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Education

- ✓ MS, Physical Chemistry, Kharazmi University - 1993
- ✓ PhD, Physical Chemistry, Shahid Beheshti University - 2002

Courses

- | | |
|-----------------------|-----------------------------|
| 1. Quantum chemistry3 | 2. Computational chemistry |
| 3. Quantum mechanics | 4. Biomolecular Recognition |

Journals Papers

2022

1. A detailed theoretical exploration on the THR-beta binding affinities and antioxidant activity of some halogenated bisphenols

Saman Zare gheslaghi, Ali Ebrahimi, Zeinab Faghih

JOURNAL OF BIOMOLECULAR STRUCTURE and DYNAMICS Volume: (40) 10835 - 10851

2. Synthesis, biological evaluation, and computational studies of some novel quinazoline derivatives as anticancer agents

Leila Emami, Soghra Khabnadideh, Zahra Faghih, Farnoosh Farahvasi, Fatemeh Zonobi, Saman Zare ghesl

BMC Chemistry Volume: (16) 1 - 14

2021

3. Identification of New Potential Cyclooxygenase-2 Inhibitors: Insight from High Throughput Virtual Screening of 18 Million Compounds Combined with Molecular Dynamic Simulation and Quantum Mechanics

Leily Heidarpour saremi, Ali Ebrahimi, Milad Lagzian

JOURNAL OF BIOMOLECULAR STRUCTURE and DYNAMICS Volume: (39) 1717 - 1734

4. Multi-stage screening to predict the specific anticancer activity of Ni(II) mixed-ligand complex on gastric cancer cells; biological activity, FTIR spectrum, DNA binding behavior and simulation studies

Leily Heidarpour saremi, Karim Dadashi Noshahr, Ali Ebrahimi, Ali Khalegian, Khatereh Abdi, Milad La

SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY Volume: (251) 119377-1 - 119377-10

5. 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

6. 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

7. Structural insights for rational design of new PIM-1 kinase inhibitors based on 3,5-disubstituted indole derivatives: An integrative computational approach

Hafez Razmazma, Ali Ebrahimi, Mohammad Hashemi

COMPUTERS IN BIOLOGY AND MEDICINE Volume: (118) 103641-1 - 103641-10

8. Pi-Stacking effects on acid capacity of p-aminobenzoic acid

Ebrahim Khalili nia, Ali Ebrahimi

STRUCTURAL CHEMISTRY Volume: (31) 1707 - 1716

9. The electrochemical properties and PIM1 kinase enzyme inhibition of some 2-(hydroxy phenyl amino) naphthalene-1,4-dione derivatives

Nahid Hesabi, Ali Ebrahimi

JOURNAL OF MOLECULAR LIQUIDS Volume: (307) 112874-1 - 112874-16

10. On Calculating the Bending Modulus of Lipid Bilayer Membranes from Buckling Simulations

Jad Eid, Hafez Razmazma, Alia Jraij, Ali Ebrahimi, Luca Monticelli

JOURNAL OF PHYSICAL CHEMISTRY B Volume: (124) 6299 - 6311

11. Insight into 6-aminopenicillanic acid structure and study of the quantum mechanical calculations of the acid-base site on gamma-Fe₂O₃@SiO₂ core-shell nanocomposites and as efficient catalysts in multicomponent reactions

, Somayeh Ostovar, Roya Behazin, Alireza Rezvani, Ali Ebrahimi, Hamid Reza Shaterian

NEW JOURNAL OF CHEMISTRY Volume: (47) 20688 - 20696

2019

12. Substituent effects on direct and indirect tautomerism of pyrimidin-2(1H)-one/pyrimidin-2-ol

Leily Heidarpour saremi, Ali Ebrahimi, Milad Lagzian

MOLECULAR SIMULATION Volume: (45) 58 - 67

13. The effects of anion approaching directions to the π - π^+ interaction

, Ali Ebrahimi

JOURNAL OF MOLECULAR LIQUIDS Volume: (276) 170 - 178

14. Ellagitannin derivatives and some conjugated metabolites: aqueous-DMSO proton affinities and acidity constants

Asiye Shahraki, Ali Ebrahimi

STRUCTURAL CHEMISTRY Volume: (30) 1343 - 1351

15. 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

16. 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

17. 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

18. Binding of ellagic acid and urolithin metabolites to the CK2 protein, based on the ONIOM method and molecular docking calculations

Asiye Shahraki, Ali Ebrahimi

NEW JOURNAL OF CHEMISTRY Volume: (43) 15983 - 15998

19. Tautomerism, Intramolecular H-bonding, Acidity and Complexation of 2,4-Dioxo-4-Phenylbutanoic Acid

Ebrahim Khalili nia, Ali Ebrahimi

Physical Chemistry Research Volume: (7) 375 - 394

2018

20. The role of chlorine substituents in lichexanthones properties the ionic and halogen bond interactions

Najmeh Mostafavi, Ali Ebrahimi

THEORETICAL CHEMISTRY ACCOUNTS Volume: (137) 117 - 128

21. The effects of cation and anion interactions on halogen bonds in the N...X...N complexes A comprehensive theoretical study

Hafez Razmazma, Ali Ebrahimi

JOURNAL OF MOLECULAR GRAPHICS and MODELLING Volume: (84) 134 - 144

22. The physicochemical properties and tyrosinase inhibitory activity of ectoine and its analogues A theoretical study

Roya Behazin, Ali Ebrahimi

Computational and Theoretical Chemistry Volume: (1130) 6 - 14

23. The estimation of H-bond and metal ion-ligand interaction energies in the G-Quadruplex M_n complexes

Najmeh Mostafavi, Ali Ebrahimi

JOURNAL OF MOLECULAR STRUCTURE Volume: (1161) 246 - 253

24. A Computational Study on the Hydride Transfer Mechanism between Nicotinamide and Menadione

Shiva Rezazadeh, Ali Ebrahimi

ChemistrySelect Volume: (3) 11977 - 11985

25. The effect of anion- interactions on the properties of pyrazinamide and some related compounds

Safie Sarhadinia, Ali Ebrahimi

Computational and Theoretical Chemistry Volume: (1124) 51 - 58

26. Mutual effects of the cation-?, anion-? and intramolecular hydrogen bond in the various complexes of 1,3,5-triamino-2,4,6-trinitrobenzene with some cations (Li⁺, Na⁺, K⁺, Mg²⁺, Ca²⁺) and anions (F⁻, Cl⁻, Br⁻)

