



علوم شیمی و نفت / شیمی تجزیه و شیمی فیزیک

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کتاب

■ کاربرد نظریه ی گروه در شیمی

ناصر صفری، منصور زاهدی

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ارتباط با صنعت

■ مطالعات تجربی بر روی خواص نوری غیر خطی ترکیبات آلی

۱۳۷۳

- Theoretical (DFT) study on the hydroxylation mechanism of Sn(IV)porphyrin: How does Sn(IV)porphyrin inhibit heme oxygenase catalysis function
Farzaneh Pourmand, Mansoor Zahedi, Naser Safari
JOURNAL OF MOLECULAR STRUCTURE, Vol.1253, 2022
- QM study of interaction between arginine amino acid and Au clusters and the effects on arginine acidity
Mina Ghiasi, Shadi Bavafa, Mansoor Zahedi
GOLD BULLETIN, Vol.54, pp. 45-57, 2021
- Separation of CH₄, H₂S, N₂ and CO₂ gases using four types of nanoporous graphene cluster model: a quantum chemical investigation
Mina Ghiasi, Parisa Zeinali, Samira Gholami, Mansoor Zahedi
JOURNAL OF MOLECULAR MODELING, Vol.27, 2021
- Theoretical study of OH⁻ nucleophilic attack on cobalt(II)-verdoheme complex
Farhad Ezadi, Homayoon Bahrami, Mansoor Zahedi
JOURNAL OF PORPHYRINS AND PHTHALOCYANINES, Vol.25, pp. 210-223, 2021
- Computational Design of New Hydroborane Fullerene-Based Pincer Ligands
Maryam Anafcheh, Mansoor Zahedi
JOURNAL OF CLUSTER SCIENCE, Vol.32, pp. 1-10, 2021
- Hydrogenation of Carbon Dioxide into Formic Acid by Aluminum Ligated NNN Pincer Fullerene Through Metal-Ligand H₂O-Assisted Pathway: A Computational Study
Maryam Anafcheh, Mansoor Zahedi
CATALYSIS LETTERS, Vol.151, pp. 1-9, 2021
- Hydroxyl bond activation of formic acid by Metal-ligand cooperation of new designed aluminum ligated pincer fullerenes
Maryam Anafcheh, Mansoor Zahedi
CHEMICAL PHYSICS, Vol.549, 2021
- Computational Design of New N-Heterocyclic Silyl Pincer Fullerenes
Maryam Anafcheh, Mansoor Zahedi
Silicon, Vol..., pp. 1-8, 2021
- BN-Substituted non-classical fullerenes containing square rings
Maryam Anafcheh, Zahra abolfathi, Mansoor Zahedi
PRAMANA-JOURNAL OF PHYSICS, Vol.95, 2021
- Diels-Alder cycloaddition of the silicon-silicon bonds at pentagon junctions of Si-doped non-IPR and SW defective fullerenes
Maryam Anafcheh, Haniyeh Khanmohammadi, Mansoor Zahedi
MONATSHFTE FUR CHEMIE, Vol.152, pp. 241-250, 2021
- Theoretical exploration of the LiF-decorated BN cages as hydrogen storage materials
Maryam Anafcheh, Mansoor Zahedi
MONATSHFTE FUR CHEMIE, Vol.152, pp. 931-938, 2021
- The effect of external electric field and metal impurities on the interaction of HF and boraphene: a computational study
Masoud Arabieh, Mansoor Zahedi
JOURNAL OF MOLECULAR MODELING, Vol.27, 2021
- Design of new pincer fullerene ligands thorough[2+3] cycloaddition of the azomethine ylides to fullerene cage: a DFT study
Maryam Anafcheh, Sara Hossein Ghanemi, Mansoor Zahedi
MOLECULAR SIMULATION, Vol.46, pp. 565-572, 2020
- Coupled Cluster and Quantum Monte-Carlo study of anionic hydrogen clusters $H(3n+1)^-$ (n odd)
Amin Gholamrezamohammadi, Saeed Nasiri, Mansoor Zahedi

■ **Quantum Monte Carlo simulations using Slater-Jastrow-backflow wave function**

Saeed Nasiri, Mansoor Zahedi

Computational and Theoretical Chemistry, Vol.1189, 2020

■ **Quantum Monte Carlo study of ground and first excited state of C, N, O, F, and Ne atoms using Slater-Jastrow-Backflow wave function**

Saeed Nasiri, Mansoor Zahedi

INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY, Vol.120, pp. 1-9, 2020

■ **Carboxylated single-walled carbon nanotubes as a semiconductor for adsorption of acrylamide in mainstream cigarette smoke**

Mehdi Yoosefian, Atef Pakpour, Mansoor Zahedi

PHYSICA E-LOW-DIMENSIONAL SYSTEMS and NANOSTRUCTURES, Vol.124, 2020

■ **Sustainable conversion of carbon dioxide to formic acid with Rh-decorated phosphorous-doped fullerenes: a theoretical study**

Maryam Anafcheh, Mansoor Zahedi

STRUCTURAL CHEMISTRY, Vol.31, pp. 1-10, 2020

■ **Towards Developing Efficient Metalloporphyrin-Based Hybrid Photocatalysts for CO₂ Reduction; An Ab Initio Study**

