

JASCO

FVS-6000

Vibrational Circular Dichroism Spectrometer An essential tool for absolute configuration of molecules

JASCO has developed the FVS-6000 high performance VCD (Vibrational Circular Dichroism) spectrometer with the most advanced DSP electronics and auto-alignment mechanism. The FVS-6000 not only allows you to easily obtain fingerprint VCD spectra, but also has several unique features such as a measurement range extension option of 4000 ~ 750 cm^{-1} . Since the CD signals in the infrared region are one or more orders of magnitude lower than ECD signals in the UV-Vis region, high sensitivity and stability are required for a VCD spectrometer. The FVS-6000 is the VCD spectrometer of choice for highly sensitive VCD measurements.



Sensitivity and Stability

● Optimized optics

The FVS-6000 employs a 28° interferometer to reduce polarization effects and reflective optics to eliminate artifacts caused by birefringence for high-quality VCD data. The isolated mount of the IR light source and the thermal control of the PEM crystal offers long-term baseline stability.

● VCD auto alignment

The auto alignment function optimizes the VCD optics to reduce linear anisotropy artifacts. No manual alignment is required when the detector and/or optical filters are exchanged.

● Lock-in detection by DSP

Phase-sensitive lock-in detection by DSP (Digital Signal Processing) with a sophisticated algorithm optimized for VCD offers drastic improvement of the S/N ratio.

● Purge capability

The optics, sample chamber and detector housing are all purgeable to obtain high-precision data free of environmental interference.

Features

● Wide band coverage

The FVS-6000 can provide spectra over a wide spectral range from 3200 ~ 850 cm^{-1} as standard. Optional detectors and filters can extend the range to 4000 ~ 750 cm^{-1} , enabling the measurement of OH and NH bands. Detectors can be easily exchanged with no manual alignment, and optical filters can be switched by a PC-controlled 6-position filter wheel.

● Narrow band mode

The narrow band mode allows measurements of small peaks at targeted absorption bands with high sensitivity by using optional band filters.

● Variety of sample cells

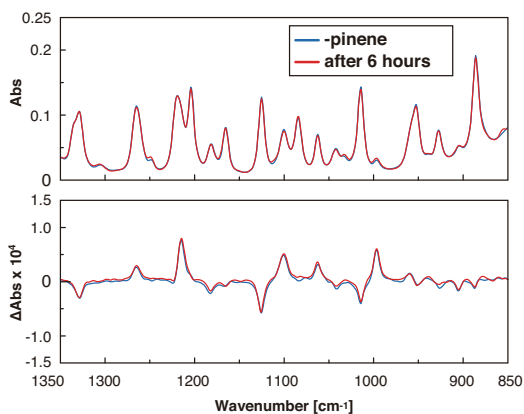
A thermostatted cell holder, 3-position sample shuttle, and range of small-volume liquid cells are available as options.

● Spectra Manager™ II

Spectra Manager II software, the cross-platform control and analysis package for all JASCO spectrometers, offers quick and easy VCD data acquisition and analysis. Theoretically calculated VCD intensities from a commercially available calculation software can be plotted as simulated spectra to be compared with the experimental data for further tertiary structure analysis of molecules.