Alireza Nowroozi, Ali Ebrahimi, Omid Rezvani rad

STRUCTURAL CHEMISTRY Volume: (29) 129 - 137

2017

27. Characterization of p-stacking interactions between aromatic amino acids and quercetagenin

Farideh Badichi akher, Ali Ebrahimi, Najmeh Mostafavi

JOURNAL OF MOLECULAR STRUCTURE Volume: (1128) 13 - 20

28. The X-...benzohydrazide complexes: the interplay between anion-p and H-bond interactions

, Ali Ebrahimi

STRUCTURAL CHEMISTRY Volume: (28) 687 - 695

29. Experimental and Theoretical Insight into the Kinetics and Mechanism of the Synthesis Reaction of 2,3-Dihydro-2-phenylquinazolin-4(1H)-one Catalyzed in Formic Acid

SayyedMostafa Habibi-Khorassani, Mehdi Shahraki, Ali Ebrahimi, Mahdieh Darijani

INTERNATIONAL JOURNAL OF CHEMICAL KINETICS Volume: (49) 157 - 172

30. The X-...benzohydrazide complexes: the interplay between anion-p and H-bond interactions

, Ali Ebrahimi

STRUCTURAL CHEMISTRY Volume: (28) -

31. Theoretical investigation of the p -p stacking interactions in substituted pyridinium ion

, Ali Ebrahimi

JOURNAL OF MOLECULAR GRAPHICS and MODELLING Volume: (77) 225 - 231

32. Tanshinone I and isotanshinone I: The effects of media, isomerization and complexation on structural and electronic parameters

, Ali Ebrahimi,

Computational and Theoretical Chemistry Volume: (1115) 276 - 283

33. 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

34. 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

35. Theoretical investigation of the π + π + stacking interactions in substituted pyridinium ion

, Ali Ebrahimi

JOURNAL OF MOLECULAR GRAPHICS and MODELLING Volume: (77) 225 - 231

36. The π - π stacking of tanshinone I and isotanshinone I with phenylalanine: The effects of isomerization, complexation and environment

, Ali Ebrahimi,

JOURNAL OF THEORETICAL and COMPUTATIONAL CHEMISTRY Volume: (16) 1750067-1 - 1750067-18

37. Experimental and Theoretical Insight into the Kinetics and Mechanism of the Synthesis Reaction of 2,3-Dihydro-2-phenylquinazolin-4(1H)-one Catalyzed in Formic Acid

SayyedMostafa Habibi Khorassani, Mehdi Shahraki, Ali Ebrahimi, Mahdieh Darijani

INTERNATIONAL JOURNAL OF CHEMICAL KINETICS Volume: (49) 157 - 172

2016

38. Kinetic Aspects of Tetrahydrobenzo[b]pyran Formation in the Presence of Fructose as a Green Catalyst: a Mechanistic Investigation

SayyedMostafa Habibi Khorassani, Mehdi Shahraki, Ali Ebrahimi, Seyedeh shadfar Pourpanah

Physical Chemistry Research Volume: (4) 379 - 390

39. A Theoretical Study of π -Stacking interactions in C-Substituted Tetrazoles

, Ali Reza Modarresi Alam, , Ali Ebrahimi

JOURNAL OF MOLECULAR GRAPHICS and MODELLING Volume: (67) 85 - 93

40. Theoretical investigation of the backbone π and π stacking interactions in substituted-benzene||3-methyl-2'-deoxyadenosine: a perspective to the DNA repair

, Ali Ebrahimi

MOLECULAR PHYSICS Volume: (114) 774 - 783

41. The influence of CH...p interaction on hydrogen bonding ability of –CONH₂ functional group of benzamide

, Ali Ebrahimi

STRUCTURAL CHEMISTRY Volume: (27) 1199 - 1209

42. H-bond and dipole–dipole interactions between water and COO functional group in methyl benzoate derivatives: Substituent and heteroatom effects

, Ali Ebrahimi

Journal of Molecular Graphics Volume: (70) 7 - 13

43. Kinetic investigation of tetrahydrobenzo[b]pyran synthesis in the presence of fructose as a catalyst via a three-component reaction: an experimental study

, SayyedMostafa Habibi Khorassani, Ali Ebrahimi

Bulgarian Chemical Communications Volume: (48) 244 - 249

44. Vibrational spectra of ?-bromo and ?-chloro derivatives of tris(acetylacetonato)chromium(III)

Fatemeh Dolati, Sayyed Faramarz Tayyari, Mohammad Vakili, Ali Ebrahimi

JOURNAL OF MOLECULAR STRUCTURE Volume: (1103) 1 - 8

45. The Nature of Halogen Bonds in [N???X???N]⁺ Complexes: A Theoretical Study

Ali Ebrahimi, Hafez Razmazma,

Physical Chemistry Research Volume: (4) 1 - 15

2015

46. The effect of intramolecular hydrogen bond on the N-glycosidic bond strength in 3-methyl-2-deoxyadenosine: A quantum chemical study

, Ali Ebrahimi, , SayyedMostafa Habibi Khorassani

STRUCTURAL CHEMISTRY Volume: () 411 - 419

47. Synthesis, characterization, X-ray crystal structure, DFT calculation and antibacterial activities of new vanadium(IV, V) complexes containing chelidamic acid and novel thiourea derivatives

, , , , Ali Ebrahimi, , , ,

JOURNAL OF INORGANIC BIOCHEMISTRY Volume: () -

48. -Stacking effects on the hydrogen bonding capacity of methyl2-naphthoate

, Ali Ebrahimi

JOURNAL OF MOLECULAR GRAPHICS and MODELLING Volume: () 115 - 122

49. Vibrational spectra of tris(acetylacetonato)chromium(III)

, , Ali Ebrahimi,

JOURNAL OF MOLECULAR STRUCTURE Volume: () 340 - 347

50. A novel high performance stopped-flow apparatus equipped with a special constructed mixing chamber containing a plunger under inert condition with a very short dead-time to investigate very rapid reactions

SayyedMostafa Habibi Khorassani, Ali Ebrahimi, Malektaher Maghsoodlou, Mehdi Shahraki, ,

Arabian Journal of Chemistry Volume: () 873 - 884

51. The influence of cations and anions on some structural and electronic properties of single-walled zigzag boron nitride and aluminum nitride nanotubes: a computational study

, Ali Ebrahimi,

STRUCTURAL CHEMISTRY Volume: () 1013 - 1024

52. Investigation of the effect of p-p stacking interaction on the properties of -CONH₂ functional group of benzamide

, Ali Ebrahimi

STRUCTURAL CHEMISTRY Volume: () -

53. Theoretical investigation of the backbone... and ... stacking interactions in substitutedbenzene||3-methyl-2-deoxyadenosine: a perspective to the DNA repair

