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* **Education**

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Chemistry

 Isfahan University of Technology, Isfahan Iran

**MSc**

 1999

Organic Chemistry

 Isfahan University of Technology, Isfahan Iran

 **Title of thesis:**

 Preparation of sulfonamides in solid state and reduction of Organic compounds with a new reducing agents(BTPPTB)

Supervisor : Prof A.R.Hajipour (Email: haji@cc.iut.ac.ir)

**Ph.D**

2005

Organic Chemistry

Isfahan University of Technology, Isfahan Iran

 **Title of thesis:**

**Application of Tetrazoles in Asymmetric Synthesis, Dynamic NMR and Quantum Mechanical Study of their Derivatives**

Supervisor: Prof. H. A. Dabbagh (Email: dabbagh@cc.iut.ac.ir)

2005-2011

Assistant Professor of Organic chemistry

 Yasouj University Yasouj, Iran

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 Assistant Professor of Organic chemistry

 Isfahan University of Technology, Isfahan, Iran

* **Research Area**
	+ Sustainable Chemistry
	+ Computational Chemistry
	+ Application of Heterogeneous Catalysts in Organic Synthesis
* **Teaching Experience**

Undergraduate courses and lab demonstration for following courses in Ilam University (2005-2006)

* + Physical Organic Chemistry
	+ Organic Chemistry
	+ Organic Chemistry Laboratory
	+ Separation and identification of organic compounds
	+ Spectrometric Identification of Organic Compound
* Teaching assistant for the course Organic chemistry in IUT., (1996-2005)
* Teaching lecturer in Yasouj University (2005-2011)
* Teaching lecturer in IUT 2012-
* **Publications**
1. Benzyltriphenylphosphonumtetrahydroborate (BTPPTB) as a selective reducing agent for reduction of aldehydes and ketones to the corresponding alcohols, A.R.Hajipour, S.E.Mallakpour and A.R.Najafi, ***phosphorus, sulfur and silicon*** ,2000, 165, 165-170.
2. An efficient and novel method for the synthesis of arylsulfonamides and sulfonic acid esters under solvent-free conditions A.R.Hajipour, S.E.Mallakpour and A.R.Najafi, Gh. Mazloumi ***Sulfur* *Letter***, 2000, 24, 137-145.
3. Benzyltriphenylphosphonumborohydride (BTPPB) as a selective reducing agent for reduction for imines, enamines , and reductive amination of aldehydes with primary and secondry amines in methanol” A.R.Hajipour, S.E.Mallakpour and A.R.Najafi, ***phosphorus, sulfur and silicon*** , 2001, 170, 197-203
4. Density Functional Theory Demonstration of Anomeric Effect and Structure: Conformational and Configurational Analysis of *N*-2-(1,4-dioxane)-*N`*-(4-methylbenzenesulfonyl)-*O*-(4-methylphenoxy) Isourea, Dabbagh H. A., Najafi Chermahini A., Modaresi-Alam A. ***Bull. Korean, Chem. Soc***. 2005, 26, 1229.
5. Ab initioand Semiempirical (AM1, PM3) Conformational and Configurational Analysis of *N*-2-(1,4-dioxane)-*N`*-(4-methylbenzenesulfonyl) -*O*-(4-methylphenoxy) Isourea , Dabbagh H. A., Najafi Chermahini A., Modaresi-Alam A. Teimouri ***Journal of Iranian Chemical Sociatey (JIC*S)**, A. 2006, 51-58.
6. Aryloxy Tetrazoles with Axial Chirality: Synthesis and Partial Resolution of 5-(1-(2-Methoxynaphthalen-1-yl)naphthalene-2-yloxy)-1H-tetrazole, Dabbagh H. A., Najafi Chermahini A., Teimouri A. ***Heteroatom Chemistry***, 2006, 17, 416-419*.*
7. A new family of bis-tetrazole (BIZOL) BINOL-type ligands, Dabbagh H. A., Najafi Chermahini A., Banibairami, S. , ***Tetrahedron Letters***, 2006, 47, 3929-3932
8. Dynamic NMR Investigation of Methyl-2,4-dimethoxysalicylate: Effect of Solvent and Temperature on Conformation, Hydrogen bonding, Chemical shift and W Coupling Dabbagh H. A., Najafi Chermahini A., Noroozi Pesyan N. *Spectrochemica Acta*, 2006, 64, 1077-1082
9. DFT and ab initio calculations of the vibrational frequencies and visible spectra of triazenes derived from cyclic amines,Hossein A. Dabbagh, Abbas Teimouri, Alireza Najafi Chermahini and Rezvan Shiasi ***Spectrochemica Acta*,** 2007**,** *67,* 437-443
10. Green and efficient diazotizationand diazocoupling reactions on Clays, Dabbagh H. A., Teimouri A. Najafi Chermahini A., ***Dyes and Pigments****,* 2007, *73, 239*-244*.*
11. Environmentally friendly efficient synthesis and mechanism of triazenes derived from cyclic amines on clays, HZSM-5 and sulfated zirconia H.A. Dabbagh, A. Teimouri, A. Najafi Chermahinic, ***Applied* Catalysis B: Environmental** 2007**,**76, 24–33.
12. Theoretical studies on tautomerism in tetrazole derivatives by polarisable continuum method (PCM). Alireza Najafi Chermahini, Masoud Nasr-Esfahani, Zeinab Dalirnasab, Hossein Abdol Dabbagh, Abbas Teimouri ***Journal of Molecular Structure: THEOCHEM*** 2007, 820, 7–11
13. Diastreoselective formation of 18-membered ring BINOL-hydrogen phosphonate dimmers - Quasi covalent hydrogen bonds? Hossein A. Dabbagh, Nader Noroozi-Pesyan,Alireza Najafi Chermahini, Brian O. Patrick, Brian R. James, ***Can. J. Chem.*** 2007**,** 85, 466-477.
14. Relation between the substituent effect and aromaticity in tetrazoles, protonated tetrazoles and tetrazolate derivatives. Alireza Najafi Chermahini, Hossein Abdol Dabbagh, Abbas Teimouri. ***Journal of Molecular Structure: THEOCHEM*** 2007, 822, 33-37.
