Chiroptical spectroscopy – Theory and Applications
LVNr 181 041

LITERATURE LIST

GENERAL RECOMMENDED READING / KEY REFERENCES

Circular dichroism and Optical Rotatory Dispersion – Principles and Application to the Investigation of the Stereochemistry of Natural Products
G. Snatzke, *Angew. Chem. Int. Ed.* **7** (1968) 14-25

Circular Dichroism and Absolute Conformation: Application of Qualitative MO Theory to Chiroptical Phenomena
G. Snatzke, *Angew. Chem. Int. Ed.* **18** (1979) 363-377

Exciton chirality method and its application to configurational and conformational studies of natural products
Nobuyuki Harada, Koji Nakanishi
Acc. Chem. Res., **1972**, 5, 257–263

Absolute configuration determination of chiral molecules in the solution state using VCD
T. B. Freedman, X. Cao, R. K. Dukor, L. A. Nafie, *Chirality* **2003**, *15*, 743-758

Exciton Chirality Method in Vibrational Circular Dichroism
T. Taniguchi, K. Monde, *J. Am. Chem. Soc.* 2012, *134*, 3695-3698

Inspecting chiral molecules by Raman optical activity spectroscopy
Václav Parchaňský, Josef Kapitán, Petr Bouř
RSC Adv., 2014,4, 57125-57136

Chiral Molecular Science: How were the absolute configurations of chiral molecules determined? "Experimental results and theories"
Nobuyuki Harada, Chirality, **29** (2017) 774–797.

Absolute Configurations of Synthetic Molecular Scaffolds from Vibrational CD Spectroscopy
C. Merten, T. Golub, N. Kreienborg, *J. Org. Chem.,* 2019, **84**, 8797

TOPICS FOR SHORT PRESENTATIONS (15 min)

TOPIC 1: AC determinations utilizing induced CD effects

A Critical Appraisal of Dimolybdenum Tetraacetate Application in Stereochemical Studies of vic-Diols by Circular Dichroism
Marcin Gorecki, Jadwiga Frelek*, J. Nat. Prod.* **83** (2020) 955−964

And related publications: *J. Org. Chem.*, **2007**, 72, 2906–2916 and J. *Org. Chem.* **2001,** *66,* 4819-4825

An Exciton-Coupled Circular Dichroism Protocol for the Determination of Identity, Chirality, and Enantiomeric Excess of Chiral Secondary Alcohols
You et al, *J. Am. Chem. Soc.* 2012, **134**, 7117−7125

TOPIC 2: Application to chiral polymers 1

A Thermal and Solvocontrollable Cylindrical Nanoshutter Based on a Single Screw-Sense Helical Polyguanidine
Tang, Novak, He, Polavarapu, *Angew. Chem.* **117** (2005) 7464-7467

Identification of the Specific, Shutter-like Conformational Reorientation in a Chiroptical Switching Polycarbodiimide by VCD Spectroscopy,
C. Merten, J. F. Reuther, J. D. DeSousa and B. M. Novak, *Phys. Chem. Chem. Phys.*, 2014, **16**, 11456--11460.

TOPIC 3: Application to chiral polymers 2

Chirality Assignment of Amines and Amino Alcohols Based on Circular Dichroism Induced by Helix Formation of a Stereoregular Poly((4-carboxyphenyl)acetylene) through Acid-Base Complexation
Eiji Yashima, Teruyuki Matsushima, and Yoshio Okamoto, *J. Am. Chem. Soc.* **1997,** *119,* 6345-6359

Further reading: *Chem Eur. J.* **10** (2004) 42-51

TOPIC 4: Cryptochirality

Determination of the Absolute Configurations of Chiral Alkanes – An Analysis of the Available Tools
Fumito Saito, Peter R. Schreiner, Eur. J. Org. Chem. doi.org/10.1002/ejoc.202000711

TOPIC 5: Complex AC determinations

Strength by Joining Methods: Combining Synthesis with NMR, IR, and Vibrational Circular Dichroism Spectroscopy for the Determination of the Relative Configuration in Hemicalide
Ewoud De Gussem, Wouter Herrebout, Simon Specklin, Christophe Meyer, Janine Cossy, Patrick Bultinck
Chem. Eur. J. 2014, 20, 17385 – 17394

Stereochemistry of the tadalafil diastereoisomers: a critical assessment of vibrational circular dichroism, electronic circular dichroism, and optical rotatory dispersion
Qui et al., *J. Med. Chem.* **56** (2013) 8903-14

TOPIC 6: Chiral Nanoparticles

Vibrational Circular Dichroism of Adsorbed Molecules: BINAS on Gold Nanoparticles
Cyrille Gautier, Thomas Bürgi, *J. Phys. Chem. C* **2010,** *114,* 15897–15902

Chiral N-Isobutyryl-cysteine Protected Gold Nanoparticles: Preparation, Size Selection, and Optical Activity in the UV-vis and Infrared
C. Gautier and T. Burgi, *J. Am. Chem. Soc.*, 2006, **128**, 11079-11087.

TOPIC 7: Chiroptical properties of cryptophanes

Unusual Chiroptical Properties of the Cryptophane-222 Skeleton
Pitrat et al. *J. Phys. Chem. B*, 2016, **120**, 12650

Chiroptical properties of cryptophane-111
T. Buffeteau et al., *Phys. Chem. Chem. Phys.*, 2017, **19**, 18303.

TOPIC 8: AC determination of natural products

Select some interesting example from this review article: J. M. Batista et al., *Studies in Natural Products Chemistry*, 2014, **41**, 383, e.g.:

1. **VCD to determine absolute configuration of natural product molecules: secolignans from Peperomia blanda**
   Felippe et al., *Org. Biomol. Chem.,* 2012, **10**, 4208

2. **Determination of the Absolute Configurations of Natural Products via Density Functional Theory Calculations of Vibrational Circular Dichroism, Electronic Circular Dichroism, and Optical Rotation: The Iridoids Plumericin and Isoplumericin**
   Stephens et al., *J. Org. Chem.* **2007**, *72*, 3521-3536

NOTE

Prepare powerpoint slides for your presentation based on the paper and *consider other references as well* - **as if you were the author of the study!** Keep in mind, the others need to understand the key problem addressed in the paper and the context of the problem.

Prepare 1 page summary of your paper as handout for the other students (should not be a simple copy of the abstract!)

Presenting a paper is mandatory for every student who needs credit points.