, Ali Ebrahimi

MOLECULAR PHYSICS Volume: (10) -

54. Mechanistic and Full Kinetic Study of the Reaction between 4-cholorobenzaldehyde, malononitrile, and dimedone uisng caffeine as agreen catalyst

, SayyedMostafa Habibi Khorassani, Ali Ebrahimi

Oriental Journal of Chemistry Volume: (31) 2107 - 2113

2014

55. ¹HNMR spectroscopic investigation of the kinetics of the equilibrium betwwen Z and E isaomers

SayyedMostafa Habibi Khorassani, Malektaher Maghsoodlou, Ali Ebrahimi

RESEARCH ON CHEMICAL INTERMEDIATES Volume: () 2729 - 2736

56. Relationship between cation-pi and anion-pi interactions: individual binding energies in the pi-M-pi-X-pi system

Ali Ebrahimi, SayyedMostafa Habibi Khorassani, Roya Behazin, , ,

MOLECULAR PHYSICS Volume: (112) 41 - 48

57. Presentation of a new index for estimation of aromaticity in halo- and cyanobenzenes: The role of potential energy in aromaticity

Ali Ebrahimi, ,

INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY Volume: () 154 - 161

58. The effects of interactions of dicarboxylic acids on the stability of the caffeine molecule: A theoretical study

, Ali Ebrahimi, SayyedMostafa Habibi Khorassani, , Roya Behazin

BULLETIN OF THE CHEMICAL SOCIETY OF JAPAN Volume: () 1116 - 1123

59. Theoretical study on the detailed repair of O6-methyl guanine to guanine by cysteine

Ali Ebrahimi, SayyedMostafa Habibi Khorassani, , Roya Behazin,

JOURNAL OF CHEMICAL SCIENCES Volume: (126) 1803 - 1813

60. Full kinetics investigation of the formation reaction of phosphonate esters in the gas-phase: a theoretical study

, SayyedMostafa Habibi Khorassani, Malektaher Maghsoodlou, Ali Ebrahimi

JOURNAL OF MOLECULAR MODELING Volume: () 1 - 19

2013

61. Intramolecular hydrogen bonding in chemoselective synthesized 2-substituted pyrrole stable phosphorus ylide GIAO AIM and NBO approaches

Mehdi Shahraki, SayyedMostafa Habibi Khorassani, Ali Ebrahimi, Malektaher Maghsoodlou

STRUCTURAL CHEMISTRY Volume: (24) -

62. Mechanistic study of the formation of a phosphonate ester containing 2 fluoroaniline

SayyedMostafa Habibi Khorassani, Ali Ebrahimi

PROGRESS IN REACTION KINETICS AND MECHANISM Volume: () 221 - 239

63. ¹H NMR kinetic investigation of the equilibrium between the Z- and E-isomers in a stable phosphorus ylide involving 2-mercaptobenzimidazole

SayyedMostafa Habibi Khorassani, Malektaher Maghsoodlou, Ali Ebrahimi

PROGRESS IN REACTION KINETICS AND MECHANISM Volume: () 295 - 304

64. Kinetic and Mechanistic Insights into the pathway leading to cyclic crystalline phosphorous ylide formation in the presence of 3-chloropentane-2,4-dione theoretical and stopped-flow approaches

Ali Ebrahimi, Niloufar Akbarzadeh- Torbati, SayyedMostafa Habibi Khorassani, Malektaher Maghsoodlou,

INTERNATIONAL JOURNAL OF CHEMICAL KINETICS Volume: (45) 596 - 612

65. Investigation of the π - π stacking interactions without direct electrostatic effects of substituents: the aromaticaromatic and aromaticanti-aromatic complexes

Ali Ebrahimi, , , Roya Behazin,

MOLECULAR PHYSICS Volume: (112) 1047 - 1056

66. Caffeine as base analogue of adenine or guanine: A theoretical study

Ali Ebrahimi, SayyedMostafa Habibi Khorassani, , ,

JOURNAL OF MOLECULAR GRAPHICS and MODELLING Volume: () 81 - 91

67. Kinetic and Mechanistic Q1 Insights into the Pathway Leading to Cyclic Crystalline Phosphorus Ylide Formation in the Presence of 3-Chloropentane-2,4-dione: Theoretical and Stopped-Flow Approaches

SayyedMostafa Habibi Khorassani, Ali Ebrahimi, Malektaher Maghsoodlou, Niloufar Akbarzadeh- Torbati

Kinetic and Related Models Volume: () -

68. Intramolecular hydrogen bonding in chemoselective synthesized 2-substituted pyrrole stable phosphorus ylide: GIAO, AIM, and NBO approaches

Mehdi Shahraki, SayyedMostafa Habibi Khorassani, Ali Ebrahimi, Malektaher Maghsoodlou, Younes Ghalan

STRUCTURAL CHEMISTRY Volume: (24) 623 - 635

69. Mechanistic study of the formation of a phosphonate ester containing 2fluoroaniline: theoretical assignment of the resulting isomer

SayyedMostafa Habibi Khorassani, Malektaher Maghsoodlou, Ali Ebrahimi, , ,

PROGRESS IN REACTION KINETICS AND MECHANISM Volume: () -

70. The Radical Cationic Repair Pathway of Cyclobutane Pyrimidine Dimer: The Effect of Sugar-Phosphate Backbone

Ali Ebrahimi, SayyedMostafa Habibi Khorassani,

PHOTOCHEMISTRY AND PHOTOBIOLOGY Volume: () 74 - 82

71. Mechanistic study of the formation of a phosphonate ester containing 2 fluoroaniline: theoretical assignment of the resulting isome

SayyedMostafa Habibi Khorassani, Malektaher Maghsoodlou, Ali Ebrahimi, Younes Ghalandarzehi, , OSMAN

PROGRESS IN REACTION KINETICS AND MECHANISM Volume: (38) 221 - 239

72. 1h NMR kinetic investigation of the equilibrium between the Z- and E-isomers in a stable phosphorus ylide involving 2 mercaptobenzimidazole

SayyedMostafa Habibi Khorassani, Malektaher Maghsoodlou, Ali Ebrahimi, , ,

PROGRESS IN REACTION KINETICS AND MECHANISM Volume: (38) 295 - 304

73. A joint experimental and theoretical investigation of kinetics and mechanistic study in a synthesis reaction between triphenylphosphine and dialkyl acetylenedicarboxylates in the presence of benzhydrazide

SayyedMostafa Habibi Khorassani, Ali Ebrahimi, Malektaher Maghsoodlou

JOURNAL OF MOLECULAR MODELING Volume: (18) -

74. NMR study and AIM analysis for assignment of the two Z- and E-isomers in phosphorane containing a 2-thiazoline-2-thiol

