

Magnetic Circular Dichroism (MCD)



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Introduction

- **MCD is the differential absorption of left and right circularly polarized light induced in a sample by strong magnetic field oriented parallel to the direction of light propagation**
- **MCD is used to observe magnetic field induced effects on optically active molecules**
- **Developed in 1930s (Theoretical explanations)**
- **Refined in 1960s**

INTRODUCTION

- ❖ **Assign transitions in the electronic absorption spectrum**
- ❖ **Determine the coordination number of the metal**
- ❖ **Can be used for both organic and inorganic systems**

INTRODUCTION

- **MCD spectroscopy is not based on resonance between spin states while NMR and EPR are**
- **MCD is based on the wavelength dependent absorption of circularly polarized light to form excited electronic states**
- **CD needs chiral centre while MCD does not**
- **MCD is complementary to UV-Vis absorption, specificity of MCD arises from three highly characteristic spectral features, the Faraday A,B and C terms**
- **Unlike EPR spectroscopy, even diamagnetic complexes exhibit an MCD signal**

WHY MCD?

❖ Sensitive Technique (**esp. near-IR**)

Has no Problems with Integer Spin

❖ Site Selectivity(**Multiple Metal Sites**)

Is not restricted to Para-magnetic Species

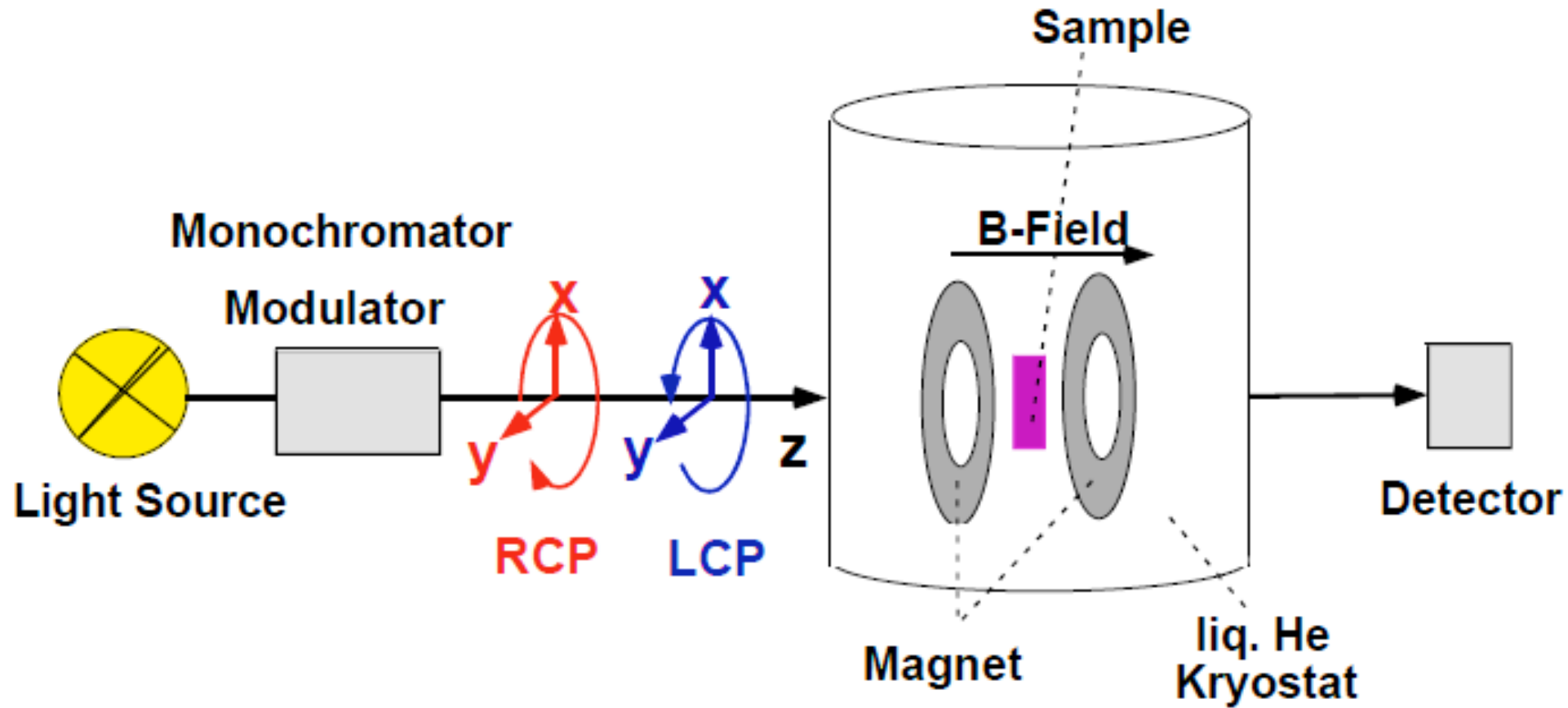
❖ Multidimensional(**B,T, λ**)

