

Ratio measurement of water ortho/para nuclear spin isomers via TDLS in the vicinity of 1.392μ

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Abstract

Water molecule exists in two nuclear spin isomers. The hydrogen atom nuclear spins could be either parallel (total spin is 1) in ortho molecule or antiparallel (total spin is 0) in para molecule. Each spin isomer has its own system of rotational levels. Optical transitions between levels of different spin isomers are strongly forbidden. Number of ortho isomer molecules is three times greater than number of para isomer molecules in the thermal equilibrium state at room temperature.

Successful separation of ortho and para water isomers was demonstrated [1]. Interest to further investigation of separation mechanisms is connected with feasible application of para-enriched water in medicine (EPR-tomography). The method of ortho/para ratio measurement used in [1] is based on microwave absorption spectroscopy in 36–38 cm^{-1} frequency interval. This technique is rather complicated and it could unlikely be used outside of physical laboratory. That's why alternative diagnostic methods are of great interest.

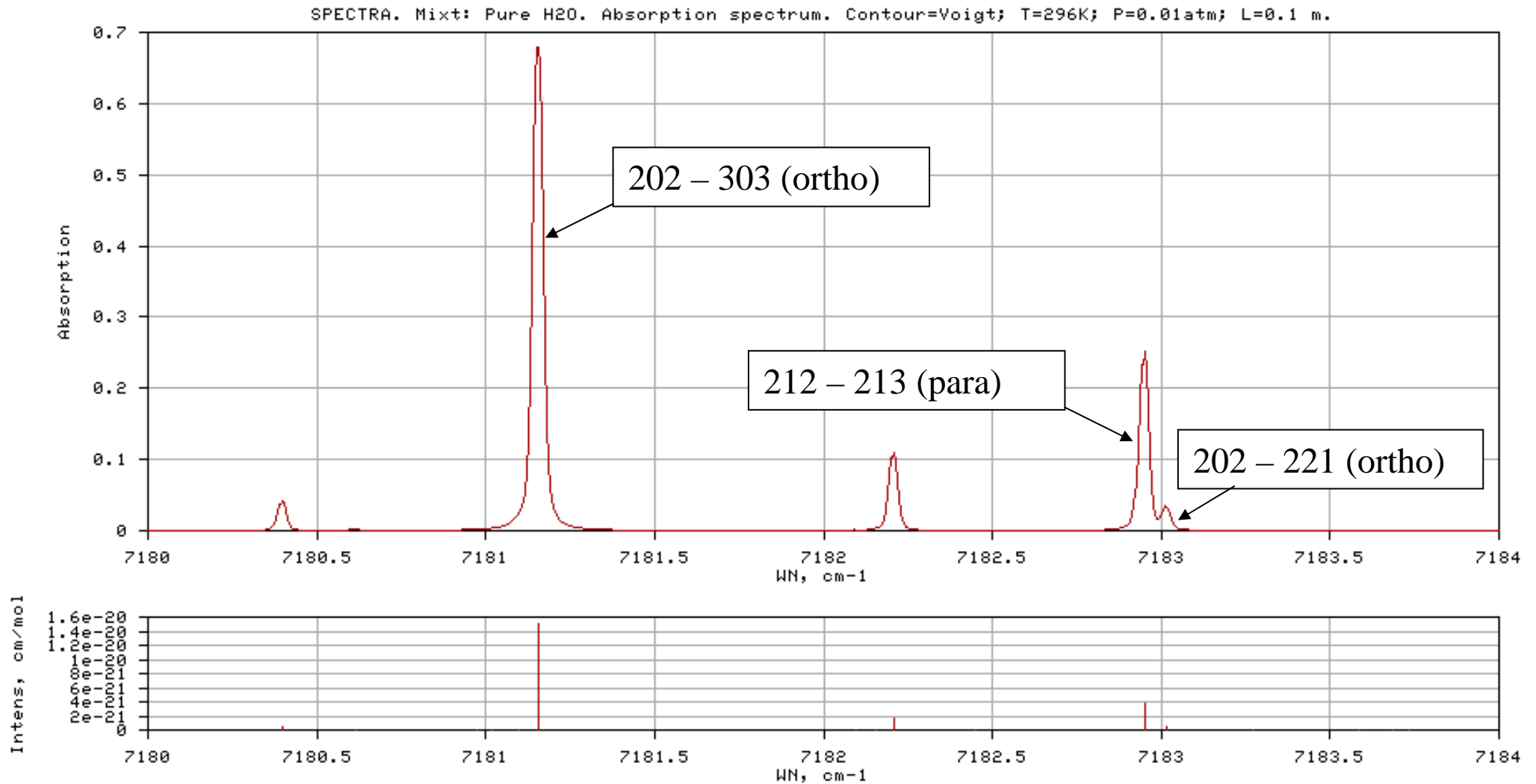
This report is concerned with further development of the method based on TDLS technique [2].

Absorption spectra of water vapor were detected and then processed using LabVIEW-based software. Ratio factors were calculated by use of integral cross section data of HITRAN-2004.

