PHYSICAL CHEMISTRY 2022

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on Fundamental and Applied Aspects of
Physical Chemistry

Organized by
The Society of Physical Chemists of Serbia

BOOK OF ABSTRACTS

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Abbreviations

PL – Plenary Lecture
SL – Section Lecture
O – Oral Presentation
P – Poster Presentation

Topics

A – Education and History
B – Spectroscopy, Molecular Structure, Physical Chemistry of Plasma
C – Kinetics, Catalysis
D – Nonlinear Dynamics, Oscillatory Reactions, Chaos
E – Electrochemistry
F – Biophysical Chemistry, EPR investigations of Bio-systems
G – Organic Physical Chemistry
H – Material Science
I – Photochemistry, Radiation Chemistry, Photonics
J – Macromolecular Physical Chemistry
K – Environmental Protection, Forensic Sciences, Geophysical Chemistry, Radiochemistry, Nuclear Chemistry
L – Phase Boundaries, Colloids, Liquid Crystals, Surface-Active Substances
M – Complex Compounds
N – Food Physical Chemistry
O – Pharmaceutical Physical Chemistry

B-11-P

MOLECULAR STRUCTURE OPTIMIZATION AND DECONVOLUTION OF COMPLEX RAMAN SPECTRUM BANDS VIBRATIONS OF INDIGO CARMINE

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ABSTRACT
Determining the complex vibrational groups for each Raman spectrum band due to substantial bands overlapping was a challenge of many researchers. Using an example of fairly complex organic molecule of indigo carmine, this work exemplifies the application of Facio software in order to give an illustration of deconvolution of complex indigo carmine Raman bands. Moreover, this work yields a better agreement of the Raman spectrum calculated of indigo carmine and experimental ones compared to the literature data. This fact makes the work important in terms of singling out the vibrational groups types in a molecule for each band in the Raman spectrum.