

# Resume

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## ***ACADEMIC EXPERIENCE***

**1991 – Present Time**

Department of chemistry

Isfahan University of Technology

Isfahan, Iran.

## ***TECHNICAL RESPONSIBILITY***

Directing graduate student (Ph. D. and Ms.) research program in the area of physical organic chemistry, computational chemistry and catalysis.

- . Chairman of the first meeting in applied catalysis.
- . Co-chairman of the fifth seminar of organic chemistry.
- . Teaching graduate and undergraduate in **all area of organic chemistry**.
- . Deputy director of research program (department of chemistry).

***PROFESSIONAL EXPERIENCE***

- . August **2002**-August **2003**                      **Visiting professor**  
**University of British Columbia**  
**Vancouver, Canada**
- . January **1987**- February **1991**                      ***SENIOR CHEMIST***  
Center for Applied Energy Research  
University of Kentucky  
Lexington Kentucky, KY  
40511-8433, USA
- . January **1986**- January **1987**    ***RESEARCH ASSOCIATE***  
Center for Applied Energy Research Laboratory  
University of Kentucky,  
3572 Iron Works Pike  
Lexington Kentucky, 40511-8433
- . January **1985**- January **1986**    ***POSTDOC RESEARCH ASSOCIATE***  
Center for Applied Energy Research Laboratory  
University of Kentucky,  
3572 Iron Works Pike  
Lexington Kentucky, 40511-8433

## ***TECHNICAL RESPONSIBILITY***

. Organic Synthesis. Synthesis of a variety of carbon-14, carbon-13, deuterium, and nitrogen 15 labeled alkane, alkenes, alcohols, ethers, esters, acids, alkylaromatics, and nitrenes from readily available and low cost starting material.

Organic analysis. Separation of isomers and purification of variety of compounds including Fischer- Tropsch synthesis products, coal liquefaction, and isotope labeled organic compound. High performance liquid chromatography (HPLC), liquid chromatography, thin layer chromatography, gas chromatography (variety of models), capillary GC Mass spectroscopy, nuclear magnetic resonance spectroscopy (proton, carbon-13, nitrogen-15, deuterium), infrared, Packard Tri-Carb Model 3330 liquid scintillation spectrometer, Packard proportional counter (model 894), radiomatic FLO-ONE/Beta detectors, and many others.

. Heterogeneous Catalysis. Use carbon-14 tracer studies to define promotion mechanism for iron Fisher-Tropsch catalysis. Prepare and test a variety of catalysts. Isotope tracer studies for the investigation of the mechanism of alcohol conversion. Use of carbon-14 and carbon-13 to investigate transalkylation and/or isomerization of alkyl aromatics with zeolites.

. Coal Liquefaction Studies. Use of isotope tracers to identify the role of solvent, hydrogen, or carbon monoxide during coal liquefaction.

. Supervised a post-doctorate research associate, graduate students, technicians, and co-op students.

. Equipment. Responsible for new equipment evaluation, operation, and maintenance.

### ***TECHNICAL RESPONSIBILITY***

. Initiate the design and operation of an apparatus for the generation and utilization of carbon-13 and carbon-14 labeled carbon dioxide to synthesis a variety of organic compounds.

. Initiate the design and operation of one atmospheric Fischer-Tropsch synthesis reactor, Use of <sup>14</sup>C-tracer studies to define promotion mechanism for the iron Fischer-Tropsch catalysis.

. Initiate the design and operation of a column for the analytical separation of compound class of Fischer-Tropsch synthesis products.

September **1981**- December **1985**

***GRADUATE STUDENT (PhD)***

Department of Chemistry

New Mexico State University

Las Cruces NM 88003

. **Thesis:** Acyl-tetrazoles (Nitrene Precursors), their equilibrium, The Nature, and Reactivity of their Ring Opening Products.

September **1979-1981**

**GRADUATE STUDENT (MS)**

East Tennessee State University

Johnson City Tennessee, 37614

September **1974-1979**

**GRADUATE STUDENT (BS)**

East Tennessee State University

Johnson City Tennessee, 37614

. **Thesis:** Kinetic Isotope Effect in the Elimination Reaction of the Alcohols with Triphenylphosphine in Carbon tetrachloride.

