Academic CV

EMPLOYMENT

Name: **Dr Mehdi Bayat**
Department of: **Inorganic Chemistry**
Faculty of Chemistry
Bu-Ali Sina University
Hamedan, Iran
Email:

EDUCATION

	Year	University
Ph.D.	2011	Bu-Ali Sina University
M.Sc	2007	Bu-Ali Sina University
B.Sc	2005	Bu-Ali Sina University

PROFESSIONAL MEMBERSHIPS

Iranian Chemical Society

SKILLS

Inorganic Chemistry, DFT Calculations, Hydrogen Bonding, Schiff Bases, Computational calculation of proton affinity as well as microscopic protonation constants of poly basic molecules in the gas phase., Computational calculation using Gaussin package and another computational software, Theoretical Chemistry, Density Functional Theory, Molecular Magnetism, Ab initio

RESEARCH

- Computational Studies on the structures and nature of metal ligand bonds in inorganic and Bio-inorganic complexes
- Studying the nature of interaction in two body and many body complexes containing van der waals interaction.
- Computational studies on the mechanism of formation of organic and inorganic compounds in both gas phase and solution.
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TEACHING

- General Chemistry I (BS.C)
- Inorganic Chemistry I (BS.C)
- Inorganic Chemistry II (BS.C)
- Group Theory in Chemistry (BS.C)
- Literature Review in Chemistry (BS.C)
- Advance Inorganic Chemistry (MS.C)
- New Topics in Inorganic Chemistry (MS.C)
- New Topics in Inorganic Chemistry (Ph.D)
-

i) Graduate M.Sc

1. Leila Ebrahimkhani(MS.C)
2. Fatemeh. Amraei(MS.C)
3. Negin Ahmadian(MS.C)
4. Elham Soltani(MS.C)
5. Shirin Kamali(MS.C)
6. Azadeh Moumivand(MS.C)

PUBLICATIONS and PRESENTATIONS

(Sort From 2016)

1. S.J. Sabounchei, A. Yousefi, M. Ahmadianpoor, A. Hashemi, M. Bayat, A. Sedghi, F.A. Bagherjeri, R.W. Gable: *A new Pd(II) complex of a sulfur ylide; Synthesis, X-ray characterization, theoretical study and catalytic activity toward the Suzuki-Miyaura reaction*. Polyhedron 06/2016; DOI:10.1016/j.poly.2016.05.046
2. Mehdi Bayat, Fatemeh Amraie, Sadegh Salehzadeh: *Theoretical Studies on Structure, Formation and Nature of bond in a Disila-, Digerma - and Distannacyclobutene Ring*. Journal of Theoretical and Computational Chemistry 04/2016; DOI:10.1142/S0219633616500322
3. Effat Kianpour, Saeid Azizian, Meysam Yarie, Mohammad Ali Zolfigol, Mehdi Bayat: *A task-specific phosphonium ionic liquid as an efficient extractant for green desulfurization of liquid fuel: An experimental and computational study*. The Chemical Engineering Journal 03/2016;

4. Seyyed Javad Sabounchei, Masoumeh Zamanian, Mahbubeh Pourshahbaz, Mehdi Bayat, Roya Karamian, Mostafa Asadbegy: *Synthesis, characterisation and theoretical and antibacterial studies of Hg(II), Cd(II) and Ag(I) complexes with a new monodentate phosphorus ylide*. Journal of Chemical Research 03/2016; 40(3):130. DOI:10.3184/174751916X14537279217786

5. S. J. Sabounchei, Mahmood Ahmadianpoor, Abed Yousefi, Ali Hashemi, Mehdi Bayat, Asieh Sedghi, Fateme Akhlaghi Bagherjeri, Robert W. Gable: *New Pd(II) Complexes of Sulfur Ylide; Synthesis, X-ray Characterization, Theoretical Study and Catalytic Activity toward Mizoroki-Heck Reaction*. RSC Advances 03/2016; DOI:10.1039/C6RA01390B

6. Hassan Keypour, Majid Rezaeivala, Ameneh Ramezani-Aktij, Mehdi Bayat, Nefise Dilek, Hüseyin Ünver: *New macrocyclic Schiff base complexes incorporating a homopiperazine unit: Synthesis of some Co(II), Ni(II),Cu(II) and Zn(II) complexes and crystal structure and theoretical studies*. Journal of Molecular Structure 02/2016; 1115. DOI:10.1016/j.molstruc.2016.02.071