15. DFT, *Ab initio* and FT-IR Studies of the Structure of Sulfonamide Triazenes H. A. Dabbagh, A. Teimouri R. Shiasi and A. Najafi Chermahini ***Journal of Iranian Chemical Sociatey (JIC*S)**, 2008, 5, 74-82.
16. Asymmetric synthesis with BINOL-Imidoyl Azides, Dabbagh H. A., Najafi Chermahini A., Teimouri A. ***Russian j. Org Chemistry****.2008, 44,1495.*
17. Theoretical studies on tautomerism of dihydropyrimidine tautomers Alireza Najafi Chermahini, Hossein Abdol Dabbagh, Abbas Teimouri. ***Journal of Molecular Structure: THEOCHEM,*** 2008,*857,* 105-110.
18. DFT and Ab initio Study of Structure of Dyes Derived from 2-Hydroxy and 2,4-Dihydroxy benzoic acids Hossein A. Dabbagh, Abbas Teimouri, Alireza Najafi Chermahini, Maryam Shahraki, ***Spectrochemica Acta*, A** 2008, 69, 449.
19. Synthesis, spectroscopic characterization and DFT calculations on [4-(Sulfonylazide)phenyl]-1-azide Abbas Teimouri, Alireza Najafi Chermahini and Mohammad Emami, ***ARKIVOC*** 2008, 172-178.
20. Density functional theory study of intermolecular interactions of cyclic tetrazole dimers Alireza Najafi Chermahini, Aseyeh Ghaedi, Abbas Teimouri, Fariborz Momenbeik Hossein A. Dabbagh ***Journal of Molecular Structure: THEOCHEM,*** 2008,*867,* 78-84.
21. Vibrational spectra and assignments using ab initio and density functional theory analysis on the structure of Biotin Mohammad Emami, Abbas Teimouri and Alireza Najafi Chermahini, ***Spectrochemica Acta*, A** 2008, 71, 1516-1524
22. Synthesis, characterization and DFT studies of a novel azo dye derived from racemic or optically active binaphthol Abbas Teimouri, Alireza Najafi Chermahini, and Mohammad Emami ***Tetrahedron***, 2008, 64, 11776
23. Spectroscopic, quantum chemical DFT/HF study and synthesis of [2.2.1] hept-2'-en-2'-amino-N-azatricyclo [3.2.1.02,4] octane, Abbas Teimouri, Mohammad Emami, Alireza Najafi Chermahini and Hossein A. Dabbagh  ***Spectrochemica Acta*, A** 2009, 71, 1749.
24. [Experimental, CIS, TD-DFT, ab initio calculations of visible spectra and the vibrational frequencies of sulfonyl azide-azoic dyes](http://www.sciencedirect.com/science?_ob=ArticleURL&_udi=B6VNG-4TRCYPG-1&_user=5388531&_coverDate=10%2F21%2F2008&_alid=811320122&_rdoc=3&_fmt=high&_orig=search&_cdi=6178&_sort=d&_docanchor=&view=c&_ct=17&_acct=C000067090&_version=1&_urlVersion=0&_userid=5388531&md5=e6c0bf964400a246c2da59bc7eb1529d) Abbas Teimouri, Alireza Najafi Chermahini, Keivan Taban, Hossein A. Dabbagh ***Spectrochemica Acta*, A** 2009, 72, 369-377.
25. Rapid and efficient diazotization and diazo coupling reactions on silica sulfuric acid under solvent-free conditions Amin Zarei, Abdol R. Hajipour, Leila Khazdooz, Bibi F. Mirjalili, Alireza Najafi Chermahini ***Dyes and Pigments****,* 2009, 81, 240-244
26. Synthesis, characterization, crystal structure, and theoretical studies on Schiff-base compound 6-[(5-Bromopyridin-2-yl)iminomethyl] phenol, Aliakbar Dehno Khalaji • Alireza Najafi Chermahini •Karla Fejfarova • Michal Dusek Struct Chem (2010) 21:153–157
27. Theoretical Studies of Hydrogen Bond Interactions in Fluoroacetic Acid Dimer, Alireza Najafi Chermahini, Mohsen Mahdavian, and Abbas Teimouri, *Bull. Korean Chem. Soc.* 2010, Vol. 31, 941-948.
28. Ab initio and DFT studies of hydrogen bond interactions in difluoroacetic acid dimer, Alireza Najafi Chermahini • Ali Moaddeli •Abbas Teimouri Struct Chem, (2010) 21:643–649
29. Clay-Catalyzed Synthesis of 5-Substituent 1-H-Tetrazoles, Alireza Najafi Chermahini, Abbas Teimouri, Fariborz Momenbeik, Amin Zarei, Zeinab Dalirnasab, Aseyeh Ghaedi, Mostafa Roosta, J. Heterocyclic Chem., 47, 913 (2010).
30. Theoretical studies on tautomerism of triazole derivatives in the gas phase and solution Hossein A. Dabbagh, Elham Rasti, Alireza Najafi Chermahini, Journal of Molecular Structure: THEOCHEM 947 (2010) 92–100
31. Studies on tautomerism in the triazoline dione Alireza Salimi Beni, Zeinab Dalirnasab, Abbas Teimouri, Alireza Najafi Chermahini, Can. J. Chem. 89: 1387–1395 (2011)
32. Synthesis of mono and bis-4-methylpiperidiniummethyl-urea as corrosion inhibitors for steel in acidic media, Abbas Teimouri, Nasrin Soltani, Alireza Najafi Chermahini Front. Chem. Sci. Eng. 2011, 5(1): 43–50
33. Simple and Efficient Synthesis of 5-Substituted 1-H-Tetrazoles Using Metal-Modified Clay Catalysts Alireza Najafi Chermahini, Abbas Teimouri, Ali Moaddeli, Heteroatom Chem. 22, 2011, 168
34. An efficient and one-pot synthesis of 2,4,5-trisubstituted and 1,2,4,5-tetrasubstituted imidazoles catalyzed via solid acid nano-catalyst, Abbas Teimouri, J. Mol. Cat. A: Chem Alireza Najafi Chermahini, 2011, 346, 39-45
35. Theoretical Studies of Hydrogen Bond Interactions in 4-Substituted Benzoic Acids Dimers, Alireza Salimi Beni\* Alireza Najafi Chermahini\*, and Hashem Shargh Journal of the Korean Chemical Society 2011, 55, 392
36. Linear free energy relationship for the anomeric effect: MP2, DFT and ab initio study of 2-substituted-1,4-dioxanes, Hossein A. Dabbagh, Marzie Naderi , Alireza Najafi Chermahini, Carbohydrate research, 2011, 346, 1047