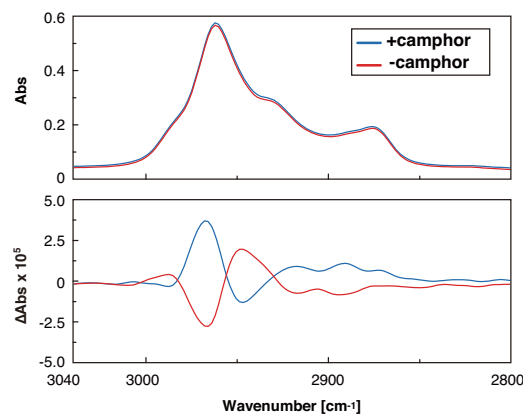
Long-term stability

VCD and IR Spectra of pinene



Narrow band mode

VCD and IR Spectra of camphor



Specifications

Instrumentation	VCD instrument
Measurement range	Standard: 3200 ~ 850 cm ⁻¹ Option: 4000 ~ 750 cm ⁻¹
Resolution	16 ~ 0.5 cm ⁻¹
Noise level (measurement conditions)	less than 8 x 10 ⁻⁶ ΔAbs (4 cm ⁻¹ , 20 min accumulation)
Light source	High intensity ceramic source, insulated mount
Detector	Standard: MCT-V (3200 ~ 850 cm ⁻¹) Option: MCT-C (1000 ~ 750 cm ⁻¹) InSb (4000 ~ 2000 cm ⁻¹)
Lock-in detection	DSP
PC communication	USB2.0 for main unit RS-232C for PEM driver
Interferometer	28° Michelson interferometer
Optical filter	Standard: 3200 ~ 2000 cm ⁻¹ , 2000 ~ 850 cm ⁻¹ (6-position automatic switching) Option: 4000 ~ 2700 cm ⁻¹ , 1000 ~ 750 cm ⁻¹ , 1850 ~ 1550 cm ⁻¹
Polarizer	KRS-5
Options	3-position automated sample shuttle Fixed liquid cell, BaF ₂ or CaF ₂ window, 25 ~ 100 μm cell path Demountable liquid cell, BaF ₂ or CaF ₂ window, including 50 and 100 μm cell spacer Temperature control cell (Peltier cooled)
Dimensions	590(W) x 670(D) x 313(H) mm
Weight	65 kg



*The VFT-4000 VCD attachment for the FT/IR-4000, 6000 Series FT-IR spectrometers is also available.

VFT-4000 VCD attachment with the FT/IR-6300 FT-IR spectrometer



● Specifications are subject to change without notice.

JASCO INTERNATIONAL CO., LTD.

4-21, Sennin-cho 2-chome, Hachioji, Tokyo 193-0835, Japan
Tel: +81-42-666-1322 Fax: +81-42-665-6512 <http://www.jascoint.co.jp/english/>
Australia, China, Hong Kong, India, Indonesia, Iran, Korea, Malaysia, New Zealand,
Pakistan, Philippines, Russia, Singapore, South Africa, Taiwan, Thailand

JASCO INCORPORATED

28600 Mary's Court, Easton, MD 21601, U.S.A
Tel: +1-800-333-5272 +1-410-822-1220 Fax: +1-410-822-7526 <http://www.jascoinc.com>
U.S.A., Canada, Costa Rica, Mexico, Puerto Rico, Argentina, Brazil, Chile, Colombia, Paraguay,
Peru, Uruguay, Guatemala

JASCO EUROPE s.r.l.

Via Luigi Cadorna 1, 23894 Cremella (Lc), Italy
Tel: +39-039-9215811 Fax: +39-039-9215835 <http://www.jasco-europe.com>

JASCO Deutschland www.jasco.de, JASCO UK www.jasco.co.uk,

JASCO France www.jascofrance.fr, JASCO Benelux www.jasco.nl,

JASCO Spain www.jasco-spain.com, JASCO Scandinavia www.jascoscandinavia.se
Italy, Germany, U.K., France, Netherlands, Belgium, Luxembourg, Spain, Sweden, Norway, Denmark,
Austria, Finland, Greece, Hungary, Poland, Portugal, Romania, Switzerland, Algeria, Cyprus,
Egypt, Israel, Jordan, Kuwait, Lebanon, Morocco, Saudi Arabia, Syria, Tunisia, Turkey,
U.A.E., Yemen

For more information, please contact:

Measurement of Vibrational Circular Dichroism spectra using the FVS-6000

< Introduction >

It is generally understood that chiral compounds have different bioactivities depending upon the absolute configuration of each compound. Some familiar examples include glutamic acid and thalidomide. L-glutamic acid demonstrates the “Umami” taste*¹, while D-glutamic acid has a bitter taste, similarly, the R form of thalidomide is a sedative, but the S form has teratogenic activity. Thus, the separation and study of chiral compounds is critical for many reasons.

The functionalities of chiral compounds have been studied for the development of advanced molecules for many applications. The study of chiral compounds has spread to several fields such as natural products, pharmaceuticals and other functional molecules, and it can be pointed out that among those studies, the structural analysis of chiral compounds is a very important topic. X-ray Diffraction (XRD), Nuclear Magnetic Resonance (NMR) and Electronic Circular Dichroism (ECD) using UV/Vis light are employed as primary methods for the structural analysis of chiral compounds. In this paper, the measurement of chiral compounds by Vibrational Circular Dichroism (VCD) using infrared light will be outlined.