7. Mahshid Saberinasab, Sadegh Salehzadeh, Yazdan Maghsoud, Mehdi Bayat: *The significant effect of electron donating and electron withdrawing substituents on nature and strength of an intermolecular Se...π interaction. A theoretical study*. Computational and Theoretical Chemistry 02/2016; 1078. DOI:10.1016/j.comptc.2015.12.009

8. Mehdi Bayat, Masoud Hatami: *Nature of the Metal-Ligand Bond in some [(CO)4 M←BIIM (R)] {M=Cr, Mo and W, R=H, F, Cl and Br} Complexes: A Theoretical Study*. Polyhedron 02/2016; 110. DOI:10.1016/j.poly.2016.02.022

9. Mehdi Bayat, Leila Ebrahimkhani, Sadegh Salehzadeh: *Where, how and how much the strength of interaction between a hydrated lanthanide cations and a π-system would be increased? A theoretical study.*. Journal of Molecular Liquids 02/2016;

10. Hassan Keypour, Amir Shooshtari, Majid Rezaeivala, Mehdi Bayat, Hadi Amiri Rudbari: *Synthesis and characterization of new Mn(II) and Cd(II) Schiff base complexes containing homopiperazine moiety: Spectral, X-ray crystal structural and theoretical studies*. Inorganica Chimica Acta 10/2015; 440. DOI:10.1016/j.ica.2015.10.027

11. Faranak Dastineh, Sadegh Salehzadeh, Mehdi Bayat, Yazdan Maghsoud: *Comparison of the selectivity of [M(12-Crown-4)]+ (M = Li+, Na+, K+) complexes for halide anions and some neutral molecules; A computational study*. Journal of Theoretical and Computational Chemistry 10/2015; 14(8). DOI:10.1142/S0219633615500571

12. Mehdi Bayat, Negin Ahmadian: *Theoretical studies on structures, stability and nature of C → E (E = Si, Sn) bond in some derivatives of bitriazole- based NHC complexes with five- membered chelate rings*. Journal of the Iranian Chemical Society 09/2015;

