

Liquid Crystals and Lighting Up Gold(III)

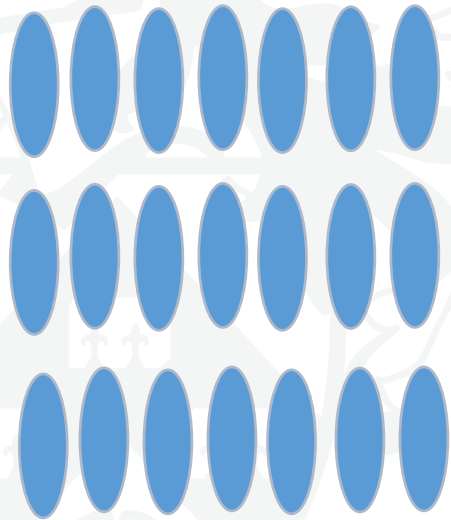
Alice Jane McEllin MChem
PhD Student, University of York

Supervisor: Professor Duncan Bruce

Topics

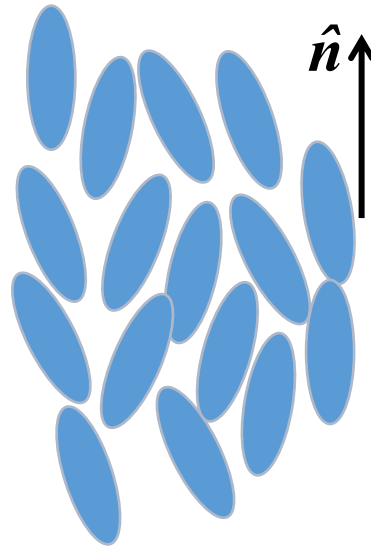
- Liquid crystals
- Organic Light Emitting Diodes (OLEDs)
- My work on gold(III)

What are liquid crystals?



Solid

T_m



Liquid Crystal

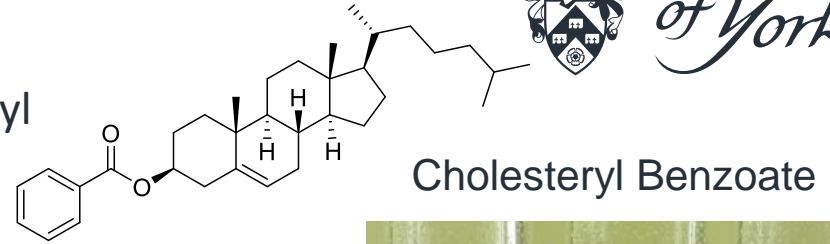
T_c



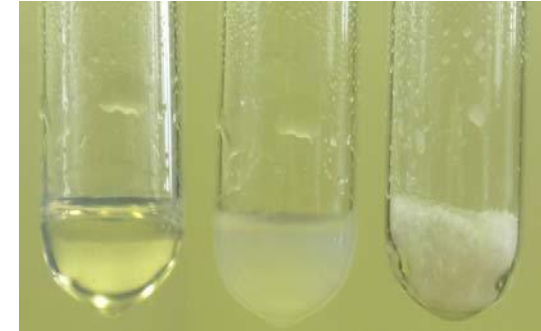
Liquid

History

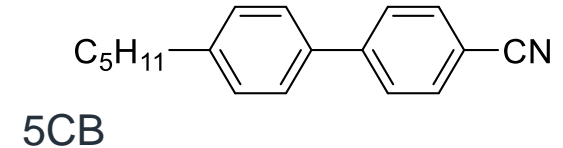
- 1st discovered in 1888 by Reinitzer: cholesteryl benzoate



- Used in prototype LCD devices in late 1960s, early 1970s

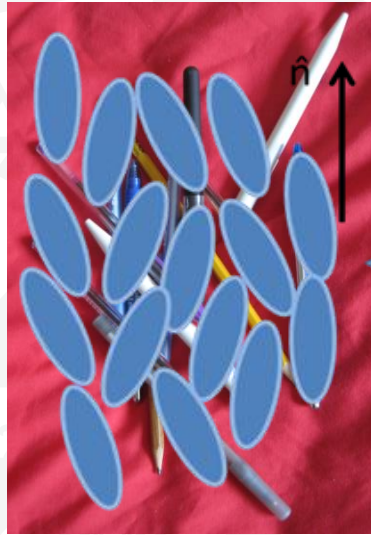


- 1972 at University of Hull: cyanobiphenyls, 4-cyano-4'-pentylbiphenyl (5CB) discovered.



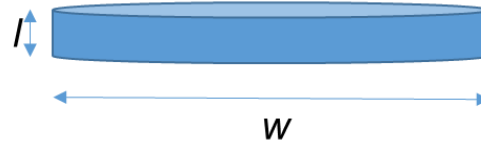
Typical Shapes?

Rod-Shaped



$$l \gg w$$

Disc-Shaped



$$w \gg l$$



Liquid Crystal Phases: Calamitic

Rod-Shaped



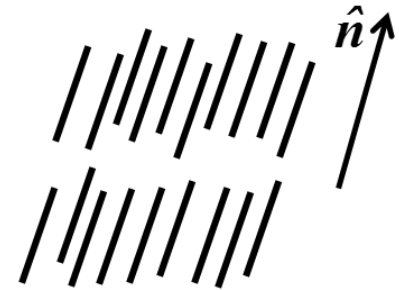
$l \gg w$



Nematic, N

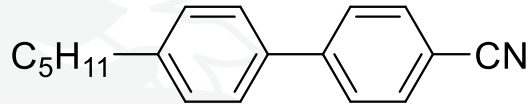


Smectic A, SmA

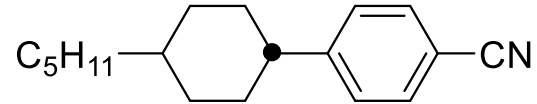


Smectic C, SmC

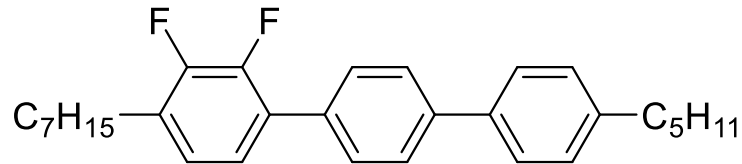
Some examples...