[1] V. I. Tikhonov, A. A. Volkov, *Science*, v. 296, p. 2363 (2002).

[2] A. I. Nadezdinskii, P. M. Omarova. *J. Mol. Spectr.*, v. 170, p. 27 (1995).

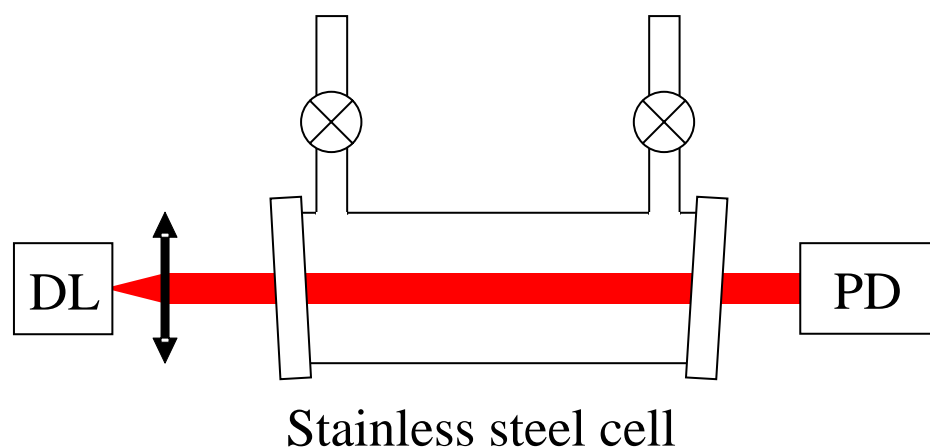
Absorption spectrum of 101 – 000 H₂O band in the vicinity of 1.392 μ



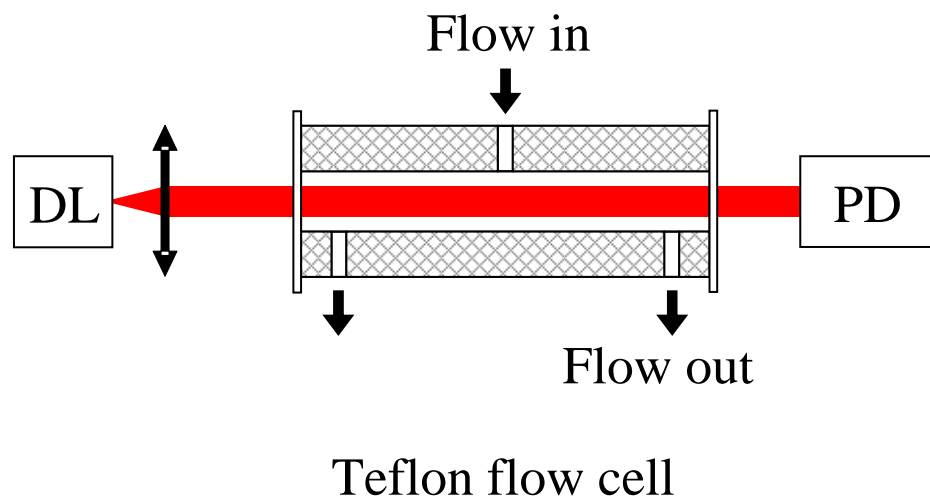
Simulated by SPECTRA Information System (<http://spectra.iao.ru/en/home/>)