### ***TEACHING RESPONSIBILITIES***

September 1981- 1985

***TEACHING ASSISTANT***

Department of Chemistry

New Mexico State University

Las Cruces NM 88003.

. Taught freshman chemistry and organic chemistry laboratories.

September 1979-1981

***TEACHING ASSISTANT***

East Tennessee State University

Johnson City Tennessee, 37614

. Taught freshman chemistry and organic chemistry laboratories.

.September **1975-1979**

**, UNDERGRADUATE STUDENT (BS)**

East Tennessee State University

Johnson City Tennessee, 37614

Chief operator for Jeol JMS-100 Mass spectrometer and JEOL-C-60H Nuclear Magnetic Resonance Spectrometer.

### ***PROFESSIONAL SOCIETIES***

. American Chemical Society (ACS), National and regional

. Iranian Chemical Society

Materials Research Society: Tri-State Catalyst Club

### ***EDUCATION***

Ph. D., Organic chemistry (minor in biochemistry), New Mexico State University, Las Cruces, NM, 1985.

M.S., Physical Organic Chemistry, East Tennessee State University, Johnson City, TN, 1981.

B.S. Chemistry and Biology, East Tennessee State University, Johnson City, TN, 1978.

### **Title of the Ms. Thesis Supervised**

1. Synthesis, stability and equilibria studies of N<sup>2</sup>-(p-toluenesulfonyl) (aryloxy) carbimidoyl azides, Gahelle S., Aban, **1994**.
2. Synthesis, stability-equilibria studies and thermal decomposition of N<sup>2</sup>-acyl-5-aryloxy tetrazoles, Karmzadeh, R., Farvardin, **1995**.
3. Synthesis of new copolymers, Mohamade varzeneh, F., Aban, **1995**.
4. Isotope effect and kinetic studies of elimination reaction of tertiary alcohols over aluminum oxide, mohamed Salehi, J., fall, **1998**.
5. Tetrazoles rearrangements and functionalization of imines by imidoyl nitrenes, Jafary Boeine, F., Summer, **1999**.
6. Functionalization of furans ring by imidoyl nitrene, Bazriz, S., Spring, **2000**.

7. Asymmetric synthesis of dioxane ring by imidoyl nitrene, conformational analysis of adduct and nucleophilic substitution of chiral imidoyl nitrene, Hoseiny, S.M., Fall, **2000**.
8. Preparation of Fischer-Tropsch Catalysts for the synthesis of light gasoline, M.S., Taymori A., Fall, **2001**.
9. X-Ray analysis of the Structure and Dehydration of Alcohols over the Mixture of Aluminum Oxide and Thorium Oxide, Yalfany M.S., Fall, **2001**.
10. Synthesis and Investigations of Alfa and Beta Binaphthoxy tetrazoles, Sodabeh BaniBirami, spring, **2002**.
11. Swern Reactions, Optimization, hydrolysis of Aryloxy tetrazoles and Synthesis of New derivative of Salicylic acids, Ali Bagheri, Fall, **2004**.
12. Synthesis, Mechanism and Quantum Chemical Studies of New Derivatives of Methyl Salicylate, Sepideh Ziaee, **2007**.
13. Evaluation of pressure and temperature effect on alumina's structure: SEM, XRD, FT-IR, Thermal Analysis, and study of elimination of secondary and tertiary alcohols. Taban, Kayvan, **2007**.
14. Synthesis, Dynamic NMR, quantum chemical studies and Conformational analysis of (4-(sulfonyl azide) phenyl)-1-azide and Products of the Reaction with Norbornene, Maryan Rezvan. **2008**.
15. XRD, SEM and Quantum Chemistry Studies of Structure, Reactivity and Stereo Selectivity of Mixed Alumina/Zirconia, Mehdi Zamani, **2008**.
16. Catalyst Promoted Synthesis of New Derivatives of Salicylic Acid from Dimethoxy benzenes and Their Theoretical Calculations and Quantum Chemical Study of Equilibria of the 5-Methoxy-1,2- Substituted Tetrazoles and Imidoyl Azides, Maryam Shahraki, **2008**.

