PHYSICAL CHEMISTRY 2010

10th International Conference on
Fundamental and Applied Aspects of
Physical Chemistry

Proceedings

The Conference is dedicated to the
100th Anniversary of the academician Pavle Savić birthday
and
20th Anniversary of the Society of Physical Chemists of Serbia

---

21-24 September 2010
B E L G R A D E

ISBN 978-86-82475-17-0
Title: Physical Chemistry 2010. (Proceedings)
Editors: S. Anić and Ž. Čupić
Published by: Society of Physical Chemists of Serbia, Studentski trg 12-16 P.O.Box 47, 11158 Beograd, 218, Srbija
Publisher: Society of Physical Chemists of Serbia
For Publisher: S. Anić, President of Society of Physical Chemists of Serbia
Printed by: "Jovan" Printing and Publishing Company; 200 Copies; Number of pages 16 + 388, **Format:** B5; Printing finished in September 2010.

Text and Layout: "Jovan"

200 - *Copy printing*

International Organizing Committee

Chairman: S. Anić (Serbia)
Vice-chairman: N. Stepanov (Russia)
B. Adnađević (Serbia)

Members:
M. Gabrovska (Bulgaria), N. Cvijetićanin (Serbia), T. Grozdić (Serbia), D. Jovanović (Serbia), M. Lalić (BiH), D. Marković (Serbia), B. Milosavljević (USA), N. Miljević (Serbia), M. Mojović (Serbia), N. Ostrovski (Serbia), C. Pona (Italy), B. Simonović (Serbia), D. Stanisavljev (Serbia), A. G. Stepanov (Russia), V. Vasić (Serbia), N. Vukelić (Serbia), V. Vukojević (Sweden)

International Scientific Committee

Chairman: Ž. Čupić (Serbia)
Vice-chairmans: V. N. Parmon (Russia)
M. Franko (Slovenia)
V. Vasić (Serbia)

Members:
A. Antić-Jovanović (Serbia), G. Bačic (Serbia), R. Cervellati (Italy), R. Compton (United Kingdom), V. Gaspar (Hungary), M. Jeremić (Serbia), A. L. Kawczyñski (Poland), Lj. Kolar-Anić (Serbia), S. Kuchanov (Russia), R. Leblanc (USA), S. Mentus (Serbia), S. Milonjić (Serbia), Lj. Morozova-Roche (Sweden), D. Moscone (Italy), J. Nedeljković (Serbia), Z. Noszticzius (Hungary), M. Perić (Serbia), V. Petruševski (Macedonia), M. Plavšić (Serbia), G. Smulevich (Italy), G. Schmitz (Belgium), I. Schreiber (Czech), P. Ševčik (Slovakia), N. Stepanov (Russia), M. Trtica (Serbia), D. Veselinović (Serbia)

Local Executive Committee

Chairman: B. Adnadjević
Vice-chairmans: S. Blagojević
A. Ivanović

Members:
A. Abu Rabi-Stanković, P. Banković, N. Begović, S. N. Blagojević, N. Cvjetičanin, M. Daković, A. Đerić, A. Ignjatović, Lj. Ignjatović, A. Jović, J. Krstić, S. Kuprešak, D. Lončarević, J. Maksimović, V. Marković, M. Milenković, M. Milojević, Z. Mojović, B. Nedić, I. Pašti, N. Pejić, A. Popović-Bjelić, M. Petković, N. Potkonjak, D. Ranković, R. Ranković, M. Stević, I. Stojković, B. Šljukić, M. Vujković

POLARIZED FT-IR STUDY OF CELL WALL OF A HARDWOOD (MAPLE BRANCH)

J. Simonović[1], J. Stevanic[2], D. Đikanović[1], J. Bogdanović Pristov[1], L. Salmén[2] and K. Radotić[1]

[1] *Institute for multidisciplinary study, Kneza Višeslava 1, 11000 Belgrade, Serbia*
[2] *Innventia, Box 5604, SE-114 86 Stockholm, Sweden*

Abstract
Mechanical and physical propreties of wood fibres are dependent on the orientation of constituent polymers (cellulose, hemicellulose, lignin). Fourier transform infrared (FTIR) microscopy was used to examine the orientation of the main wood polymers in transversal and longitudinal direction of the isolated cell wall of the maple branch. The polarised FTIR measurements indicated that glucomannan and xylan appear to have parallel orientation with regard to the orientation of cellulose. Lignin has also parallel orientation.

