

74
V58



ELSEVIER

Volume 68 September 2013

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

Vibrational spectroscopic study of poly(dimethylsiloxane)-ZnO nanocomposites L. Bistričić (Zagreb, Croatia), V. Borjanović (Zagreb, Croatia and Raleigh, NC, USA), L. Mikac and V. Dananić (Zagreb, Croatia).....	1
Spectroscopic analysis of pigments and inks in manuscripts: I. Byzantine and post-Byzantine manuscripts (10–18th century) I. Nastova, O. Grupče, B. Minčeva-Šukarova (Skopje, Republic of Macedonia), M. Ozcataı (Afyonkarahisar, Turkey) and L. Mojsoska (Ohrid, The Former Yugoslav Republic of Macedonia).....	11
Temperature dependence of the microstructure of 1-butyl-3-methylimidazolium tetrafluoroborate in aqueous solution H. Wang, J. Wang and L. Zhang (Xinxiang, PR China).....	20
Label free non-invasive imaging of topically applied actives in reconstructed human epidermis by confocal Raman spectroscopy F.D. Fleischli, S. Mathes and C. Adhart (Wädenswil, Switzerland).....	29
High-pressure Raman scattering of MgMoO ₄ M.N. Coelho, P.T.C. Freire (Fortaleza, Brazil), M. Maczka (Wrocław, Poland), C. Luz-Lima (Teresina, Brazil), G.D. Saraiva (Quixadá, Brazil), W. Paraguassu (Belém, Brazil), A.G. Souza Filho (Fortaleza, Brazil) and P.S. Pizani (São Carlos, Brazil).....	34
Effect of thermal annealing on the microstructure of P3HT thin film investigated by RAIR spectroscopy L. An, Y. Duan, Y. Yuan, L. Zhou and J. Zhang (Qingdao City, People's Republic of China).....	40
Immobilised gold nanostars in a paper-based test system for surface-enhanced Raman spectroscopy D. Mehn, C. Morasso, R. Vanna, M. Bedoni, D. Prosperi and F. Gramatica (Milan, Italy).....	45
Synchronous ATR infrared and NIR-spectroscopy investigation of sepiolite upon drying V.J. Bukas, M. Tsampodimou, V. Gionis and G.D. Chryssikos (Athens, Greece).....	51
DFT study of Raman spectra of phosphorus-containing dendrimers built from thiophosphoryl core V.L. Furer, A.E. Vandyukov (Kazan, Russia), J.P. Majoral, A.M. Caminade (Toulouse, France) and V.I. Kovalenko (Kazan, Russia).....	61
Observation of sub-surface phenyl rings in polystyrene with vibrationally resonant sum-frequency generation A.D. Curtis, A.R. Calchera, M.C. Asplund and J.E. Patterson (Provo, UT, USA).....	71
Vibrational spectra and factor group analysis of rare-earth chromium borates, RCr ₃ (BO ₃) ₄ , with R = La–Ho E.Yu. Borovikova, E.A. Dobretsova, K.N. Boldyrev, V.S. Kurazhkovskaya, V.V. Maltsev and N.I. Leonyuk (Moscow, Russia).....	82
Distribution of species in Na ₂ O–CaO–B ₂ O ₃ glasses as probed by FTIR H. Doweidar, G. El-Damrawi (Mansoura, Egypt) and M. Al-Zaibani (Mansoura, Egypt and Amran, Yemen).....	91
Characterization and quantification of secondary metabolite profiles in leaves of red and white clover species by NIR and ATR-IR spectroscopy A. Krämer, G. Gudi (Berlin, Germany), N. Weiher, M. Gierus (Kiel, Germany), W. Schütze (Quedlinburg, Germany) and H. Schulz (Berlin, Germany).....	96
Selective determination of mercury (II) ion in water by near-infrared diffuse reflection spectroscopy with the aid of preconcentration and multivariate calibration F. Liu, W. Cai and X. Shao (Tianjin, PR China).....	104
Structural and optical characterization of type II In _{0.14} Ga _{0.86} As _{0.13} Sb _{0.87} /GaSb heterostructure doped with zinc grown by liquid phase epitaxy J. Díaz-Reyes (Tepetitla, Mexico), J.G. Mendoza-Alvarez, P. Rodríguez-Fragoso, M. Galván-Arellano (México, Mexico), E. López-Cruz (Puebla, Mexico) and J.L. Herrera-Pérez (México, Mexico).....	109
Raman spectroscopic study on classification of cervical cell specimens S. Rubina (Kharghar, India), M. Amita, D. Kedar K., R. Bharat (Parel, India) and C.M. Krishna (Kharghar, India).....	115
Infrared and Raman spectra of magnesium ammonium phosphate hexahydrate (<i>struvite</i>) and its isomorphous analogues. IX: Spectra of protiated and partially deuterated cubic magnesium caesium phosphate hexahydrate V. Stefov (Skopje, Macedonia), Z. Abdija (Skopje, Macedonia and Tetovo, Macedonia), M. Najdoski (Skopje, Macedonia), V. Koleva (Sofia, Bulgaria), V.M. Petruševski (Skopje, Macedonia), T. Runčevski, R.E. Dinnebieer (Stuttgart, Germany) and B. Šoptrajanov (Skopje, Macedonia).....	122
Investigation of Raman and infrared phonon modes in case of barium bismuth tantalate (BaBi ₂ Ta ₂ O ₉) Archana and H.C. Gupta (New Delhi, India).....	129

