

CURRICULUM di **BENCIVENNI LUIGI**

RICERCATORE UNIVERSITARIO CONFERMATO in servizio presso il
Dipartimento di
Chimica dell'Università di Roma

Insegnamenti:

Precedentemente: Chimica Teorica, Chimica Quantistica, Teoria
delle Vibrazioni molecolari; Chimica Computazionale,
Tecnologie Informatiche Chimiche, Laboratorio di Chimica
Fisica (Spettroscopia)

Attualmente: Corsi di dottorato interni al dipartimento di
chimica

Settore della ricerca: Chimica Fisica (CHIM 02)

ELENCO DI ALCUNE PUBBLICAZIONI

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

JOURNAL OF CHEMICAL PHYSICS Volume: 145 Issue: 2
Article Number: 024507
DOI: 10.1063/1.4956459
Published: JUL 14 2016

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
DOI: 10.1016/j.chemphys.2016.03.027
Published: JUL 1 2016

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

APPLIED SPECTROSCOPY

, Volume 69, Number 12, 2015

, 1472-1486

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

Struct Chem (2013) 24:933-943 DOI 10.1007/s11224-013-0206-4

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

From ISRN Physical Chemistry (2012), 243741, 11 pp..

Language: English, Database: CAPLUS

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

Author(s): Guidoni, Leonardo; Gontrani, Lorenzo; Bencivenni, Luigi; JOURNAL OF PHYSICAL CHEMISTRY Volume: 113 Issue: 1

Pages: 353-359 DOI: 10.1021/jp809076t Published: JAN 8 2009

Dimerisation of urea in water solution: a quantum mechanical investigation

Author(s): Ramondo, Fabio; Bencivenni, Luigi; Caminiti, Ruggero;

Source: PHYSICAL CHEMISTRY CHEMICAL PHYSICS Volume: 9 Issue:
18 Pages: 2206-2215 DOI: 10.1063/b617837e Published: 2007

Gas phase dissociation of H₂SO₄: A computational study

Author(s): Brutti, S.; Bencivenni, L.; Barbarossa, V.; et al.

Source: JOURNAL OF CHEMICAL THERMODYNAMICS Volume: 38 Issue:
11 Pages: 1292-1300 DOI: 10.1016/j.jct.2006.02.009 Published:
NOV 2006

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

Author(s): Zazza, Costantino; Grandi, Andrea; Bencivenni,
Luigi;

Source: JOURNAL OF MOLECULAR STRUCTURE-THEOCHEMÂ Volume: 764
Issue: 1-3 Pages: 87-93 DOI: 10.1016/j.theochem.2006.02.019
Published: MAY 30 2006

Computational and vibrational spectroscopy study of the
microclusters of C_{2v} symmetry urea molecule in the(1)A
electronic ground state

Author(s): Spoliti, M; Perrone, G; Bencivenni, L;

Source: JOURNAL OF MOLECULAR STRUCTURE-THEOCHEMÂ Volume: 756
Issue: 1-3 Pages: 113-126 DOI: 10.1016/j.theochem.2005.07.021
Published: DEC 9 2005

A density functional theory study of hexafluoropropene: low-
lying singlet excited states and primary photodissociation
channel

Author(s): Zazza, C; Bencivenni, L; Aschi, M

Source: CHEMICAL PHYSICS LETTERS Volume: 399 Issue: 1-3
Pages: 184-189 DOI: 10.1016/j.cplett.2004.10.012 Published:
NOV 21 2004

FTIR spectra and density functional calculations of carbonylic
complexes of chromium in argon and nitrogen cryomatrices

Author(s): Bencivenni, L; Dobos, S; Cesaro, S N;

Source: VIBRATIONAL SPECTROSCOPYÂ Volume: 36 Issue: 1 Pages:
57-63 DOI: 10.1016/j.vibspec.2004.02.010 Published: OCT 18
2004

On the performance of time-dependent density functional theory
and polarizable continuum model in the study of aqueous
formaldehyde

Author(s): Zazza, C; Bencivenni, L; Grandi, A;
Source: JOURNAL OF MOLECULAR STRUCTURE-THEOCHEMÂ Â Volume: 680
Issue: 1-3 Pages: 117-120 DOI: 10.1016/j.theochem.2004.05.006
Published: JUL 5 2004

Energy-dispersive X-ray diffraction on thin films and its
application to superconducting samples

Author(s): Albertini, VR; Paci, B; Meloni, S;
Source: JOURNAL OF APPLIED CRYSTALLOGRAPHY Volume: 36 Pages:
43-47 DOI: 10.1107/S0021889802018319 Part: Part 1 Published:
FEB 2003

Hydrogen bonding in barbituric and 2-thiobarbituric acids: a
theoretical and FT-IR study

Author(s): Ramondo, F; Pieretti, A; Gontrani, L;
CHEMICAL PHYSICS Volume: 271 Issue: 3 Pages: 293-308 DOI:
10.1016/S0301-0104(01)00440-2 Published: SEP 15 2001