13. Eslam Salahifar, Davood Nematollahi, Mehdi Bayat, Amir Mahyari, Hadi Amiri Rudbari: *Regioselective Green Electrochemical Approach to the Synthesis of Nitroacetaminophen Derivatives*. Organic Letters 09/2015; 17(19). DOI:10.1021/acs.orglett.5b01837
14. Mehdi Bayat, Masood Hatami, Hassan Keypour, Sadegh Salehzadeh: *Ab Initio and DFT studies on the Structures, Binding energies and Nature of Bonds in X2Y3 Metal Clusters(X+=Li+, Na+ and K+; Y32-=Zn32-, Cd32- and Hg32-)*. Journal of Theoretical and Computational Chemistry 07/2015;
15. Mehdi Bayat, Negin Ahmadian: *Bis-N-heterocyclic carbene in stabilized [bis-NHC(R) → EBr2H2] (E = Si to Pb) (R = H, F, Cl, Br, CH3, CF3) complexes: A theoretical study*. Polyhedron 04/2015; DOI:10.1016/j.poly.2015.04.032
16. Seyyed Javad Sabounchei, Mahbubeh Pourshahbaz, Sadegh Salehzadeh, Mehdi Bayat, Roya Karamian, Mostafa Asadbegy, Hamid Reza Khavasi: *New Chlorine Bridged Binuclear Silver(I) Complexes of Bidentate Phosphorus Ylides: Synthesis, Spectroscopy, Theoretical and Anti-Bacterial Studies*. Polyhedron 01/2015; DOI:10.1016/j.poly.2014.09.030
17. Sadegh Salehzadeh, Yasin Gholiee, Mehdi Bayat: *The significant role of the solvent in high selectivity of symmetrical calix[4]tubes for potassium ion in solution: A DFT study*. Computational and Theoretical Chemistry 09/2014; 1048. DOI:10.1016/j.comptc.2014.09.013
18. Mehdi Bayat, Sadegh Salehzadeh, Sameneh Hokmi, Yasin Gholiee, Fereshteh Yaghoobi: *Regioselective Diels–Alder reaction of 2-phosphaindolizine with some 1,3-butadiene derivatives (RCHCHCHCH2, R = F, Cl, CH3 and SiH3): A theoretical study*. Journal of Organometallic Chemistry 09/2014; 767:54–59. DOI:10.1016/j.jorganchem.2014.05.020
19. Hassan keypour, Mozhdeh Liyaghati-Delshad, Majid Rezaeivala, Mehdi Bayat: *Synthesis, characterization, antibacterial activities and theoretical studies of Mn(II) and Cd(II) complexes with new macrocyclic Schiff-base ligands incorporating a phenanthroline head unit*. Journal of the Iranian Chemical Society 07/2014; 12(4). DOI:10.1007/s13738-014-0520-9
20. Sadegh Salehzadeh, Fereshteh Yaghoobi, Mehdi Bayat: *Theoretical studies on the interaction of some endohedral fullerenes {[X@C60]− (X=F−, Cl−, Br−) or [M@C60] (M=Li, Na, K)} with [Al(H2O)6]3+ and [Mg(H2O)6]2+ cations*. Computational and Theoretical Chemistry 04/2014; 1034:73-79. DOI:10.1016/j.comptc.2014.01.033
21. Javad Seyyed Sabounchei, Sepideh Samiee, Mahbubeh Pourshahbaz, Sadegh Salehzadeh, Mehdi Bayat, Davood Nematollahi, Roya Karamian, Mostafa Asadbegy: *Synthesis and characterisation of Hg(II) complexes including bidentate phosphorus ylides*. Journal of Chemical Research 01/2014; 38(1). DOI:10.3184/174751914X13863254117794
22. Hadi Beiginejad, Davood Nematollahi, Mehdi Bayat, Fahimeh Varmaghani, Ali Nazaripour: *Experimental and Theoretical Analysis of the Electrochemical Oxidation of Catechol and Hydroquinone Derivatives in the*

Presence of Various Nucleophiles. Journal of The Electrochemical Society 12/2013; 160(10). DOI:10.1149/2.037310jes

23. Sadegh Salehzadeh, Mehdi Bayat, Yasin Gholiee: *A theoretical study on the importance of steric effects, electronic properties, interaction and solvation energies in the 'host–guest' chemistry of protonated azacryptands and halide anions*. Tetrahedron 11/2013; 69(44):9183-9191. DOI:10.1016/j.tet.2013.08.064
24. Sadegh Salehzadeh, Mehdi Khalaj, Saeed Dehghanpour, Mehdi Bayat: *Synthesis and Structure of [Hg2(L)2](NO3)2 (L(4-nitrophenyl)pyridin-2-ylmethylene-amine) a theoretical study on Hg–Hg bond in this and linear Hg2X2 (XF, Cl, Br, I, Ph) complexes*. Journal of the Iranian Chemical Society 10/2013; 11(1). DOI:10.1007/s13738-013-0268-7
25. Seyyed Javad Sabounchei, Mohammad Panahimehr, Sadegh Salehzadeh, Mehdi Bayat, Hamid Reza Khavasi, David Morales-Morales: *Structural, Theoretical, and Spectroscopic Study of Mercury(II) Complexes of two New Unsymmetric Phosphorus Ylides*. Phosphorus, sulfur, and silicon and the related elements 10/2013; 188(12). DOI:10.1080/10426507.2013.779274
26. Davood Nematollahi, Hadi Beiginejad, Fahimeh Varmaghani, Mehdi Bayat: *Efficient Factors on the Hydrolysis Reaction Rate of Some Para-Aminophenol Derivatives in Acidic pHs*. Journal of The Electrochemical Society 09/2013; 160(8). DOI:10.1149/2.084308jes
27. Davood Nematollahi, Hadi Beiginejad, Fahimeh Varmaghani, Mehdi Bayat, Hamid Salehzadeh: *Efficient Factors on the Reaction Rate and Site-Selectivity in Sulfonylation of Catechol and Hydroquinone Derivatives: Experimental and Theoretical Studies*. Journal of The Electrochemical Society 04/2013; DOI:10.1149/2.001307jes
28. Hassan Keypour, Nasibeh Rahpeyma, Majid Rezaeivala, Parisa Arzhangi, Mehdi Bayat, Laura Valencia, Yalcin Elerman, Orhan Büyükgüngör: *Synthesis and structural characterization of a new Schiff base macrocyclic ligand containing a piperazine head unit and its metal complexes. Crystal structure of the Co(II) complex*. Polyhedron 02/2013; 51(1). DOI:10.1016/j.poly.2012.12.020
29. Seyyed Javad Sabounchei, Mehdi Sarlakifar, Mahbubeh Pourshahbaz, Sadegh Salehzadeh, Mehdi Bayat, Hamid Reza Khavasi, Fatemeh Akhlaghi Bagherjeri, Collete Boscovic: *Structural, Theoretical and Multinuclear NMR Study of a New Polymeric Mercury(II) Complex with an Ambidentate Phosphorus Ylide*. Journal of Inorganic and Organometallic Polymers and Materials 12/2012; DOI:10.1007/s10904-012-9793-6
30. Hadi Beiginejad, Davood Nematollahi, Mehdi Bayat: *Electrochemical oxidation of hematoxylin – Part 1: Experimental and theoretical studies in an aqueous acidic medium*. Journal of Electroanalytical Chemistry 07/2012; 681. DOI:10.1016/j.jelechem.2012.05.022