SayyedMostafa Habibi Khorassani, Ali Ebrahimi, Malektaher Maghsoodlou

Arabian Journal of Chemistry Volume: () -

75. Cooperativity of CH/p and hydrogen bond interactions in HF...Py\X1benX2 complexes

, Ali Ebrahimi,

Journal of the Iranian Chemical Society JICS Volume: () 991 - 998

76. The influence of cation-p and anion-p interactions on the strength and nature of N...H hydrogen bond

Ali Ebrahimi, , SayyedMostafa Habibi Khorassani,

Computational and Theoretical Chemistry Volume: () 48 - 55

2011

77. Chemoselective Synthesis of Stable Phosphorus Ylides from 6-Azauracil and Mechanistic Investigation of the Reaction by UV Spectrophotometry

SayyedMostafa Habibi Khorassani, Malektaher Maghsoodlou, Ali Ebrahimi

PHOSPHORUS SULFUR AND SILICON AND THE RELATED ELEMENTS Volume: (1384) -

78. The impact of protonation and deprotonation of 3-methyl-2 -deoxyadenosine on N-glycosidic bond cleavage

Ali Ebrahimi

PHYSICAL CHEMISTRY CHEMICAL PHYSICS Volume: () The impact -

79. Effect of protonation on individual hydrogen bonds in the 8-oxoguanine-cytosine base pair NMR NBO and AIM analyses

Ali Ebrahimi

MOLECULAR PHYSICS Volume: (109) -

80. Establishing a new conductance stopped-flow apparatus to investigate the initial fast step of reaction between 1 1 1-trichloro-3-methyl-3-phospholene and methanol under a dry inert atmosphere

Ali Ebrahimi

ANALYST Volume: () -

81. Dynamic ^1H NMR study around the carbon-carbon single bond partial carbon-carbon double bond in the two particular phosphorus ylides and in an enaminoester

Ali Ebrahimi

MAGNETIC RESONANCE IN CHEMISTRY Volume: () -

82. Efficient Synthesis of Stable Phosphonate Ylides and Phosphonate Esters Reaction Between Activated Acetylenes and Triphenylphosphite in the Presence of Sulfonamide and Heterocyclic NH-Acids

Ali Ebrahimi

COMBINATORIAL CHEMISTRY and HIGH THROUGHPUT SCREENING Volume: () -

83. Effects of Sugar Ring Puckering Anti-Syn Interconversion and Intramolecular Interactions on N-Glycosidic Bond Cleavage in 3-Methyl-2'-deoxyadenosine and 2'-Deoxyadenosine

Ali Ebrahimi

Journal of the Iranian Chemical Society JICS Volume: (8) -

84. Theoretical NMR study Kinetics and a mechanistic investigation of the reaction between triphenylphosphine dialkyl acetylenedicarboxylates and acetyl acetone

Ali Ebrahimi

Scientia Iranica Volume: (18) -

85. Theoretical NMR study kinetics and a mechanistic investigation of the reaction between triphenylphosphine dialkylacetylenedicarboxylates and acetyl acetone

Malektaher Maghsoodlou, Ali Ebrahimi, SayyedMostafa Habibi Khorassani

Scientia Iranica Volume: (18) -

86. efficient synthesis of stable phosphonate ylides and phosphonate esters

Malektaher Maghsoodlou, SayyedMostafa Habibi Khorassani, Reza Heydari, Ali Ebrahimi

COMBINATORIAL CHEMISTRY and HIGH THROUGHPUT SCREENING Volume: (14) -

2010

87. F-H...N hydrogen bonds Influence of substituent and hybridization of nitrogen on H-bond properties and two-bond ^{19}F - ^{15}N spin-spin coupling constants ($2h_{\text{JF-N}}$)

Ali Ebrahimi, SayyedMostafa Habibi Khorassani

CHEMICAL PHYSICS LETTERS Volume: () -

88. The effect of CH_3 , F and NO_2 substituents on the individual hydrogen bond energies in the adenine-thymine and guanine-cytosine base pairs

Ali Ebrahimi, SayyedMostafa Habibi Khorassani

JOURNAL OF COMPUTER-AIDED MOLECULAR DESIGN Volume: () -

89. The role of cation- interactions in ethylenic complexes A theoretical NMR study

Ali Ebrahimi, SayyedMostafa Habibi Khorassani

CHEMICAL PHYSICS LETTERS Volume: () -

90. The O...H Intramolecular Hydrogen Bond in 4-X-2-Hydroxybenzaldehydes The Relationships Between Geometrical Parameters Estimated Binding Energies and NMR Data

Ali Ebrahimi, SayyedMostafa Habibi Khorassani

INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY Volume: () -

91. A Facile Synthesis and Theoretical Study of Novel Stable Heterocyclic Phosphorus Ylides Containing A 2 4-Dimethyl-3-Acetyl Moiety

SayyedMostafa Habibi Khorassani, Ali Ebrahimi, Malektaher Maghsoodlou

PHOSPHORUS SULFUR AND SILICON AND THE RELATED ELEMENTS Volume: () -

92. NMR study and AIM analysis for the ylide rotamers from the reaction between triphenylphosphine and dialkyl acetylenedicarboxylates in the presence of 2-mercapto-1-methylimidazole

SayyedMostafa Habibi Khorassani, Ali Ebrahimi, Malektaher Maghsoodlou

Journal of Sulfur Chemistry Volume: (31) -

93. Study of Reaction between Activated Acetylenes and N N -Diethyl-2-thiobarbituric Acid in the Presence of Isocyanides or Triphenylphosphine

, Malektaher Maghsoodlou, Nourallah Hazeri, Reza Heydari, SayyedMostafa Habibi Khorassani, Ali Ebrah

HETEROATOM CHEMISTRY Volume: () -

94. Kinetics and Mechanism Investigation of the Reaction between Triphenylphosphine Di-tert-butyl Acetylenedicarboxylate and OH-Acid

SayyedMostafa Habibi Khorassani, Ali Ebrahimi, Malektaher Maghsoodlou

CHINESE JOURNAL OF CHEMISTRY Volume: () -

95. Quantum mechanical calculation for determination of more stable isomer of phosphorous ylide involving an indol

SayyedMostafa Habibi Khorassani, Ali Ebrahimi, Malektaher Maghsoodlou

Iranian Journal of Organic Chemistry Volume: (2) -

96. Effect of CH₃CO functional group on the molecular and electronic properties of BN_{43zz} nanotube A computational chemistry study