VCD is a method to measure the difference of absorbance intensity between left-hand and right-hand circularly polarized light as shown in Figure 1. It is an advantage of VCD that this method can be applied to almost all organic compounds in the same way as infrared (IR) spectroscopy. In addition, by comparing the measurement results with calculated results by ab-initio molecular orbital calculations, the absolute configuration of the sample can be determined. However, since the peak intensity of VCD spectra are 1,000 – 10,000 times weaker than that of standard IR spectra, spectroscopic instruments with high sensitivity and stability with very small baseline fluctuations are required. The FVS-6000 VCD system has a high sensitivity detector, suitable optical filter technology and a thermostatted Photoelastic Modulator (PEM) to accurately measure the weak VCD peaks. The measurement results of typical chiral compounds and hemoglobin as a model protein using the FVS-6000 are reported.

*¹ Umami taste is the fifth taste sensation in addition to sweet, acid, salty and bitter taste.

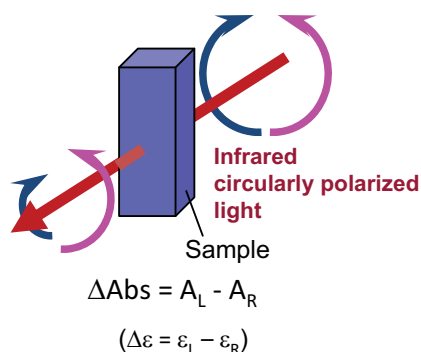


Fig. 1.
Principles of VCD spectroscopy



Fig. 2.
External view of the FVS-6000

< Measurement results >

Figures 3 through 6 illustrate the measurement results for alpha-pinene; 1,1-Bi-2-naphthol; proline and hemoglobin, respectively. Both IR and VCD spectra can be obtained by the FVS-6000. The identification of the absolute configuration of chiral compounds can be determined from both the IR and the VCD spectra as well as the analysis of the molecular structure.

Figure 3 demonstrates the IR and VCD spectra of alpha-pinene which is a typical standard sample to validate a VCD instrument system. IR spectra of the R- and S- form of alpha-pinene are completely overlapped, while their VCD spectra are symmetric, clearly identifying each alpha-pinene enantiomer. Since the peak shapes of the VCD spectra obtained illustrate typical alpha-pinene spectra, it is confirmed that high quality VCD spectra can be measured by the FVS-6000.

Figure 4 outlines measurement results for 1,1-Bi-2-naphthol which is used as a ligand for transition-metal catalyzed asymmetric synthesis and is a precursor for chiral ligands such as BINAP. The small peaks due to the anisotropy factor 'g value' (VCD peak/IR peak) around 1600 and 1500 cm^{-1} attributed to the benzene ring are clearly shown. These results demonstrate that the FVS-6000 is a very effective system for evaluation of chiral compounds which have similar structures.

Figure 5 illustrates the measurement results of proline which is one of the amino acids. Good, symmetrical VCD spectra were obtained for the D- and L- forms. Since amino acids demonstrate different bioactivities between the D- and L- forms, studies regarding structure and bioactivity are increasingly popular. Liquid samples can be easily measured by VCD instrumentation so the structural analysis of amino acids can be performed under similar to physiological conditions.

Figure 6 contains the measurement results for hemoglobin. Hemoglobin is known as a spherical model protein which contains rich alpha-helix structures, and in addition, its VCD spectrum shape is very different from that of concanavalin A, which contains a rich beta-sheet structure.

The addition of VCD spectral results to information obtained from ECD and IR spectra can provide much more accurate secondary structure analysis of proteins in solvents. We also believe that VCD can also be a powerful tool for the analysis of DNA and chiral polymers other than proteins.

In this paper, the standard performance and measurement results of typical chiral compounds using the FVS-6000 were reported and we believe the FVS-6000 can be an essential and indispensable tool for analysis of chiral compounds.

Measurement condition

Model name:	FVS-6000
Resolution:	4 cm^{-1}
Detector:	MCT-V
Accumulation:	1000 (alpha-pinene and 1,1'-Bi-2-naphthol), 2500 (proline), 2000 (hemoglobin)

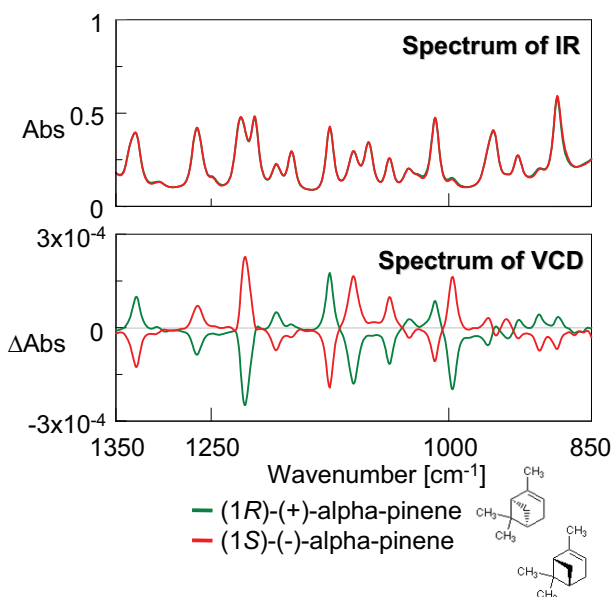


Fig. 3. Spectra of alpha-pinene
(neat, 50 μm pathlength BaF_2 liquid cell)