37. Zeolite and sulfated zirconia as catalysts for the synthesis of 5-substituted 1H-tetrazoles via [2+3] cycloaddition of nitriles and sodium azide Abbas Teimouri, Alireza Najafi Chermahini, Polyhedrone, 2011, 30. 2606
38. MP2, DFT and ab initio calculations on thioxanthone, Alireza Salimi Beni, Alireza Najafi Chermahini, Hashem Sharghi, Setareh Mirzaei Monfared, Spectrochimica Acta Part A 82 (2011) 49–55
39. Theoretical studies on tautomerism of tetrazole 5-thion, Alireza Najafi Chermahini Abbas Teimouri •Alireza Salimi Beni, **Struct. Chem.** 2011, 22, 175-181
40. One-pot Green Synthesis of Pyrrole Derivatives Catalyzed by Nano Sulfated Zirconia as a Solid Acid Catalyst, Abbas Teimouri, Alireza Najafi Chermahini, **Chinese Journal of Chemistry**, 2012, 30, 372-376.
41. Synthesis, Crystal Structure and Conformational Studies of Schiff-Base Compound 2-{[4-(Phenyldiazenyl)Phenyl] Iminomethyl}-5-Bromophenol, Aliakbar Dehno Khalaji, Karla Fejfarova Michal Dusek, Alireza Najafi Chermahini, **J Chem Crystallogr**, 2012, 42, 136-140
42. Application of modified clays in diazotization and azo coupling reactions in water, Alireza Najafi Chermahini, Maryam Doukheh, Hassan Zadeh Hassan, Mehdi Bostanian, **Journal** **of Industrial and Engineering Chemistry** 18 (2012) 826–833
43. A simple and efficient one-pot three-component synthesis of propargylamines using Bismuth (III) chloride Abbas Teimouri, Alireza Najafi Chermahini, M. Narimani, **Bulletin of Korean Chemical Society**, 2012, 33, 1556-1560.
44. Stereoselective (exo-specific) synthesis, dynamic 1H NMR and quantum chemical conformational and configurational analysis of norbornene-aziridine-E-imidoyl system, Hossein A. Dabbagh, Alireza Najafi Chermahini**, J. Iran. Chem. Soc**. 2012, 9, 339-348.
45. Relation between the substituent effect and aromaticity in imidazole derivatives: A comparative study [Chermahini, A.N.](http://www.scopus.com/authid/detail.url?authorId=14048076300&eid=2-s2.0-84864291509)[Hosseinzadeh, B.](http://www.scopus.com/authid/detail.url?authorId=55307448100&eid=2-s2.0-84864291509) [Beni, A.S.](http://www.scopus.com/authid/detail.url?authorId=18133713500&eid=2-s2.0-84864291509)[Teimouri, A.](http://www.scopus.com/authid/detail.url?authorId=21733846400&eid=2-s2.0-84864291509), [**Computational and Theoretical Chemistry**](http://www.scopus.com/source/sourceInfo.url?sourceId=21000196008&origin=recordpage) 2012, 994, 97-104
46. Theoretical Studies on Tautomerism of Imidazole-2-selenone, A.N. Chermahini, Alireza Najafi Chermahini, Hossein Farrokhpour, Abbas Teimouri, Fatemah Pourmoghaddas, **Struct. Chem.** 2013, 24, 1215-1227
47. Investigation into the regioisomeric composition of some tetrazolopyrimido[4,5- E] [1,3,4] thiadiazines: 1H-NMR studies, Nikpour, M. Sabaghian, A.J., Atashi, S., Chermahini, A.N. [***J. Chem. Soc. Pakistan***](http://www.scopus.com/source/sourceInfo.url?sourceId=23349&origin=recordpage)*,* 2012, 34, 958-962
48. The green synthesis of new azo dyes derived from salicylic acid derivatives catalyzed via Baker’s yeast and solid acid catalysis, Abbas Teimouri , Alireza Najafi Chermahini, Mohammad Hasan Ghorbani, **Chemija,** 2013, 24, 59-66
49. Theoretical studies on the effect of substituent in the proton transfer reaction of 4-substituted pyrazoles, Alireza Najafi Chermahini, Abbas Teimouri, Alireza Salimi Beni Fatemah Dordahan, [**Computational and Theoretical Chemistry**](http://www.scopus.com/source/sourceInfo.url?sourceId=21000196008&origin=recordpage) 2013, 1008, 67-73
50. An efficient and one-pot synthesis of benzimidazoles, benzoxazoles, benzothiazoles and quinoxalines catalyzed via nano-solid acid catalysts **J. Mol. Cat. A Chem.** A. Teimouri, H. Salavati, A. N. Chermahini O. L. Ghorbanian. 2013, 373, 38-45
51. The green synthesis of Xanthenedione and Dihydropyrimidone derivatives catalyzed by nano-crystalline solid acid catalysts” Abbas Teimouri, Alireza Najafi Chermahini, Leila Ghorbanian, **Chemija**, 2013, 24, 223-233.
52. Theoretical studies on the tautomerism of tetrazole selenone, Alireza Najafi Chermhini, Mostafa Abedi, Hossein Farrokhpour, Abbas Teimouri, Bahareh Reisi, **J Mol Model**, 2013, 19, 4377-4386
53. Enantiomeric separation of D- and L-lactic acid enantiomers by use of nanotubular cyclicpeptides: A DFT study, Fereshte Shahangi, Alireza Najafi Chermahini, Hossein A. Dabbagh, Abbas Teimouri, Hossein Farrokhpour [**Computational and Theoretical Chemistry**](http://www.scopus.com/source/sourceInfo.url?sourceId=21000196008&origin=recordpage) 2013, 1020, 163-169
54. Theoretical studies on the reactivity of mono-substituted imidazole ligands Alireza Najafi Chermahini, Behzad Hosseinzadeh, Alireza Salimi beni, Abbas Teimouri, **Struct Chem** 2014, 25, 583-592.
55. Nano-Alumina Sulfuric Acid: An Efficient Catalyst for the Synthesis of α-Aminonitriles Derivatives, Abbas Teimouri, Alireza Najafi Chermahini, leila Ghorbanian, **World Academy of Science, Engineering and Technology** 79 2013, 1302-1305
56. Synthesis of functionalized piperidines by one-pot multi-component reaction using nano-crystalline solid acid catalysts, Abbas Teimouri, Alireza Najafi Chermahini, leila Ghorbanian, **Bulg. Chem. Commun.** 2014,46, 523-529.