Schematic of ortho/para ratio measurements

Method: direct absorption measurement with sweep integration

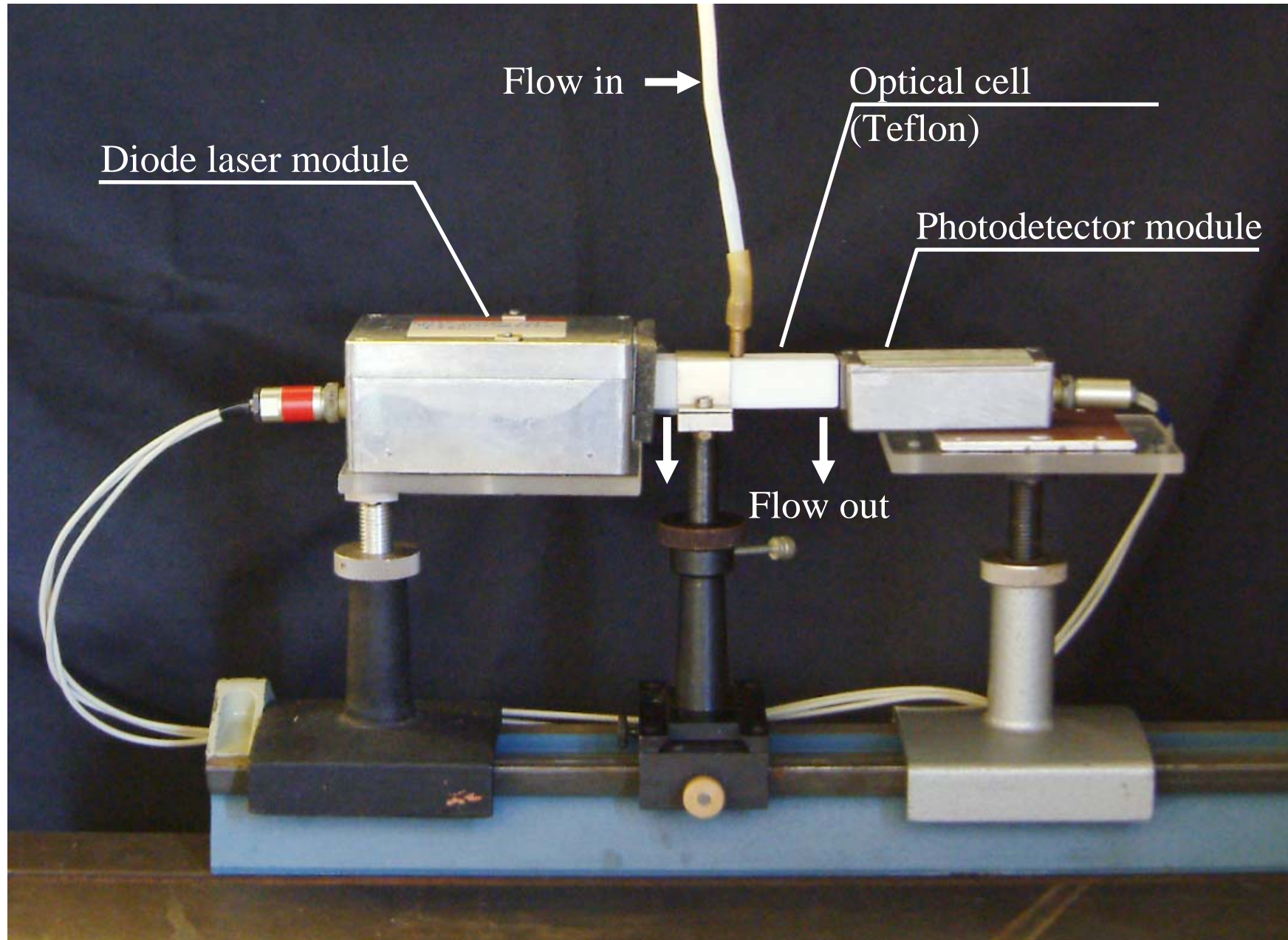


Stationary measurement: stainless steel cell ($L = 12$ cm) with glass windows is filled with water vapor at different pressures



Flow measurement: water in gas-carrier (dry N_2 or air) is pumped through the Teflon cell ($L = 9$ cm) with polyethylene film windows. Total pressure in the cell ~ 1 atm.

General view of the experimental setup

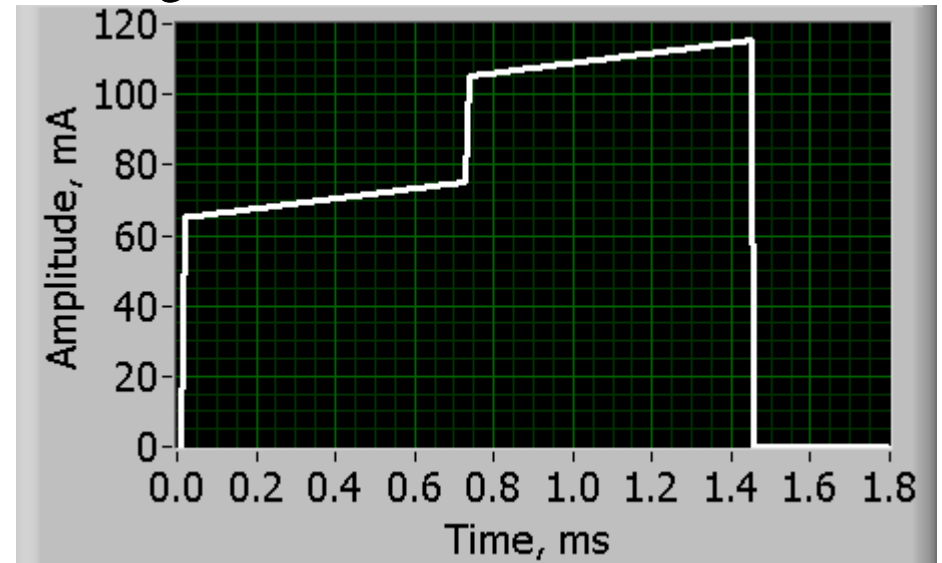


Diode laser parameters and operating mode

Laser type	DFB diode laser with integrated Peltier cooler
Manufacturer	Laser Components GmbH
Model	SPECDILAS-D
Wavelength	1391 nm
Linewidth	< 20 MHz
SMSR*	< -40 dB

