Curriculum Vitae

A Brief Description

Nasser L. Hadipour

Date of Birth: **1948**

Place of Birth: **Iran**

Nationality: **Iranian**

Ph.D: **Physical Chemistry 1985 University of Massachusetts at Amherst**

MSc: **Physics 1983 University of Massachusetts at Amherst**

MSc: **Chemistry 1981 Northeastern University at Boston**

BSC: **Chemistry 1976 Sharif University of Technology, Tehran, Iran**

Post Doctorate: **1985 – 1986 City University of New York**

Visiting Fellow at Institute of Chemistry, Academia Sinica of Taiwan (Sept. 2007- Sept. 2008)

Permanent Position:

Professor of Physical Chemistry

Department of Chemistry

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Teaching Experience:

A) Taught Undergraduate Courses:

- Physical Chemistry I & II (Used Texts: Ira N. Levine, P. W. Atkins, and etc.)

- Elementary Quantum Chemistry (Used Text: Ira N. Levine, up to Chapter 6)

- Basic Molecular Spectroscopy (Used Text: W. Banvel)

- General Chemistry I & II

B) Taught Graduate Courses (Master and Ph.D in Physical Chemistry):

- Advanced Physical Chemistry (Used Texts: H. Callen, F. Wall, and etc.)

- Quantum Chemistry I, II & III (Used Texts: Ira. N. Levine, S. Gasirowicz,P.

W. Atkins, and etc.)

- Statistical Thermodynamics I & II (Used Texts: F. Reif, D. McQuarri, T. Hill,

and etc.)

- Molecular Spectroscopy (Used Text: Ira N. Levine)

- NMR Spectroscopy (Used Text: C. P. Slichter, and etc.)

Research Interests:

The main goal of our 8 members (5 Ph.D and 3 M.Sc. students) research group is study of *hydrogen-bonds in crystalline phases*. Our tools include calculation of nuclear quadrupole resonance (NQR) and nuclear magnetic shielding parameters using *ab initio* and DFT methods.

We perform these studies on:

1- Nucleic acid bases

2- Chitin and Chitosans

3- Histidin rich protein II and its complex with heme (the fundamental protein

responsible for oxidation of iron(II) of heme in malaria disease)

4- Molecular dynamic investigation of the repetitive segments of Hhistidin rich

protein II.

5-Nanotubs

List of Publications:

[59] ^{15}N Chemical Shift Calculations and Natural Bonding Orbital Analyses of (Benzamide)n=1-6 Clusters

M.D. Esrafili, J. Beheshtian, N.L. Hadipour, *Journal of Theoretical and Computational Chemistry*, **in press**.

[47] Role of spin state on the geometry and nuclear quadrupole resonance parameters in hemin complex

H. Behzadi, M. D. Esrafili, D. van der spoel, G. Parsafar, N. L. Hadipour, *Biophysical Chemistry* **2008**, 134, 200-206.

[46] DFT calculations of oxygen, nitrogen and hydrogen NMR parameters to study the C-H···O hydrogen bond in crystalline structure of 4-methylpyridine-N-oxide

M. Mirzaei, N.L. Hadipour, *Polish Journal of Chemistry* **2008**, 82, 1091-1096

[45] Density Functional Theory Study of Boron Nitride Nanotubes: Calculations of

the N-14 and B-11 NQR Parameters.

Z. Bagheri, M. Mirzaei, N. L. Hadipour, and M. R. Abolhassani, *Journal of Computational and Theoretical Nanoscience* **2008**, 5, 614-618

[44] Density functional study of zigzag BN nanotubes with equivalent ends

M. Mirzaei, N. L. Hadipour, A. Seif, M. Giahi, *Physica E: Low-Dimensional Systems and Nanostructures* **2008**, 40, 3060-3063

[43] A computational NQR study on the hydrogen-bonded lattice of cytosine-5-

acetic acid

M. Mirzaei and N. L. Hadipour, *Journal of Computational Chemistry* **2008**, 29, 832-838.

[42] Study of hydrogen bonds in N-methylacetamide by DFT calculations of oxygen, nitrogen, and hydrogen solid-state NMR parameters

M. Mirzaei, N. L. Hadipour, *Structural Chemistry* **2008**, 19, 225-232

[41] Density Functional Theory Study of N-H···O, O-H···O and C-H···O Hydrogen-

Bonding Effects on the ^{14}N and ^{2}H Nuclear Quadrupole Coupling Tensors of N-Acetyl-

Valine.