Azar Ostovan, Nick Papior, Mansoor Zahedi, Alireza Z. Moshfegh

PHYSICAL CHEMISTRY CHEMICAL PHYSICS, Vol.22, pp. 23128-23140, 2020

■ **Addition of borazine to boron nitride nanotubes: [2+2] cycloaddition or bond cleavage**

Maryam Anafcheh, Elaheh Ahmadi, Mansoor Zahedi

MONATSHFTE FÜR CHEMIE, Vol.150, pp. 1019-1024, 2019

■ **QM/MM study of the conversion of biliverdin into verdoheme by heme oxygenase**

Fatemehsadat Alavi, Mansoor Zahedi, Naser Safari, Ulf Ryde

THEORETICAL CHEMISTRY ACCOUNTS, Vol.138, 2019

■ **Formation of boron nitride islands in the graphene nanoflakes: A DFT study**

Maryam Anafcheh, Narges khodaei, Mansoor Zahedi

MATERIALS CHEMISTRY AND PHYSICS, Vol.223, pp. 164-170, 2019

■ **N-N bond cleavage and ring expansion at the surface of exchange and substitutional antisite defective boron nitride nanotubes by boron cluster: A density functional theory study**

Maryam Anafcheh, Nasrin Shahbaz, Mansoor Zahedi

PRAMANA-JOURNAL OF PHYSICS, Vol.93, 2019

■ **A novel mechanism of heme degradation to biliverdin studied by QM/MM and QM calculations**

Fatemehsadat Alavi, Mahin Gheydi, Mansoor Zahedi, Naser Safari, Ryde Ulf

DALTON TRANSACTIONS, Vol.47, pp. 8283-8291, 2018

■ **Thiozonation and thiozonolysis of triatomic sulfur (S₃) on the C₇₀ fullerene: A DFT study**

Maryam Anafcheh, Fereshteh Naderi, Mansoor Zahedi

STRUCTURAL CHEMISTRY, Vol.29, pp. 1299-1306, 2018

■ **Incorporation of topological defects and atomic impurities on the carbon nanotube surface: A DFT study of AD-dimer defects**

Maryam Anafcheh, Fereshteh Naderi, Mansoor Zahedi

HETEROATOM CHEMISTRY, Vol.29, 2018

■ **Polarizability of the Si₆₀H₆₀ Derivatives Containing Epoxide Moieties (Si₆₀H₆₀2_nO_n with n up to 30) A DFT Study**

Maryam Anafcheh, Fereshteh Naderi, Fatemeh Ektefa, Reza Ghafouri, Mansoor Zahedi

JOURNAL OF CLUSTER SCIENCE, Vol.29, pp. 889-896, 2018

■ **Activation modelling of - and -class of carbonic anhydrase with amines and amino acids Proton transfer process**

within the active site from thermodynamic point of view

Mina Ghiasi, Somaye Hemati, Mansoor Zahedi
Computational and Theoretical Chemistry, Vol.1109, pp. 42-57, 2017

■ **Quantum Mechanical Approach for the Catalytic Mechanism of Dinuclear Zinc Metallo--lactamase by Penicillin and Cephalixin Kinetic and Thermodynamic Points of View**

Mina Ghiasi, Noohi Bahareh, Mansoor Zahedi
Physical Chemistry Research, Vol.5, pp. 709-725, 2017

■ **QM/MM Study of the Conversion of Oxophlorin into Verdoheme by Heme Oxygenase**

Fatemehsadat Alavi, Mansoor Zahedi, Naser Safari, Ulf Ryde
JOURNAL OF PHYSICAL CHEMISTRY B, Vol.121, pp. 11427-11436, 2017

■ **Density functional theory studies on the conversion of hydroxyheme to iron-verdoheme in the presence of dioxygen**

Mahin Gheydi, Naser Safari, Mansoor Zahedi
DALTON TRANSACTIONS, Vol.46, pp. 2146-2158, 2017

■ **Fullerene-C60 and crown ether doped on C60 sensors for high sensitive detection of alkali and alkaline earth cations**

Fatemeh Alipour Zagharzi, Mansoor Zahedi, Adeleh Mola, Saboor Abedini, Sattar Arshadi, Saeed Ahmadzadeh, Nazanin Etminan, Omran Younesi, Elham Rahmanifar, Mehdi Yoosefian
PHYSICA E-LOW-DIMENSIONAL SYSTEMS and NANOSTRUCTURES, Vol.87, pp. 51-58, 2017

■ **A benchmark study of Li₂ Li₂ - LiH and LiH - Quantum Monte-Carlo and Coupled-Cluster computations**

Saeed Nasiri, Mansoor Zahedi
Computational and Theoretical Chemistry, Vol.1114, pp. 106-117, 2017

■ **Coupled Cluster and Quantum Monte-Carlo potential energy curves of the ground state of Be₂ and Be₂ molecules**

Saeed Nasiri, Mansoor Zahedi
Computational and Theoretical Chemistry, Vol.1112, pp. 27-36, 2017

■ **Synthesis structural characterization QSAR and docking studies of a new binuclear nickel (II) complex based on the flexible tetradentate N-donor ligand as a potent antibacterial and anticancer agent**

Azizolla Beheshti, Faezeh Hashemi, Fatemeh Behavndi, Mansoor Zahedi, Maryam Kolahi, Hossein Motamedi, Peter Mayer
INTERNATIONAL JOURNAL OF BIOLOGICAL MACROMOLECULES, Vol.104, pp. 1107-1123, 2017