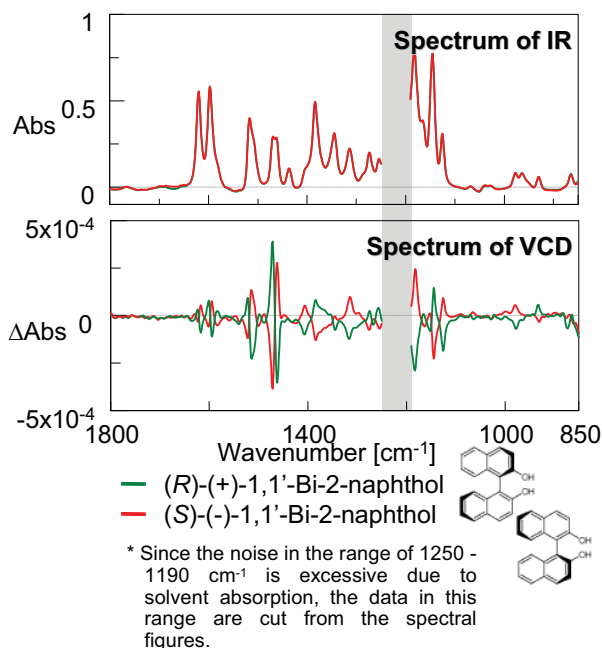


Fig. 4. Spectra of 1,1'-Bi-2-naphthol
(solvent: CHCl_3 , concentration: 0.162 M, 50 μm pathlength BaF_2 liquid cell)

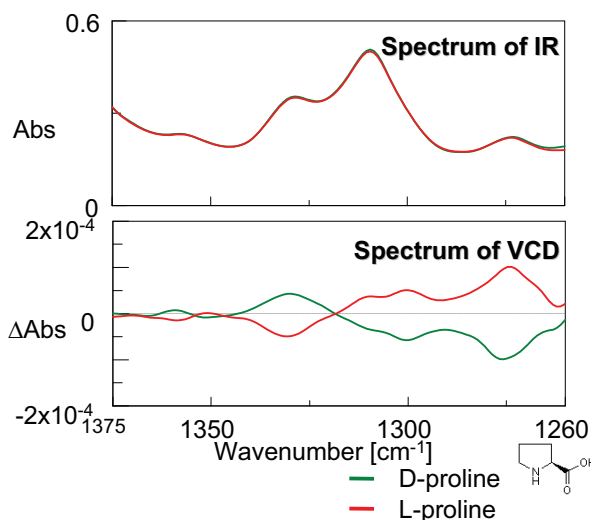


Fig. 5. Spectra of proline
(solvent: D_2O , concentration: 0.9 M, 25 μm pathlength CaF_2 liquid cell)

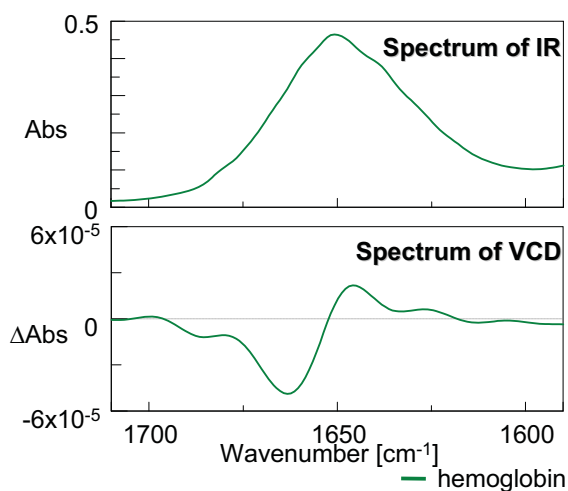


Fig. 6. Spectra of hemoglobin
(solvent: D_2O , concentration: 50 mg/mL , 25 μm pathlength CaF_2 liquid cell)