, Alireza Nowroozi, Ali Ebrahimi

JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM Volume: () -

97. NMR Study Theoretical Calculations for Assignment of the Z- and E-Isomers and Kinetics Investigation of Stable Phosphorus Ylides Involving a 2-Mercapto-4 6-dimethyl Pyrimidine

SayyedMostafa Habibi Khorassani, Ali Ebrahimi, Malektaher Maghsoodlou

HETEROATOM CHEMISTRY Volume: () -

98. Theoretical Study and Synthesis of the Reaction Between Triphenylphosphine Dialkyl Acetylenedicarboxylates and 2-Aminobenzimidazole 2-Hydroxy-3-Nitropyridine or 1 2 3 4-Tetrahydrocarbazol

SayyedMostafa Habibi Khorassani, Malektaher Maghsoodlou, Ali Ebrahimi, Reza Heydari, Nourallah Hazer

COLLECTION OF CZECHOSLOVAK CHEMICAL COMMUNICATIONS Volume: (75) -

99. The effect of CH₃ F and NO₂ substituents on the individual hydrogen

Ali Ebrahimi, SayyedMostafa Habibi Khorassani, Hadi Esmaeeli Darmian

JOURNAL OF COMPUTER-AIDED MOLECULAR DESIGN Volume: (24) 409 - 416

2009

100. Development of Eclipsed and Staggered Forms in Some Hydrogen Bonded Complexes

Ali Ebrahimi,

INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY Volume: () -

101. Relationship between calculated NMR data and intermolecular hydrogen bond properties in X-pyridine HF

Ali Ebrahimi,

CHEMICAL PHYSICS Volume: () -

102. The role of H... interaction on some calculated NMR data

Ali Ebrahimi,

CHEMICAL PHYSICS LETTERS Volume: () -

103. Interaction between uracil nucleobase and phenylalanine amino acid the role of sodium cation in stacking

Ali Ebrahimi,

THEORETICAL CHEMISTRY ACCOUNTS Volume: () -

104. Dynamic ¹H NMR study around the heteroaryl carbon and carbon carbon single bonds and also around carbon carbon double bond in a particular phosphorous ylide involving a 2-methyl indole

SayyedMostafa Habibi Khorassani, Malektaher Maghsoodlou, Ali Ebrahimi

TETRAHEDRON LETTERS Volume: () -

105. Theoretical Study An Efficient Synthesis Route to And Kinetic Investigation of Stable Phosphorus Ylides Derived from Benzamide

SayyedMostafa Habibi Khorassani, Ali Ebrahimi, Malektaher Maghsoodlou, Hamideh Saravani, , , , Zoh

PROGRESS IN REACTION KINETICS AND MECHANISM Volume: () -

106. One-pot three-component reaction of aromatic isocyanides and dialkyl acetylene dicarboxylates in the presence of aryl aldehydes A convenient synthesis of highly hindered aminofurans

Nourallah Hazeri, Malektaher Maghsoodlou, SayyedMostafa Habibi Khorassani, Ali Ebrahimi

Iranian Journal of Organic Chemistry Volume: () -

107. Theoretical kinetics and mechanism investigation of the reaction between triphenylphosphine di-tert-butyl acetylenedicarboxylate and OH-acid

SayyedMostafa Habibi Khorassani, Ali Ebrahimi, Malektaher Maghsoodlou

Iranian Journal of Organic Chemistry Volume: () -

108. A facile synthesis and theoretical study of novel stable heterocyclic phosphorus ylides containing 2 4-dimethyl-3-acetyl pyrrole

SayyedMostafa Habibi Khorassani, Malektaher Maghsoodlou, Ali Ebrahimi

Iranian Journal of Organic Chemistry Volume: () -

109. AIM analysis for the ylide rotamers from the reaction between triphenylphosphine and dialkyl acetylenedicarboxylates in the presence of 2-pyrrolecarbaldehyde

SayyedMostafa Habibi Khorassani, Ali Ebrahimi, Malektaher Maghsoodlou

Iranian Journal of Organic Chemistry Volume: () -

110. Antiaromaticity affects on the response of single walled armchair carbon nanotube to tension

, Ali Ebrahimi, SayyedMostafa Habibi Khorassani,

JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM Volume: () -

111. Substituent Effect On Intramolecular Hydrogen Bonding in 2-Hydroxybenzaldehyde

Ali Ebrahimi, SayyedMostafa Habibi Khorassani,

INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY Volume: () -

112. SYNTHESIS OF STABLE PHOSPHORUS YLIDES FROM 6-CHLORO-2-BENZOXAZOLINONE AND KINETIC INVESTIGATION OF THE REACTIONS BY UV SPECTROPHOTOMETRY

, , SayyedMostafa Habibi Khorassani, Ali Ebrahimi, Malektaher Maghsoodlou,

PROGRESS IN REACTION KINETICS AND MECHANISM Volume: (34) -

113. The effect of carbon hybridization and halogen-acceptor type on some calculated NMR data in C-X H-F hydrogen bonds

Ali Ebrahimi, SayyedMostafa Habibi Khorassani

CHEMICAL PHYSICS LETTERS Volume: (483) -

114. Estimation of individual binding energies in some dimers involving multiple hydrogen bonds using topological properties of electron charge density

Ali Ebrahimi, SayyedMostafa Habibi Khorassani

CHEMICAL PHYSICS Volume: (365) -

115. Cooperativity of π -stacking and hydrogen bonding interactions and substituent effects on X-ben pyr H-F complexes

Ali Ebrahimi, SayyedMostafa Habibi Khorassani

PHYSICAL CHEMISTRY CHEMICAL PHYSICS Volume: (11) -

2008

116. Density functional calculations of response of single-walled armchair carbon nanotubes to axial tension

Ali Ebrahimi, ,

COMPUTATIONAL MATERIALS SCIENCE Volume: () -

117. Anion- interactions CP-corrected vs. standard optimization AIM and NBO analyses

Ali Ebrahimi, SayyedMostafa Habibi Khorassani,

MOLECULAR SIMULATION Volume: (34) -

118. Kinetic study and mechanism. investigation of the reactions between triphenylphosphine dialkyl acetylenedicarboxilates and NH-acid such as 2-aminobenzimidazole by UV

SayyedMostafa Habibi Khorassani, Malektaher Maghsoodlou, Ali Ebrahimi, , , Mehdi Shahraki

International Journal of Chemical Sciences Volume: (6) -

119. A comparison of C-C rotational barrier in 2 staffane 2 tetrahedrane and ethane

Ali Ebrahimi, SayyedMostafa Habibi Khorassani, ,

CHEMICAL PHYSICS LETTERS Volume: () -

120. Biologically Active Benzoxazolinone in Reaction with Triphenylphosphine Dialkyl Acetylenedicarboxilates and Theoretical Study on the Kinetic and Mechanism Investigation of the Reactions