31. Seyyed Javad Sabounchei, Mehdi Sarlakifar, Sadegh Salehzadeh, Mehdi Bayat, Mahbubeh Pourshahbaz, Hamid Reza Khavasi: *Structural, theoretical and multinuclear NMR study of mercury(II) and silver(I) complexes with two new ambidentate phosphorus ylides*. Polyhedron 05/2012; 38(1):131–136. DOI:10.1016/j.poly.2012.02.034

32. Mehdi Bayat, Sadegh Salehzadeh, Gernot Frenking: *Energy decomposition analysis of the metal-imine bond in [(CO)4M–SB] (M = Cr, Mo, W; SB: RHCN–CH2CH2–NCHR)*. Journal of Organometallic Chemistry 01/2012; 697(1):74–79. DOI:10.1016/j.jorganchem.2011.10.024

33. Mehdi Bayat, Fereshteh Yaghoobi, Sadegh Salehzadeh, Samaneh Hokmi: *A theoretical study on the interaction of [Al(H2O)6]3+ and [Mg(H2O)6]2+ cationswith fullerene (C60), coronene and benzene p-systems*. Polyhedron 09/2011; 30(17). DOI:10.1016/j.poly.2011.08.017

34. Mehdi Bayat, Moritz von Hopffgarten, Sadegh Salehzadeh, Gernot Frenking: *Energy decomposition analysis of the metal–oxime bond in [M{RC(NOH)C(NO)R}2] (M = Ni(II), Pd(II), Pt(II), R = CH3, H, F, Cl, Br, Ph, CF3)*. Journal of Organometallic Chemistry 09/2011; 696(18):2976–2984. DOI:10.1016/j.jorganchem.2011.05.009

35. Sadegh Salehzadeh, Mehdi Bayat: *A theoretical study on the formation of "1 + 1" versus "2 + 2" macrocyclic Schiffbase complexes in the absence of coordinated anions*. Journal of Molecular Structure THEOCHEM 07/2011; 971(1-3). DOI:10.1016/j.comptc.2011.05.034

36. Sadegh Salehzadeh, Mehdi Bayat: *Computational evidence of preferred energy and preferred binding energy in the formation of ''1 + 1'' versus ''2 + 2'' macrocyclic Schiff base complexes*. Journal of Molecular Structure THEOCHEM 03/2011; 965(1). DOI:10.1016/j.comptc.2011.01.036

37. Sadegh Salehzadeh, Mehdi Bayat: *Theoretical Studies on the Structure and Protonation of Cu(II) Complexes of a Series of Tripodal Aliphatic Tetraamines: Good Correlations with the Experimental Data*. Journal of Computational Chemistry 10/2010; 31(13):2371-80. DOI:10.1002/jcc.21530