C 24.0 N 35.0 Iso

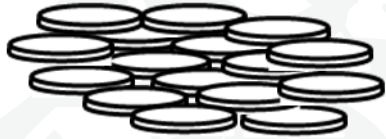


C 31.0 N 55.0 Iso

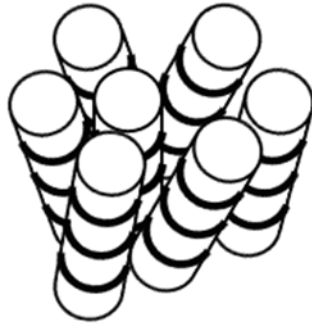


C 56.0 SmC 105.5 SmC 131.0 N 136.0 Iso

Liquid Crystal Phases: Discotic



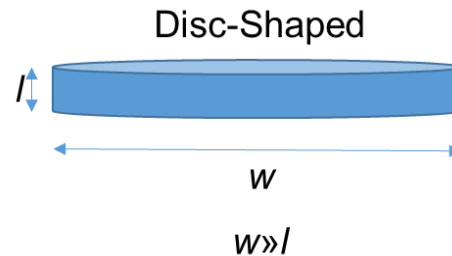
Discotic Nematic, N_D



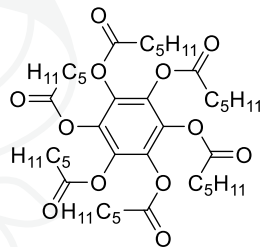
Columnar Nematic, N_{Col}



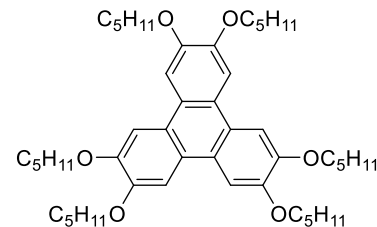
Hexagonal Columnar, Col_h



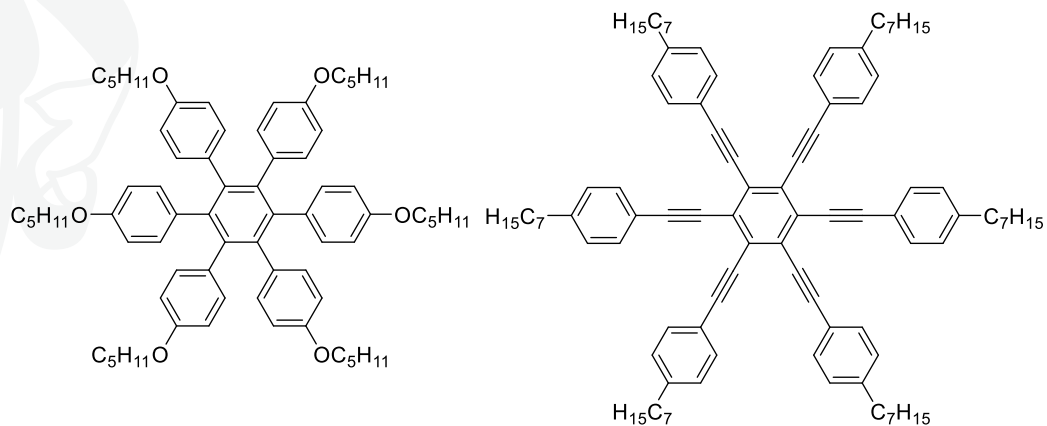
Some examples...



C 68.3 Col_r 86.0 Iso



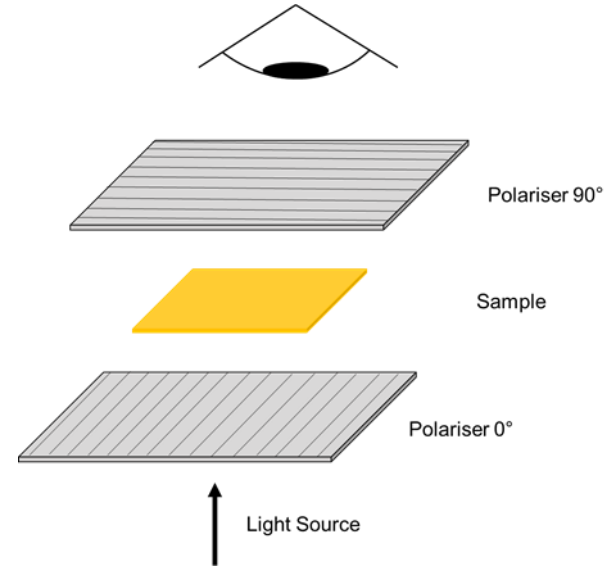
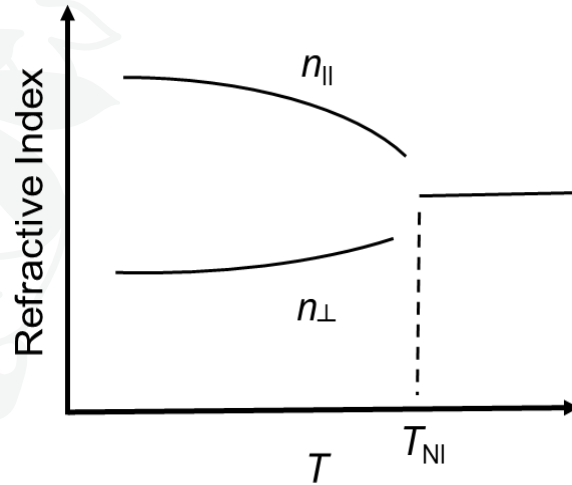
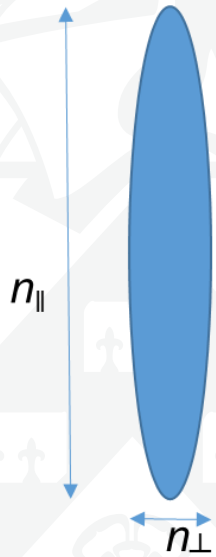
C 69.0 Col_h 122.0 Iso