Use of Raman spectroscopy to determine the kinetics of chemical transformation in yogurt production R. Rodríguez, S. Vargas, M. Estevez (Querétaro, Mexico), F. Quintanilla, A. Trejo-Lopez (Campus Querétaro, Mexico) and A.R. Hernández-Martínez (Querétaro, Mexico).....	133
DFT and Raman spectroscopy of porphyrin derivatives: Tetraphenylporphine (TPP) M. Aydin (Samsun, Turkey).....	141
Surface-enhanced Raman scattering measurements on silver nanoparticles covered with differently formed platinum films S. Wojtysiak and A. Kudelski (Warsaw, Poland).....	153
Study of the dependence of the photoacoustic signal amplitude from methane on different collisional partners N. Barreiro, A. Peuriot, V. Slezak (Villa Martelli, Argentina) and G. Santiago (Buenos Aires, Argentina).....	158
Vibrational spectra of fluorene, 1-methylfluorene and 1,8-dimethylfluorene S. Chakraborty, P. Das (Bangalore, India), S. Manogaran (Kanpur, India) and P.K. Das (Bangalore, India).....	162
Trace gas detection of benzene, toluene, <i>p</i> -, <i>m</i> - and <i>o</i> -xylene with a compact measurement system using cantilever enhanced photoacoustic spectroscopy and optical parametric oscillator C.B. Hirschmann (Oulu, Finland), S. Sinisalo, J. Uotila (Turku, Finland), S. Ojala and R.L. Keiski (Oulu, Finland).....	170
Laser-induced transformation of stibnite (Sb_2S_3) and other structurally related salts P. Makreski, G. Petruševski, S. Ugarković and G. Jovanovski (Skopje, Macedonia).....	177
Double beryllium iodate dihydrates, $\text{M}_2\text{Be}(\text{IO}_3)_4 \cdot 2\text{H}_2\text{O}$ ($\text{M} = \text{K}, \text{NH}_4^+, \text{Rb}$): Preparation, X-ray powder diffraction and vibrational spectra V. Karadjova, D. Kovacheva and D. Stoilova (Sofia, Bulgaria).....	183
Ion-polymer complexation and ion-pair formation in a polymer electrolyte PEO:LiPF ₆ containing an ionic liquid having same anion: A Raman study S.K. Chaurasia, R.K. Singh and S. Chandra (Varanasi, India).....	190
Infrared microspectroscopy of Oral Squamous Cell Carcinoma: Spectral signatures of cancer grading S. Sabbatini, C. Conti, C. Rubini (Ancona, Italy), V. Librando (Catania, Italy), G. Tosi and E. Giorgini (Ancona, Italy).....	196
Synchrotron infrared microspectroscopy study of the orientation of an organic surfactant on a microscopically rough steel surface K. Lepková, W. van Bronswijk, V. Pandarinathan and R. Gubner (Perth, Australia).....	204
Quantification of the inorganic phase of the pelagic aggregates from an iron contaminated lake by means of Raman spectroscopy V. Ciobotă, S. Lu, N. Tarcea, P. Rösch, K. Küsel and J. Popp (Jena, Germany).....	212