Studies the Ground and Excited States at the same time

❖ Does not require Isotopic Enrichment and is not restricted to certain elements

❖ Needs minimal sample

THE MCD EXPERIMENT

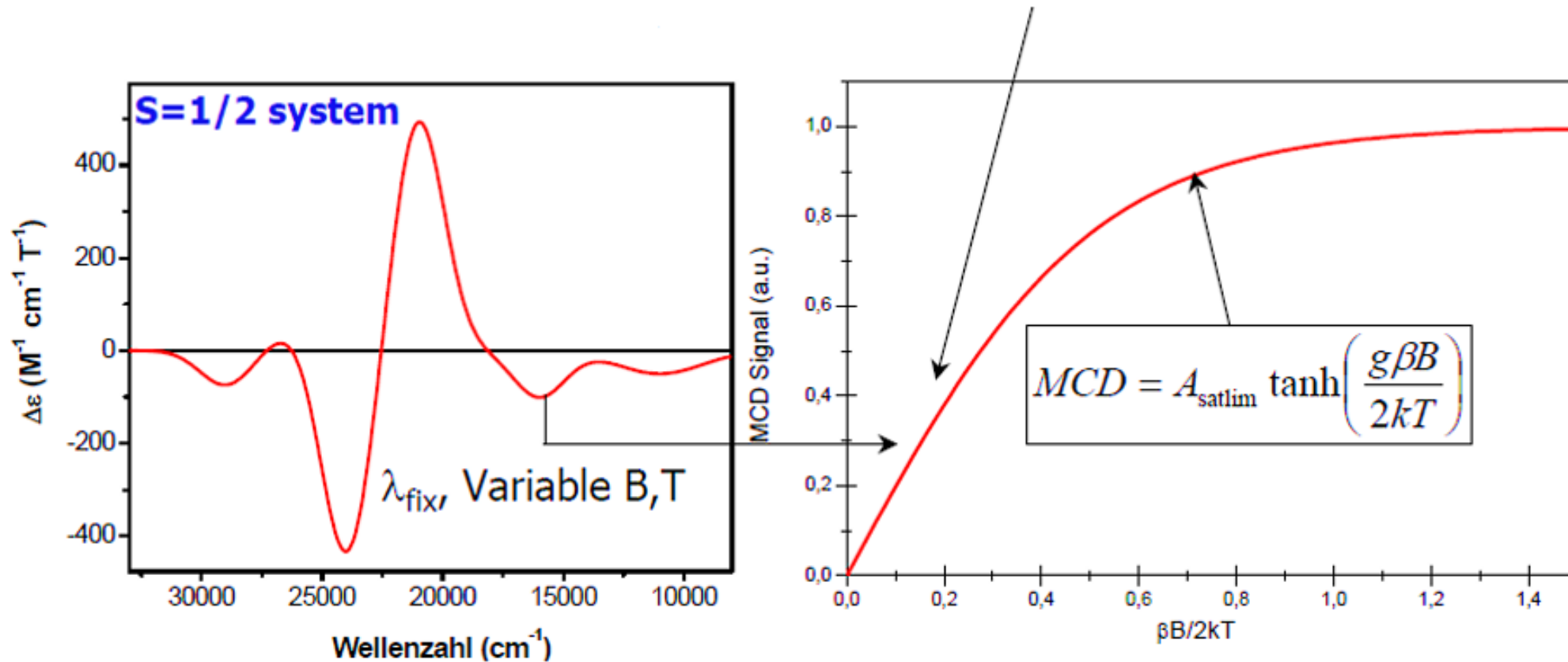