■ **Chlorofluorofullerenes (CFFs)**

Maryam Anafcheh, Fereshteh Naderi, Zahra Khodadadi, Fatemeh Ektefa, Reza Ghafouri, Mansoor Zahedi
STRUCTURAL CHEMISTRY, Vol.28, pp. 1707-1716, 2017

■ **Computational study for the circular redox reaction of N₂O with CO catalyzed by fullerometallic cations C₆₀Fe and C₇₀Fe**

Maryam Anafcheh, Fereshteh Naderi, Zahra Khodadadi, Fatemeh Ektefa, Reza Ghafouri, Mansoor Zahedi
JOURNAL OF MOLECULAR GRAPHICS and MODELLING, Vol.72, pp. 50-57, 2017

■ **The Theoretical and Experimental Studies on Oxidation of Straight Chain Amino Acids in Moderately Concentrated Sulfuric Acid Medium**

Homayoon Bahrami, Gholamreza Jaferian, , Mansoor Zahedi, Ali Akbar Moosavi-Movahedi
INTERNATIONAL JOURNAL OF CHEMICAL KINETICS, Vol.48, pp. 647-659, 2016

■ **Tracing the Fingerprint of Chemical Bonds within the Electron Densities of Hydrocarbons A Comparative Analysis of the Optimized and the Promolecule Densities**

Zahra Alimohammadi Keyvani, Shant Shahbazian, Mansoor Zahedi
CHEMPHYSICHEM, Vol.17, pp. 3260-3268, 2016

■ **Exploration of the binding properties of the human serum albumin sites with neurology drugs by docking and molecular dynamics simulation**

Fatemehsadat Alavi, Rahim Ghadari, Mansoor Zahedi
Journal of the Iranian Chemical Society JICS, Vol.14, pp. 19-35, 2016

■ **To What Extent are Atoms in Molecules Structures of Hydrocarbons Reproducible from the Promolecule Electron Densities**

Zahra Alimohammadi Keyvani, Shant Shahbazian, Mansoor Zahedi
CHEMISTRY-A EUROPEAN JOURNAL, Vol.22, pp. 5003-5009, 2016

■ **Theoretical calculation and prediction for experimental design to obtain spin crossover complexes**

Farshid Shahbazi raz, Maryam Adineh Arehjan, Naser Safari, Mansoor Zahedi
INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY, Vol.116, pp. 1179-1186, 2016

■ **AlSi2P nanotubes a theoretical study**

Reza Ghafouri, Fatemeh Ektefa, Mansoor Zahedi
STRUCTURAL CHEMISTRY, Vol.27, pp. 525-533, 2016

■ **Evaluation of the effect of the chiral centers of Taxol on binding to b-tubulin A docking and molecular dynamics simulation study**

, Fatemehsadat Alavi, Mansoor Zahedi
COMPUTATIONAL BIOLOGY AND CHEMISTRY, Vol.56, pp. 33-40, 2015

■ **Boron-nitride ad-unit and carbon ad-dimer defects in the boron nitride nanotubes**

, , , Mansoor Zahedi
JOURNAL OF PHYSICS AND CHEMISTRY OF SOLIDS, Vol.79, pp. 7-13, 2015

■ **A DFT comparative study of single and double SO2 adsorption on Pt-doped and Au-doped single-walled carbon nanotube**

, Mansoor Zahedi, , Samira Naserian Moghani
APPLIED SURFACE SCIENCE, Vol.349, pp. 864-869, 2015

■ **Comparison of the effects of sucrose molecules on alcohol dehydrogenase folding with those of sorbitol molecules on alcohol dehydrogenase folding using molecular dynamics simulation**

Homayoon Bahrami, Mansoor Zahedi
Journal of the Iranian Chemical Society JICS, Vol.12, pp. 1973-1982, 2015

■ **Theoretical study of the substituent effects on O H BDE of trans-resveratrol derivatives in water and benzene NBO analysis of intramolecular hydrogen bonds**

Elyas Nazarpour Noshadi, Mansoor Zahedi, Erik Klein
STRUCTURAL CHEMISTRY, Vol.26, pp. 47-59, 2015

■ **Characterization of hydrogen bonds in the End-Functionalized Single-Wall Carbon nanotubes A DFT Study**

, , Mansoor Zahedi
NANO, Vol.10, 2015

■ **Accurate potential energy curves of Li2 and LiH A Quantum Monte-Carlo (QMC) study**

Saeed Nasiri, Mansoor Zahedi
CHEMICAL PHYSICS LETTERS, Vol.634, pp. 101-107, 2015

■ **QM study of complexation between natural bilirubin and poly-terthiophene carboxylic acid Mn(II) as a biosensor Temperature and interferences effect**

Mina Ghiasi, Masoumeh Molaei, Mansoor Zahedi
JOURNAL OF THEORETICAL and COMPUTATIONAL CHEMISTRY, Vol.14, 2015

■ **Stone Wales defect formation in the zigzag and armchair BC2N nanotubes ADFT study**

, , Mansoor Zahedi
PHYSICA E-LOW-DIMENSIONAL SYSTEMS and NANOSTRUCTURES, Vol.58, pp. 94-100, 2014

