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vibrational spectroscopy of determining parameters of the molecular force field from given experimental data formulated within different models particularly joint treatment of experimental data on vibrational spectra and results of quantum mechanical calculations within new approaches is considered"

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April 21st, 2020 - two methodological approaches to inverse problems solu tion with the help of neural networks are considered ex periment based and model based their merits draw backs and characteristics of their use are discussed suc cessful application of neural networks for solution of three inverse problems in laser spectroscopy of water media is re'

'raman scattering
May 26th, 2020 - raman scattering or the raman effect ?r??m?n is the inelastic scattering of photons by matter meaning that there is an exchange of energy and a change in the light s direction typically this involves vibrational energy being gained by a molecule as incident photons from a visible laser are shifted to lower energy''a general algorithm to solve

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'stable numerical methods of solving certain inverse

May 7th, 2020 - it is essential that Z_s and Z should be closed sets bounded in the subset the majority of methods of solving inverse problems of vibrational spectroscopy are intended for solving eqs 2 and 3 i e for those cases when only the frequencies of the vibrations of the molecules are used as experimental

data'

'analytical solution of the inverse spectroscopic problem

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June 1st, 2020 - solving inverse problems arising in vibrational spectra data processing and includes classical theory of small vibrations molecular force fields and experimental sources of information mathematical model of molecular vibrations formulation of inverse vibrational problem generalized coordinates in normal coordinate

analysis'

'lecture 1 describing inverse problems

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incl earthquake location
lecture 24 exemplary inverse problems
incl vibrational problems
the inverse problem is to determine the number and position of sources from observations of the position of the sediments matlab'

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analytical solution of the inverse spectroscopic problem

February 11th, 2020 - the inverse problem of spectroscopy of vibrational transitions of diatomic molecules was analytically solved on the basis of wave functions of the morse oscillator an example of the determination of the transition dipole moment function by intensities of several lines of molecule vibrational rotational spectra measured experimentally was considered'

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May 5th, 2020 - in the first 1986 edition of this book inverse problems in vibration were interpreted strictly problems concerning the reconstruction of a unique undamped vibrating system of a specified type from specified vibratory behaviour particularly specified natural frequencies and or natural mode'

'inverse photoemission spectroscopy

April 20th, 2020 - inverse photoemission spectroscopy is a surface science technique used to study the unoccupied electronic structure of surfaces thin films and adsorbates a well collimated beam of electrons of a well defined energy It 20 eV is directed at the sample these electrons couple to high lying unoccupied electronic states and decay to low lying unoccupied states with a subset of these transitions being radiative'

'osa inverse problem in diffuse reflectance spectroscopy

June 4th, 2020 - in diffuse reflectance spectroscopy the kubelka munk equations have been used

extensively these equations provide simple solutions to the inverse problem of obtaining information on the scattering and absorption cross sections from reflected light proof is provided that the basic kubelka munk equation $dR \times Sdx \ r^2 \times 2ar \times 1$ should be replaced by the equation $dR \times Sdx \ r^2 \times 2'$

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April 15th, 2020 - this volume aims to provide a consistent mathematical and physical treatment of empirical data processing in vibrational spectroscopy based on the modern theory of nonlinear ill posed problems it focuses on the mathematical formulation of model constraints and the use of experimental data'

'inverse problems of molecular spectra data processing

May 19th, 2020 - the main of them the general inverse problem of structural chemistry for free molecules is nonlinear inverse problem of molecular vibrations the modern view on this problem joins the study of molecular force field and geometry restoration using all available experimental data vibrational ir and raman spectroscopy electron diffraction etc'

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