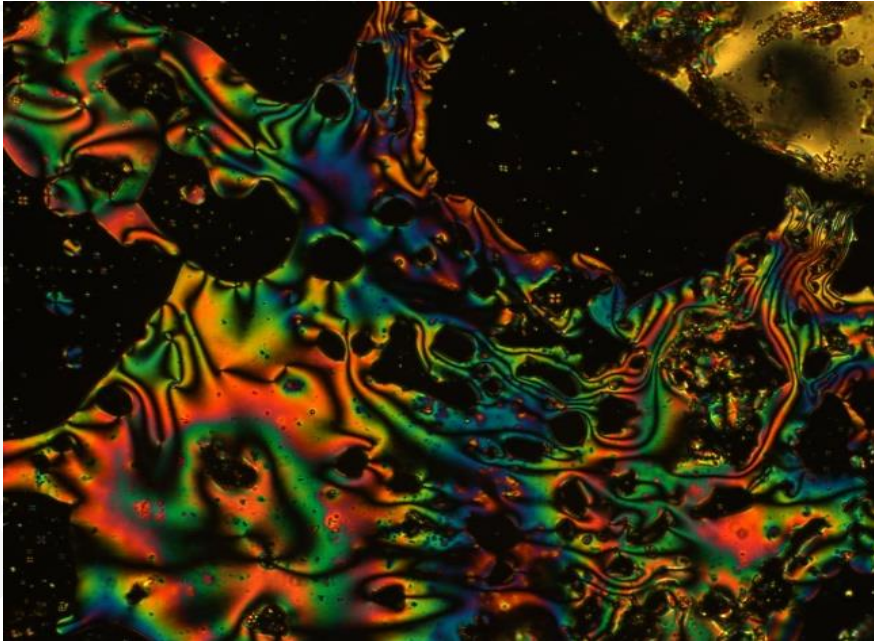
C 68.0 Col_r 97.0 Iso

C 98.2 N_D 131.2 Iso

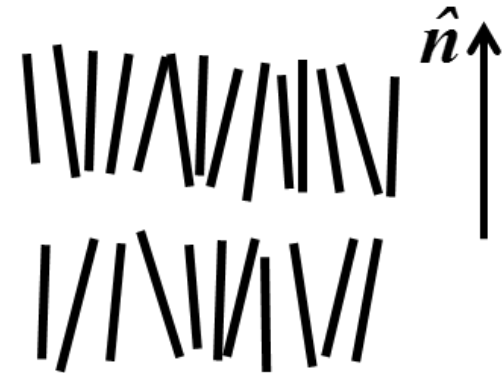
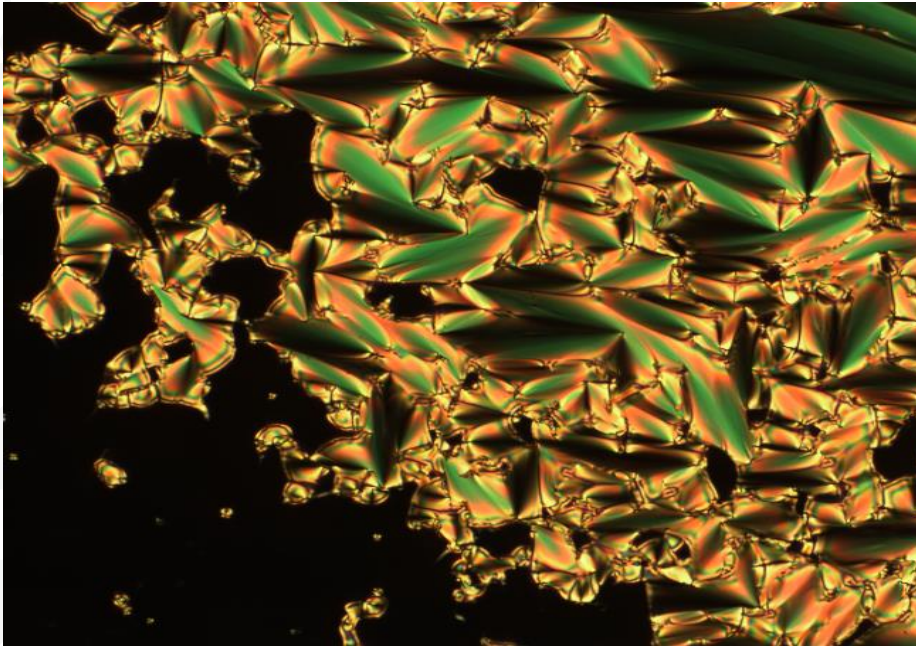
Birefringence



Nematic Texture



Smectic A Texture

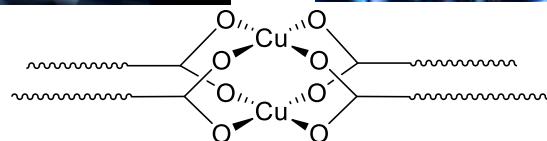
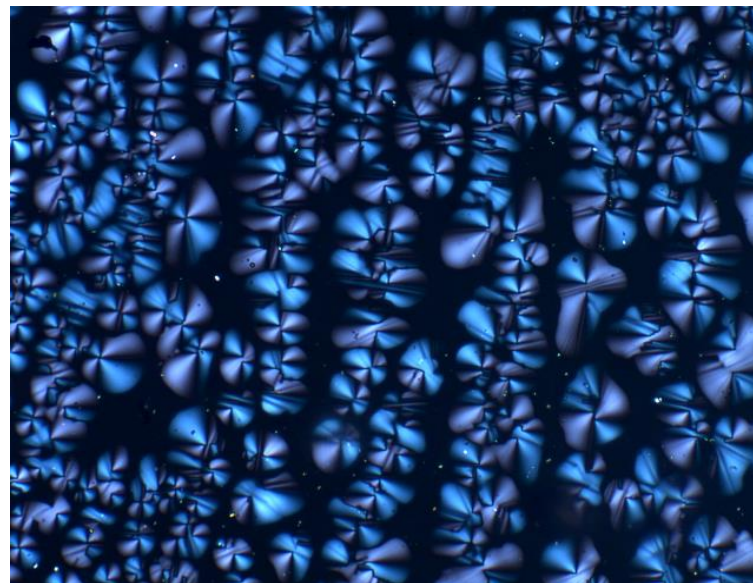
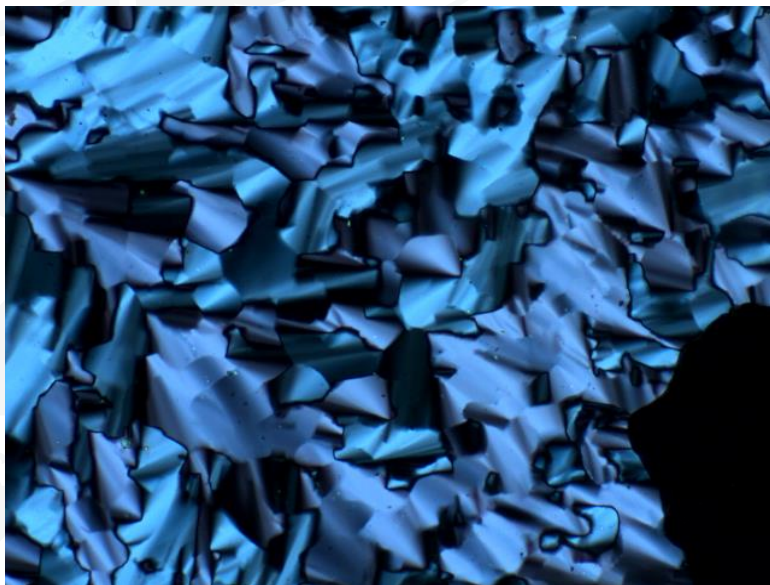