■ **COMPLEXATION OF NANOSCALE ENZYME INHIBITOR WITH CARBONIC ANHYDRASE ACTIVE CENTER A QUANTUM MECHANICAL APPROACH**

, , Mansoor Zahedi
STRUCTURAL CHEMISTRY, Vol.55, pp. 393-404, 2014

■ **A computational study on the mechanism and the transition states of the cyclization of 1-trifluoromethyl-1,3-dicarbonyl compounds with azides to form 1,2,3-triazoles**

Rahim Ghadri Karkaj, Mansoor Zahedi

■ **Chameleonic Nature of Hydroxyheme in Heme Oxygenase and Its Reactivity A Density Functional Theory Study**

Mahin Gheydi, Naser Safari, Mansoor Zahedi
INORGANIC CHEMISTRY, Vol.53, pp. 2766-2775, 2014

■ **Fully and partially exohydrogenated Si80 fullerene cage a DFT study**

, , Mansoor Zahedi
STRUCTURAL CHEMISTRY, Vol.24, pp. 575-581, 2013

■ **DUAL-LEVEL DIRECT DYNAMICS STUDIES ON THE HYDROGEN ABSTRACTION REACTION OF CF3CHF3 (HFC-227ea) WITH Cl ATOM**

, Mansoor Zahedi
JOURNAL OF THEORETICAL and COMPUTATIONAL CHEMISTRY, Vol.12, pp. 1-15, 2013

■ **A Theoretical Study on the Enthalpies of Homolytic and Heterolytic N-H Bond Cleavage in Substituted Melatonin in the Gas-Phase and Aqueous Solution**

, , Erik KLEIN, Mansoor Zahedi
ACTA CHIMICA SLOVENICA, Vol.60, pp. 43-55, 2013

■ **Interaction Modes and Absolute Affinities of α -Amino Acids for Mn²⁺ A Comprehensive Picture**

Mohammadhasan Khodabandeh, Hamidreza Raeesi Harooni, , Karim Zare, Mansoor Zahedi, gills ohanessian
CHEMPHYSICHEM, Vol.14, pp. 1733-1745, 2013

■ **Phenomenal Properties of Gold Nanoclusters with No Chemical Interaction with O₂ Field Effect and Electron Pumping**

Ali Moghaddasi, Mansoor Zahedi
Journal of Physical Chemistry C, Vol.117, pp. 20893-20904, 2013

■ **Investigation of origin of stereo-selectivity of BF₃·Et₂O-promoted allylboration of aldehydes in the presence of (R)-pinanediol by computational method**

Rahim Ghadri Karkaj, , Ahmad Shaabani, Mansoor Zahedi
Computational and Theoretical Chemistry, Vol.999, pp. 28-33, 2012

■ **Effect of Axial Ligand on the Electronic Configuration Spin States and Reactivity of Iron Oxophlorin**

Mahin Gheydi, Naser Safari, Mansoor Zahedi
INORGANIC CHEMISTRY, Vol.51, pp. 7094-7102, 2012

■ **Synthesis of a New Class of Highly Functionalized Phosphorus Ylides Containing Heterocyclic Compounds**

Ahmad Shaabani, Sajjad Keshipour, Morteza Aghaee, Mohammadhasan Khodabandeh, Mansoor Zahedi
CHINESE JOURNAL OF CHEMISTRY, Vol.30, pp. 1893-1900, 2012

■ **Protective effect of rutin (vitamin p) against heme oxidation A quantum mechanical approach**

, , , Mansoor Zahedi
Computational and Theoretical Chemistry, Vol.996, pp. 28-36, 2012

■ **A theoretical elucidation of coordination properties of histidine and lysine to Mn²⁺**

Hamidreza Raeisi Harooni, Mohammadhasan Khodabandeh, Karim Zare, Mansoor Zahedi
INTERNATIONAL JOURNAL OF MASS SPECTROMETRY, Vol.313, pp. 47-54, 2012

■ **Structure and Redox Behavior of Iron Oxophlorin and Role of Electron Transfer in the Heme Degradation Process**

Mahin Gheydi, Naser Safari, Mansoor Zahedi
INORGANIC CHEMISTRY, Vol.51, pp. 12857-12866, 2012

■ **Carbonic anhydrase inhibitors A quantum mechanical study of interaction between some antiepileptic drugs with active center of carbonic anhydrase enzyme**

, , , Mansoor Zahedi
Computational and Theoretical Chemistry, Vol.992, pp. 59-69, 2012

■ **Comparative DFT Study To Determine if -Oxoaldehydes Precursors are for Pentosidine Formation**

Rasool Nasiri, Martin J. Field, Mansoor Zahedi

■ **Density Functional Theory (B3LYP) Study of Substituent Effects on O H Bond Dissociation Enthalpies of trans-Resveratrol Derivatives and the Role of Intramolecular Hydrogen Bonds**

Elyas Nazarpour Noshadi, Mansoor Zahedi,
JOURNAL OF ORGANIC CHEMISTRY, Vol.22, pp. 10093-10104, 2012

■ **Theoretical Study of Site Dependency on Charge Transfer at Au(111) Nanoclusters**

Ali Moghaddasi, Mansoor Zahedi, Philip Watson
Journal of Physical Chemistry C, Vol.116, 2012

■ **Kinetics and mechanism of the permanganate-induced autocatalytic dehydration reaction of L-g-amino-n-butyric acid to give 2-pyrrolidone through a radical intermediate in moderately concentrated acidic medium**