17. Preparation, structure analysis (XRD, SEM, BET, FT-IR), reactivity and selectivity of mixed Alumina with H<sub>2</sub>SO<sub>4</sub>, HNO<sub>3</sub> or NaNO<sub>2</sub> and Ab initio, MP2, DFT investigation of Anomeric Effect and Non-bonding interactions of Cyclohexane and 1,4-Dioxane derivatives, Marziye Naderi Beni, **2008**.
- 18, Catalyst promoted synthesis of salicylic acid from anisole and Quantum chemical study of new derivative of salicylic acid and methyl benzoates, Rzvvan Shiasi, **2009**.
19. Investigation of environmental effect on mixed oxides of iron and alumina performance in dehydration reaction of secondary and tertiary alcohols, Mohammad Yousefi Ghasabeh, **2009**.
20. Investigation of temperature, air and nitrogen atmosphere effect on mixed oxides of nickel and alumina performance in dehydration reaction of secondary and tertiary alcohols, Mohammad Toulabi, **2012**.
21. Synthesis of New Derivatives of Ortho Acetaminophen, Ionic Liquid Promoted On it , Methylation of Anisole And Quantum Chemical Study With Conformational Analysis of Di-Amino, Di-Nitro and Amino-Nitro Ethane, Rezvan Ghadiri, **2011**.
22. Synthesis of New Derivatives of Acetaminophen, Ionic Liquid Promoted Acylation of anisolee And Quantum Chemical Study With Conformational Analysis of Di-hydroxy, Di-thiol and si-silyl Ethane, **Mahta Mousavi, 2011**.
23. Synthesis of di-salicylates, evaluation of Catalyst effect and ionic liquid on alkylation and acylation of hydroquinone and Quantum chemical study of phenyl sulfonyl azide, phenyl sulfonyl nitrene and the Mechanism of their reaction, Maryam Balanian, **2012**.
23. Synthesis of di-salicylates, evaluation of catalyst effect and ionic liquid on alkylation and acylation of dimethoxy benzene and quantum chemical study of the 18-member ring dimmers, Shirin Shabani, **2012**.



24. Quantum chemical study of  $\gamma$ -Alumina surface, Freshteh Shangy, **2012**.
25. Effect of vacuum and nitrogen atmosphere on Al<sub>2</sub>O<sub>3</sub>-Ni-Co structure, reactivity and selectivity of amination of ethanol and dehydration of 1-octanol and FFT study of 100 surface Al<sub>2</sub>O<sub>3</sub>-Ni-Co structure with adsorbed ethanol, Hossein Morthagi, **2012**.
26. Synthesis and characterization of mixed  $\gamma$ -alumina-BIBOL, dehydration of alcohol and DFT calculation of BINOL over  $\gamma$ -alumina (100) and (110) surfaces, Mehdi Reiesi-Hasani, **2013**.

### **Title of the Ph. D. Thesis Supervised**

1. Studies of Elimination and substitution reactions of tertiary alcohols with triphenylphosphine, polystyryl diphenylphosphine and (-)-menthol diphenylphosphine, Faghihi K., Fall, **1999**.
2. The synthesis of the new aryloxyimidoyl azides, imidoyl-N-2-amino-1,4-dioxane and their Dynamic NMR studies, Modarresi-Alam, A.R., Fall, **1999**.
3. Kinetics and Mechanism of the Equilibria of the N-Alkylcarboxylate-5-aryloxy Tetrazoles and Aryloxytetrazole-Azoic Dyes and New Acrylamide Derivative: Synthesis, Free Radical Polymerization, Reactivity Ratios and  $Q$  and  $e$  Values, Yagoub Mansoori, Fall, **2000**.
4. New Applications NMR and X-ray investigation of the structure of Aryloxy tetrazoles and Binaphthyl Hydrogen Phosphonate, Nader Noroozi-Pesyan, spring, **2004**.
5. **BINOL**-aryloxy tetrazoles as Chiral Pool in Asymmetric Synthesis; DFT Computational analysis of Anomeric Effect and Binaphthyl-Bistrazoles, Alireza Najafi, Fall, **2005**.