* in operating mode

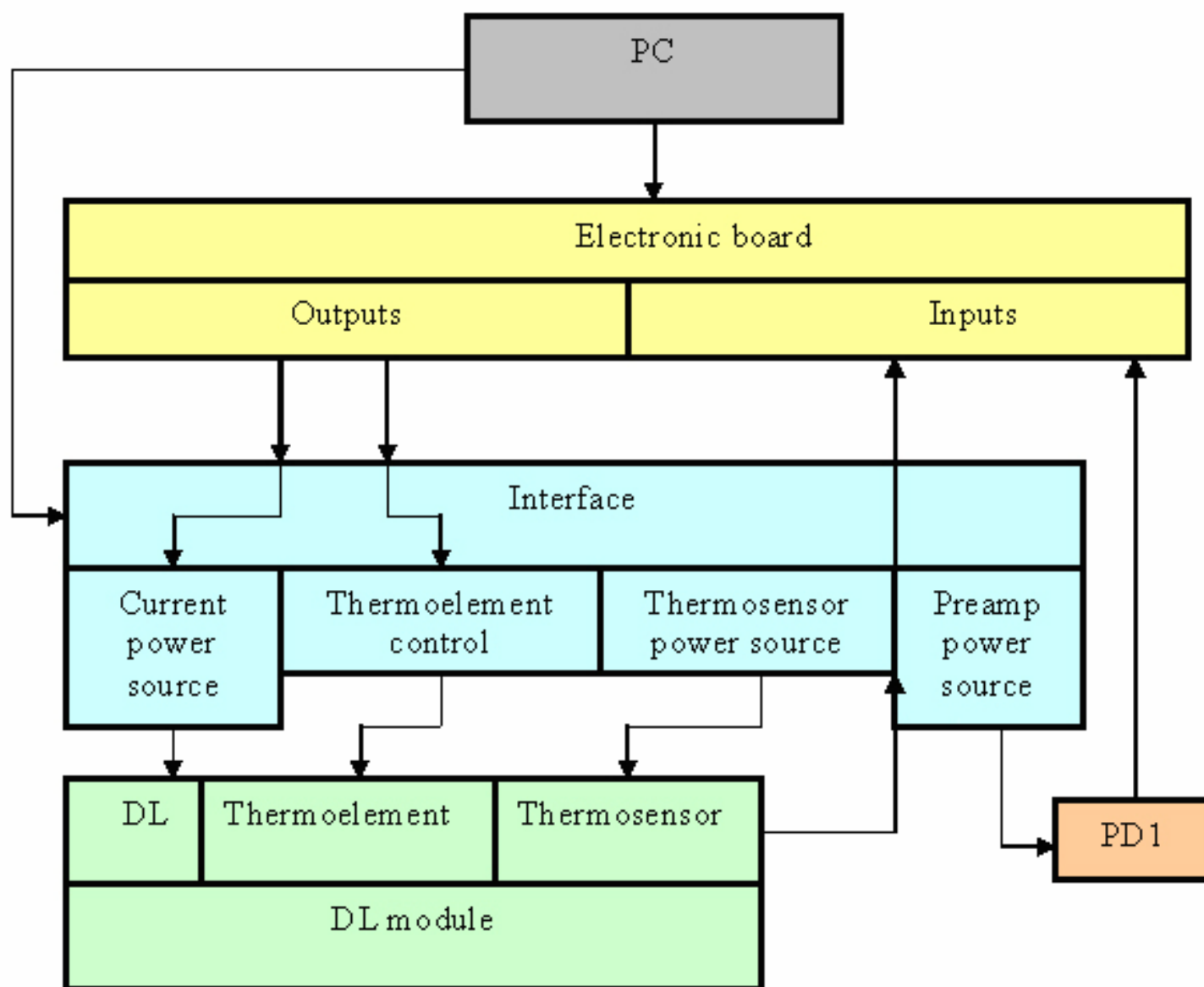
Driving current waveform:



