

Structural and vibrational study of 2-MethoxyEthylAmmonium Nitrate (2-OMeEAN): Interpretation of experimental results with ab initio molecular dynamics

By:Campetella, M; Bovi, D; Caminiti, R ; Guidoni, L ; Bencivenni,; Gontrani, L

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Chloromethyl-oxirane and chloromethyl-thiirane in liquid phase: A joint experimental and quantum chemical study

Campetella, M; Bencivenni, L ; Caminiti, R ; Zazza, C ; Di Trapani, S ; Martino, A ; Gontrani,

CHEMICAL PHYSICS Volume: 473 Pages: 24-31

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FTIR spectra and density functional theory P.E.D. assignments of oxiranes

in Ar matrix at 12 K

L.Gontrani, S. Nunziante Cesaro, S. Stranges, L. Bencivenni  
A. Pieretti

Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy 120 (2014) 558-567

Two Different Models to Predict Ionic-Liquid Diffraction

Patterns: Fixed-Charge versus Polarizable Potentials

Marco Campetella, Lorenzo Gontrani, Francesca Leonelli, Luigi Bencivenni, and  
Ruggero Caminiti  
ChemPhysChem 2015, 16, 197 - 203

Comprehensive Infrared Study of Tetryl, Dinitrotoluene, and Trinitrotoluene Compounds

Adriana Puiu,Gianfranco Giubileo,Stella Nunziante Cesaro,  
Luigi Bencivenni  
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Tautomerism in liquid 1,2,3-triazole: a combined energy-dispersive X-Ray diffraction, molecular dynamics and FTIR study

Author(s): Bellagamba, Marco; Bencivenni, Luigi; Gontrani, Lorenzo; Guidoni, Leonardo; Sadun, Claudia  
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Combined FTIR matrix isolation and density functional studies of indole-3-pyruvic acid molecule. Spectroscopic evidence of gas-phase tautomerism

Author(s): Bencivenni, Luigi; Margonelli, Andrea; Mariani, Alessandro; Pieretti, Andrea; Nunziante Cesaro, Stella  
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Overcoming the Inadequacy of X-ray Powder Diffraction in Reliable Hydrogen Location with the Aid of First Principles Calculations: Crystal Structure Determination of Orotaldehyde Monohydrate

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Gas phase dissociation of H<sub>2</sub>S<sub>0</sub>4: A computational study

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On the performance of gradient-corrected approximation functionals and polarizable continuum model in the study of 1,2,3-triazine in water

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