57. [Synthesis of triazenes by using aryl diazonium silica sulfates under mild conditions](http://www.sciencedirect.com/science/article/pii/S0143720813004002), Amin Zarei, Leila Khazdooz, Hamidreza Aghaei, Ghobad Azizi, Alireza Najafi Chermahini, Abdol R. Hajipour, **Dyes and Pigments**, 2014, 101, 295-302.
58. Selective complexation of alkali metal ions and nanotubular cyclopeptides A DFT study Alireza Najafi Chermahini, Mehdi Rezapour, Abbas Teimouri, **J. Incl. Phenom. Macro.** 2014, 79, 205-214.
59. Theoretical studies on proton transfer reaction of 3(5)-substituted pyrazoles Alireza Najafi Chermahini, Abbas Teimouri, **J. Chem. Sci.** 2014, 126, 273-281
60. Three component coupling catalyzed by Nickel (II) chloride hexahydrate: synthesis of α-amino phosphonates. Abbas Teimouri, Alireza Najafi Chermahini, Mehdi Narimani **Chiang Mai Journal of Science.,** 2015, 42, 228
61. Fabrication and characterization of silk/forsterite composites for tissue engineering applications Abbas Teimouri, Leila Ghorbanian, Alireza Najafi Chermahini, R. Emadi, **Ceramics International**, 2014, 6405-6411.
62. Theoretical study on structure, conformation, stability and electronic transition of C4 and C5 anions of ascorbic acid stereoisomers Hossein A. Dabbagh, Fatemeh Azami, Hossein Farrokhpour, Alireza Najafi Chermahini, **J. Mol. Struct.** 2014, 1061, 69-75.
63. A periodic density functional theory study of tetrazole adsorption on anatase surfaces: Ability of tetrazole ring for application in dye-sensitized solar cells, Alireza Najafi Chermahini, Behzad Hosseinzadeh, Alireza Salimi Beni, Abbas Teimouri,Mahmood Moradi, **J. Mol. Mod.** 2014, 20, 1-10
64. DFT and MP2 study of intermolecular interaction of 5-amino tetrazole and hydrazine: Enthaply of formation of hydrazinium 5-amino tetrazolate in the gas phase, Alireza Najafi Chermahini, Hossein Farrokhpour, Mohammadbagher Eghbalsaid, Abbas Teimouri **Propellants, Explosives, Pyrotechnics,** 2014, 39, 496-503
65. Anti-inflammatory drugs interacting with Zn(II) metal ion based on thiocyanate and azide ligands: Synthesis, spectroscopic studies, DFT calculations and antibacterial assays Hossein Chiniforoshan, Leila Tabrizi, Morteza Hadizade, Mohammad R. Sabzalian, Alireza Najafi Chermahini, Mehdi Rezapour, ***Spectrochemica Acta*, A** 2014, 128, 183-190
66. Synthesis, characterization and application of various types of alumina and nano-γ-alumina sulfuric acid for the synthesis of 2,5-disubstituted 1,3,4-oxadiazoles, Abbas Teimouri, Hossien Salavati, Alireza Najafi Chermahini, **Acta Chimica Slovenica,** 2014, 61, 51-58
67. Theoretical studies on the reactivity of thiazole derivatives Behzad Hosseinzadeh, Alireza Najafi Chermahini, Alireza Salimi Beni, Abbas Teimouri, **Monatshefte fur Chemie,** 2014, 145, 1769-1776
68. A complete scheme of tautomerism on diacetylmonoxime in the gas and solution phases: a DFT study, Abdol Reza Hajipour, Morteza Karimzadeh, Saman Jalilvand, Hossein Farrokhpour, Alireza Najafi Chermahini, [**Computational and Theoretical Chemistry**](http://www.scopus.com/source/sourceInfo.url?sourceId=21000196008&origin=recordpage), 2014, 2014, 1045, 10-21.
69. Characterization and catalytic properties of molybdenum oxide catalysts supported on ZrO2-γ-Al2O3 for ammoxidation of toluene Abbas Teimouri, Bahareh. Najari, Alireza Najafi Chermahini, Hossein Salavati, Mohsen. Fazel, **RSC Advanced**, 2014, 4, 37679-37686.
70. UV-VIS, NMR and FT-IR spectra of tautomers of vitamin C. Experimental and DFT calculations Hossein A. Dabbagh, Fatemeh. Azami, Hossein Farrokhpour, Alireza Najaﬁ Chermahini **J Chil Chem Soc**, **2014**, 59, 2588-2594
71. Theoretical studies of Urea adsorption on single wall boron-nitride nanotubes, Alireza Najafi Chermahini, Abbas Teimouri, Hossein Farrokhpour, **Applied Surface Science**, 2014, 320, 231-236
72. Metal ion binding of s-block cations and nanotubular cyclic (proline)4: A theoretical study, Zahra Jafari Chermahini,Alireza Najafi Chermahini, Hossein A. Dabbagh, Abbas Teimouri, **Struct. Chem**., **2015** Accepted for Publication.
73. Silver nanoparticles with 4,4′-dicyanamidobiphenyl Ligand: Synthesis, photoluminescent and electroluminescent properties and DFT calculations Leila Tabrizi, Hossein Chiniforoshan, Sara Bahmanpour Khalesi, Abdol R. Hajipour,Alireza Najafi Chermahini, Morteza Karimzadeh. **J Mol. Struct**, 2015, 1082, 56-61.
74. Catalytic conversion of glucose to 5-hydroxymethylfurfural (HMF) using nano-POM/nano-ZrO2/nano-γ-Al2O3 Abbas Teimouri, Mitra. Mazaheri, Mahmoud Fazel-Najafabadi, Alireza Najafi Chermahini, Hossien Salavati, Fariborz. Momenbeik, **Journal of the Taiwan Institute of Chemical Engineers**, 2015, 49, 40-50
75. Selective complexation of alkaline earth metal ions with nanotubular cyclopeptides: DFT theoretical study Fereshte Shahangia, Alireza Najafi Chermahini, Hossein Farrokhpour, Abbas Teimouri, **RSC Advances**, 2015, 5, 2305-2317
76. Synthesis and characterization of Chitosan/montmorillonite/ZrO2 nanocomposite and its application as adsorbent for removal of fluoride, Abbas Teimouri, Shima Ghanavati Nasab, Mahmoud Fazel Najafabadi, Alireza Najafi Chermahini, **RSC Advances**, 2015, 5, 6771-6781
