

Application Note #11

Rapid Kinetic and Spectroscopy instruments

ORD (Optical Rotatory Dispersion) accessory using the MOS450 AF/CD spectrometer

Theory:

Optical Rotation is used extensively in the quantification and characterization of chiral molecules (such as sugars and polymers) for many years [1,2]. Optical Rotation depends on the wavelength of the irradiating light. The wavelength dependence of the optical rotation is called Optical Rotatory Dispersion (ORD). The effect results in a rotation of the polarization plane of linearly polarized light after passing through a sample.



Figure 1: Simplified measurement set-up in ORD

CD (Circular Dichroism) and ORD.

CD and ORD are two polarimetric techniques that can differentiate two enantiomeres of chiral compounds. ORD and CD are two techniques relatively similar as both involve the same chiroptical technique.

CD involves the measurement of absorption, i.e., the differential absorption of left- and right-handed circularly polarized radiation. This result in CD occurs in the vicinity of an absorption band. This technique is important in the determination of secondary structure elements of peptides, proteins, polynucleotides, etc.

ORD involves the measurement of a plane polarized light rotation which can be detected in the whole wavelength range. ORD measurements can be done sequentially across a wavelength range where light is absorbed. The ORD spectra will give a monotonous signal in the case of a sample that does not absorb. It is well known from the literature that when a sample has a chromophore (absorption band) adjacent to the chiral center, then anomalous ORD is found. When an absorption band is scanned, an S-shaped ORD curve is produced. This anomalous rotation is called the Cotton Effect [3]. Indirectly, ORD spectra can be transformed in CD spectra through the Kronig-Kramers relation [4].

The figure below displays the relationship between an absorption spectrum, a CD and an ORD spectrum.

The positive or negative cotton effects are shown on the figure below.



Figure a): Absorbance spectrum of a camphor solution Figure b) ORD (red) and CD (purple) spectra of CSA (1S)-(+)-10camphorsulphonic acid Figure c) ORD (red) and CD (purple) spectra of CSA (1S)-(-)-10camphorsulphonic acid solution and positive cotton effect

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ORD accessory for MOS450AF/CD: easy of use and reliability

The ORD accessory kit is an upgrade to the MOS450AF/CD. This eliminates the need to equip your lab with a standard polarimeter and thus, saves money. With the ORD accessory, a spectrum is recorded quickly without any mechanical rotation of the detector and without any limitations regarding the wavelength, as would be encountered with a standard polarimeter. Installation of the accessory is very quick and requires only few seconds. A polarizer is set in front of the detector (PM tube) at 45° and a rotatable ring is installed around the PM tube (to firmly position the polarizer at 45° before b eing able to take the measurement). The vertical polarized light is produced by the MOS-450 AF/CD using a PEM (PhotoElastic Modulator), and the deviation of the polarized light is measured by the PM tube.

The figure below shows an ORD spectrum of a camphor solution (0.9 mg/mL) and exhibits the cotton effect.



Figure 2: CSA (1S)-(-)-10-camphorsulphonic acid (0.9 mg/mL) in 1cm cuvette in water spectrum is displayed in both CD and ORD. Each plot has been performed using the MOS-450AF/CD from Bio-Logic SAS (France) at a fast sampling rate. Plot is only takes a few seconds.

Advantage of the accessory:

- No need to buy a new device
- Fast adaptation of the accessory on your existing CD spectrometer (MOS450AF/CD)
- Possibility to follow the ORD measurement at a single wavelength or sweep a defined wavelength range
- No need for an additional detector! The PM tube provided as standard with the MOS450AF/CD is perfectly suited for the ORD measure

References:

- [1] J. Chem. Phys. 25, 467 (1956); William Moffitt, Optical Rotatory Dispersion of Helical Polymers
- [2] J. Chem. Educ., 1964, 41 (6), p 308 Robert E. Lyle and Gloria G. Lyle A brief history of polarimetry
- [3] Physical chemistry for the biosciences, Raymond Chang
- [4] J. Phys. Radium 22, 3 (1961) 179-191, N.G. Van Kampen, François Lurçat