38. Mehdi Bayat, Sadegh Salehzadeh: *Author's personal copy Theoretical studies on the proton affinities of four different series of nano-size diamines and designing strong superbases based on fullerene(C 60) molecule*. Journal of Molecular Structure THEOCHEM 08/2010;

39. Seyyed Javad Sabounchei, Vida Jodaian, Sadegh Salehzadeh, Sepideh Samiee, Alireza Dadrass, Mehdi Bayat, Hamid Reza Khavasi: *Synthesis of New Phosphonium Ylides Containing Thiophene and Furan Rings and Study of Their Reaction with Mercury(II) Halides: Spectral and Structural Characterization*. Helvetica Chimica Acta 06/2010; 93(6). DOI:10.1002/hlca.200900305

40. Sadegh Salehzadeh, Yasin Gholi Ee, Mehdi Bayat: *Complete gas-phase proton microaffinity analysis of five linear tetraamines containing two*

ethylenediamine residues. Journal of Molecular Structure THEOCHEM 05/2010; 952(1-3). DOI:10.1016/j.theochem.2010.04.019

41. Seyyed Javad Sabounchei, Sepideh Samiee, Sadegh Salehzadeh, Zabihollah Bolboli Nojini, Mehdi Bayat, Elisabeth Irran, Marina Borowski: *New mononuclear mercury(II) complexes of a bifunctionalized ylide containing five-membered chelate ring: Spectral and structural characterization*. Inorganica Chimica Acta 04/2010; 363(14). DOI:10.1016/j.ica.2010.05.004
42. Sadegh Salehzadeh, Mehdi Bayat, Leila Davoodi, Reza Golbedaghi, Vida Izadkhah: *Synthesis and characterization of A heptadentate (N4O 3) schiff base ligand and associated La(III), Sm(III) and Gd(III) complexes, and A theoretical study*. Bulletin of the Chemical Society of Ethiopia 03/2010; 24(1):59-66. DOI:10.4314/bcse.v24i1.52961
43. Seyyed Javad Sabounchei, Sepideh Samiee, Sadegh Salehzadeh, Mehdi Bayat, Zabihollah Bolboli Nojini, David Morales-Morales: *Synthesis, characterization, and structural studies of mercury(II) complexes of new bidentate phosphorus ylide*. Inorganica Chimica Acta 02/2010; 363(6). DOI:10.1016/j.ica.2010.01.024
44. Sadegh Salehzadeh, Yasin Gholiee, Mehdi Bayat: *Prediction of Microscopic Protonation Constants of Polybasic Molecules Via Computational Methods: A Complete Microequilibrium Analysis of Spermine*. International Journal of Quantum Chemistry 01/2010; 111(14):3608-3615. DOI:10.1002/qua.22927
45. Mahdi Rezaei Sameti, Mehdi Bayat, Sadegh Salehzadeh: *The DFT study of hydrogen bonding and thermodynamic parameters of (CH 3 OH) n (H 2 O)m (n, m = 1–8) clusters at different temperatures*. Arabian Journal of Chemistry 01/2010; 100. DOI:10.1016/j.arabjc.2011.02.003
46. Sadegh Salehzadeh, Amir Shooshtari, Mehdi Bayat: *Good correlation between the calculated gas-phase first proton macroaffinities of some triazacycloalkanes ([X]aneN 3 , X = 9–12) with their protonation constants in solution*. Journal of Molecular Structure THEOCHEM 08/2009; 911(1-3). DOI:10.1016/j.theochem.2009.07.002
47. Sadegh Salehzadeh, Mehdi Bayat, Fereshteh Yaghoobi: *Theoretical studies on proton affinities of H 2 N–(CH 2) n –NH 2 (n = 2À10) diamines at gas phase. Good correlation with protonation constants in solution*. Journal of Molecular Structure THEOCHEM 05/2009; 906(1-3). DOI:10.1016/j.theochem.2009.04.003
48. Sadegh Salehzadeh, Amir Shooshtari, Mehdi Bayat: *Theoretical studies on the first proton macroaffinity of Ni(II), Cu(II), Zn(II) and Cd(II) complexes of four triazacycloalkanes ([X]ane N-3, X=9-12): good correlations with the formation constants in solution*. Dalton Transactions 05/2009; DOI:10.1039/b822260f
49. Sadegh Salehzadeh, Fereshteh Yaghoobi, Mehdi Bayat: *Illustration of all species and all microspecies involved in full protonation steps of spermine*

and determination of corresponding most abundant and most stable conformers, a gas phase theoretical study. Chemical Physics 04/2009; 361(1-2). DOI:10.1016/j.chemphys.2009.05.002

