



Alireza Nowroozi Associate Professor

Faculty : Science

Departments : Chemistry

Phone : +9854 - 31136331

Email : anowroozi@chem.usb.ac.ir

Address : Dept.of Chemistry, Faculty of Science, University of Sistan and Baluchestan, Daneshgah Ave., Zahedan, Iran.

Education

- ✓ B.Sc, Pure Chemistry, University of Mazandaran - 1990
- ✓ MS, Physical Chemistry, Ferdowsi University of Mashhad - 1995
- ✓ PhD, Physical Chemistry, Ferdowsi University of Mashhad - 2003

Courses

- | | |
|-----------------------------------|---|
| 1. quantum chemical | 2. thermodynamic statics 1 |
| 3. molecular spectroscopy | 4. Advanced physical chemistry |
| 5. Quantum chemistry3 | 6. attitude physical chemistry subjects |
| 7. new topis in physics chemistry | 8. physical chemistry 1 |

Journals Papers

2021

1. A detail investigation of synergistic effects between the intramolecular hydrogen bond and pi-electron delocalization in 3-hydroxy prop-2-en thial and its derivatives

Alireza Nowroozi, M. R. Housaindokht, Ebrahim Nakhahae sobhie

STRUCTURAL CHEMISTRY Volume: (32) 709 - 718

2. The cooperativity and diminutive effects between the cation- π and aerogen bond in some complexes of heterocyclic rings

Sadeghali Bavafa, Alireza Nowroozi, Ali Ebrahimi

MOLECULAR PHYSICS Volume: (119) 1 - 13

2020

3. Ab initio study of aerogen-bonds between some heterocyclic compounds of benzene with the noble gas elements (Ne, Ar, and Kr)

Sadeghali Bavafa, Alireza Nowroozi, Ali Ebrahimi

STRUCTURAL CHEMISTRY Volume: (31) 435 - 445

4. On the performance of molecular tailoring approach for estimation of the intramolecular hydrogen bond energies of RAHB systems: a comparative study

ABBASALI KEYKHAEI, Alireza Nowroozi

STRUCTURAL CHEMISTRY Volume: (31) 423 - 433

2019

5. Comparative study of resonance-inhibited hydrogen bonded (RIHB) systems with different atoms involved: the leading role of π -planarity

, Alireza Nowroozi

MOLECULAR PHYSICS Volume: (117) 1 - 11

6. The influence of 5-fluorouracil anticancer drug on the DNA base pairs; a quantum chemical study

Ebrahim Nakhahae, Alireza Nowroozi, Fateme Ravari

JOURNAL OF BIOMOLECULAR STRUCTURE and DYNAMICS Volume: (37) 1 - 19

7. A Comprehensive Theoretical Study of Amide Resonance, Intramolecular Hydrogen Bonding, and pi-Electron Delocalization in Diformyl and Dithioformyl Amine

Seyede Samira Hosseini, Alireza Nowroozi, Ebrahim Nakhaei, Abbas Heshmati Jannat Magham

Russian Journal of Physical Chemistry A Volume: (93) 2053 - 2060

8. Competition Between the Intramolecular Hydrogen Bond and the π -Electron Delocalization in Some RAHB Systems: A Theoretical Study

Ramin Rafat, Alireza Nowroozi

JOURNAL OF STRUCTURAL CHEMISTRY Volume: (60) 755 - 762

9. Quantum chemical study of the nature of interactions between the boraphosphinine and alumaphosphinine with some of the mono- and divalent cations: cation- π or cation-lone pair?

Sadeghali Bavafa, Alireza Nowroozi, Ali Ebrahimi

STRUCTURAL CHEMISTRY Volume: (30) 1887 - 1898

10. Complexes of damirone A/C, batzelline A/D, makaluvamine O and makaluvone with guanidinium and magnesium cations: a theoretical study

, Ali Ebrahimi, Alireza Nowroozi

STRUCTURAL CHEMISTRY Volume: (30) 1635 - 1646

11. Theoretical insight to intermolecular hydrogen bond interactions between methyl N-(2-pyridyl) carbamate and acetic acid: substituent effects, cooperativity and energy decomposition analysis

, Ali Ebrahimi, Alireza Nowroozi

Bulgarian Chemical Communications Volume: (51) 224 - 233

2018

12. Mutual effects of the cation- π , anion- π and intramolecular hydrogen bond in the various complexes of 1,3,5-triamino-2,4,6-trinitrobenzene with some cations (Li^+ , Na^+ , K^+ , Mg^{2+} , Ca^{2+}) and anions (F^- , Cl^- , Br^-)