6. Synthesis, Reactions, Quantum Chemical Study and Structure of Azo dyes and Triazenes Containing sulfonyl azides or Sulfonyl Amides, Abbass Timouri, **2006**.
7. Investigation of the influence of organic acids and/or bases on morphology of aluminananostructures and Quantum chemical conformational analysis, structure, NMR and hydrogen bonding of hydrazinoturns and Studies of tautomerism, effect of solvent and substitution of triazole derivatives, Elham Rasty, **2011**.
8. Quantum chemical study of group III oxides nanocapsuls for gas storage and influence of diketene on modification of metanol to gasoline conversion over zeolite ZSM-5 and its mechanism, Mehdi Zamani, **2013**.
9. Degradation of vitamin C in the presence of water and ZnO nanoparticles and computational study of isomerization, Fatemeh Azami, **2014**.
10. Synthesis, characterization, application and theoretical investigations of alumina/boria nanocomposites and borazine-melamine polymer for hydrogen storage, Maryam Shahraki, **2014**.

### **Funded Research Projects**

1. Functionalization of pheny rings by imidoyl nitrenes II. Cycloaddition or electrophilic aromatic substitution.
2. Stereoselective synthesis of alkenes by triphenylphosphine in tetrachloromethane.
3. Isotope effect and kinetic studies of the reaction of tetiary alcohols with triphenylphosphine in tetrachloromethane.

4. Funcionalization of phenyl rings by imidoyl nitrenes III. Effect of resonance, steric, and inductive on reactivity or selectivity of nitrene, and stability of their precursors.
5. New transition state model for elimination reaction of alcohols over aluminum oxide and thorium oxide.
6. Experimental and AM1 Demonstration of Anomeric Effect, Structure, Dynamic NMR, X-Ray Conformational and Configurational Analysis of N-2-(1,4-Dioxane)-N`-(p-methylbenzenesulfonyl)-O-(p-methylphenoxy) isourea.
7. Preparation of Fischer-Tropsch Catalysts for the synthesis of light gasoline.
8. Novel Synthesis, X-ray, and Quantum Mechanical calculations of 1-(Methylthiomethyl)-5-(40nitrophenoxy)tetrazoles.
9. An XRD and fourier-transformed infrared spectroscopy investigation of single and mixed  $\gamma$ -alumina and thorium oxide.
10. Dynamic NMR Investigation of Methyl-2,4-dimethoxysalicylate: Effect of Solvent and Temperature on Conformation, Hydrogen bonding.

## **BOOKS**

- 1 *Principles of Organic Chemistry*, Dabbagh, H.A.; Malakpour S; Amirkhizi, M.H. **IUT Press, 1998.**
- 2 *Principles of Physical Organic Chemistry Part one: Structure*, Dabbagh, H.A. **Arkan Press, 2004.**
- 3 *Name Reactions and mechanisms in Organic Chemistry*, Dabbagh A. Hossein, Hossein Etedali, Mehdi Zamani, **Jungle Press, 2009.**

# PUBLICATIONS

1. Nature of intramolecular interactions of vitamin C in view of interacting quantum atoms: the role of hydrogen bond cooperativity on geometry, Saeid Ebrahimi, Hossein A. Dabbagh and Kiamars Eskandar, **Phys. Chem. Chem. Phys.**, **2016**, 18, 18278—18288.i
2. 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, and Abbas Teimouri, **ChemistrySelect** **2016**, 3, 430–433.
3. Production of 5-hydroxymethylfurfural from fructose using a spherically fibrous KCC-1 silicacatalyst, Alireza Najafi Chermahini, Fereshte Shahangi, Hossein A. Dabbagh and Mohammad Saraji, *RSC Adv.*, **2016**, 6, 33804.
4. Surface modification of  $\gamma$ -alumina by  $\text{NaNO}_2$ ,  $\text{NaNO}_3$ ,  $\text{HNO}_2$ ,  $\text{HNO}_3$  and  $\text{H}_2\text{SO}_4$ : A DFT-D approach Mehdi Zamani, Hossein A. Dabbagh, 6(3), **2016**, Iranian Journal of Catalysis, 345-353.
5. Fluorine substituent effect on the adsorption of acetic acid derivatives( $\text{CH}_3\text{-nFnCO}_2\text{H}$ ) on anatase  $\text{TiO}_2(1\ 0\ 0)$  and  $(1\ 0\ 1)$  surfaces, surfacesMasoume Rezaeia, Alireza Najafi Chermahinia, Hossein A. Dabbagha, Abbas Teimouri, **Applied Surface Science** 357 (2015) 1260–1267.