Smectic A, SmA

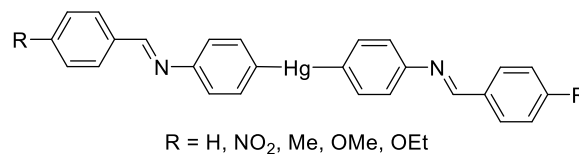
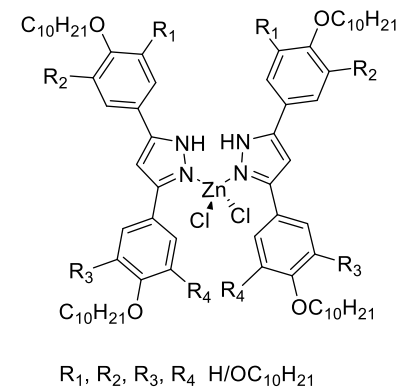
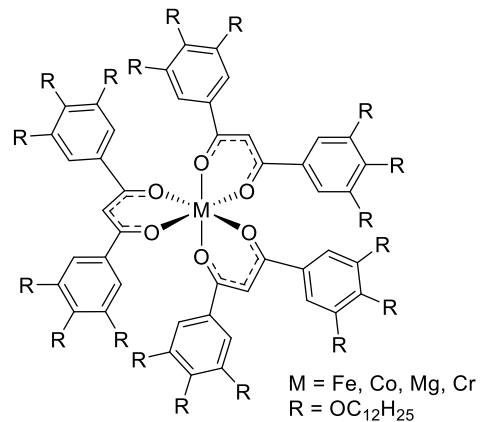
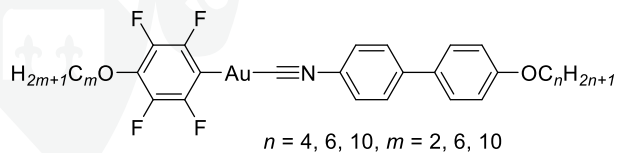
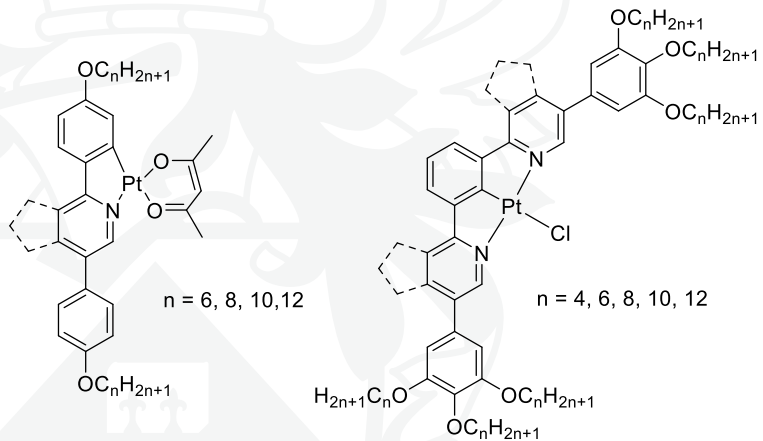
Hexagonal Columnar Texture