Introduction
Cell wall can be considered as a nano-composite in which cellulose, lignin and hemicelluloses are interconnected in a specific manner. Structural organisation of the cell wall and related polymers is important for both mechanical properties of plants and chemical reactions occurring in the wall space, especially in the response to stress. By using imaging FT-IR microscopy, run in transmission mode and at different polarisation modes (from 0° to 90°), it is possible to follow the chemical variability and the orientation of cell wall polymers [1]. The orientation of cellulose, glucomannan, xylan and lignin, as essential components of the wood, were analysed by iFTIR with regard to the sample axis.

Materials and methods
The purified isolated cell wall material was obtained from maple (*Acer sp*.) branches by methanol extraction and subsequent purification using a series of solvents (phosphate buffer, 1% Triton X-100, 1M sodium chloride, distilled water, methanol, acetone) [2]. FTIR microscopy measurements were carried out using a Spectrum Spotlight 400 FTIR Imaging System (Perkin Elmer Inc, Shelton, CT, USA). Spectral resolution: 8 cm^{-1}; spectral range: from 1800 cm^{-1} to 720 cm^{-1}. Polarisation: the incident IR radiation was polarised by a gold wire grid polariser from 0° to 90° polarisation in relation to the fibre orientation with intervals of 5°. The sample was mounted on the sample stage as parallel as possible to the orientation of the 0° polarisation. The IR spectra were processed by the software Spotlight 1.5.1, HyperView 3.2 and Spectrum 6.2.0 (Perkin Elmer Inc., Shelton, CT, USA) [1].

Results and discussion
From the in-depth study of polymer orientation, three areas from the sample were selected. The transmission spectra recorded at 0° and 90° polarisation modes were

processed using a ratio function to produce an orientation spectrum ($R = T_{0°} / T_{90°}$), where R is ratio spectra, T_0^o is the transmission spectra recorded at 0° and $T_{90°}$ is transmission spectra recorded at 90°. Spectral signals related to absorptions from cellulose, hemicellulose (glucomannan and xylan) and lignin in the wavenumber range between 1800 cm^{-1} and 720 cm^{-1} can be identified. Figure 1 a) shows average absorbance spectra at 0° and 90° polarization angle and Figure 1b) shows the average orientation spectra for the maple branch cell wall. In Figure 1b), the positive signals indicate that their corresponding functional groups are arranged in a more parallel orientation to the fibre axis, and the negative signals indicate that their corresponding functional groups are arranged in a perpendicular orientation to the fibre axis.

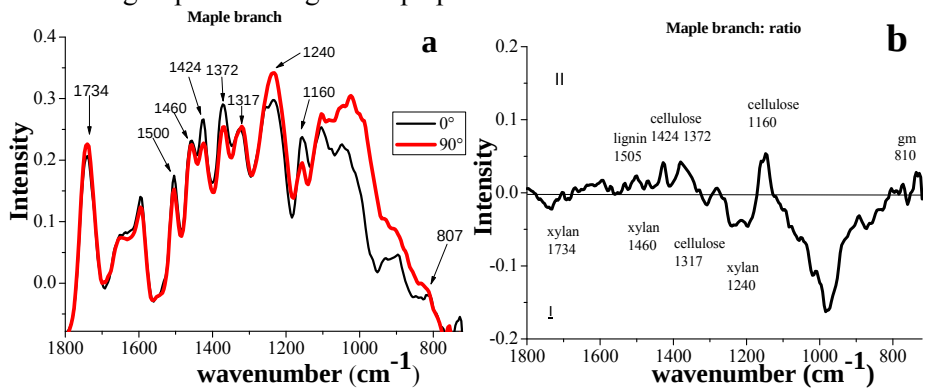

Fig.1. a) Average absorbance spectra of maple branch cell wall at 0° and 90° polarization angle; b) The average orientation spectra of maple branch cell wall.