M. D. Esrafili, H. Behzadi, and N. L. Hadipour *Biophysical Chemistry* **2008**, 133, 11-18.

[40] Density functional calculations of oxygen, nitrogen and hydrogen electric field gradient and chemical shielding tensors to study hydrogen bonding properties of peptide group (O=C-NH) in crystalline acetamide

Z. Samadi, M. Mirzaei, N.L. Hadipour, S. Abedini Khorami, *Journal of Molecular Graphics and Modelling* **2008**, 26, 977-981

[39] Density functional calculations of ^{14}N and ^{11}B NQR parameters in the H-capped

(6,0) and (4,4) single-walled BN nanotubes.

M. Mirzaei and N. L. Hadipour, *Physica E: Low-Dimensional Systems and Nanostructures* **2008**, 40, 800-804.

[38] Synthesis and structural characterization of diorganotin(IV) complexes with 2,6-pyridinedicarboxylic acid

A.Azadmehr, M.M. Amini, N. Hadipour, H.R. Khavasi, H.-K. Fun, C.-J. Chen, *Applied Organometallic Chemistry* **2008**, 22, 19-24

[37] Density functional theory study of binding energies, ^{7}Li nuclear magnetic shielding, and electric field gradient tensors on the small clusters of LinHm ($m \leq n \leq 4$)

M.D. Esrafili, F. Elmi, N. L. Hadipour, *Journal of Theoretical and Computational Chemistry* **2007**, 6, 959-973.

[36] Theoretical investigation of hydrogen bonding effects on oxygen, nitrogen, and ydrogen chemical shielding and electric field gradient tensors of chitosan/HI salt

S. Khodaei, N. L. Hadipour, M.R. Kasaai, *Carbohydrate Research* **2007**, 342, 2396-2403

[35] A density functional study of ^{14}N NQR parameters of imidazole derivatives and extrapolation to PfHRP2-Fe3+-PPIX complex

Sareh M. Nasseri, Nasser L. Hadipour and Alireza Mohebbi, Journal of Molecular Structure: THEOCHEM **2007**, 820, 48-52.

[34] Influence of N-H…O and O-H…O hydrogen bonds on the ^{17}O, ^{15}N and ^{13}C

chemical shielding tensors in crystalline acetaminophen: A density functional theory

study.

Mehdi D. Esrafili, Hadi Behzadi and Nasser L. Hadipour, *Biophysical Chemistry* **2007**, *128,* 38-45**.**

[33] Study of Hydrogen Bonds in 1-Methyluracil by DFT Calculations of Oxygen,

Nitrogen, and Hydrogen Quadrupole Coupling Constants and Isotropic Chemical Shifts.

M. Mirzaei, N. L. Hadipour *Chemical Physics Letters*, **2007**, *438, 304-307*.

[32] Investigation of the effects of ionic hydrogen bonds (C=O-...H-C and + N-H…-O=C) in crystalline DL-Proline by ab initio and DFT calculated NQR parameters.

S. M. Nasseri, N. L. Hadipour, A. Mohebbi, *Journal of Molecular Structure,* **2007***,*846, *119-122.*

[31] A Theoretical Study of ^{17}O, ^{14}N and $_{2}$H Nuclear Quadrupole Coupling Tensors in the Real Crystalline Structure of Acetaminophen

H. Behzadi, M. D. Esrafili, N. L. Hadipour, *Chemical Physics* **2007**, 333, 97-104.

[30] Influence of C-Doping on the B-11 and N-14 Quadrupole Coupling Constants in Boron-Nitride Nanotubes: A DFT Study.