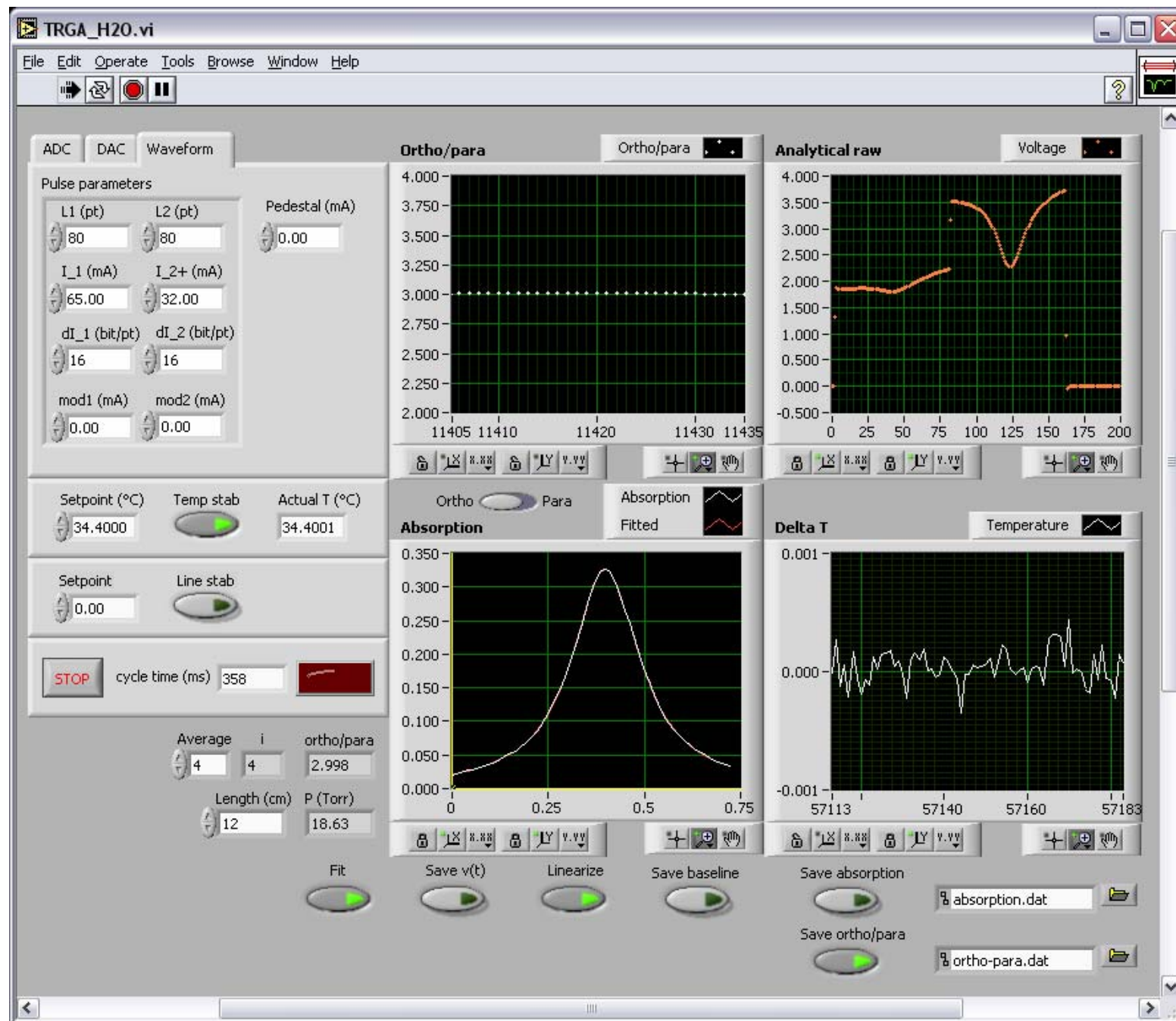
Operating temperature: 34.4°C

Peak optical power: 15 mW

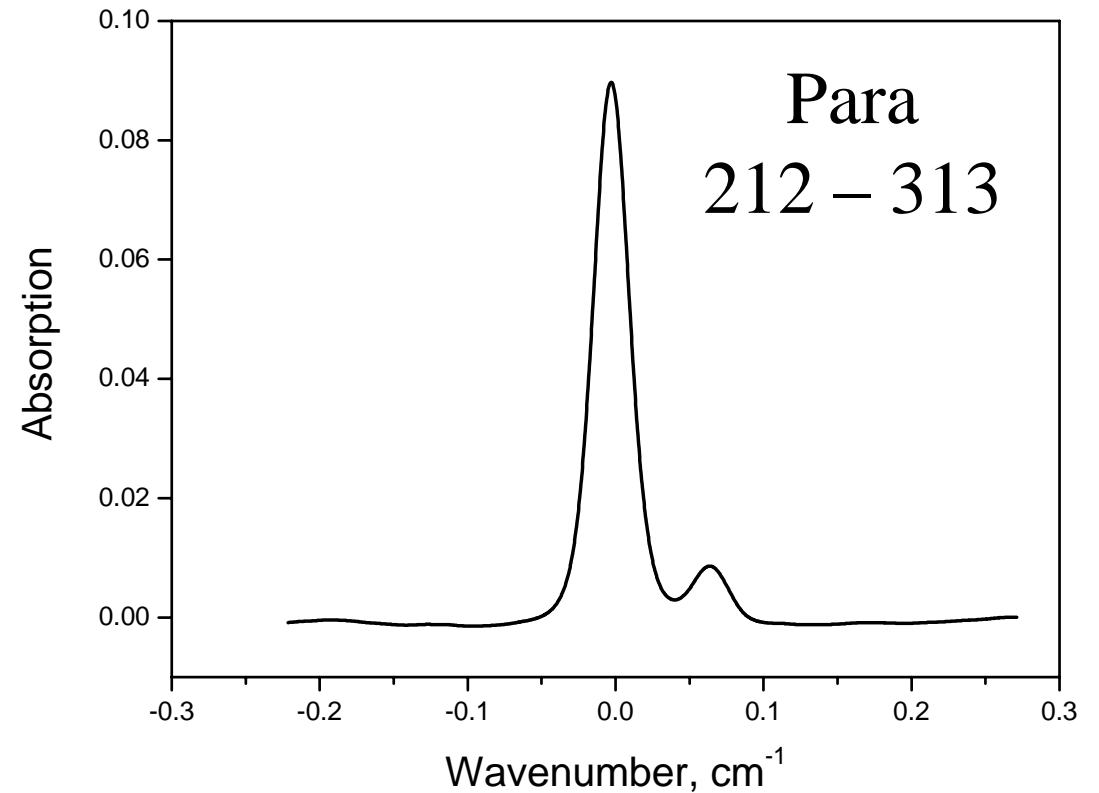
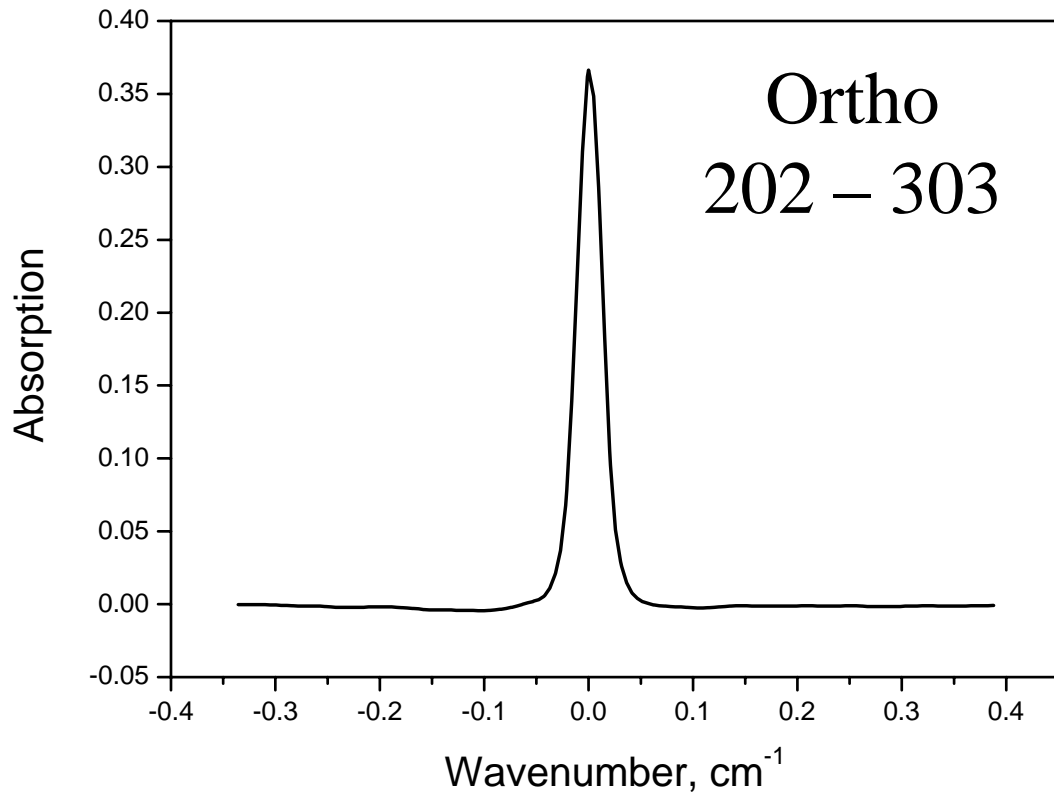