77. A theoretical study on the interaction of amphetamine and single-walled carbon nanotubes Hamid Hafizi, Alireza Najafi Chermahini, Gholamhossein Mohammadnezhad, Abbas Teimouri, **Applied Surface Science**, 2015, 329, 87-93
78. Complexation of all-cis cyclo(L-Pro)3 and alkali metal cations: A DFT study. Zahra Jafari Chermahini, Alireza Najafi Chermahini, Hossein A Dabbagh, Abbas Teimouri, **Journal of Inclusion Phenomena and Macrocyclic Chemistry**, 2015, 81, 465-473
79. Tautomerism and mechanism of intramolecularproton transfer both in the gas phase and micro-hydrated solvent: Biuret as a case study,AR Hajipour, A.N. Chermahini., M Karimzadeh, M. Rezapour **Struct Chem** 2015, 26, 159-169
80. Nano-composite of Silk fibroin-Chitosan/Nano ZrO2 for tissue engineering applications: Fabrication and morphology, Abbas Teimouri, Raheleh Ebrahimi, Rahmatollah Emadi, Batool Hashemi Beni, Alireza Najafi Chermahini, **International Journal of Biological Macromolecules,** 2015, 76, 292-302
81. Dissociation, absorption and ionization of some important sulfur oxoanions (S2O n 2-n= 2, 3, 4, 6, 7 and 8), M Abedi, H. Farrokhpour, S Farnia, A Najafi Chermahini, **J Mol Struct.** 2015, 1093, 125-134
82. Application of functionalized mesoporous silica catalyst for the synthesis of tetrazoles Alireza Najafi Chermahini, Masoud Khani Omran, Hossein A. Dabbagh, Gholamhossein Mohammadnezhad, Abbas Teimouri, **New Journal of Chemistry**, 2015, 39, 4814-4820.
83. Fabrication and characterization of POM/ZrO2/silk fibroin composites scaffold, Abbas Teimouri, Abbas Teimouria, Leila Ghorbanian, Hossien Salavati, Alireza Najafi Chermahini, **Materials Letters, 2015**, 157, 85-88
84. Novel organic dyes with anchoring group of barbituric/thiobarbituric acid and their application in dye-sensitized solar cells, Behzad Hosseinzadeha, Alireza Salimi Beni, Alireza Najafi Chermahini, Raheleh Ghahary, Abbas Teimouri, **Synthetic Metals**, 2015, 209, 1-10
85. Protein-ligand interaction study of signal transducer smoothened protein with different drugs: Molecular docking and QM/MM calculations, Hossein Farrokhpour, Vahid Pakatchian, Abdol R. Hajipour, Fatemeh Abyar, Alireza Najafi Chermahini and Farzaneh Fakhari, **RSC Advances**, 2015, 5, 68829-68838
86. Preparation, characterization, degradation and biocompatibility of different silk fibroin based composite scaffolds prepared by freeze-drying method for tissue engineering application, Abbas Teimouria, Mohammad Azadia, Rahmatollah Emadi , Jalil Lari, Alireza Najafi Chermahini, **Polymer Degradation and Stability**, 2015, 121, 18-29
87. Fluorine substituent effect on the adsorption of acetic acid derivatives (CH3-n FnCO2H) on Anatase TiO2 (100) and (101) surfaces Masoume Rezaei, Alireza Najafi Chermahini, Hossein A. Dabbagh, Abbas Teimouri, **Appl. Sur. Sci**. 2015, 357, 1260-1267
88. New Tetrazole-Based Organic Dyes for Dye-Sensitized Solar Cells Zahra Jafari Chermahini,Alireza Najafi Chermahini, Hossein A Dabbagh, Abbas Teimouri, **J. Chem. Energy**, 2015,
89. Selective complexation of s-block cations and nanotubular silk type cyclopeptides: A DFT study, Abbas Teimouri, Batoul Najari, Alireza Najafi Chermahini, Hossein Farrokhpour, **J. Chinese Chemical Society**, 2015,
90. A DFT-D study on the interaction between lactic acid and single-wall carbon nanotubes Alireza Najafi Chermahini, Abbas Teimouri, Hossein Farrokhpour, **RSC Advances**, 2015,
91. Synthesis and characterization of organic dyes bearing new electron-withdrawing group for dye-2 sensitized solar cells A. Salimi Beni, M. Zarandi, A. R. Madramb, Y. Bayat, A. Najafi Chermahini, R. Ghahary, **Electrochimica Acta,** 2015, 186, 504-511
92. The effect of deformation and intermolecular interaction on the absorption spectrum of 5-aminotetrazole and hydrazine: A computational molecular spectroscopy study on hydrazinium 5-aminotetrazolate H. Farrokhpour , A. Dehbozorgi, M. Manassir, A. Najafi Chermahini, **Journal of Molecular Structure** 2016, 1107 121-136
93. Amino-functionalized mesoporous silica as solid base catalyst for regioselective aza-Michael reaction of aryl tetrazolesAlireza Najafi Chermahini, Mahboobeh Azadi, Elham Tafakori, Abbas Teimouri Mohammadreza Sabzalian, **J. Porous Mater.** 2016
94. Comparing the ion affinity of two ionophores: Theoretical study of alkali earth metal ion-nano tubular cyclic peptide complexes, Alireza Najafi Chermahini, Zahra Jafari Chermahini, **J. Mol. Liquid**. 2016, 214, 101-110
95. Theoretical study of microhydrated cyclo(L-pro)4-alkali cation complexes Zahra Jafari Chermahini, Alireza Najafi Chermahini, **Computational and Theoretical Chemistry,** 2016, 1078, 37-46
96. The Catalytic Conversion of Fructose into 5-Hydroxymethylfurfural Over Acid-Functionalized KIT-6, an Ordered Mesoporous Silica Hamid Hafizi, Alireza Najafi Chermahini, Mohammad Saraji, Gholamhossein Mohammadnezhad, **Chem. Eng. J.** 2016, 294, 380-388
97. One-pot synthesis of ethyl-3-aryl-2-(1H-tetrazol-5-yl)acrylates and 3-(1H-tetrazol-5-yl) coumarins via tandem [2+3] dipolar cycloaddition reaction-Knoevenagel condensation Zahra Jafari Chermahini, Alireza Najafi Chermahini, Hossein A Dabbagh, Abbas Teimouri, **ChemistrySelect** 2016, 1, 430-433