6. New tetrazole-based organic dyes for dye-sensitized solar cells, Zahra Jafari Chermahinia, Alireza Najafi Chermahini, Hossein A Dabbagh, Abbas Teimouri, **Journal of Energy Chemistry**, 24 (2015) 770–778.
7. 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. J chem.** 2015, 39, 4114.
8. Complexation of all-cis cyclo(L-Pro)<sub>3</sub> and alkali metal cations: A DFT study, Zahra Jafari Chermahini • Alireza Najafi Chermahini • Hossein A. Dabbagh • Abbas Teimouri, **J Incl Phenom Macrocycl Chem** (2015) 81:465–473.
9. Metal ion binding of s-block cations and nanotubular cyclic (proline)<sub>4</sub>: A theoretical study Zahra Jafari Chermahini • Alireza Najafi Chermahini • Hossein A. Dabbagh • Abbas Teimouri, **Struct Chem** (2015) 26:675–684.
10. Theoretical Investigation of the Ability of Borazine-Melamine Polymer as a Novel Candidate for Hydrogen Storage Applications, Abdol Hossein Dabbagh, Maryam Shahraki and Hossein Farrokhpour, **Physical Chemistry Chemical Physics**, 2014, 10519-10530.
11. Experimental and theoretical study of racemization, stability and tautomerism of vitamin C stereoisomers, Hossein A. Dabbagh, Fatemeh Azami, **Food Chemistry**, 164 (2014) 355–362.
12. 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, **Journal of Molecular Structure**, 2014, 1061, 69–75.

13. 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.
14. Vibrational and UV Spectroscopic Analysis of C<sub>20</sub> Carbon Nanostructures, M. Zamani, A. Motahari, H. A. Dabbagh, H. Farrokhpour, **Nano Analysis**, **2014**,
15. Computational note on chemoselectivity of alcohols adsorption over  $\gamma$ -alumina(100) surface, Hossein A. Dabbagh, Mehdi Zamani **Nano Analysis**, **2014**,
16. The influence of ester additives on the properties of gasoline, H.A. Dabbagh, F. Ghobadi, M.R. Ehsani, M. Moradmamand, **Fuel**, **2013**, .104, 216–223.
17. Mesoporous nano rod-like  $\gamma$ -alumina synthesis using phenol–formaldehyde resin as a template, Hossein A. Dabbagh, Maryam Shahraki, **Microporous and Mesoporous Materials** **2013**, 175, 8–15.
18. The nature of resonance and hyperconjugation for cyclic  $\beta$ -silyl substituted carbocations: NBO, NRT, EDA, and NMR studies, Hossein A. Dabbagh, Mehdi Zamani & Sara Fakhraee, **Res Chem Intermed**, **2013**, 39, 2011–2033.
19. Gas Storage of Simple Molecules in Boron Oxide, Mehdi Zamani, Hossein A. Dabbagh, Hossein Farrokhpour, **International J. of Quantum Chemistry**, **2013**, 113, 2319–2332.
20. Density functional theory study of structure and bonding of water on alumina nanotube, Hossein A. Dabbagh, Mehdi Zamani, **Computational Materials Science**, **2013**, 79 (2013) 781–788.
21. Quantitative analysis of intermolecular forces for hydrogen bond driven self-assembly of resorcinol and bis(pyridine) substituted ethylene cocrystals, before