50. Sadegh Salehzadeh, Amir Shooshtari, Mehdi Bayat: *On the Effects of Methods and Basis-Set in Studying of Proton Macroaffinity of Metal Complexes of Some Triazacycloalkanes*. Asian Journal of Chemistry 01/2009;
51. Vida Izadkhah, Sadegh Salehzadeh, Leila Davoodi, Reza Golbedaghi, Mehdi Bayat: *La(III) complex of assymetrical heptadentate (N4O3) Schiff base*. Asian Journal of Chemistry 01/2009; 21(1):787-794.
52. Sadegh Salehzadeh, Mehdi Bayat, Michael D Ward: *First Reported Correlation between the Calculated Gas-Phase Proton Macroaffinities of Some Metal Complexes with Their Measured Formation Constants in Solution: Zn(II) Complexes of a Series of Tripodal Aliphatic Tetraamines*. The Journal of Physical Chemistry A 06/2008; 112(17):4090-4. DOI:10.1021/jp709603r
53. Seyyed Javad Sabounchei, Hassan Nemattalab, Sadegh Salehzadeh, Sima Khani, Mehdi Bayat, Hamid Reza Khavasi: *Structural, theoretical and multinuclear NMR study of mercury(II) complexes of phosphorus ylides: Mono and binuclear complexes*. Polyhedron 05/2008; 27(8). DOI:10.1016/j.poly.2008.03.009
54. Seyyed Javad Sabounchei, Hassan Nemattalab, Sadegh Salehzadeh, Sima Khani, Mehdi Bayat, Harry Adams, Michael D Ward: *Synthesis and characterization of binuclear mercury(II) complexes of phosphorus ylides, X-ray analysis and multinuclear NMR measurements*. Inorganica Chimica Acta 04/2008; 362(1). DOI:10.1016/j.ica.2008.03.015
55. Seyyed Javad Sabounchei, Hassan Nemattalab, Sadegh Salehzadeh, Mehdi Bayat, Hamid Reza Khavasi, Harry Adams: *New mono and binuclear mercury(II) complexes of phosphorus ylides containing DMSO as ligand: Spectral and structural characterization*. Journal of Organometallic Chemistry 04/2008; 693(11). DOI:10.1016/j.jorganchem.2008.02.025
56. Vida Izadkhah, Sadegh Salehzadeh, Reza Golbedaghi, Mehdi Bayat, Leila Davoodi: *Synthesis and Theoretical Study of Gadolinium(III) Complex of Heptadentate (N 4 O 3) Tripodal Schiff Base Ligand*. Asian Journal of Chemistry 12/2007; 19(7):5505-5512.
57. Sadegh Salehzadeh, Mehdi Bayat: *A Comparison between the Experimental and Theoretical Investigations on Carbon-13 Isotropic Shielding Constants of Some Tripodal Tetraamine Ligands*. Chinese Journal of Chemistry 10/2007; 54(5). DOI:10.1002/jccs.200700164
58. Sadegh Salehzadeh, Mehdi Bayat, Mehdi Hashemi: *Complete Gas-Phase Proton Microaffinity Analysis of Two Bulky Polyamine Molecules*. The Journal of Physical Chemistry A 09/2007; 111(33):8188-92. DOI:10.1021/jp072882v

59. Sadegh Salehzadeh, Mehdi Bayat: *Three new defined proton affinities for polybasic molecules in the gas-phase: Proton microaffinity, proton macroaffinity and proton overallaffinity*. Chemical Physics Letters 07/2006; 427(4-6). DOI:10.1016/j.cplett.2006.06.088

Book Chapters

Mohammad Ali Zolfigol, Mehdi Bayat, Vahid Khakyzadeh: *Opportunity, Weakness and New Horizons in Chemistry of I.R.Iran*. Iranian Chemical Society Newsletter, 9 edited by Mohammad Reza Iravani, 07/2012: chapter 1: pages 3-17; Iranian Chemical Society.