98. A DFT approach for simple and solvent assisted-proton movement: Biurea as a case of study Abdol Reza Hajipour, Sirous Ghorbani, Morteza Karimzadeh, Saeideh Jajarmi, Alireza Najafi Chermahini, **Computational And Theoretical** Chemistry 2016, 1078, 37-46
99. A comparative MP2 study between water and acid assisted-proton transfer: Allophanic acid as a case of study Abdol Reza Hajipour, Morteza Karimzadeh, Sirous Ghorbani,a Hossein Farrokhpour, Alireza Najafi Chermahini, **Struct Chem** 2016, 27, 1345-1362
100. Production of 5-hydroxymethylfurfural from fructose using spherically fibrous KCC-1 silica catalyst Alireza Najafi Chermahini, Fereshte Shahangi, Hossein A. Dabbagh, Mohammad Saraji, **RSC Advances**, 2016, 6, 33804-33810
101. Adsorption of some important tautomers of 5-amino tetrazole on the (001) and (101) surfaces of anatase: Theoretical Study, Alireza Najafi Chermahini, Hossein Farrokhpour, Abbas Zeinodini, **J Mol Struct** 2016, 1121, 203-214
102. Theoretical studies on the adsorption of 5-aminotetrazole on single-walled carbon nanotubes Alireza Najafi Chermahini, Kamran Kermannezhad, Masoume Rezaei, **J. Chines Chem.** **Soc**. 2016, 63, 716-724
103. Enantiomeric discrimination of leucine enantiomers by nanotubular cyclic peptides: DFT and ONIOM calculation of the absortion spectra of guested enantiomers Fereshte shahangi, Alireza Najafi Chermahini, Hossein Farrokhpour, Hossein A. Dabbagh, **J Inc Phen Macrocycl Chem.** 2016, 85, 329-339
104. Application of amine-functionalized MCM-41 as pH-sensitive nano container for controlled release of 2-mercaptobenzoxazole corrosion inhibitor Kamran Kermannezhad, Alireza Najafi Chermahini\*, Mohamad Mohsen Momeni, Behzad Rezaei, **Chem. Eng. J.** 2016, 306, 849-857
105. Chitosan/Zeolite Y/Nano ZrO2 nanocomposite as an adsorbent for the removal of nitrate from the aqueous solution, Abbas Teimouri, Shima Ghanavati nasab, Niaz Vahdatpoor, Saeed Habibollahi, Hossein Salavati, Alireza Najafi Chermahini, **International Journal of Biological Macromolecules**, 2016, 93, 254-266
106. Density functional theory of tautomerism and water-assisted proton transfer of glycoluril, Alireza Salimi Beni, Masoume Aazari, Alireza Najafi Chermahini, Maryam Zarandi **Russian Journal of Physical Chemistry A** 90 (9), 1859-1868
107. Theoretical Modeling of the Chirality Discrimination of Enantiomers by Nanotubular Cyclic Peptides using Gas Phase Photoelectron Spectroscopy: An ONIOM Spectroscopic Calculations, H Farrokhpour, S Karachi, A Najafi Chermahini **The Journal of Physical Chemistry A,** 2016,120, 6780-6791
108. Intermolecular interaction of guanidine and 2H-tetrazole: Enthalpy formation of guanidinium tetrazolate in the gas phaseMohammad Reza Afyouni,Hossein Farrokhpour\*, Alireza Najafi Chermahini, **Computaional and Theoretical Chemistry,** 2016, 1094, 42-46
109. Density functional theory of tautomerism and water-assisted proton transfer of glycoluril, Alireza Salimi Beni, Masoumeh Aazari, Alireza Najafi Chermahini, Maryam Zarandi, **Russian Journal of Physical Chemistry** A 2016, 90 (9), 1859-1868
110. Design and fabrication of novel chitin hydrogel/chitosan/nano diopside composite scaffolds for tissue engineering Athar Moatary, Abbas Teimouri, Mehdi Bagherzadeh, Alireza Najafi Chermahini, R Razavizadeh, **Ceramics International**, 2017
111. Interaction of lactic acid and silicon-doped single-walled carbon nanotubes: A DFT study, Alireza Najafi Chermahini, Abbas Teimouri, **J. Chines Chem. Soc.** 2017,
112. Green and selective oxidation of cyclohexane over vanadium pyrophosphate supported on mesoporous KIT-6, Masoume Rezaei, Alireza Najafi Chermahini, Hossein A. Dabbagh, **Chemical Engineering Journal** 2017, **In Press**
113. The effects of second electron acceptor group on the performance of tetrazole-based nanocrystalline TiO2 sensitizers in DSSCs Zahra Jafari Chermahini, Alireza Najafi Chermahini\*, Hossein A. Dabbagh, Behzad Rezaei, Neda Irannezhad, **Spectrochimica Acta A**, 2017, In Press
114. Theoretical study on the bridge comparison of TiO2 nanoparticle sensitizers based on phenoxazine in dye-sensitized solar cells Zahra Jafari Chermahini, Alireza Najafi Chermahini, **Theoretical Chemistry Accounts**, 2017, In Press
115. Transport Behavior of the Enantiomers of Lactic Acid through Cyclic Peptide Nanotube: Enantiomer Discrimination H Farrokhpour, A Mansouri, A Najafi Chermahini **The Journal of Physical Chemistry** C, 2017
116. The catalytic effect of Al-KIT-5 and KIT-5-SO3H on the conversion of fructose to 5-hydroxymethylfurfural AN Chermahini, H Hafizi, N Andisheh, M Saraji, A Shahvar **Research on Chemical Intermediates**, 1-15,
117. Synthesis of new dyes containing double tetrazole groups for sensitization of TiO2 nanoparticles in dye-sensitized solar cells ZJ Chermahini, AN Chermahini, HA Dabbagh, B Rezaei, N Irannejad **Journal of the Iranian Chemical Society**, 1-8
118. Adsorption modes of 1, 3-thiazol-2-amine on the TiO2 (001) and (101) anatase surfaces H Farrokhpour, M Vazifeh, AN Chermahini, **Structural Chemistry**, 1-12