Electrical Block-scheme



Front panel of the LabVIEW control program



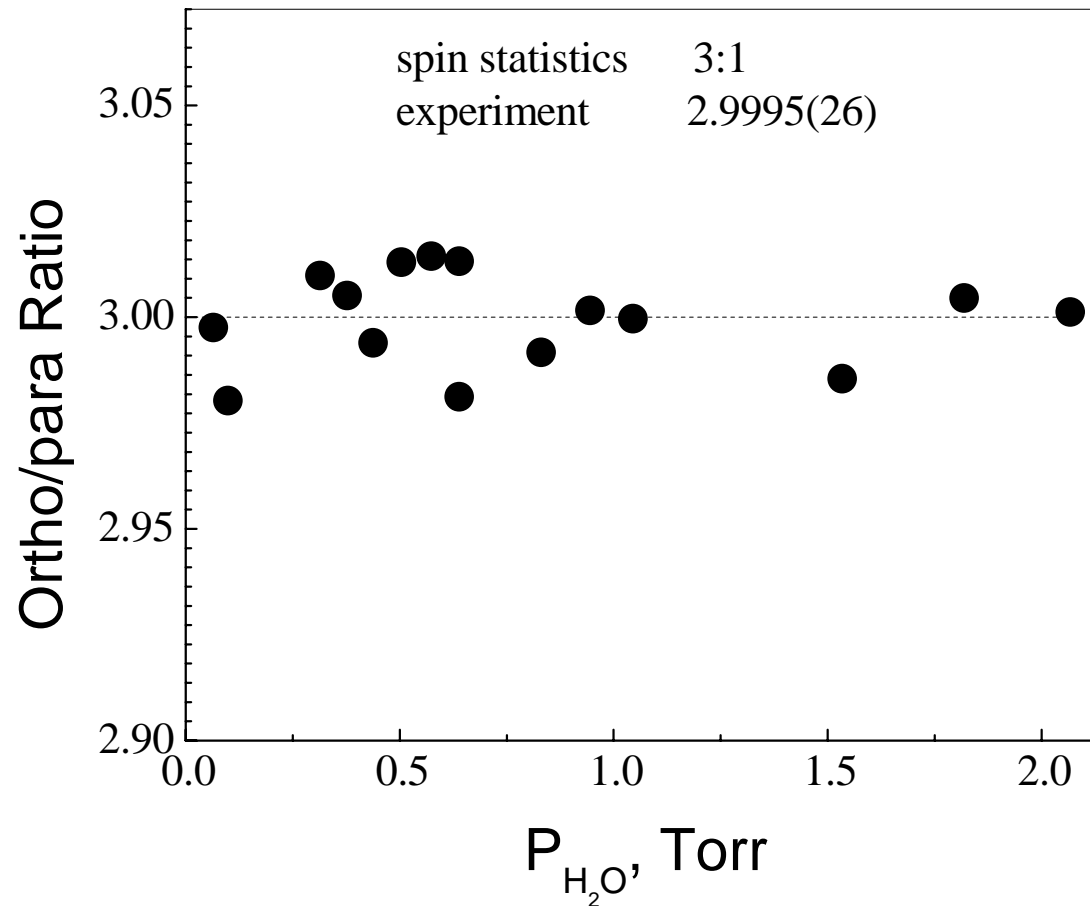
Experimental spectra of ortho and para lines