SayyedMostafa Habibi Khorassani, Ali Ebrahimi, Malektaher Maghsoodlou,

Biomedical pharmacology Journal Volume: (1) -

121. Synthesis Dynamic ^1H NMR and Theoretical Study of Aryl-Nitrogen Single Bond Rotational Energy Barriers in Highly Functionalized 4H-Chromenes

, Nourallah Hazeri, SayyedMostafa Habibi Khorassani, Malektaher Maghsoodlou, Ali Ebrahimi, , ,

ARKIVOC Volume: (xvii) -

122. A facile synthesis dynamic ^1H NMR and theoretical study of novel stable heterocyclic phosphorus ylides containing a tetrazole ring

, , Ali Ebrahimi, Malektaher Maghsoodlou, SayyedMostafa Habibi Khorassani,

ARKIVOC Volume: (xvii) -

123. Interaction between some anions and deficient olefinic and aromatic centers

Ali Ebrahimi, SayyedMostafa Habibi Khorassani,

JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM Volume: () -

124. Kinetic study and mechanism investigation of the reactions between triphenylphosphine dialkyl acetylene dicarboxylates and NH-acid such as Harman

SayyedMostafa Habibi Khorassani, Malektaher Maghsoodlou, Ali Ebrahimi, , ,

Oriental Journal of Chemistry Volume: (1) -

2007

125. The study of counterion effect on the reactivity of nucleophiles in some SN2 reactions in gas phase and solvent media (ISI)

Ali Ebrahimi, SayyedMostafa Habibi Khorassani,

JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM Volume: () -

126. Theoretical study of the influence of para- and meta-substituents on X-pyridine HF hydrogen bonding (ISI)

Ali Ebrahimi, SayyedMostafa Habibi Khorassani,

CHEMICAL PHYSICS Volume: () -

127. Comparison between standard and counterpoise-corrected optimization using some hydrogen and halogen bonded systems (ISI)

Ali Ebrahimi, SayyedMostafa Habibi Khorassani,

MOLECULAR PHYSICS Volume: () -

128. Spectrophotometric Kinetic Studies of the Reaction between Triphenylphosphine Dialkyl Acetylenedicarboxylates and NH-Acids (ISI)

SayyedMostafa Habibi Khorassani, Malektaher Maghsoodlou, Ali Ebrahimi, , ,

asian journal of chemistry (MSRT BLACKLIST) Volume: () -

129. Kinetic Investigation of the Reactions Between Triphenylphosphine Dialkyl Acetylenedicarboxylates and NH-Acid such as 5 6-Dimethyl Benzimidazole by the UV Spectrophotometry Technique (ISI)

SayyedMostafa Habibi Khorassani, Malektaher Maghsoodlou, Ali Ebrahimi, , ,

Scientia Iranica Volume: () -

130. Kinetic investigation of the reactions between triphenylphosphine dialkyl acetylenedicarboxylates and NH-acid such as 7-azaindole by the UV spectrophotometry (ISI)

SayyedMostafa Habibi Khorassani, Malektaher Maghsoodlou, Ali Ebrahimi, , ,

INDIAN JOURNAL OF CHEMISTRY SECTION A-INORGANIC BIO-INORGANIC PHYSICAL THEORETICAL and ANALYTICAL CHEMISTRY Volume: () -

131. Kinetics and Mechanism of the Reactions Between Triphenylphosphine Dialkyl Acetylenedicarboxylates and a NH-Acid Pyrazole by UV Spectrophotometry (ISI)

SayyedMostafa Habibi Khorassani, Malektaher Maghsoodlou, Ali Ebrahimi, ,

JOURNAL OF SOLUTION CHEMISTRY Volume: () -

132. Kinetic investigation of the reactions between triphenylphosphine dialkyl acetylenedicarboxylates and SH-acid such as 2-Thiazoline-2Thiol Or 2-Mercaptobenzoxazole by the UV spectrophotometry

SayyedMostafa Habibi Khorassani, Malektaher Maghsoodlou, Ali Ebrahimi

Scientia Iranica Volume: () -

2006

133. UV Spectrophotometric Study of the Kenetics and Mechanism of the Reactions between Triphenylphosphine Dialkl Acetylenedicarboxylates and NH-Acid (ISI)

SayyedMostafa Habibi Khorassani, Malektaher Maghsoodlou, Ali Ebrahimi, ,

Journal of the Iranian Chemical Society JICS Volume: () -

134. Kinetic Investigation of the Reaction between Triphenylphosphine Dialkyl Acetylenedicarboxylate and Carbazole by the UV Spectrophotometry Technique (ISI)

SayyedMostafa Habibi Khorassani, Malektaher Maghsoodlou, Ali Ebrahimi, , , ,

PHOSPHORUS SULFUR AND SILICON AND THE RELATED ELEMENTS Volume: () -

135. Kinetic Investigation of the Reactions between Triphenylphosphine Dialkyl Acetylenedicarboxylates and NH-acids such as Indol Derivatives by UV spectrophotometry (ISI)

SayyedMostafa Habibi Khorassani, Malektaher Maghsoodlou, , Ali Ebrahimi,

asian journal of chemistry (MSRT BLACKLIST) Volume: () -

136. Evaluation of the origin of rotational barrier in NH₂-X (X NO NS) (ISI)

, Ali Ebrahimi, ,

JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM Volume: () -

137. Topological and natural population analyses of gas-phase identity SN₂ reactions of some methyl halides Backside attack (ISI)

Ali Ebrahimi, , SayyedMostafa Habibi Khorassani, ,

CHEMICAL PHYSICS LETTERS Volume: () -

138. Characterization of conformers of non-ionized proline on the basis of topological and NBO analyses Can nitrogen be a donor of hydrogen bond (ISI)

Ali Ebrahimi, , SayyedMostafa Habibi Khorassani, ,

CHEMICAL PHYSICS Volume: () -

139. Determination of gas-phase nucleophilicities and electrophilicities using B HX bond critical point properties of AIM analysis (ISI)

Ali Ebrahimi, , SayyedMostafa Habibi Khorassani,

CHEMICAL REVIEWS Volume: () -

140. Kinetic Investigation of the Reactions Between Triphenylphosphine Dialkyl Acetylenedicarboxylates and NH-Acid such as Benzimidazole