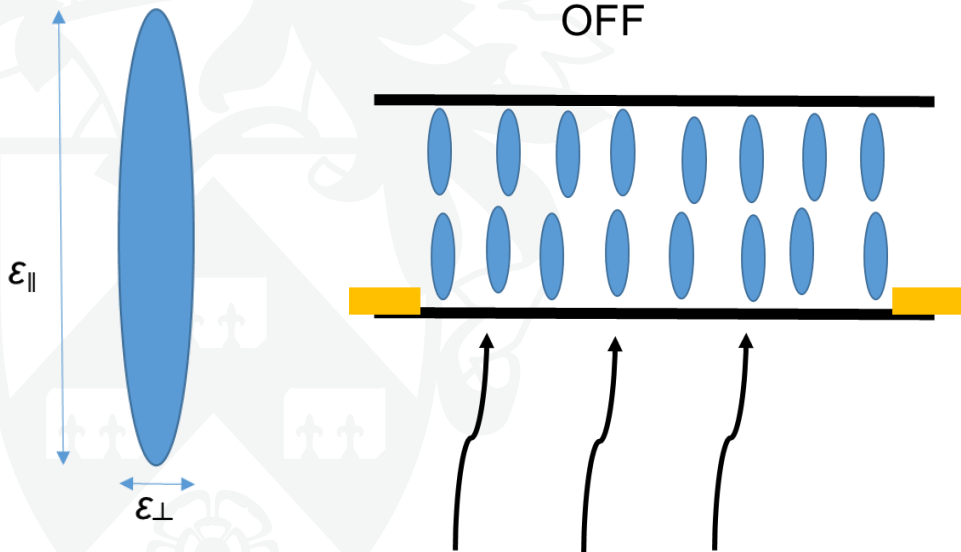
Hexagonal Columnar, Col_h



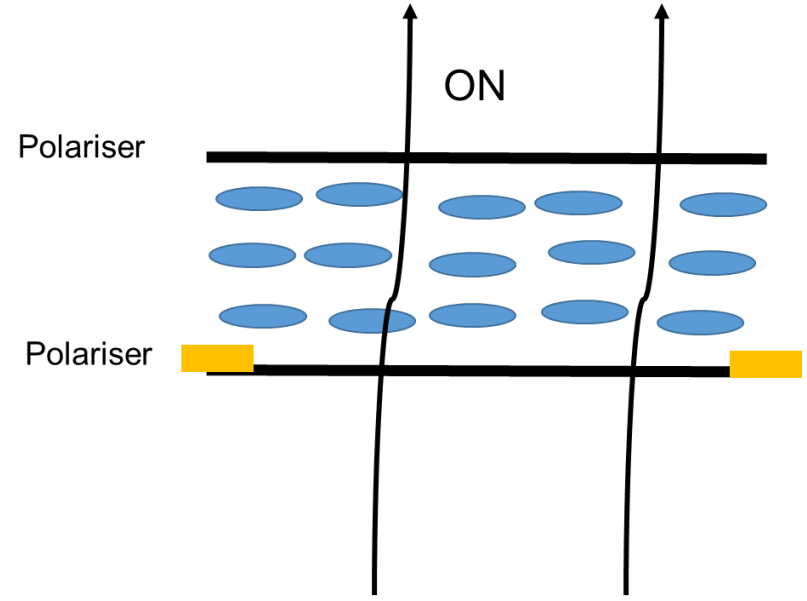
Metallomesogens



Liquid Crystal Displays



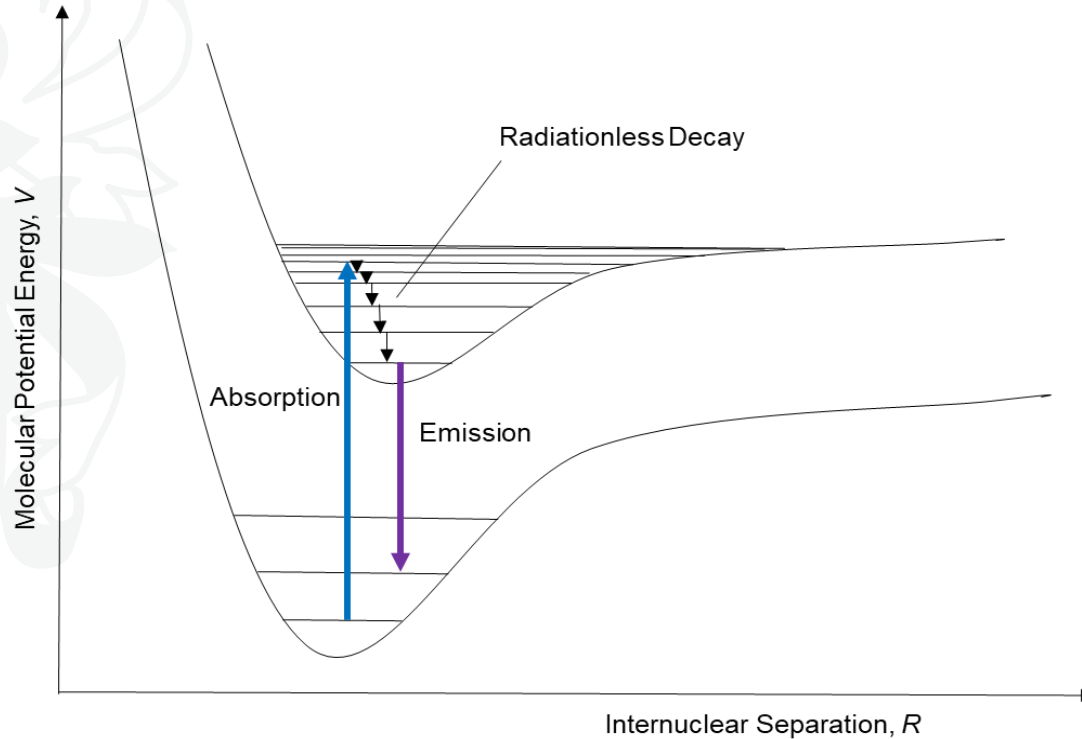
$$\Delta\epsilon = \epsilon_{\parallel} - \epsilon_{\perp}$$



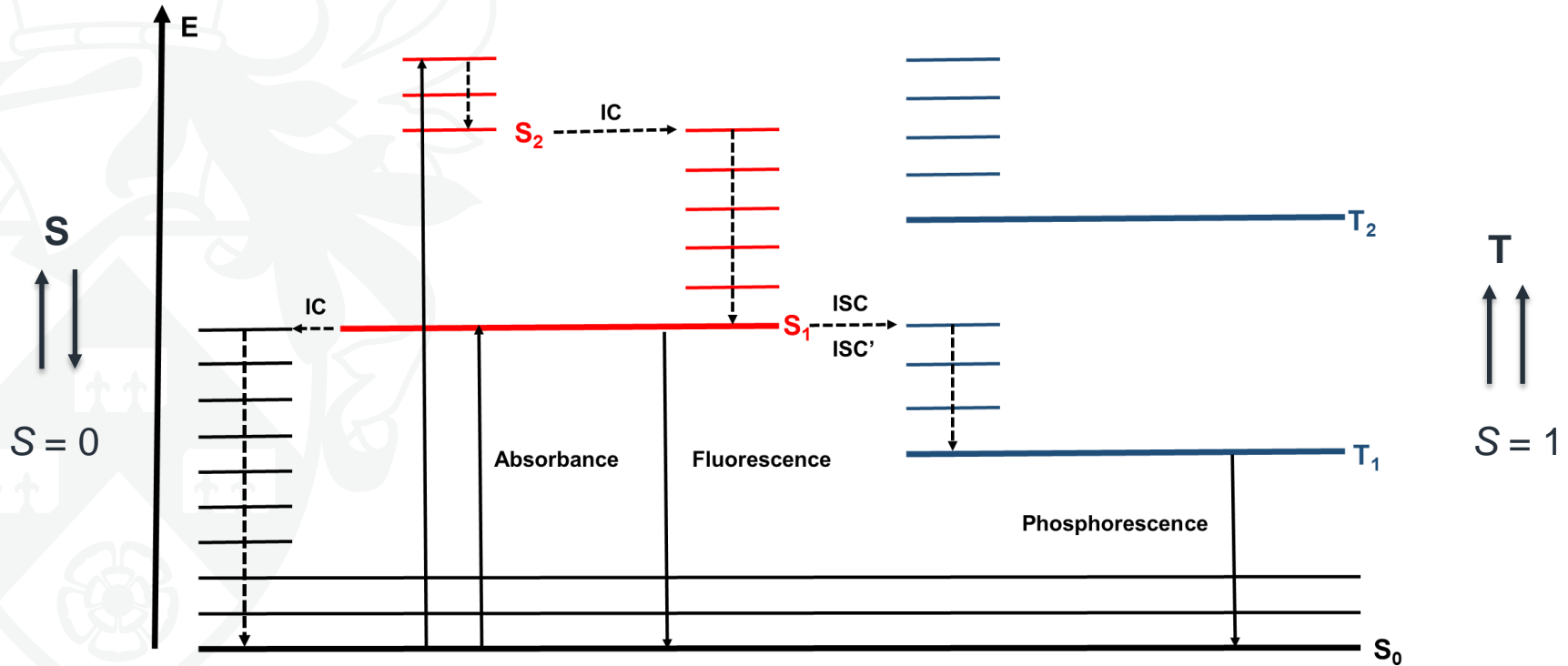
Organic Light Emitting Diodes (OLEDs)