Experiment conditions:

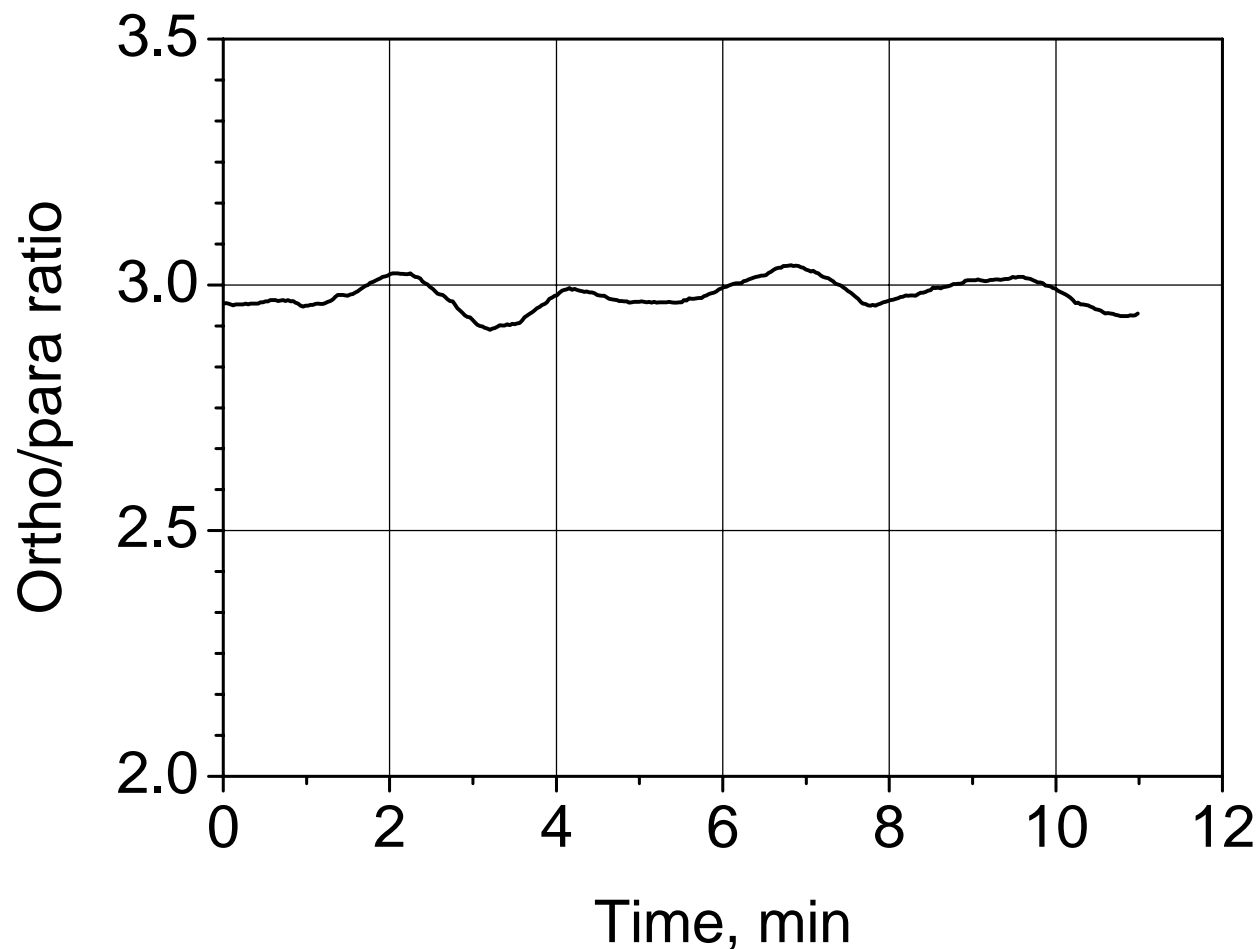
$$P_{\text{total}} = 0.05 \text{ atm}, P_{\text{H}_2\text{O}} = 0.9 \text{ Torr}, L = 12 \text{ cm}$$