Alireza Nowroozi, Ali Ebrahimi, Omid Rezvani rad

STRUCTURAL CHEMISTRY Volume: (29) 129 - 137

13. A comprehensive theoretical study of conformational analysis, intramolecular hydrogen bond, π -electron delocalization, and tautomeric preferences in 2-selenoformyl-3-thioxo-propionaldehyde

Ramin Rafat, Alireza Nowroozi

STRUCTURAL CHEMISTRY Volume: (29) 1057 - 1065

14. Solvent effects on the molecular stability, intramolecular hydrogen bond, and π -electron delocalization in the simple RAHB systems with different donors and acceptors: a quantum chemical study

Ramin Rafat, Alireza Nowroozi

STRUCTURAL CHEMISTRY Volume: () 1 - 9

15. Boron nitride nanotubes for delivery of 5-fluorouracil as anticancer drug: a theoretical study

, Alireza Nowroozi

APPLIED SURFACE SCIENCE Volume: (428) 500 - 513

16. The hydrogen-bonded complexes of the 5-fluorouracil with the DNA purine bases: a comprehensive quantum chemical study

Ebrahim Nakhaei, Alireza Nowroozi, Fateme Ravari

STRUCTURAL CHEMISTRY Volume: (29) 69 - 80

17. Kinetic study, structural analysis and computational investigation of novel xerogel based on drug-PEG/SiO₂ for controlled release of enrofloxacin

Azra Ebadi, A.A. Rafati, Sadeghali Bavafa, Alireza Nowroozi

JOURNAL OF MOLECULAR LIQUIDS Volume: (266) 733 - 742

2017

18. intermolecular hydrogen bonds between 1,4-benzoquinones and HF molecule: Synergetic effects, reduction potentials and electronaffinities

, Ali Ebrahimi, Alireza Nowroozi

JOURNAL OF MOLECULAR GRAPHICS and MODELLING Volume: (77) 86 - 93

19. The effects of structural properties on the methylglyoxal scavenging mechanism of flavonoid aglycones: A quantum mechanical study

Shiva Rezazadeh, Ali Ebrahimi, Alireza Nowroozi

Computational and Theoretical Chemistry Volume: (1118) 26 - 38

20. DFT and TD-DFT study of the enol and thiol tautomers of 3-thioxopropanal in the ground and first singlet excited states

Kolsoom Shayan, Alireza Nowroozi

JOURNAL OF THEORETICAL and COMPUTATIONAL CHEMISTRY Volume: (16) 1750034 - 1750056

21. Evaluation the origin of conformational preferences in trifluoroacetylacetaldehyde by detail analysis of the intramolecular hydrogen bond and π -electron delocalization in the ground and first excited states

, Alireza Nowroozi

JOURNAL OF STRUCTURAL CHEMISTRY Volume: (58) 1251 - 1261

22. A comparative study of cooperative effects between the intramolecular hydrogen bond and cation- π interaction in various complexes of ortho-aminobenzaldehyde with its thio and seleno analogous

Alireza Nowroozi, Omid Rezvani rad

THEORETICAL CHEMISTRY ACCOUNTS Volume: (136) 1 - 9

23. Interplay between the intramolecular hydrogen bonds and cation- π interactions in various complexes of salicylaldehyde, thiosalicylaldehyde and selenosalicylaldehyde with Li⁺, Na⁺, K⁺, Mg

Omid Rezvani rad, Alireza Nowroozi

MOLECULAR PHYSICS Volume: (115) 784 - 794

24. A comprehensive theoretical study of mutual interactions between the intramolecular hydrogen bond and π -electron delocalization of RAHB units with the benzene rings in salicylaldehyde and ortho-aminobenzaldehyde with their thio and seleno analogues

Omid Rezvani rad, Alireza Nowroozi

STRUCTURAL CHEMISTRY Volume: (28) 1141 - 1149

2016

25. On the performance of resonance assisted hydrogen bond theory in malonaldehyde derivatives

, Alireza Nowroozi

Computational and Theoretical Chemistry Volume: (1096) 27 - 32

26. A comparative study of two-ring resonance-assisted hydrogen bond systems

Alireza Nowroozi, , ,

STRUCTURAL CHEMISTRY Volume: (27) 829 - 838

27. Study on the interaction of metallocene catalysts with the surface of carbon nanotubes and its influence on the catalytic properties. 1. Investigation of possible complex structures and the influence on structural and electronic properties