Homayoon Bahrami, Mansoor Zahedi, Moghaddas Bigdeli, ,
PROGRESS IN REACTION KINETICS AND MECHANISM, Vol.36, 2011

■ **Cross-Linking Mechanisms of Arginine and Lysine with -Dicarbonyl Compounds in Aqueous Solution**

Rasool Nasiri, Martin J. Field, Mansoor Zahedi, Ali Akbar Mousavi Movahedi
JOURNAL OF PHYSICAL CHEMISTRY A, Vol.115, pp. 13542-13555, 2011

■ **DFT/B3LYP Study of the Substituent Effect on the Reaction Enthalpies of the Individual Steps of Single Electron Transfer-Proton Transfer and Sequential Proton Loss Electron Transfer Mechanisms of Chroman Derivatives Antioxidant Action**

Meysam Najafi, Mansoor Zahedi, kaveh haghghi mood, erik klein
Computational and Theoretical Chemistry, Vol.969, pp. 1-12, 2011

■ **DFT/B3LYP study of the solvent effect on the reaction enthalpies of homolytic and heterolytic OAH bond cleavage in mono-substituted chromans**

Meysam Najafi, Mansoor Zahedi, Erik Klein
Computational and Theoretical Chemistry, pp. 16-28, 2011

■ **Kinetics and mechanism of the KMnO₄-oxidative catalysed condensation reaction of L-proline to a diketopiperazine**

, Mansoor Zahedi, Homayoon Bahrami, Khosro Jadidi
PROGRESS IN REACTION KINETICS AND MECHANISM, Vol.36, pp. 95-119, 2011

■ **DFT/B3LYP study of the substituent effects on OAH bond dissociation enthalpies of chroman derivatives in the gas phase and solvent environment**

Elyas Nazarpour Noshadi, Mansoor Zahedi, Meysam Najafi
Computational and Theoretical Chemistry, Vol.965, pp. 114-122, 2011

■ **An in silico study on the ring-size effect in ring enlargement Bellus-Claisen rearrangement**

Rahim Ghadri Karkaj, Mansoor Zahedi, , Ahmad Shaabani
Computational and Theoretical Chemistry, Vol.981, pp. 25-30, 2011

■ **theoretical investigation of interaction of sorbitol molecules with alcohol dehydrogenase in aqueous solution using molecular dynamics simulation**

Homayoon Bahrami, Mansoor Zahedi, , ,
CELL BIOCHEMISTRY AND BIOPHYSICS, Vol.59, pp. 79-88, 2011

■ **A new mixed-ligand complex of copper(II) containing N-(2-pyridylmethyl)-2-pyrazinecarboxamide (NPyPzCa) Synthesis molecular and crystal structure and properties of Cu(NPyPzCa)(NO₃)(DMSO)**

Hamidreza Khavasi, Koroush Sasan, Shahin Sowlati Hashjin, Mansoor Zahedi
COMPTES RENDUS CHIMIE, Vol.14, pp. 563-567, 2011

■ **Theoretical studies on models of lysine-arginine cross-links derived from -oxoaldehydes a new mechanism for glucosepane formation**

Rasool Nasiri, Mansoor Zahedi, Jamet Helene, Ali Akbar Moosavi-Movahedi
JOURNAL OF MOLECULAR MODELING, Vol.18, 2011

■ **dft/ b3lyp study of the substituent effect on o-h bond dissociation enthalpies of chroman derivatives in the gas**

phase and solvent environment

Meysam Najafi, Mansoor Zahedi, Elyas Nazarpour Noshadi, ,
Computational and Theoretical Chemistry, Vol.965, pp. 114-122, 2011

■ theoretical investigation of the ring opening process of verdoheme to biliverdin in the presence of dioxygen

Naser Safari, Mahin Gheydi, Mansoor Zahedi
JOURNAL OF MOLECULAR MODELING, pp. 1401-1413, 2010

■ a new chromium (iii) complex containing n-(2 pyridylmethyl)-2- pyrazinecarboxamide (npypzca) synthesis molecular and crystal structure and theoretical electron density analysis

Hamidreza Khavasi, Rohollah Firoozi Asl, Koroosh Sasan, Mansoor Zahedi
SOLID STATE SCIENCES, Vol.12, pp. 1960-1965, 2010

■ a theoretical elucidation of glucose interaction with hsa domains

Rasool Nasiri, Mansoor Zahedi, Homayoon Bahrami, ,
JOURNAL OF BIOMOLECULAR STRUCTURE and DYNAMICS, Vol.28, 2010

■ A new chromium (III) complex containing N-(2-pyridylmethyl)-2-pyrazinecarboxamide (NPyPzCa) Synthesis molecular and crystal structure and theoretical electron density analysis

Hamidreza Khavasi, Rohoullah Firouzi, Koroosh sasan, Mansoor Zahedi
SOLID STATE SCIENCES, Vol.12, pp. 1960-1965, 2010

■ effect of the axial ligands on the structure and reactivity of tin verdoheme in the ring opening process

, Homayoon Bahrami, Mansoor Zahedi, Naser Safari
INORGANICA CHIMICA ACTA, Vol.363, pp. 1577-1586, 2010

