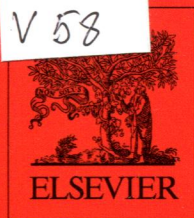


TUM
V 58

Volume 75 November 2014 ISSN 0924-2031



VIBRATIONAL SPECTROSCOPY

An International Journal devoted to Applications of
Infrared and Raman Spectroscopy

Editors

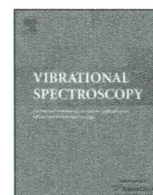
G. KERESZTURY (Budapest, Hungary)

H.M. HEISE (Iserlohn, Germany)

D. MCNAUGHTON (Melbourne, Australia)

Available online at www.sciencedirect.com

ScienceDirect



Contents

DFT study of structure, IR and Raman spectra of phosphorus-containing dendron with azide functional group V.L. Furer, A.E. Vandyukov (Kazan, Russia), J.P. Majoral, A.M. Caminade, S. Gottis, R. Laurent (Toulouse, France) and V.I. Kovalenko (Kazan, Russia).....	1
Adsorption of CO on various M@Pt core-shell nanoparticles: Surface-enhanced infrared absorption and DFT studies S. Wojtyśiak, M. Kamiński, J. Krajczewski, P. Dłużewski and A. Kudelski (Warsaw, Poland).....	11
FTIR and quantum chemical study of LiBr solvation in acetonitrile solutions A.M. Erkabaev, T.V. Yaroslavtseva, S.E. Popov and O.V. Bushkova (Ekaterinburg, Russia).....	19
Complementary optical and neutron vibrational spectroscopy study of bromanilic acid: 2,3,5,6-tetramethylpyrazine (1:1) cocrystal K. Łuczyńska (Warsaw, Poland and Dubna, Russian Federation), K. Druźbicki (Dubna, Russian Federation and Poznan, Poland), K. Lyczko and W. Starosta (Warsaw, Poland).....	26
A novel approach to investigate vascular wall in 3D: Combined Raman spectroscopy and atomic force microscopy for aorta <i>en face</i> imaging M. Pilarczyk, A. Rygula, A. Kaczor, L. Mateuszuk, E. Maślak, S. Chlopicki and M. Baranska (Krakow, Poland).....	39
Vibrational properties and DFT calculations of formamidine-templated Co and Fe formates E. Kucharska, J. Hanuza, A. Ciupa, M. Mączka and L. Macalik (Wroclaw, Poland).....	45
Study on the cesium Tutton compounds, Cs ₂ M(XO ₄) ₂ ·6H ₂ O (M = Mg, Co, Zn; X = S, Se): Preparation, X-ray powder diffraction and infrared spectra V. Karadjova, D. Kovacheva and D. Stoilova (Sofia, Bulgaria).....	51
Interaction of sodium and potassium ions with PEO-PPO copolymer investigated by FTIR, Raman and NMR X. Li, K. Huang, Y. Xu and H. Liu (Beijing, PR China).....	59
Vibrational relaxation study of C=O stretching mode of liquid <i>N,N</i> -dimethylformamide: Comparative study with theoretical calculation Th.G. Devi (Nirjuli, India).....	65
Synthesis and characterization of porous WO ₃ –SnO ₂ nanomaterials: An infrared study of adsorbed pyridine and dimethyl methylphosphonate Y. El-Sayed, N. Abu-Farha and S. Kanan (United Arab Emirates).....	78
Cardiolipin containing liposomes are fully ionized at physiological pH. An FT-IR study of phosphate group ionization D. Malyska, L.A. Pandiscia and R. Schweitzer-Stenner (Philadelphia, PA, USA).....	86
Raman and infrared vibrational modes of tricosane paraffin under high pressure M.A. Puerto and N.M. Balzaretto (Av. Bento Goncalves, Brazil).....	93
Polarized Raman study on the lattice structure of BiFeO ₃ films prepared by pulsed laser deposition Y. Yang, Y.B. Yao, Q. Zhang and X.X. Zhang (Saudi Arabia).....	101
Importance of weak interactions and conformational equilibrium in <i>N</i> -butyl- <i>N</i> -methylpiperidinium bis(trifluoromethanesulfonyl) imide room temperature ionic liquids: Vibrational and theoretical studies M. Shukla (Varanasi, India), H. Noothalapati, S. Shigeto (Hsinchu, Taiwan) and S. Saha (Varanasi, India).....	107
Performance of an optical stabilization system at NSLS beamline U12IR R.J. Smith, E. Stavitski and G.L. Carr (Upton, NY, USA).....	118
Modeling infrared beam lines with Shadow and Zemax T. May and A. Duffy (Saskatoon, Canada).....	123
Further insights into the assessment of cell cycle phases by FTIR microspectroscopy D.E. Bedolla, S. Kenig, E. Mitri, P. Storici and L. Vaccari (Basovizza, Italy).....	127
Synchrotron FTIR microscopy of synthetic and natural CO ₂ –H ₂ O fluid inclusions M.K. Nieuwoudt (Auckland, New Zealand), M.P. Simpson (Taupo, New Zealand), M. Tobin and L. Puskar (Clayton, Australia).....	136
Fine-scale determination of OH in radiation-damaged zircon using Synchrotron Fourier Transform Infra Red spectroscopy (FTIR) and Attenuated Total Reflectance (ATR) W. van Bronswijk and R.T. Pidgeon (Bentley, Australia).....	149

