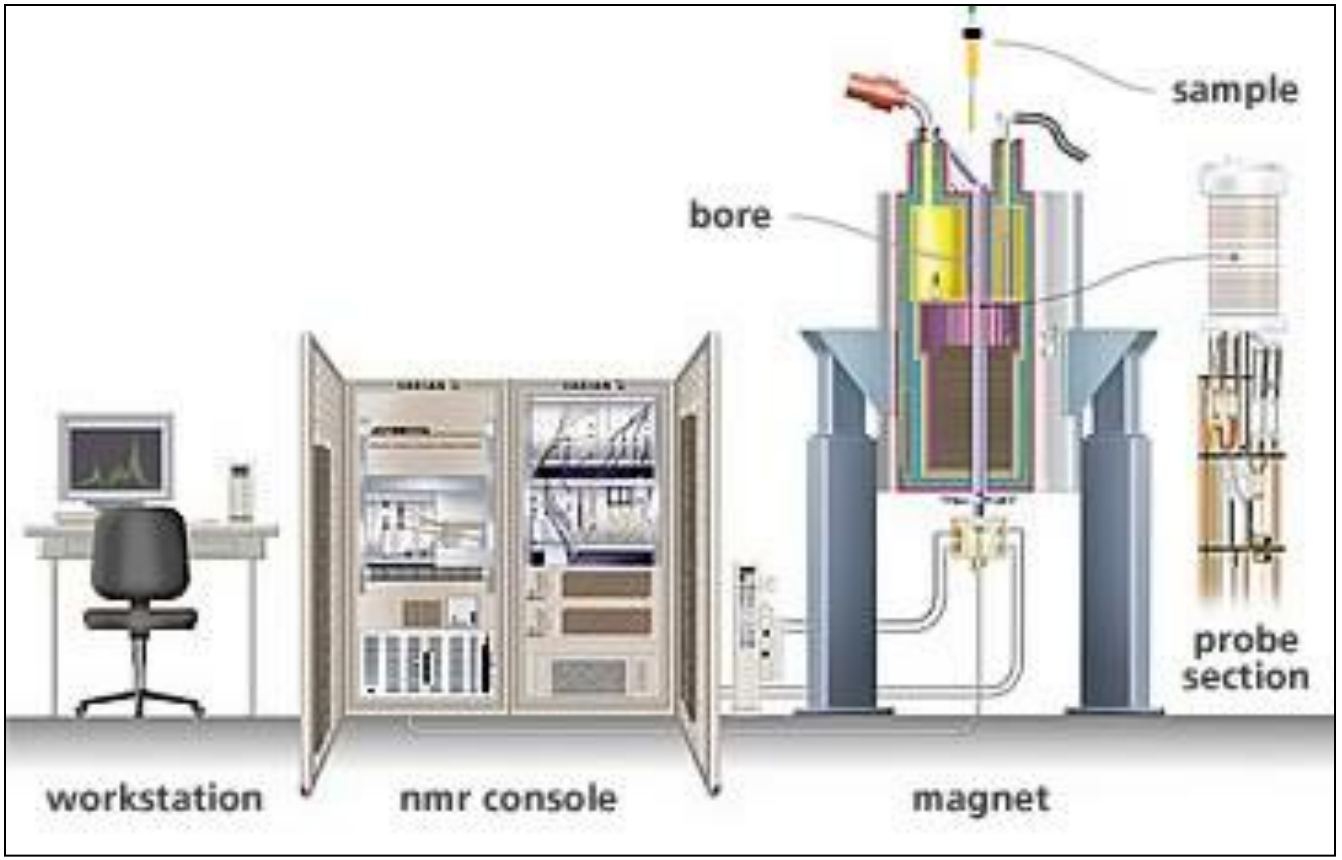


6 - Métodos Ressonantes

Ressonância Magnética Nuclear

Espectros RMN, Deslocamento químico.

Relaxação Nuclear. Aplicações.



Varian Inc

Bruker

Métodos Ressonantes

Ressonância Paramagnética Eletrônica

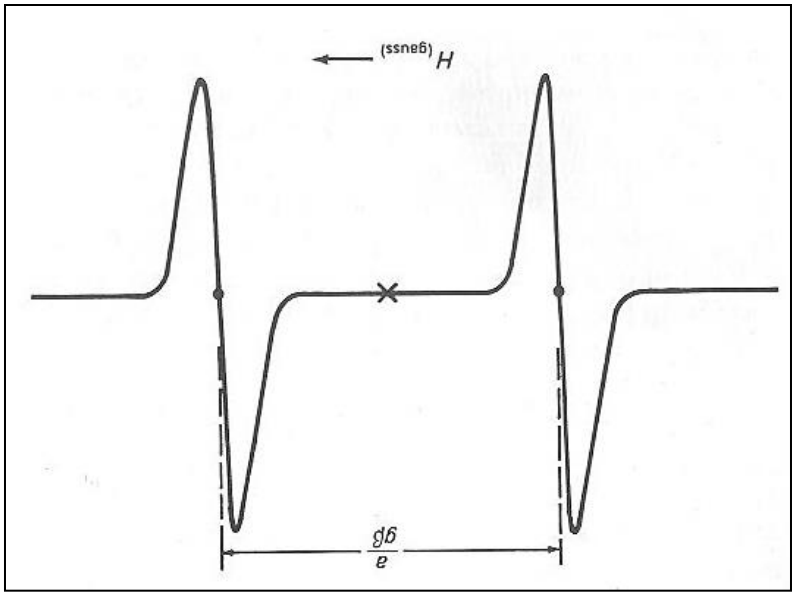
(*RPE, ESR*)

-Espectros hiperfinos;

-Espectros de íons metálicos;

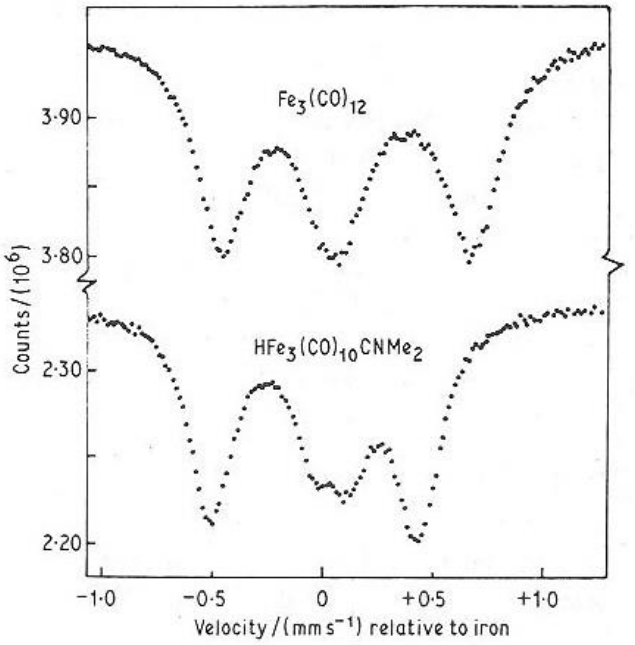
- Hamiltoniano de Spin.

- Radicais livres. Marcadores de spin.



6 - Métodos Ressonantes

Espectroscopia Mossbauer



The Mössbauer spectra of $Fe_3(CO)_{12}$ and $HFe_3(CO)_{10}CNMe_2$.

Univ. Coimbra, Portugal