- and after [2 + 2] dimerization, **Struct Chem**, **2013**, DOI 10.1007/s11224-012-0197-6.
22. DFT investigation of endohedral boron oxide nanocapsules: Encapsulation of He, Ne, Ar, H, N, and Cl atoms, Hossein A. Dabbagh, Mehdi Zamani, Hossein Farrokhpour, **Chemical Physics** , **2012**, 393, 86-95.
  23. DFT, NBO, and NRT analysis of alkyl and benzyl b-silyl substituted cations: carbenium ion vs. silylium ion, Hossein A. Dabbagh • Mehdi Zamani • Sara Fakhraee, **Res Chem Intermed**, **2012**, 38:1551–1570.
  24. Stereoselective (*exo*-Specific) Synthesis, Dynamic <sup>1</sup>H NMR and Quantum Chemical Conformational and Configurational Analysis of Norbornene-Aziridine-*E*-Imidoyl Systems, Hossein A. Dabbagh, and Ali Reza Najafi-Chermahini, **J IRAN CHEM SOC** , **2012**, 9:339–348.
  25. Conformational Stability and Rotational Energy Barrier of RC<sub>60</sub>—C<sub>60</sub>R dimers: Hyperconjugation vs. Steric Effect, H. A. Dabbagh, M. Zamani, H. Mortaji, **J IRAN CHEM SOC**, **2012**, 9:205-223.
  26. Catalytic conversion of alcohols over alumina–zirconia mixed oxides: Reactivity and selectivity, Hossein A. Dabbagh, Mehdi Zamani, **Applied Catalysis A: General**, **2011**, 404, 141–148.
  27. Formation of  $\gamma$ -alumina nanorods in presence of alanine, Hossein A. Dabbagh, Elham Rasti , Mohammad S. Yalfani, Francesc Medina, **Materials Research Bulletin**, **2011**, 46, 271-277.
  28. 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, 1047–1056.

29. Nanoscale surface study and reactions mechanism of 2-butanol over the  $\gamma$ -alumina (100)surface and nanochannel: ADFT study Hossein A. Dabbagha, Mehdi Zamania, BurtronH.Davis, *Journal of Molecular Catalysis A: Chemical*, **2010**, 33, 54-68.
30. Effects of vacuum and calcination temperature on the structure, texture, reactivity, and selectivity of alumina: Experimental and DFT studies Hossein A. Dabbagh, Keivan Taban, Mehdi Zamani, *Journal of Molecular Catalysis A: Chemical*, **2010**, 55–68.
31. Influence of B, Ga and In impurities in the structure and electronic properties of alumina nanoball Hossein A. Dabbagh, Mehdi Zamani, Hossein Farrokhpour, Mansoor Namazian , Hossein Etedali Habibabadi , *Chemical Physics Letters*, **2010**, 485, 176–182.
32. DFT, ab initio, NMR, and NBO analyses of Na-substituted hydrazino acetamides: Experimental vs theoretical values, Hossein A. Dabbagh, Elham Rasti, Philippe Le Grel, Alexandre Hocquet, *Tetrahedron*, **2010**, 66, 2322–2330.
33. Conformational analysis and intramolecular/intermolecular interactions of *N,N'*-dibenzylideneethylenediamine derivatives, Hossein A. Dabbagh, Mehdi Zamani, Hossein Farrokhpour, Mohammad Hossein Habibi, Kazem Barati, *Journal of Molecular Structure*, **2010**, 169-185.
34. 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*, **2010**, 92–100.
35. DFT and ab initio potential energy scan and hydrogen bond analysis of Na-substituted hydrazino acetamides: Characterization of the “hydrazinoturn”