, Alireza Nowroozi

JOURNAL OF ORGANOMETALLIC CHEMISTRY Volume: (818) 154 - 162

28. The first singlet excited state (S1) intramolecular hydrogen bond of malonaldehyde derivatives: a TD-DFT and CIS study

, Alireza Nowroozi

STRUCTURAL CHEMISTRY Volume: (27) 1769 - 1780

2015

29. Computational investigation on the intramolecular resonanceinhibited hydrogen bonding: a new type of interaction versus the RAHB model

, Alireza Nowroozi

THEORETICAL CHEMISTRY ACCOUNTS Volume: (134) 1 - 11

2014

30. Conformation Analysis and Computation of Energy Barrier to Rotation about C-N Bond in Para-Methylphenyl Carbamate and its Solvent Dependence in Comparison with tertiary Carbamates and tertiary Amides

Ali Reza Modarresi Alam, Alireza Nowroozi, ,

journal of molecular structure Volume: (1076) 299 - 307

31. Hydrogen adsorption on SiC nanotube under transverse electric field

, , Alireza Nowroozi

physics letters a Volume: (378) 2549 - 2552

32. A comprehensive theoretical study of tautomeric and conformeric preferences intramolecular hydrogen bonding and π -electron delocalization in α -selenoaminoacrolein with its thio and oxo analogs

Alireza Nowroozi, , ,

structural chemistry Volume: (25) 1359 - 1368

33. Exploring the correlation between the π -electron delocalization and intramolecular hydrogen bond in malonaldehyde derivatives a quantum chemical study

Alireza Nowroozi, ,

structural chemistry Volume: (25) 1415 - 1422

34. How to estimate the intramolecular hydrogen-bond energy of complex RAHB systems A theoretical study

Alireza Nowroozi,

structural chemistry Volume: (25) 215 - 220

35. OH O and OH S intramolecular interactions in simple resonance-assisted hydrogen bond systems a comparative study of various models

Alireza Nowroozi, ,

structural chemistry Volume: (25) 251 - 258

36. A comprehensive theoretical study of tautomeric and conformeric preferences, intramolecular hydrogen bonding, and p -electron delocalization in β -selenoaminoacrolein with its thio and oxo analogs

Alireza Nowroozi, , ,

STRUCTURAL CHEMISTRY Volume: () 1359 - 1368

37. Conformation analysis and computation of energy barrier to rotation about CAN bond in para-methylphenyl carbamate and its solvent dependence in comparison with tertiary carbamates and tertiary amides

Ali Reza Modarresi Alam, Alireza Nowroozi, , ,

JOURNAL OF MOLECULAR STRUCTURE Volume: () 299 - 307

38. OHO and OHS intramolecular interactions in simple resonance-assisted hydrogen bond systems: a comparative study of various models

Alireza Nowroozi, ,

STRUCTURAL CHEMISTRY Volume: () 251 - 258

39. Exploring the correlation between the p-electron delocalization and intramolecular hydrogen bond in malonaldehyde derivatives; a quantum chemical study

Alireza Nowroozi, ,

STRUCTURAL CHEMISTRY Volume: () 1415 - 1422

2013

40. Conformational analysis tautomeric preference intramolecular hydrogen bonding and solvent effect on dinitrosamine A quantum chemical study

Alireza Nowroozi,

international journal of quantum chemistry Volume: (113) 1026 - 1033

41. Conformational Analysis, Tautomeric Preference, Intramolecular Hydrogen Bonding, and Solvent Effect on Dinitrosamine: A Quantum Chemical Study

, Alireza Nowroozi

INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY Volume: () 1026 - 1033

2012

42. A quantum chemical study of conformational and tautomeric preferences intramolecular hydrogen bonding and π -electron delocalization on dinitrosomethane in gas phase and water solution

, Alireza Nowroozi, ,

structural chemistry Volume: (23) 1941 - 1951

43. A comparative study of open-close and related rotamers methods to evaluate the intramolecular hydrogen bond energies in 3-imino-propen-1-ol and its derivatives

, Alireza Nowroozi, , ,

international journal of quantum chemistry Volume: (112) 1384 - 1391

44. A quantum chemical study of conformational and tautomeric preferences, intramolecular hydrogen bonding and p-electron delocalization on dinitrosomethane; in gas phase and water solution

, Alireza Nowroozi, ,

STRUCTURAL CHEMISTRY Volume: () 1941 - 1951

2010

45. Effect of CH₃CO functional group on the molecular and electronic properties of BN43zz nanotube A computational chemistry study

, Alireza Nowroozi, Ali Ebrahimi

journal of molecular structure-theochem Volume: () -

46. [Ab initio and DFT computational studies on molecular conformations and intramolecular hydrogen bonding in 3-mercapto-but-2-enethial](#)