**Seminars**

**a) Posters**

Presentation of more than 25 papers.

 **b) Oral Presentation**

* 1. Synthesis and partial resolution of aryloxy tetrazoles with axial chirality, 10th Iranian Seminar of Organic Chemistry Isfahan University of Technology, Isfahan, 2005
	2. Semiempirical study of the aromaticity and electronic properties of aryloxy tetrazoles. 14th Iranian Seminar of Organic Chemistry University of Zabol , Zabol, 2008

**Workshops**:

* + - Application of Infrared Spectroscopy in Organic Chemistry, [Institute for Advanced studies in Basic Sciences, Zanjan, winter 2000.](http://www.iasbs.ac.ir/)
		- Application of NMR in Organic Chemistry, [Institute for Advanced studies in Basic Sciences, Zanjan, Winter 2001.](http://www.iasbs.ac.ir/)
	+ **STUDENTS**
	+ ⯁ Ms Students
1. Ghaedi A. (Yasouj University)
2. Dalirnasab Z. (Yasouj University)
3. Safikhani N. (Yasouj University)
4. Moaddeli, A. (Yasouj University)
5. Mahdavian M. (Yasouj University)
6. Jamshidi S. (Tarbiat Moallem Azarbayejan University)
7. Mazaheri A. (Yasouj University)
8. Doukheh M. (Yasouj University)
9. Bostanian M. (Yasouj University)
10. Zadehassan H. (Yasouj University)
11. Reisi B. (Yasouj University)
12. Pourmoghddas F. (Yasouj University)
13. Askarian Motlagh M. (Yasouj University)
14. Taffakori E. (Yasouj University)
15. Fattahi Sonia (IUT)
16. Khani Masoud(IUT)
17. Azadi Mahboubeh (IUT)
18. Hafizi Hamid
19. Kermannezhad Kamran

⯁PhD students

* + 1. Jafari Chermahi Zahra (Supervisor)
		2. Rasti Elham. (Advisor)
	+ **STUDENTS CURRENTLY ADVISED:**
* **PhD students**
	+ - 1. Shahangi Fereshte
1. Rezaei Masoume
2. Mohamadbagheri Zahra