M. Mirzaei, N. L. Hadipour, and M. R. Abolhassani *Z. Naturforsch.,* **2007**, *62**a***, 1.

[29] Density Functional Theory Investigation of Hydrogen Bonding Effects on the Oxygen, Nitrogen and Hydrogen Electric Field Gradient and Chemical Shielding Tensors of Anhydrous Chitosan Crystalline Structure

M. D. Esrafili, F. Elmi, N. L. Hadipour, *Journal Physical Chemistry A* **2007***, 111,* 963.

[28] Investigation of C-H...O=C and N-H...O=C Hydrogen-Bonding Interactions in Crystalline Thymine by DFT Calculations of O-17, N-14 and H-2 NQR Parameters

M. Mirzaei, N. L. Hadipour, and K. Ahmadi *Biophysical Chemistry* **2007,** *125*,414.

[27] A Density Functional Study of $_{17}$O, $_{14}$N and $_{2}$H Electric Field Gradient Tensors in the Real Crystalline Structure of _-Glycine

H. Behzadi, N. L. Hadipour, and M. Mirzaei *Biophysical Chemistry* **2007,** *125,* 179.

[26] The C−H...O Hydrogen Bonding Effects on the $_{17}$O Electric Field Gradient and Chemical Shielding Tensors in Crystalline 1-Methyluracil: A DFT Study

T. Partovi, M. Mirzaei, and N. L. Hadipour, *Z. Naturforsch.* **2006,** *61a,* 383.

[25] A Systematic Investigation of Hydrogen-Bonding Effects on the ^{17}O, ^{14}N and ^{2}H Nuclear Quadrupole Resonance Parameters of Anhydrous and Monohydrated Cytosine Crystalline Structures: A Density Functional Theory Study

M. Mirzaei, F. Elmi, and N. L. Hadipour *Journal of Physical Chemistry B* **2006,** *110,* 10991.

[24] An Investigation of Hydrogen-Bonding Effects on the Nitrogen and Hydrogen Electric Field Gradient and Chemical Shielding Tensors in the 9-Methyladenine Real Crystalline Structure: A Density Functional Theory Study

M. Mirzaei and N. L. Hadipour *Journal of Physical Chemistry A* **2006,** *110,* 4833.

[23] Correlation between NQR Parameters and Residue Size of Aliphatic Amino Acids and their Dimers

A. Ghaderi, H. Sabzyan, N. L. Hadipour *Biophysical Chemistry* **2006***, 12,* 62.

[22] Structural Elucidation of $\{[(CH_3)_2SnCl_2 \cdot H_2O]_2 \cdot 18\text{-crown-}6\}_n$ and its Hydrogen Bonding in Solution by HMBC Spectroscopy

M. Amini, A. Azadmher, N. L. Hadipour *Journal of Inclusion Phenomena and Macrocyclic Chemistry* **2006**, *54 No. 1-2,* 77.

[21] A Study on the Intermolecular Hydrogen Bonds of -Glycylglycine in Its Actual Crystalline Phase Using ab Initio Calculated ^{14}N and ^{2}H Nuclear Quadrupole Coupling Constants

F. Elmi and N. L. Hadipour, *Journal of Physical Chemistry A* **2005**, *109*, 1729.

[20] The Role of Charge Distribution on the Antimalarial Activity of Artemisinin Analogues

M. A. Rafiee, N. L. Hadipour, H. Naderi-manesh *Journal of Chemical Information and*

Modeling **2005,** *45*, 366.

[19] Ab initio Calculations of the Nuclear Quadrupole Coupling Constants of BH_n = $_{2,4}X^+$ (X = NH_3, PH_3, H_2O, H_2S)

T. Partovi, M. A. Rafiee, N. L. Hadipour *Z. Naturforsch.* **2005,** *60**a**,* 37.

[18] A Correlation Study of Quinoline Derivatives and their Pharmaceutical Behavior by ab initio Calculated NQR Parameters

M. A. Rafiee, N. L. Hadipour, H. Naderi-manesh *Journal of Computer-Aided Molecular Design* **2004,** *18,* 215.

[17] A Study of Hydrogen Bond of Imidazole and its 4-Nitro Derivative by ab initio and DFT Calculated NQR Parameters