The relative absorbance spectra are presented (Figure 2) as specific absorption peaks ($RA = (I_p - I_{min}) / (I_{max} - I_{min})$) where RA is relative absorbance, I_p is intensity of the absorbed IR radiation at a given angle of the polarisation, P, I_{max} is maximal intensity observed for a given vibration and I_{min} is minimal intensity observed for a given vibration. These relative absorbance values were presented in relation to the angle of the incident IR polarisation (from 0° to 90°).

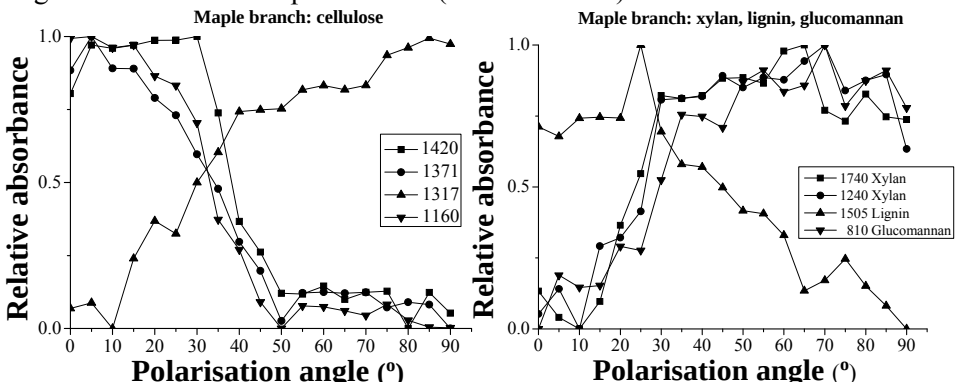

Fig.2. The relative absorbance of IR specific absorption wavenumbers plotted against the polarisation angle for the different wood polymers for maple branch.

Tree vibration peaks of cellulose, the antisymmetric C-O-C bridge stretching vibration at 1160 cm^{-1}, the C-H bending vibration at 1370 cm^{-1} and the C-OH bending vibration of the CH_2-OH group at 1424 cm^{-1} was found to be oriented parallel to the fibre axis. The cellulose vibration (CH_2 wagging vibration at 1317 cm^{-1} oriented perpendicular to the cellulose chain was also found. Hemicelluloses (xylan - vibrations at 1734 cm^{-1}, 1240 cm^{-1}, and glucomannan - vibration at 810 cm^{-1}) are parallel with the longitudinal axis of the isolated cell wall of maple. A lignin vibration, i.e. the C=C aromatic ring vibrations at 1505 cm^{-1} showed a positive signal [3-5].

Conclusion

One can be concluded that both hemicelluloses are arranged in paralel with the cellulose microfibrils. These components show anisotropic behaviour. Lignin is also oriented parallel to the fibre axis in the cell wall.

Acknowledgements

This work was supported by Ministry of Science of Republic Serbia (Project #143043) and COST Action FP0802.

Reference

[1] J. S. Stevanic, L. Salmén, Holzforschung, 2009, **63**, 497-503.

[2] M. Chen et al, Phytochem. Anal., 2000, **11**, 153-159.

[3] R. H. Marchessault, Pure Appl. Chem., 1962, **5**, 107-129.

[4] R. H. Marchessault, C. Y. Liang, J. Polym. Sci., 1962, **59**, 357-378.

[5] M. Åkerholm et all, Carbohydr. Res., 2004, **339**, 569-578.