New experimental set-ups for studying nanoconfined water on the AILES beamline at SOLEIL S. Dalla Bernardina, F. Alabarse, A. Kalinko, P. Roy, M. Chapuis, N. Vita (Gif-sur-Yvette, France), R. Hienerwadel, C. Berthomieu (Saint-Paul-lez-Durance, France), P. Judeinstein, J.-M. Zanotti (Gif Sur Yvette, France), J.L. Bantignies, J. Haines, J. Catafesta (Montpellier, France), G. Creff (Ave Valrose, France), L. Manceron and J.-B. Brubach (Gif-sur-Yvette, France)	154
Observation of radially polarized terahertz radiation generated by a sub-picosecond electron beam Y. Taira, R. Kuroda (Tsukuba, Japan), M. Kumaki (Tokyo, Japan), M. Tanaka, H. Toyokawa (Tsukuba, Japan) and H. Tomizawa (Sayo, Japan)	162
3D FT-IR imaging spectroscopy of phase-separation in a poly(3-hydroxybutyrate)/poly(L-lactic acid) blend M. Unger (Milwaukee, WI, USA and Esslingen a. N., Germany), J. Sedlmair (Madison, WI, USA), H.W. Siesler (Essen, Germany) and C. Hirschmugl (Milwaukee, WI, USA)	169
Wing wettability of <i>Odonata</i> species as a function of quantity of epicuticular waxes S.H. Nguyen, H.K. Webb, J. Hasan (Hawthorn, Australia), M.J. Tobin (Clayton, Australia), D.E. Mainwaring, P.J. Mahon (Hawthorn, Australia), R. Marchant, R.J. Crawford and E.P. Ivanova (Clayton, Australia).....	173
Polarised infrared microspectroscopy of edge-oriented graphene oxide papers M.D. Frogley (Chilton, UK), C. Wang (London, UK), G. Cinque (Chilton, UK) and A.H. Barber (London, UK)	178
Characterization of THz radiation generated by ultra-short bunch from energy chirping cell attached RF electron gun Y. Koshiba, K. Sakaue, M. Mizugaki, M. Washio (Tokyo, Japan), R. Kuroda, T. Takatomi and J. Urakawa (Ibaraki, Japan)	184
Concept for a single-shot mid-infrared spectrometer using synchrotron radiation U. Schade, E. Ritter, P. Hegemann, E.F. Aziz and K.P. Hofmann (Berlin, Germany).....	190
Simulation of photon intensity distributions to facilitate the design of beamlines at accelerator-based IR/THz sources P. Rieger, Y.-L. Mathis, B. Gasharova and D. Moss (Karlsruhe, Germany).....	196
Qualitative spectroscopic characterization of the matrix–silane coupling agent interface across metal fibre reinforced ion exchange resin composite membranes L.F. Dumée (Waurm Ponds, Australia and Werribee, Australia), F.-M. Allieux (Waurm Ponds, Australia), R. Reis (Waurm Ponds, Australia and Werribee, Australia), M. Duke, S. Gray (Werribee, Australia), M. Tobin, L. Puskar (Clayton, Australia), L. He, P. Hodgson and L. Kong (Waurm Ponds, Australia)	203
Far-infrared studies on Nafion and perfluoroimide acid (PFIA) and their alkali salts A.D.O. Bawagan (Ottawa, Canada), S.J. Hamrock, M. Schaberg (St Paul, MN, USA), I. Yousef (Allan, Jordan), E. Ritter and U. Schade (Berlin, Germany).....	213