- 1907: silicon carbide (SiC) first example of electroluminescence
- 1955: acridine orange and quinacridone first organic example
- 1960: first OLED at Dow Chemicals
- 1987: Tang and Van Slyke developed first practical device from tris(8-hydroxyquinolato)aluminium(III) (Green)

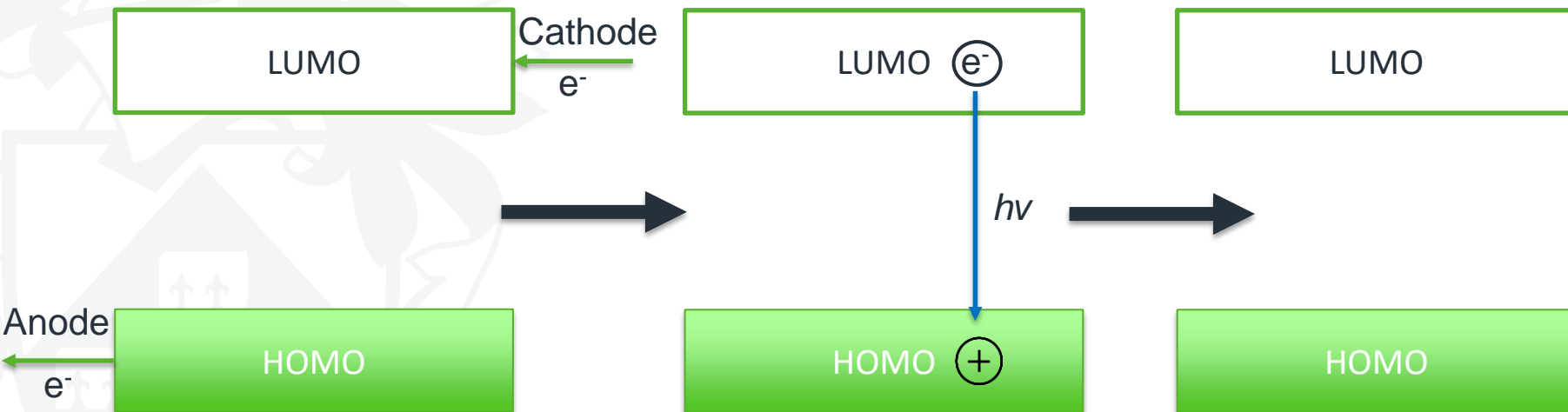
Absorption and emission of Light



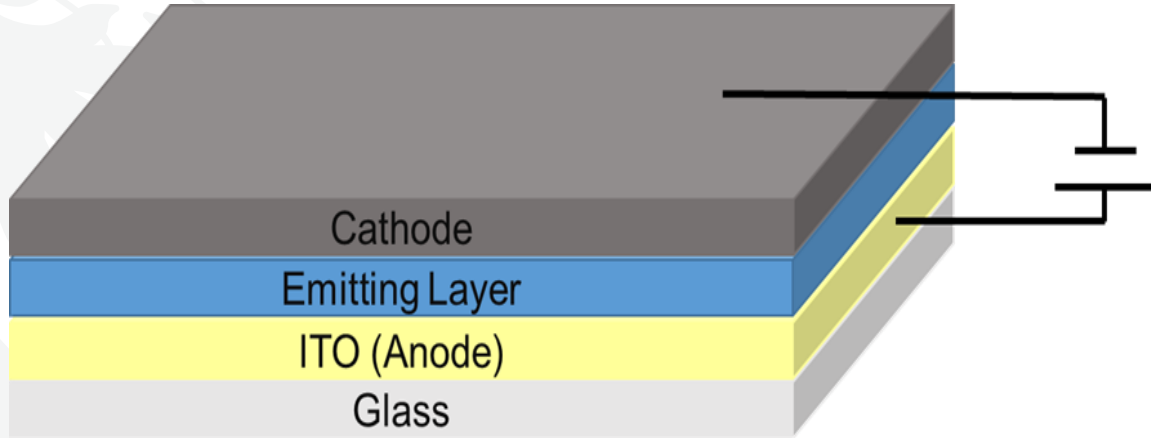
Jabłoński diagram



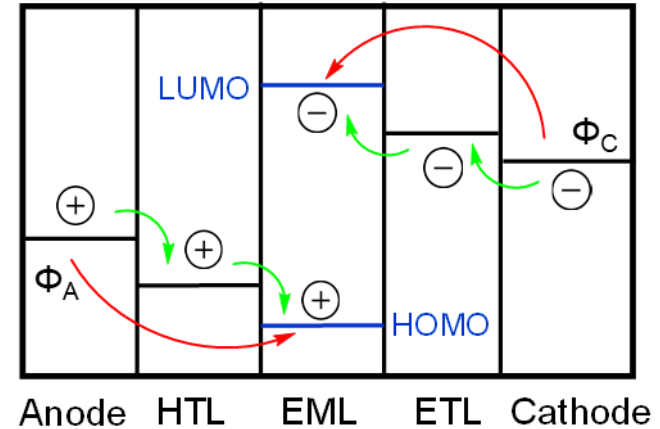
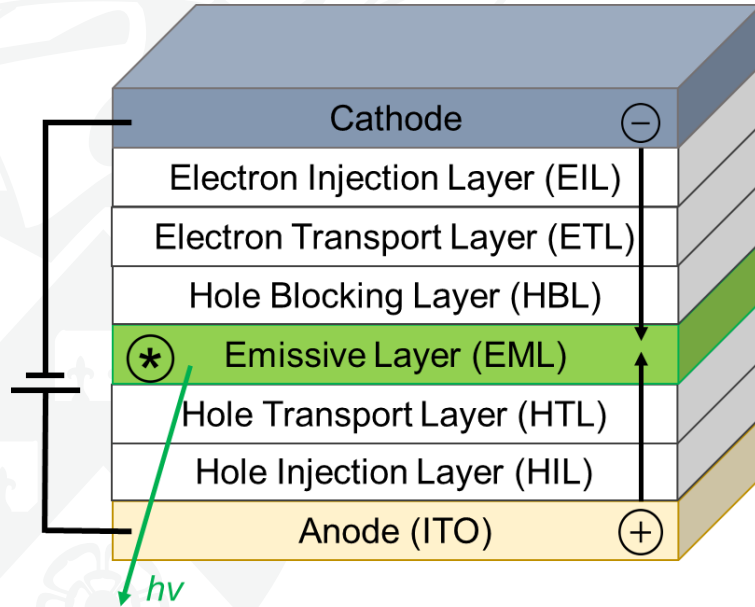
OLEDs