APPLICATIONS

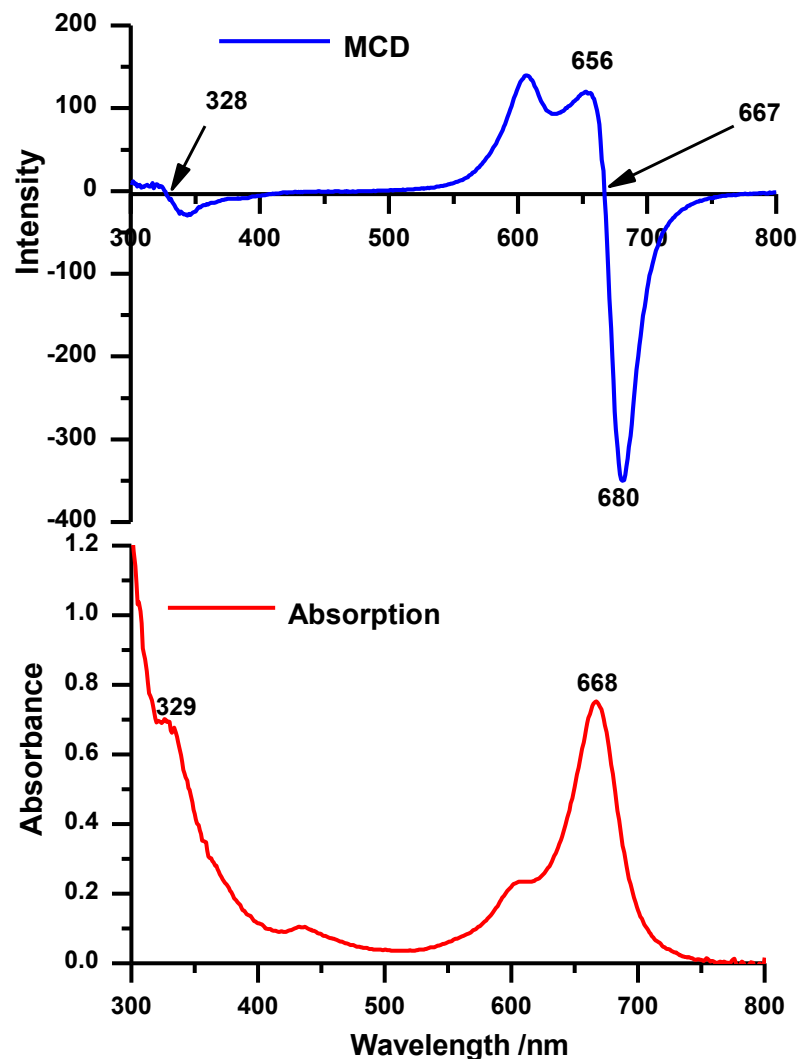
- ❖ **Biological systems (haem & myoglobin)**
- ❖ **Biological chromophores (vitamin B12 & Chlorophylls)**
- ❖ **Porphyrin**
- ❖ **BODIPY**
- ❖ **Phthacyanines**