SayyedMostafa Habibi Khorassani, Malektaher Maghsoodlou, Ali Ebrahimi

Chemistry Volume: (181) -

141. NBO and AIM Analysis of the Anomeric Effect in Fluoromethanthiol

, Ali Ebrahimi, SayyedMostafa Habibi Khorassani

JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM Volume: () -

2005

142. Anomeric effect and rotational barrier in fluoromethanol A theoretical study

, Ali Ebrahimi

JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM Volume: () -

143. AIM and NBO analyses of N-N rotational barrier in monocyclic nitrosamine compounds

, Ali Ebrahimi, ,

CHEMICAL PHYSICS LETTERS Volume: () -

144. Restricted rotation in Six-membered cyclic nitrosamine compounds an ab initio and DFT study and NBO analysis

, , Ali Ebrahimi,

JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM Volume: () -

145. Kinetic Investigation of the Reaction between Triphenylphosphine Dialkyl Acetylenedicarboxylates and sh-acid such as 2-thiazoline -2-thiol or 2-mercaptobenzoxazole by uv spectrophotometry

SayyedMostafa Habibi Khorassani, Malektaher Maghsoodlou, Ali Ebrahimi, , ,

PROGRESS IN REACTION KINETICS AND MECHANISM Volume: () -

2004

146. Determination of Activity Coefficients Osmotic Coefficients and Excess Gibbs Free Energies of HC1 in N N-Dimethylformamide-Water Mixed Solvent Systems by Potentiometric Measurements

Ali Ebrahimi,

JOURNAL OF CHEMICAL AND ENGINEERING DATA Volume: () -

147. The characterization of stationary points in the potential energy surface of difluoromethane dimmer

Ali Ebrahimi, SayyedMostafa Habibi Khorassani,

JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM Volume: () -

148. Quantum Mechanical Study of Tautomerism of Methimazole Methimazole-I2 Complexes

, Ali Ebrahimi, SayyedMostafa Habibi Khorassani

JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM Volume: () -

149. the dimer of trimethylene sulfide with some hydrogen and halogen bond donors a theoretical study

Ali Ebrahimi, , SayyedMostafa Habibi Khorassani

JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM Volume: () -

150. The Dimmers of Trimethylene Sulfide With Some Hydrogen and Halogen Bond Donors a theoretical Study

Ali Ebrahimi, , SayyedMostafa Habibi Khorassani

JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM Volume: () -

2003

151. Natural bond orbital (NBO) population analysis of the highly strained .

Ali Ebrahimi

JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM Volume: () -

152. Natural bond orbital (NBO) population analysis of the highly strained central bond in 1.1.1 propellane and some 1.1.1 heteropropellane compounds

Ali Ebrahimi, ,

JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM Volume: () -

2001

153. Alkyl migration in vinylidene acetylene rearrangement reactions investigation of structural activation thermodynamic energies and kinetics properties by density functional theory based method

Ali Ebrahimi, ,

JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM Volume: () -

154. Nitrogen-inversion in some aziridine type compounds structural and kinetic investigations by ab initio methods

Ali Ebrahimi, ,

JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM Volume: () -

155. Ab initio calculations of energetic and structural properties of the single-atom peri-bridged naphthalene compounds

, Ali Ebrahimi,

JOURNAL OF MOLECULAR STRUCTURE Volume: () -

156. Restricted rotation in five-membered cyclic nitrosamine compounds DFT investigation of structural energetic and kinetics properties

, Ali Ebrahimi,

JOURNAL OF MOLECULAR STRUCTURE Volume: () -

2000

157. FInvestigation of structural properties of heteropropellane compounds by ab initio methods

Ali Ebrahimi, ,

JOURNAL OF CHEMICAL RESEARCH-S Volume: () -

Conferences Papers

2017

1. Identification of new potential human aldose reductase inhibitors by high throughput virtual screening technique in databases of natural compounds

1st International Joint Conference on New Trends In Biotechnology

Leily Heidarpour saremi, Ali Ebrahimi, Milad Lagzian

2. Identification of new potential leads for cyclooxygenase 2 inhibition by high throughput virtual screening technique on UNPD database

1st International Joint Conference on New Trends In Biotechnology

Leily Heidarpour saremi, Ali Ebrahimi, Milad Lagzian

2010

3. NMR study on protonated 8OG C base paris DFT calculation

9th Iran Biophysical Chemistry Conference

Ali Ebrahimi,

2008

4. Effect of Time on selective elimination of antimony from electrolyte of Sarcheshmeh copper refinery by Duolite C467 ion exchange resins

IICC

Abdolreza Samimi, Ali Ebrahimi, , ,

5. Effect of temperature on elimination of floating slime from Sarcheshmeh copper refinery using MX2 ion exchange resins

IICC

Abdolreza Samimi, Ali Ebrahimi, , ,

6. Theoretical Study of the Kinetics and Mechanism of the Reactions Between Triphenylphosphine Dialkylacetylenedicarboxylates and N-H Asid

14th Iranian Seminar of Organic Chemistery

SayyedMostafa Habibi Khorassani, Ali Ebrahimi

7. Kinetics study and mechanism investigation of the reactions between triphenylphosphine dialkyl acetylenedicarboxilates and NH-acids such as Harman

14th Iranian Seminar of Organic Chemistery

SayyedMostafa Habibi Khorassani, Ali Ebrahimi

8. Reactivity of Ions and ion Pairs in uncleophilic Subsitution Reaction

14th Iranian Seminar of Organic Chemistery

Ali Ebrahimi

2005

9. The study of counterion effects on the reactivity of nucleophiles in some gas-phase SN2 reactions

14th European Symposium on Organic Chemistry

Ali Ebrahimi, , SayyedMostafa Habibi Khorassani, Malektaher Maghsoodlou

10. Kinetic investigation of the reaction between triphenylphosphine dialkyl acetylenedicarboxylate and carbazole by the UV spectrophotometry technique

14th European Symposium on Organic Chemistry

SayyedMostafa Habibi Khorassani, Ali Ebrahimi, , Malektaher Maghsoodlou

11. NBO and AIM analyses of N-N Rotational Barrier in Cyclic Thionitrosamine

14th European Symposium on Organic Chemistry

, Ali Ebrahimi, SayyedMostafa Habibi Khorassani, Malektaher Maghsoodlou

12. New T-spiroiminolactone Synth-esis by Reaction Between alkyl or arylisocyanides and 10 phenan throline-5 6-dione in the presence of acetylenic esters

14th European Symposium on Organic Chemistry

Malektaher Maghsoodlou, SayyedMostafa Habibi Khorassani, Ali Ebrahimi,

13. The study of Electronic Effects on The Reactivity of ion and ion Pairs

8th Physical Chemistry Seminar

Ali Ebrahimi, , SayyedMostafa Habibi Khorassani

14. Theoretical Study of Gas Phase Indentity SN2 Reaction of some ion Pairs Eith Methyl Chloride

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15. Characterization of nonionized proline conformers on the basis of topological and NBO analysis...