Simple OLED Device

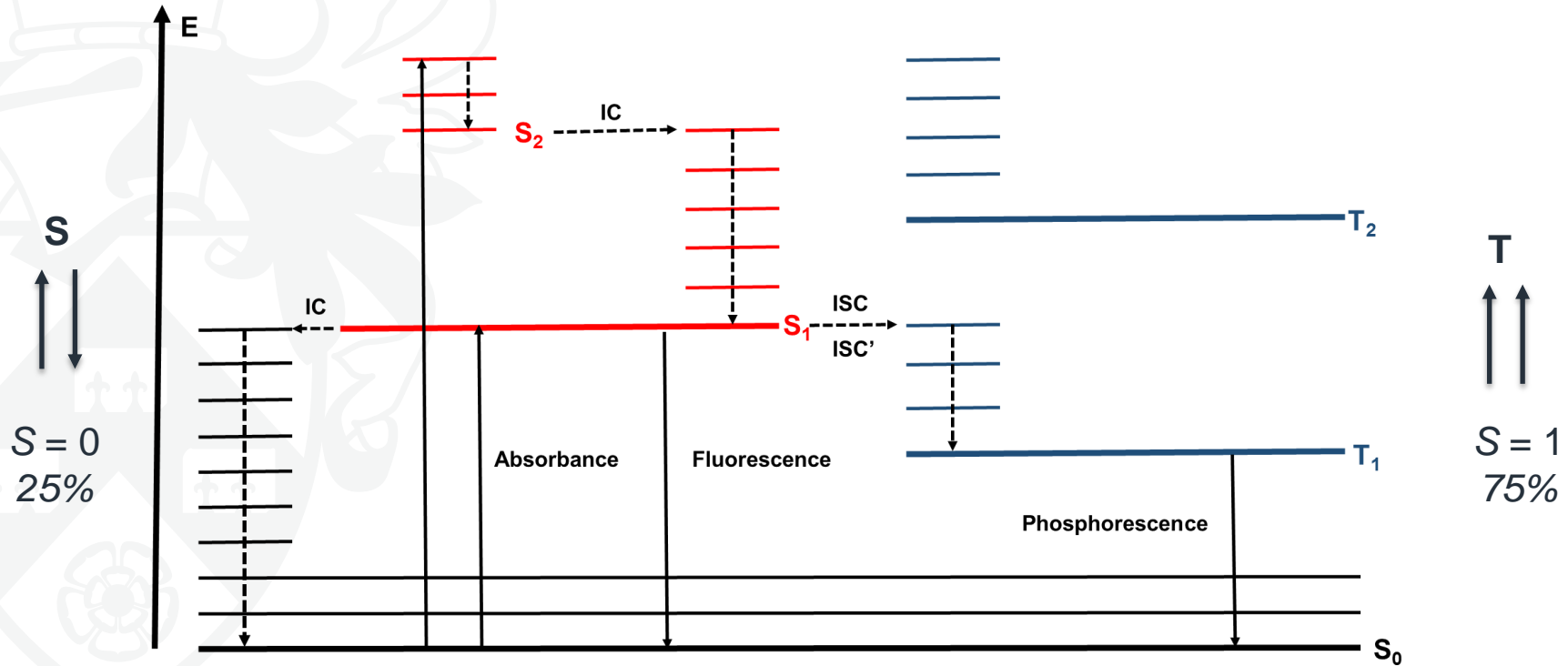


What OLEDs Actually Look Like...





Why triplet emitters?



LCDs vs OLEDs

Advantages of OLEDs

- Faster Response Time
- Improved Colour Contrast
- Thinner
- No Backlight Required
- Lower Power Consumption
- Improvements in Viewing Angle and Contrast ratio

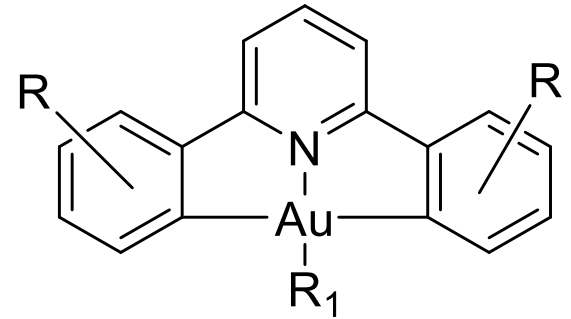
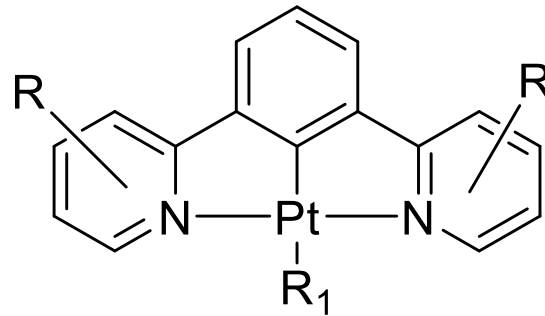
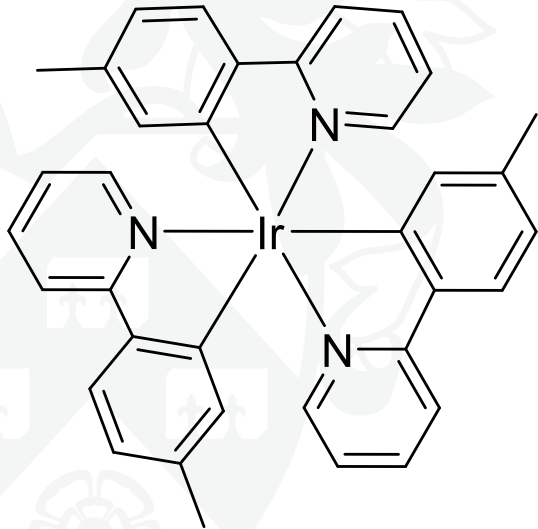
Disadvantages of OLEDs

- Operational Lifetime Shorter
- Colour Decay
- Lower Resolution
- Manufacturing Cost High
- Non-Recyclable