THEORY OF MCD

$$\frac{\Delta \mathcal{A}_{l-r}}{E} = 152.5 Bcl \left[\mathcal{A}_l \left(-\frac{df}{dE} \right) + \left(B_0 + \frac{C_0}{kT} \right) f \right]$$



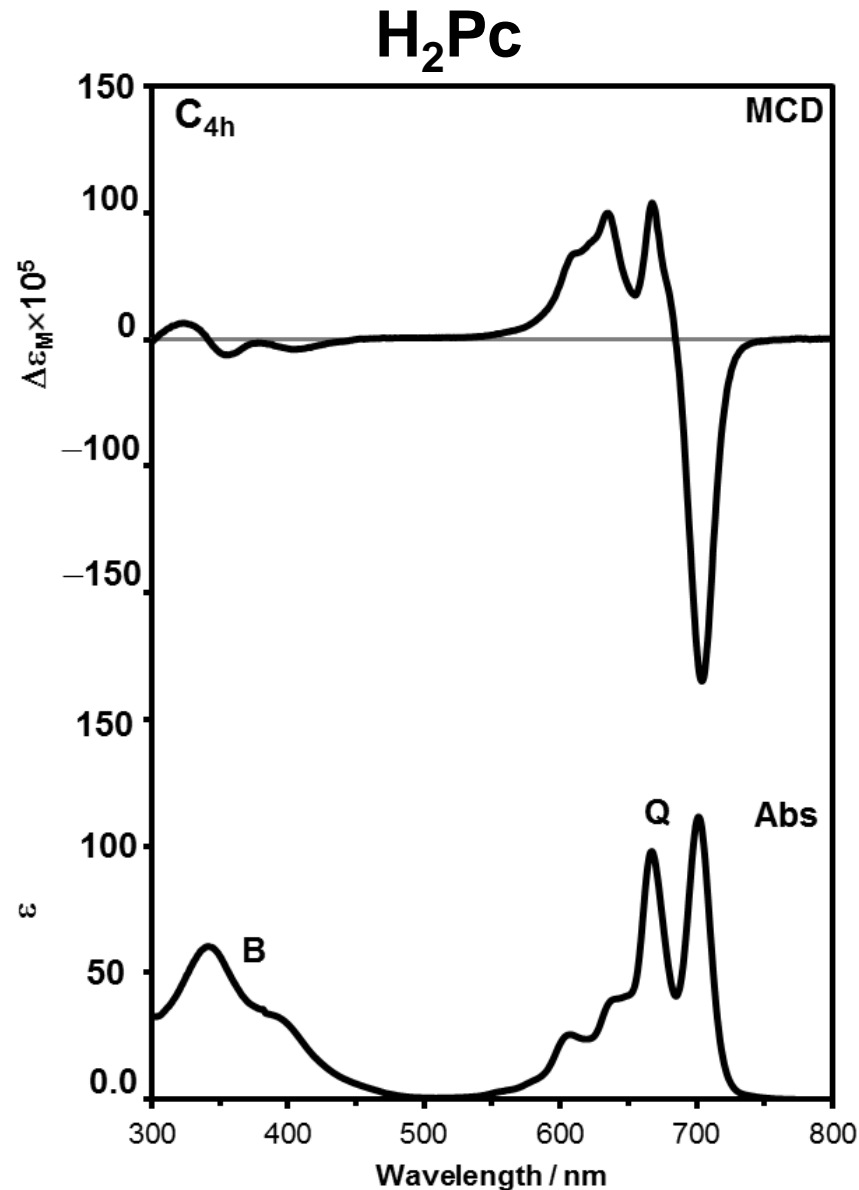
FARADAY A-TERM



A-term describes the breaking of degeneracies of the ground state and the excited state of the molecule

Electronic absorption and MCD spectra of CoTPPc in DMF

FARADAY B-TERM



**B-term describes the
field induced mixing
of the electronic
states**

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