■ complexation of glycine by manganese (II) in the gas phase a theoretical study

Mohammadhassan Khodabandeh, , Mansoor Zahedi,
INTERNATIONAL JOURNAL OF MASS SPECTROMETRY, Vol.291, pp. 73-83, 2010

■ Theoretical investigation of interaction of sorbital molecules with alcohol dehydrogenase in aqueous solution using molecular dynamics simulation

Homayoon Bahrami, Mansoor Zahedi, , ,
CELL BIOCHEMISTRY AND BIOPHYSICS, Vol.59, pp. 79-88, 2010

■ kinetics and mechanism of the dehydration reaction of sarcosine to a bislactame through diacyclopentoxide intermediate in strong acidic medium

Homayoon Bahrami, , Maryam Keshavarzi, Mansoor Zahedi, Ayoob Bazgir,
INTERNATIONAL JOURNAL OF CHEMICAL KINETICS, pp. 690-703, 2009

■ Linear regression analysis of molecular energy properties for poly heterocyclic compounds

Rohollah Firoozi Asl, Mansoor Zahedi
JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, pp. 35-40, 2009

■ quantum chemical investigation of intramolecular thione -thiol tautomerism of 1,2,4-triazole -3- thione and its disubstituted derivatives

, Homayoon Bahrami, Zahra Zolmajd Haghighi, Mansoor Zahedi
JOURNAL OF MOLECULAR MODELING, 2009

■ Ab initio studies of BN-acenes and cyclo BN-acenes electronic properties and their dependence on the molecular size and the number of electrons

Rohollah Firoozi Asl, Shahin Sowlati Hashjin, Mansoor Zahedi
JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, pp. 1-7, 2009

■ KINETICS AND MECHANISM OF THE PERMANGANATE - INDUCED OXIDATIVE CATALYTIC CONDENSATION OF SARCOSINE TO A DIKETOPIPERAZINE

Zahra Khati Dizabadi, Mahdi Davari Dolatabadi, Homayoon Bahrami, Mansoor Zahedi
PROGRESS IN REACTION KINETICS AND MECHANISM, Vol.34, pp. 453-478, 2009

■ theoretical investigations on the hydrolysis pathway of tin verdoheme complexes elucidation of tin s ring opening inhibition role

, Homayoon Bahrami, Mansoor Zahedi, Naser Safari

■ **linear regression analysis of molecular energy properties for poly heterocyclic compounds**

Rohollah Firoozi Asl, Mansoor Zahedi

JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, Vol.906, pp. 35-40, 2009

■ **how tin metal prevents verdoheme ring opening comparative study of various nucleophiles**

, Homayoon Bahrami, Mansoor Zahedi, Naser Safari

JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, Vol.908, pp. 1-11, 2009

■ **Noninnocent effect of axial ligand on the heme degradation process a theoretical approach to hydrolysis pathway of verdoheme to biliverdin**

Parisa Rajabali Jamaat, Naser Safari, , , Mansoor Zahedi

JOURNAL OF BIOLOGICAL INORGANIC CHEMISTRY, Vol.13, pp. 121-132, 2008

■ **Introduction of a novel additivity scheme coincidence with homodesmicity concept for (CH)_xN_y (x y 6) molecules**

Rohollah Firoozi Asl, Mansoor Zahedi

JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, pp. 1-7, 2008

■ **Polyacenes electronic properties and their dependence on molecular size**

Rohollah Firoozi Asl, Mansoor Zahedi

JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, pp. 7-15, 2008

■ **conclusive evidence for delayed autocatalytic behavior of Mn(II) ions at a critical concentration**

Homayoon Bahrami, Mansoor Zahedi

Journal of the Iranian Chemical Society JICS, Vol.5, pp. 535-545, 2008

■ **theoretical study on the kinetics and mechanism of the reaction of cyclohexyl isocyanide and 1,1,1,5,5,5-hexafluoropentane-2,4-dione using dft method**

Ahmad Shaabani, , , Mansoor Zahedi, Homayoon Bahrami

JOURNAL OF THEORETICAL and COMPUTATIONAL CHEMISTRY, Vol.7, pp. 1227-1250, 2008

■ **Conclusive evidence on the insensitivity of additive rules to the combinational details of exchange and correlation functional in hybrid DFT methods**

Rohollah Firoozi Asl, Mansoor Zahedi

INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY, Vol.108, pp. 1-11, 2008

■ **A Theoretical Elucidation of Bilirubin Interaction With HSA's Lysines First Electrostatic binding Site in IIA Subdomain**

Homayoon Bahrami, Mansoor Zahedi, , ,

BIOPHYSICAL CHEMISTRY, Vol.125, pp. 357-387, 2007

■ **An ab initio quantum chemical comparative study of possible additive rules and linear relations in parent and extended sulfur diimide families**

Shant Shahbazian, , Mansoor Zahedi

THEORETICAL CHEMISTRY ACCOUNTS, Vol.117, pp. 153-161, 2007

■ **Theoretical investigations of the hydrolysis pathway of verdoheme to biliverdin**

, Naser Safari, , Mansoor Zahedi

JOURNAL OF INORGANIC BIOCHEMISTRY, Vol.101, pp. 385-395, 2007

■ **The concept of Chemical bond Some like it fuzzy but others concrete**

Mansoor Zahedi

Foundations of Chemistry, 2006

■ **Theoretical Investigations of the Reactivity of Verdoheme Analogues Opening of the Planar Macrocycle by Amide Dimethyl Amide and Hydroxide Nucleophiles to Form Helical Biliverdin Type Complexes**