The determination of the Fe content in natural sphalerites by means of Raman spectroscopy A. Buzatu, N. Buzgar (Iași, Romania), G. Damian (Iași, Romania and Baia Mare, Romania), V. Vasilache and A.I. Apopei (Iași, Romania).....	220
Application of vibrational spectroscopy techniques for material identification from fire debris T.J. Kerr, K.L. Duncan and L. Myers (Kingston, Jamaica).....	225
Vibrational co-assignment of the calculated frequencies in the ground and two lowest excited electronic states Y.N. Panchenko (Moscow, Russian Federation).....	236
On the complex refractive index of N-doped TiO_2 nanospheres and nanowires in the terahertz spectral region P. Bawuah, P. Silfsten (Joensuu, Finland), A. Sarkar (Umeå, Sweden), K. Kordas (Oulu, Finland), J.-P. Mikkola (Umeå, Sweden and Åbo-Turku, Finland) and K.-E. Peiponen (Joensuu, Finland).....	241
Surface-enhanced Raman scattering of 4-aminobenzenethiol on silver nanoparticles substrate E. de Barros Santos, F.A. Sigoli and I.O. Mazali (Campinas, Brazil).....	246
Pressure-induced crystal-amorphous transformation in $\text{Y}_2\text{Mo}_3\text{O}_{12}$ A.C. Torres Dias (Fortaleza, Brazil), C. Luz Lima (Teresina, Brazil), W. Paraguassu (Belém, Brazil), K. Pereira da Silva, P.T.C. Freire, J. Mendes Filho (Fortaleza, Brazil), B.A. Marinkovic (PUC-Rio, Brazil), K.J. Miller, M.A. White (Halifax, Canada) and A.G. Souza Filho (Fortaleza, Brazil).....	251
A conformational study of hydroxylated isoflavones by vibrational spectroscopy coupled with DFT calculations N.F.L. Machado, L.A.E. Batista de Carvalho (Coimbra, Portugal), J.C. Otero (Málaga, Spain) and M.P.M. Marques (Coimbra, Portugal).....	257
The spectroscopic characterization of the sulphate mineral ettringite from Kuruman manganese deposits, South Africa R.L. Frost, A. López, Y. Xi (Brisbane, Australia), R. Scholz, G.M. da Costa, R.M.F. Lima and A. Granja (Ouro Preto, Brazil).....	266
Synthesis and characterization of imine-modified silicas obtained by the reaction of essential oil of <i>Eucalyptus citriodora</i> , 3-aminopropyltriethoxysilane and tetraethylorthosilicate L.M.P. Montenegro, J.B. Griep, F.C. Tavares, D.H. de Oliveira, D. Bianchini and R.G. Jacob (Pelotas, Brazil).....	272
Micro-Raman mapping on an anatase TiO_2 single crystal with a large percentage of reactive (0 0 1) facets G. Zeng (China and Beijing, China), K.-K. Li (Beijing, China), H.-G. Yang (Shanghai, China) and Y.-H. Zhang (Beijing, China).....	279