Alireza Nowroozi

Journal of Sulfur Chemistry Volume: (31) -

47. [The effects of substitutions on structure electron density resonance and intramolecular hydrogen bonding strength in 3-mercapto-propenethial](#)

Alireza Nowroozi

journal of molecular structure-theochem Volume: (960) -

48. [Intramolecular Hydrogen Bonding in Structural Conformers of 2-Amino Methylene Malonaldehyde AIM and NBO Studies](#)

Alireza Nowroozi

international journal of quantum chemistry Volume: (110) -

2009

49. [Hydrogen Bonding in Acetylacetaldehyde Theoretical Insights from the Theory of Atoms in Molecules](#)

Alireza Nowroozi,

international journal of quantum chemistry Volume: () -

50. [The Gas Phase Hydrogen-Bonded Dimers of HOCL A High-Level Quantum Chemical Study](#)

, Alireza Nowroozi

international journal of quantum chemistry Volume: () -

51. [Interaction Between NH₂NO and H₂O₂ A Quantum Chemistry Study](#)

, Alireza Nowroozi

international journal of quantum chemistry Volume: () -

52. [Conformational and Tautomeric Preferences in 3-Aminoacrylaldehyde A Theoretical Study](#)

Alireza Nowroozi,

international journal of quantum chemistry Volume: () -

53. [The Competition Between the Intramolecular Hydrogen Bond and \$\pi\$ -Electron Delocalization in Trifluoroacetylacetone A Theoretical Study](#)

Alireza Nowroozi,

international journal of quantum chemistry Volume: () -

54. Cyanisde uptake from wastewater by modified natrolite zeolite-iron oxyhydroxide system
Application of isotherm and kinetic models

Meissam Noroozifar, Alireza Nowroozi

journal of hazardous materials Volume: () -

55. Hydrogen Bonding in Acetylacetaldehyde Theoretical Insight from the Theory of atoms in Molecules

Alireza Nowroozi, A.F jalbout, , , M Sadeghi, A De Leon,

international journal of quantum chemistry Volume: () -

56. Molecular Structure and Vibrational Assignment of Chloro Acetylacetone A Density Functional Theory Study

A.F Jalbout, M Ali Nasiri, , , Alireza Nowroozi, A De Leon

international journal of quantum chemistry Volume: () -

57. The Gas Phase Hydrogen-Bonded Dimers of HOGI High-Level Quantum Chemical Study

, Alireza Nowroozi,

international journal of quantum chemistry Volume: () -

2008

58. Theoretical study of solvent effects on the conformational preference in GH2FWH (W 0 S) using PCM and IPCM methods

, Alireza Nowroozi, ,

journal of molecular liquids Volume: () -

2006

59. Vibrational assignment structure and intramolecular hydrogen bond study of 3-amino-1-phenyl-2-buten-1-one

Alireza Nowroozi

spectrochimica acta part a-molecular and biomolecular spectroscopy Volume: () -

60. Intramolecular hydrogen bond molecular structure and vibrational assignment of tetra-acetyethane A density functional study (ISI)

, Alireza Nowroozi, ,

spectrochimica acta part a-molecular and biomolecular spectroscopy Volume: () -

61. Strong intramolecular hydrogen bond in triformylmethane ab-initio AIM and NBO study (ISI)

Alireza Nowroozi,

journal of molecular structure-theochem Volume: () -

62. Molecular structure and vibrational assignment of (trifluoroacetyl) acetone A density functional study

, Alireza Nowroozi, ,

journal of molecular structure Volume: () -

2005

63. The presentation of an approach for estimational the intramolecular hydrogen bond strength in conformational study of α -Aminocrolein

Alireza Nowroozi, ,

journal of molecular structure-theochem Volume: () -

64. Density functional theory study of the Fourier transform infrared and Raman spectra of Cu(II) bis-acetylacetone

, Alireza Nowroozi, ,

spectrochimica acta part a-molecular and biomolecular spectroscopy Volume: () -

65. Vibrational assignment and structure of 3-(4-methoxyphenyl) pentane-2 4-dione

, , Alireza Nowroozi

journal of molecular structure-theochem Volume: () -

Conferences Papers

2008

1. Characterization of Hydrogen Bonding by Quantum the Theory of Atoms in Molecules (QTAIM)

9th European Conference on Research in Chemical Education

, Alireza Nowroozi

2. NBO Software A Powerful Tool in Chemical Education

9th European Conference on Research in Chemical Education

Alireza Nowroozi,