, Mansoor Zahedi, Naser Safari

JOURNAL OF INORGANIC BIOCHEMISTRY, Vol.100, pp. 1449-1461, 2006

■ **the role of observables and non-observables in chemistry a critique of chemical language**

, Mansoor Zahedi

■ **Delayed Autocatalytic Behavior of Mn(II) Ions at a Critical Ratio The Effect of Structural Isomerism on Permanganic Oxidation of L-norleucine**

Mansoor Zahedi, Homayoon Bahrami

INTERNATIONAL JOURNAL OF CHEMICAL KINETICS, Vol.38, pp. 1-11, 2006

■ **Calorimetric and binding dissections of HSA upon interaction with bilirubin**

, , Mansoor Zahedi, , , Homayoon Bahrami, ,

PROTEIN JOURNAL, Vol.25, pp. 193-201, 2006

■ **towards a complete basis set limit of hartree_ fock method correlation-consistent versus polarized-consistent basis sets**

, Mansoor Zahedi

THEORETICAL CHEMISTRY ACCOUNTS, Vol.113, pp. 152-160, 2005

■ **modeling of biliverdin reduction process regio-specificity and H-bonding**

Mansoor Zahedi, , Naser Safari

CHEMICAL PHYSICS, Vol.310, pp. 179-187, 2005

■ **Toward complete basis set limit of Hartree-Fock method Correlation consistent versus polarized consistent basis sets**

Mansoor Zahedi

THEORETICAL CHEMISTRY ACCOUNTS, Vol.113, 2005

■ **autoacceleration/degradation of electrochemical polymerization of substituted anilines**

, Mansoor Zahedi, , ,

POLYMER, Vol.46, pp. 11476-11483, 2005

■ **An Ab initio Investigation of Sulfur Diimides Stability of Various Conformers and Conformational Analysis. PART III. The effect of moieties (X) on the SN2H(X) hierarchy**

Mansoor Zahedi

JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, Vol.673, 2004

■ **Kinetics and Mechanism of the Oxidation of L- -Amino-n-Butyric Acid in Moderately Concentrated Sulfuric Acid Medium**

Mansoor Zahedi

CANADIAN JOURNAL OF CHEMISTRY, Vol.82, 2004

■ **Kinetics and Mechanism of the Autocatalytic Oxidation of L-Asparagine in Moderately Concentrated Sulfuric Acid Medium**

Mansoor Zahedi

KINETICS AND CATALYSIS, Vol.45, 2004

■ **A Theoretical Investigation of Electronic Ground State of Parent Sulfur Diimide (PSD)**

Shant Shahbazian, Mansoor Zahedi, Ng SW

JOURNAL OF MOLECULAR SPECTROSCOPY, Vol.223, 2004

■ **An Ab initio Quantum Chemical Study of Cumulative Double Bonds Stability of Various Conformers and Charge Distribution Analysis PART I. XY2H2 Hierarchy (X O S Se and Y N P As)**

Mansoor Zahedi

JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, Vol.683, 2004

■ **Prediction of Novel Complexation of porphine and BF3 Is it a 1 1 or 1 2 species**

Mansoor Zahedi

CHEMICAL PHYSICS, Vol.301, pp. 1-7, 2004

■ **Unique1 2 adduct formation of meso-tetraarylporphyrins and meso -tetraalkylporphyrins with BF3 a spectroscopic and ab initio study**

, Mansoor Zahedi, , , Naser Safari, Hamidreza Khavasi,

NEW JOURNAL OF CHEMISTRY, Vol.28, pp. 1600-1607, 2004

■ **Unique 1 2 adduct formations of meso-tetra-arylporphyrins and -alkylporphyrins with BF₃ a spectroscopic and ab initio study**

Mansoor Zahedi
NEW JOURNAL OF CHEMISTRY, Vol.28, 2004

■ **Prediction of novel complexation of porphine and BF₃ Is it 1 1 or 1 2 species**

Mansoor Zahedi, Hamidreza Khavasi, , Naser Safari,
CHEMICAL PHYSICS, Vol.301, 2004

■ **An ab initio/hybrid (ONIOM) investigation of biliverdin isomers and metal biliverdin analogue complexes**

Naser Safari, Mansoor Zahedi, Homayoon Bahrami, Shant Shahbazian, Seik Weng Ng
JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, Vol.633, 2003

■ **An Ab initio/Hybrid (ONIOM) Investigation of Biliverdin Isomers and Metal-Biliverdin Analogue Complexes**

Mansoor Zahedi
JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, Vol.633, 2003

■ **An Ab initio Investigation of Sulfur Diimides Stability of Various Conformers and Conformational Analysis. PART I. Parent Sulfur Diimide**

Mansoor Zahedi
JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, Vol.629, 2003

■ **An Ab initio Investigation of Sulfur Diimides Stability of Various Conformers and Conformational Analysis. PART II. Dimethyl Sulfur Diimides (DMSD)**

Mansoor Zahedi
JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, Vol.636, 2003

■ **Theoretical Studies of Biliverdin Energetics of the Reduction Pathways to Bilirubin**