8th Physical Chemistry Seminar

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16. Nitration Mechanism of 1 8 methanonaphthalene a theorical study

8th Physical Chemistry Seminar

, Ali Ebrahimi

17. analysis of N-N Rotational Barrier in Cyclic Nitrosamine Compounds A theoretical Study

8th Physical Chemistry Seminar

, Ali Ebrahimi

18. Restricted Rotation in Cyclic Thionitrosamine Compounds A theoretical Study

8th Physical Chemistry Seminar

, Ali Ebrahimi

19. Hydrogen Bonded Dimmer of 1H-Imidazole-2-Carbaldehyde

11th Iranian Seminar Organic Chemistry

Ali Ebrahimi, , SayyedMostafa Habibi Khorassani, Malektaher Maghsoodlou

20. The Effect of Hydrogen Bonding on the Stability of 1,1,4,4-Tetrafluoro-Butane

11th Iranian Seminar Organic Chemistry

Ali Ebrahimi, , SayyedMostafa Habibi Khorassani

21. Reactivity of Ions and ion Pairs in The nucleophilic Substitution of Unactivated Vinylic Carbon Along The Plane and Out of Plane S_N2 Pathways

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Ali Ebrahimi, , SayyedMostafa Habibi Khorassani

22. Potential Energy Surfaces of The Gas Phase S_N2 Reaction Nuc CH₃Br--- Reactivity of Ions And Ion Pairs

11th Iranian Seminar Organic Chemistry

Ali Ebrahimi, , SayyedMostafa Habibi Khorassani

23. Kinetic investigation of the reaction between triphenylphosphine dialkyl acetylenedicarboxylate and indazole by the UV spectrophotometry technique

8th Physical Chemistry Seminar

SayyedMostafa Habibi Khorassani, Ali Ebrahimi

24. Kinetic investigation of the reaction between triphenylphosphine dialkyl acetylenedicarboxylate and 3-methylindole by the UV spectrophotometry technique

8th Physical Chemistry Seminar

SayyedMostafa Habibi Khorassani, Ali Ebrahimi

25. A steric effect and rotational barrier in fluoromethanethiol a theoretical study

11th Iranian Seminar Organic Chemistry

, Ali Ebrahimi, Malektaher Maghsoodlou

26. Kinetic investigation of the reaction between triphenylphosphin dialkyletyendicarboxylate and 4-methylimidazole by UV Spectrophotometry technique

11th Iranian Seminar Organic Chemistry

SayyedMostafa Habibi Khorassani, Ali Ebrahimi

27. Anomeric Effect and Rotational Barrier Fluoro-Methanthiol A Theoretical Study

11th Iranian Seminar Organic Chemistry

, Ali Ebrahimi, Malektaher Maghsoodlou

2004

28. Kinetic investigation of the reaction between triphenyl phosphin dialkyle acetylendicarboxylat and 2-Acetylpyrrol by the UV Spectrophotometry

14th Iranian chemistry chemical Engineeing congress

SayyedMostafa Habibi Khorassani, Ali Ebrahimi

2003

29. The C _ F . H_C anti Hydrogen bond in the gas phase a theoritical study

Ali Ebrahimi

30. N5 -donor interactions a NBO and AIM study

The Third Physical Chemistry Seminar

Ali Ebrahimi, , SayyedMostafa Habibi Khorassani

31. Kinetic investigation of the reaction between triphenylphosphin dialkyletyendicarboxylate and payroll from study of the effects of acid-base catalysis micellisation and solvent on the rate of the reaction by UV Spectrophotometry technique

The third physical chemistry seminar held by iranian universities faculty

SayyedMostafa Habibi Khorassani, , Ali Ebrahimi,

32. Theoretical study of restricted Rotation in six membered Cyclic Nitrosamine compounds

The third physical chemistry seminar held by iranianuniversitiesfaculty

, Ali Ebrahimi

2002

33. Theoretical study of dimmers of trimethylene sulfide with ClF and F2

10th Iranian Seminar of Organic Chemistry

Ali Ebrahimi, , SayyedMostafa Habibi Khorassani

34. The dimmers of trimethylene sulfide with HF and HCl a thtoretical study

Ali Ebrahimi, , SayyedMostafa Habibi Khorassani

35. DFT Ab initio study in the interconversion and decomposition of furanones

SayyedMostafa Habibi Khorassani, Ali Ebrahimi

36. Theoretical study of interconversion and decomposition of furanones

Ali Ebrahimi, SayyedMostafa Habibi Khorassani,

37. Theoretical study of the heteropropellanel

The First Physical-Chemistry Conference Held By the I Iranian Universities Faculty

Ali Ebrahimi, , Malektaher Maghsoodlou,

38. Kinetic investigation of the reaction between triphenylphosphine Dialkyl ethylenedicarboxylate and pyrrol from study of the effects of acid-base catalysis micellisation and solvent on the rate of the reaction by UV Spectrophotometry technique.

SayyedMostafa Habibi Khorassani, Ali Ebrahimi,

39. Further kinetic investigation and solvent effects on the rate of the reaction between sodium hydroxide and carbon acids such as nitroalkanes by UV spectrophotometry technique

40. Ab initio study of the single-atom peri-bridged naphthalenes

The First Physical-Chemistry Conference Held By the Iranian Universities Faculty

, Ali Ebrahimi, Malektaher Maghsoodlou,

41. The stability of some bridgehead carbocations And DFT Study

The 10th Iranians seminar of organic chemistry

, Ali Ebrahimi

42. AIM(Atom In Molecules) study of restricted rotation in some of five-membered cyclic nitrosamine compounds

, Ali Ebrahimi

43. Semi-Empirical Study of Tautomerism in Some Substituted Anthraquinolines

, , Ali Ebrahimi

44. Stability of carbodiimides type compounds A density functional theory investigation

4th physical chemistry seminar-kish

, Ali Ebrahimi

45. THEORETICAL STUDY OF TAUTOMERISM OF METHIMAZOLE

2nd Int . conf . on chemistry its application

, Ali Ebrahimi

46. THE C-F...H-C ANTI-HYDROGEN BOND IN THE GAS PHASE A THEORETICAL STUDY

2nd Int . conf . on chemistry its application

, Ali Ebrahimi, SayyedMostafa Habibi Khorassani

Research Project

2003

1. The Study of tautomerism of methimazol vapour phase by using abinitic computational methods

, Ali Ebrahimi - 2003

2000

2. Detemination of activity and osmotic coefficient & Piterz parameters in the mixture of solvent with

, Ali Ebrahimi - 2000