- hydrogen bonding pattern, Hossein A. Dabbagh, Elham Rasti, Alexandre Hocquet,, Philippe Le Grel, **Journal of Molecular Structure: THEOCHEM**, **2009**, 911, 92–97.
36. Dynamic <sup>1</sup>H-NMR demonstration of anomeric effect and structure: conformational and configurational analysis of *N*-2-(1,4-dioxane)-*N*-(*p*-methylbenzenesulfonyl)-*O*-(*p*-methylphenoxy) isourea, Ali Reza Modarresi-Alam and Hossein A. Dabbagh, **Turk J Chem**, **2009**, 33, 607 – 619.
37. Experimental and CIS, TD-DFT, ab initio calculations of visible spectra and the vibrational frequencies of sulfonyl azide-azoic dyes Abbas Teimouria, Alireza Najafi Chermahini, Keivan Taban, Hossein A. Dabbagh **Spectrochimica Acta Part A**, **2009**, 72, 369–377.
38. Spectroscopic, quantum chemical DFT/HF study and synthesis of [2.2.1]hept-2-en-2-amino-*N*-azatricyclo [3.2.1.0<sup>2,4</sup>] octane Abbas Teimouria, Mohammad Emami, Alireza Najafi Chermahini, Hossein A. Dabbagh, **Spectrochimica Acta Part A**, **2009**, 1749–1755.
39. DFT and Ab initio Study of Structure of Sulfonamide Triazenes, H. A. Dabbagh, A. Teimouri and R. shiasi, **Journal of Iranian Chemical Society**, **2008**, 5 (V1), 74-82.
40. Insertion Reaction of Reactive Azo sulfonyl nitrene Dye with Model Hydrocarbons and Hetero-hydrocarbons. Hossein A. Dabbagh\*, Abbas Teimouri, and Alireza Najafi Chermahini, **R Journal of Organic Chemistry**, **2008**, 1464–1470.
41. 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**, 857, 78-84.
42. Theoretical studies on tautomerism of dihydropyrimidine tautomers Alireza Najafi Chermahini, Hossein A. Dabbagh, Abbas Teimouri, **Journal of Molecular Structure: THEOCHEM**, **2008**, 857, 105–110.
43. Stereoslective Asymmetric Application of BINOL-Imidoyl Azides, H. A. Dabbagh, and A. Najafi Chermahini' *R Journal of Organic Chemistry*, **2008**, 1471–1477.
44. *p*-Toluenesulfonic acid a useful and selective reagent for the oxidation of benzoin to benzil under solvent-free condition Nader Noroozi-Pesyan,, Abdul Hossein Dabbagh, *J. Iran. Chem. Res.* **2008**, 123-127.
45. 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 Chermahini, *Journal of Applied Catalysis B: Environmental.*, **2007**, 76, 24-33.
46. Diastereoselective formation of 18-membered ring, BINOL-hydrogen phosphonate dimers: quasi-covalent hydrogen-bonds? Hossein A. Dabbagh, Nader Noroozi-Pesyan, Ali R. Najafi-Chermahini, Brian O. Patrick, and Brian R. James, *Canadian J. of Chemistry*, **2007**, 85, 466-474.
47. Green and efficient diazotization and diazo coupling reactions on clays Hossein A. Dabbagh\*, Abbas Teimouri, Alireza Najafi Chermahini, *Dyes and Pigments* **2007**, 73, 239-244.
48. 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, *Spectrochimica Acta Part A*, **2007**, 67, 437-443.
49. 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, *Spectrochimica Acta Part A* **2007**, 449-459.
50. Synthesis, Characterization and Free Radical Polymerization of New Acrylamide-Based Monomer Containing (1H)-Tetrazole: A Thermal Investigation and Derivatization of the Homopolymer H. A. Dabbagh, Y. Mansoori, *Russian J. Org. Chem.* **2007**, 43, 6, 890-897.
51. Theoretical studies on tautomerism of 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.
52. 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.
53. DFT, ab initio and Experimental NMR study of methyl-2,4-dimethoxysalicylate in vacuo and in solvent, Hossein A. Dabbagh, Sepideh Ziaee Rad, Alireza Najafi Chermahini, *Spectrochimica Acta Part A*, Re submitted.
54. A new family of bis-tetrazole (**BIZOL**) **BINOL**-type ligands, Hossein A. Dabbagh, Alireza Najafi-Chermahini and Soodabeh Banibairami, submitted to *Tetrahedron Lett*, **2006**, 47, 3929-3932.

55. Ab initio and Semiempirical Conformational and Configurational Analysis of N-2-(1,4-Dioxane)-N'-(p-methylbenzenesulfonyl)-O-(p-methylphenoxy) isourea, Hossein A. Dabbagh; Alireza Najafi; Ali Reza Modarresi-Alam, submitted to *Journal of Iranian Chemical Society*, **2006**, 3, 51-58.
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# Oral Presentations

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4. Experimental and Density Functional Theory Investigation of the Role of Oxygen sites of  $\gamma$ -Alumina on Selective Dehydrogenation and/or Dehydration

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