Liquid Crystalline OLEDs

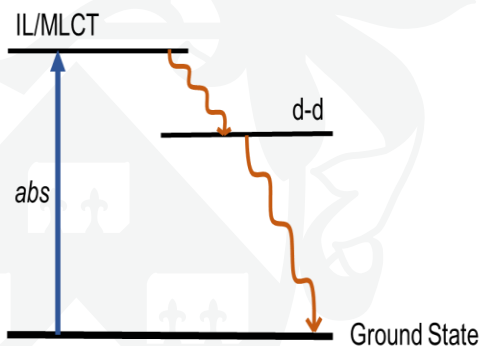
- Increased Molecular Ordering
- Lowers Drive Voltage
- Chains Act as Spacers Mitigating Self-quenching
- Fluid Nature Allows Dynamic Effects and Self-healing
- Potential Polarised Emission

Real world examples

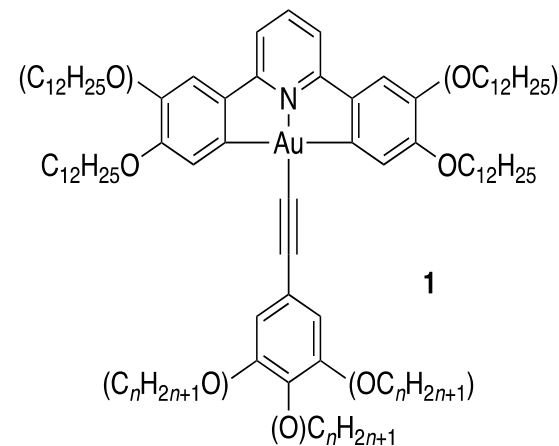
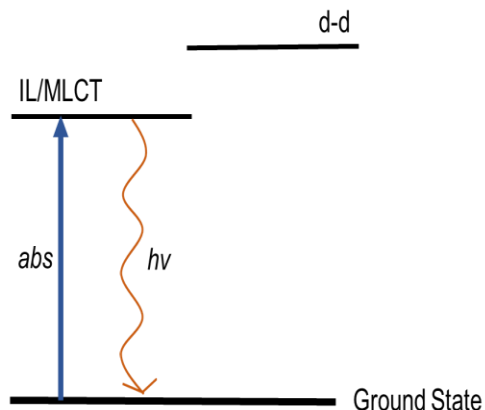


C[^]N[^]C Gold(III) Alkynyl Complexes

Weak Ligand Field



Strong Ligand Field



Note from the CSTS:

We have removed some slides which contain confidential information, we hope that once the information has been formally published we will be able to upload the complete presentation.

The video of the talk has also been edited to remove the confidential material.

Thank you for your understanding, we are sure you appreciate that lectures from the cutting edge of science sometimes include confidential IP!

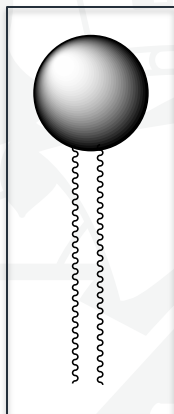
Acknowledgements



- Supervisor: Professor Duncan Bruce
- IPM, DFT: Dr Jason Lynam
- Previous Work on Gold(III) Complexes: Dr Rachel Parker
- MChem Student: Liam Curtis
- X-ray Structures: Dr Adrian Whitwood and Theo Tanner
- Mass Spectrometry: Karl Heaton
- Elemental Analysis: Dr Graeme McAllister
- NMR help and training: Miss Heather Fish, Alexander Heyam
- DFT help: Dr Luke Wilkinson, Fraser Arnold
- The rest of E214 lab

- Funding from Department of Chemistry, University of York
- Johnson Matthey for generous gifts of gold(III) salts.
- Use of the Viking Cluster, high performance compute facility provided by University of York

What are liquid crystals?



Liquid Crystals

Lyotropic

Thermotropic

Low MW

High MW

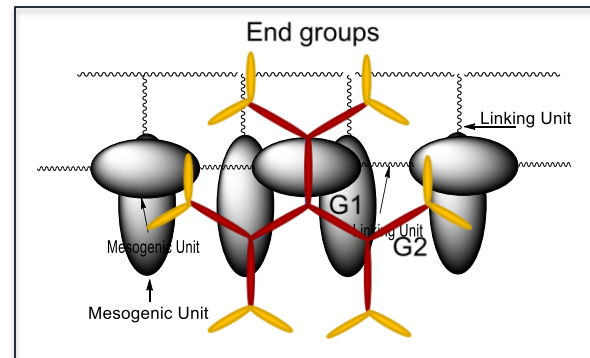
Calamitic

Discotic

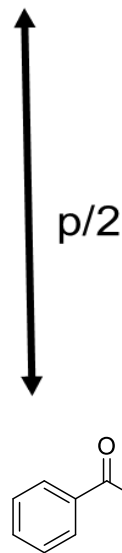
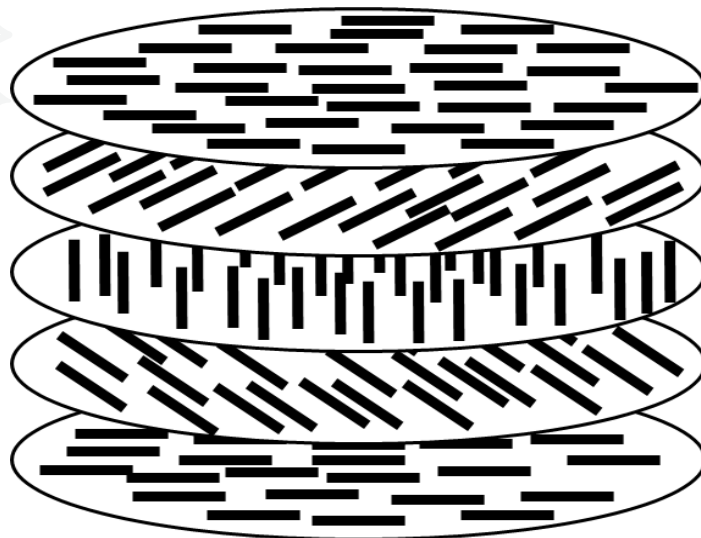
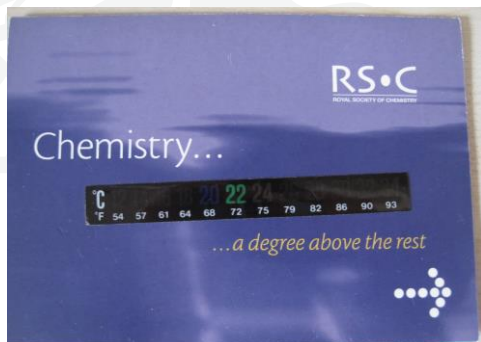
Side Chain Polymer

Main Chain Polymer

Dendrimer



Liquid Crystal Phases: Chiral Nematic



Cholesteryl Benzoate

Chiral Nematic Texture