Stationary ortho/para ratio measurement



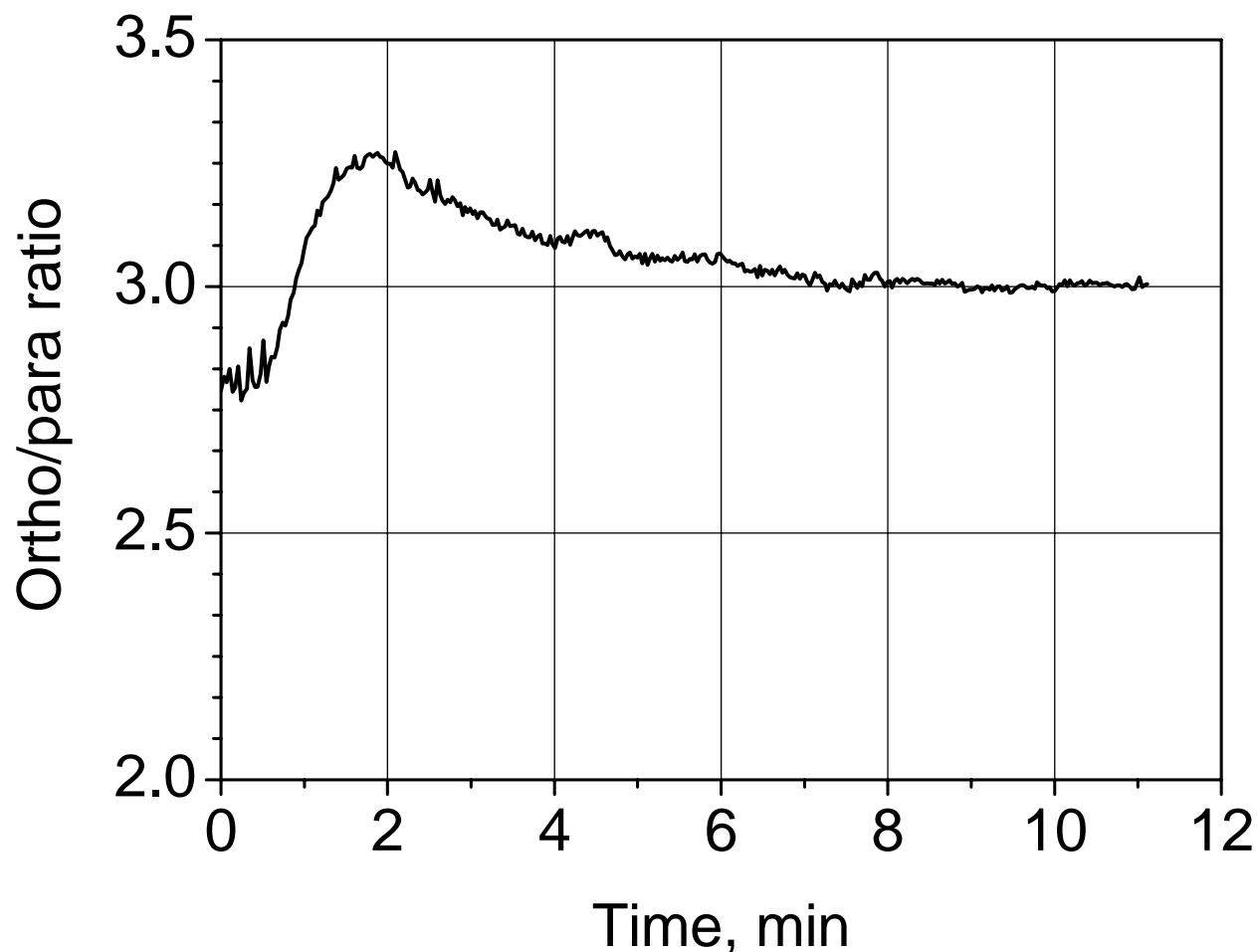
Experiment conditions: stainless steel cell with glass windows ($L = 12$ cm) is evacuated and then filled with water vapor. Measurement is taken after pressure stabilization. Each point corresponds to separate experiment.

Measurement of ortho/para ratio in flow cell



Experiment conditions: saturated water vapor in nitrogen at total pressure 1 atm is fed to the Teflon flow cell ($L = 9$ cm).

Measurement of spin-selective sorption dynamics



Experiment conditions: saturated water vapor in nitrogen at total pressure 1 atm is passed through activated charcoal column and then fed to the Teflon flow cell ($L = 9$ cm).