Mansoor Zahedi
JOURNAL OF MOLECULAR MODELING, Vol.8, 2002

■ **Stability Factors Among Fullerene C₆₀ Complete Set Isomers**

Mansoor Zahedi
indain j.chem, Vol.41B, 2002

■ **SEMIEMPIRICAL MOLECULAR ORBITAL CALCULATIONS OF CONFIGURATIONAL PROPERTIES OF DIHALOGENATED SULFUR DIIMIDES**

Mansoor Zahedi, Ahmad Shaabani,
INDIAN JOURNAL OF CHEMISTRY SECTION B-ORGANIC CHEMISTRY INCLUDING MEDICINAL CHEMISTRY, Vol.40b, 2001

■ **Semiempirical Molecular Orbital Calculation of Azobenzene Stability Study of Isomers and Mechanism of E/Z Isomerization**

Mansoor Zahedi
JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, Vol.506, 2000

■ **Semiempirical Molecular Orbital Calculations of Biliverdin Study the Dynamics and Energetics of the Self-association of a Two-Electron Oxidation Product**

Mansoor Zahedi
JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, Vol.531, 2000

■ **Semiempirical molecular orbital calculations of biliverdin Study of dynamics and energetics of the self-association of a two-electron oxidation product**

Naser Safari, Mansoor Zahedi, S Haddadpour
Theoretical Chemistry, Vol.531, pp. 79-79, 2000

■ **SEMIEMPIRICAL MOLECULAR ORBITAL CALCULATION OF AZOBENZENE STABILITY STADY OF ISOMERS AND MECHANISM OF E/Z ISOMERIZATION**

Ahmad Shaabani, Mansoor Zahedi
JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, Vol.506, 2000

■ **Resonance Stabilization Study of Some Fullerenes C_n (20 ≤ n ≤ 88) Is n = 32 a Magic Number**

Mansoor Zahedi

■ SEMIEMPIRICAL MOLECULAR ORBITAL CALCULATIONS OF BILIVERDINE TABILITY STUDY OF VARIOUS ISOMERS AND CONFORMATION ANALYSIS

Mansoor Zahedi, Ahmad Shaabani, Naser Safari

JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, Vol.425, 1998

■ Semiempirical Molecular Orbital Calculations of Biliverdin Stability study of Various Isomers and Conformation Analysis

Mansoor Zahedi

JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, Vol.452, 1998

■ Non-adiabatic Interactions in Excited C₂H Molecules and Their Relationship to C₂ Formation in Comets

Mansoor Zahedi

ASTROPHYSICS AND SPACE SCIENCE, Vol.236, 1996

■ Dissociation Dynamics in the Photolysis of C₂H₂ and C₂H at 193.3 nm

Mansoor Zahedi

A Chemical Festschrift MIT Press Cambridge Mass, 1994

■ 266nm CH₃I Photodissociation CH₃ Spectra and Population Distributions by Coherent Raman Spectroscopy

Mansoor Zahedi

j.chem.phys, Vol.6, 1994

■ Use of Seeded Nd YAG Lasers for High Resolution Spectroscopy

Mansoor Zahedi

OPTICS LETTERS, 1993

■ Rate Constant for CN Reactions with Hydrocarbons and the Product HCN Vibrational Populations Examples of Heavy-Light-Heavy Abstraction Reaction

Mansoor Zahedi

j.chem.phys, Vol.96, 1992

■ High Resolution Study of The v₁ Vibration of CH₃ by Coherent Raman Photofragment Spectroscopy

Mansoor Zahedi

j.chem.phys, Vol.96, 1992

بررسی نظری مکانیسم کاتالیستی و مهار آنتی بیوتیک های بتالاکتام بامتالوبتالاکتامها در حلال ها و دماهای مختلف با استفاده از محاسبات

■ مکانیک کوانتومی

منصور زاهدی، Bahare Noohi، مینا غیائی

نشریه علوم دانشگاه خوارزمی، نسخه ۱۴، صفحات: ۲۳۹-۲۵۸، ۱۳۹۳

مقالات علمی ارائه شده در همایش ها

■ Theoretical investigations of the hydrolysis pathway of verdoxheme to biliverdin effect of axial ligand

Naser Safari, Parisa Rajabali Jamaat, , Mansoor Zahedi

13th international conference on biological inorganic chemistry, pp.220-220

■ Theoretical Study on the role of axial ligand in the Hydrolysis Pathway of Verdoxheme to Biliverdine

, Parisa Rajabali Jamaat, , Naser Safari, Mansoor Zahedi

9th Iranian Inorganic Chemistry Conference, pp.160-160

■ SEMIEMPIRICAL MOLECULAR ORBITAL CALCULATION OF AZOBENZENE STABILITY STADY OF ISOMERS AND MECHANISM OF E/Z ISOMERIZTION

Ahmad Shaabani, Mansoor Zahedi

The 5th World Congress of Theoretically Oriented Chemists

■ SEMIEMPIRICAL MOLECULAR ORBITAL CALCULATION OF BILIVERDINE STABILITY STADY OF VARIOUS ISOMERS AND CONFORMATIONAL ANALYSIS

پایان نامه ها و رساله های دکتری

بررسی مکانیسم تخریب هیم و تبدیل آن به بیلی وردین و وردوهیم و مطالعات اثرات آنزیم – بروتئین با استفاده از شبیه سازی دینامیک مولکولی

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