S. K. Amini, N. L. Hadipour, F. Elmi *Chemical Physics Letters* **2004,** *391, 95.*

[16] Self-association study of methanol in CCl4 by FT-NMR spectroscopy

H. Shekaari, H. Modarres, N. Hadipour *Iranian Journal of Science and Technology* **2004***, 28*, 701

[15] Thermodynamic Investigation on Self-Association of Alcohols in Carbon Tetrachloride by FT-NMR Spectroscopy

H. Shekaari, H. Modarress, N. Hadipour *Journal of Physical chemistry A* **2003,** *107*, 1891.

[14] Investigation Hydrogen-Bonding Capabilities of Modified Amide Groups Using Calculated Nuclear Quadruple Coupling Constants

F. Elmi, N. L. Hadipour, F. Safinezhad *Chemical Physics Letters* **2003***, 375,* 273.

[13] A New Method for Distinguishing Between Al_2X_6 (X=Cl, Br) Conformers Based on ab initio Calculated Nuclear Quadrupole Coupling Constants

N. L. Hadipour , F. Elmi *Chemical Physics Letters* **2003,** *371,* 56.

[12] A Theoretical Study (ab-initio) on Various Structures of {CH_3N_2 +$(H_2)_{n=1-9}$} by Calculating NQR Parameters

N. L. Hadipour, M. A. Rafiee, M. Javaheri *Chemical Physics Letters* **2002,** *366,* 578.

[11] ab initio Calculations of NQR ^{35}Cl Frequency in Organo-Germanium Chlorides and its Dependency on Ge–O Distance

N. L. Hadipour, M. A. Rafiee, M. Javaheri, M. K. Mousavie *Chemical Physics Letters* **2002,** *356,* 445.

[10] Semi-Empirical Quantum Mechanical Calculations of Electronic Distribution and NQR Parameters of Bromine Atoms in Some Organic and Inorganic Compounds

N. L. Hadipour , S. Javadian *Journal of Molecular Structure* **2000,** *525,* 129.

[9] Quantitation of Model Digestive Mixtures by ^{13}C NMR

D. Wang, N. L. Hadipour, E. A. Jerlin, R. E. Stark *Journal of Lipid Research* **1992,** *33,* 431.

[8] A Deuterium NQR Study of Imidazolidone, Imidazolidone Hemihydrate, Phthalimide, and Benzamide

R. O. Day, N. L. Hadipour, J. L. Ragle *Journal of Magnetic Resonance,* **1986,** *67,* 466.

[7] Deuterium NQR spectra: dipolar interaction between two quadrupolar nuclei.

N. Hadipour, J. L. Ragle *Z. Naturforsch* **1985***, 40**a**, 355.*

[6] Deuterium NQR study and X-ray structural determination of 2-imidazolidon.

N. Hadipour, R. O. Day, J. L. Ragle *Journal of crystal spectroscopy research* **1985**.

[5] Deuterium NQR Study of Phenylphosphonic Acid and Two Ternary Cocrystals of Pyridine, Catechol, and Phenylphosphonic Acid

R. O. Day, N. Hadipour, J. L. Ragle *Journal of Magnetic Resonance* **1984,** *59,* 373.

[4] Deuterium Double-Transition Quadrupole-Resoname Spectra and the Structures of Catechol, Resorcinol, and Hydroquinone

R. O. Day, N. Hadipour, J. L. Ragle *Journal of Magnetic Resonance* **1984,** *57,* 369.

[3] Assignment of the Deuteron NQR Spectrum of Hydroquinone-(O)-D_2

N. Hadipour and J. L. Ragle *Journal of Molecular Structure* **1983,** *111,* 17.

[2] Effect of Electric Fields on the Thermal Decomposition of Calcium Carbonate

K. J. D. Mackenzie and N. Hadipour *Thermochimica Acta* **1980,** *35,* 227.

[1] Formation Kinetics of Portland Clinker Phases III B- Dicalcium Silicate and Tricalcium Silicat

N. L. Hadipour, K. J. D. Mackenzie *Trans. J. Br. Ceram. Soc.* **1978***,77(6),* 168.