**عناوین پایان نامه های کارشناسی ارشد راهنمایی شده**

* + 1. مطالعه نوارآرایی واکنش بنزیل بنزیلیک اسید با روش هارتری فاک و تئوری عاملیت دانسیته در حلالهای آلی علیرضا نجفی چرمهینی، علیرضا سلیمی بنی، آرزو مظاهری 1389
		2. تهیه تترازولها با استفاده از کائولین به عنوان کاتالیزور سازگار با محیط زیست و مطالعه اثر استخلاف روی پیوند هیدروژنی در دیمرهای تترازول علیرضا نجفی چرمهینی، مسعود نصر اصفهانی، آسیه قایدی 1387
		3. تهیه تترازولها با استفاده از کاتالیزور مونت موریلونیت K10 و بررسی تاتومریسیم 1-H و 2H در مشتقات تترازولها علیرضا نجفی چرمهینی، فریبرز مومن بیک، زینب دلیر نسب 1387
		4. سنتز کالیکس[4] رزورسینارنها در شرایط بدون حلال و مطالعه تئوری تعادلات تترازول-تترازولون بهادر کرمی، علیرضا نجفی چرمهینی و نیلوفر صفی خانی محمودی 1387
		5. تهیه و مطالعه رنگهای آزوی جدی بر پایه چارا آمینو فنیل ایمیدازول و محاسبات تئوری آنها علیرضا نجفی چرمهینی، مسعود نصر اصفهانی حسن زاده حسن 1390
		6. سنتز مشتقات تترازول با استفاده از خاک مونتموریلونیت-K10 اصلاح شده و مطالعه پیوند هیدروژنی در دیمرهای در فلئورو استیک اسید علیرضا نجفی چرمهینی، بهادر کرمی، علی معدلی 1388
		7. بررسی تعادلات و آروماتیسیتی تیول-تیون در مشتقات اکسازول-2-تیول و اکسازول-2-تیون مهرداد مهکام، علیرضا نجفی چرمهینی، سعادت جمشیدی 1389
		8. تهیه و مطالعه رنگهای آزوی جدید بر پایه پارا آمینو فنیل تترازول و محاسبات تئوری بر روی آنها علیرضا نجفی چرمهینی، بهادر کرمی، مریم دوخه 1389
		9. تهیه و مطالعه رنگهای آزوی جدید بر پایه 3- آمینو فنیل تترازول و بررسی پیوند هیدروژنی فلئورو استیک اسید. علیرضا نجفی چرمهینی، علیرضا سلیمی بنی، محسن مهدویان 1388.
		10. تبدیل ترکیبات تیوکربونیل به ترکیبات کربونیل توسط ید، یدومونوکلرید و تنگستو سیلیسیلیک اسید مسعود نصر اصفهانی، علیرضا نجفی چرمهینی، ساره مرادی 1387.
		11. سنتز تعدادی از رنگهای جدید بر پایه 3-هیدروکسی-N(1H-تترازول-5-ایل)-2-نفتامید و مطالعات تئوری بر روی تاتومری 1H-ایمیدازول2(3H) سلنون ، علیرضا نجفی چرمهینی، مسعود نصر اصفهانی، فاطمه پورمقدس 1390
		12. سنتز رنگدانه های با کارایی بالا بر پایه 3-هیدروکسی-2-نفتوئیک اسید و 5-آمینو تترازول و مطالعات تئوری بر روی ایزومرهای تترازول-5-سلنون علیرضا نجفی چرمهینی، علیرضا سلیمی بنی، بهاره رییسی، 1390
		13. سنتز تعدادی از رنگهای آزوی جدید مشتقات تیوزانتون علیرضا سلیمی بنی، علیرضا نجفی چرمهینی، زهرا جعفری چرمهینی 1389.
		14. دی آزوتاسیون و سنتز تعدادی از رنگهای آزو با استفاده از خاک مونت موریلونیت-K10 اصلاح شده به عنوان کاتالیزور علیرضا نجفی چرمهینی، علیرضا سلیمی بنی، مهدی بستانیان 1389
		15. سنتز ایمیدازولهای سه و چهار استخلافی با استفاده از کاتالیزور ایتریوم نیترات شش آبه در شرایط بدون حلال و گرمایی بهادر کرمی، علیرضا نجفی چرمهینی، فاطمه محمد پور دهقانی 1389
		16. سنتز مشتقات کومارین با استفاده از لوییس اسیدهای ایتریوم (III) نیترات شش آبه و زیرکونیوم اکسی کلرید هشت آبه نشانده شده بر روی سیلیکاژل تحت شرایط حرارتی و بدون حلال بهادر کرمی، علیرضا نجفی چرمهینی، مهتاب کیانی 1389
		17. سنتز تک مرحله ای ایمیدهای خطی نا متقارن در حضور پارا تولوئن سولفونیک اسید تحت شرایط حرارتی و آلتراسونیک مسعود نصر اصفهانی، علیرضا نجفی چرمهینی، نجمه فیلوان ترکمن 1389
		18. جداسازی و شناسایی همزمان قندها بعد از مشتق سازی با 4-آمینو فنوکسی تترازول به روش کروماتوگرافی مایع فاز معکوس و آشکار سازی فلورسانس، فریبرز مومن بیک، علیرضا نجفی چرمهینی، غلامعلی بهمنی 1388
		19. سنتز تعدادی از مشتقات تیوزانتون با استفاده از واکنشگرهای آلومینا متان سولفونیک اسید، مونت موریلونیت K-10 متان سولفونیک اسید و هتروپلی اسید و مطالعات ساختاری آنها علیرضا سلی بنی، علیرضا نجفی چرمهینی، ستاره میرزایی منفرد 1388
		20. سنتز مشتقات 4-آریل-3،4-دی هیدروپیریمیدین-2-(1H) اون تیون در حضور کاتالیزور نیترات کبالت (II) شش آبه و سنتز مشتقات پلی هیدروکینولین در حضور نیترات باریوم ، مسعود نصر اصفهانی، علیرضا نجفی چرمهینی، مریم عاقل میررضایی 1390