

NBO 2013 - 1352 references  
Compiled by Ariel Andrea on 4/3/2014

- Aal, S. A.; Shalabi, A. S.; Halim, W. S. A.  
*Interaction of O-2 and N-2 molecules with Au deposited on regular and defective CaO (001) surfaces: Density functional calculations*  
Thin Solid Films, (545): 341-352 2013.
- Abarenkov, I. V.; Boyko, M. A.; Sushko, P. V.  
*Localized directed orbitals representing chemical bonds in ion-covalent crystals*  
International Journal of Quantum Chemistry, (113): 1868-1876 2013.
- Abdel-Ghani, N. T.; E-Ghar, M. F. A.; Mansour, A. M.  
*Novel Ni(II) and Zn(II) complexes coordinated by 2-arylaminoethyl-1H-benzimidazole: Molecular structures, spectral, DFT studies and evaluation of biological activity*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (104): 134-142 2013.
- Abe, M.; Watanabe, S.; Tamura, H.; Boinapally, S.; Kanahara, K.; Fujiwara, Y.  
*Substituent Effect on Reactivity of Triplet Excited State of 2,3-Diazabicyclo 2.2.1 hept-2-enes, DBH Derivatives: alpha C-N Bond Cleavage versus beta C-C Bond Cleavage*  
Journal of Organic Chemistry, (78): 1940-1948 2013.
- Abney, C. W.; Liu, S. B.; Lin, W. B.  
*Tuning Amidoximate to Enhance Uranyl Binding: A Density Functional Theory Study*  
Journal of Physical Chemistry A, (117): 11558-11565 2013.
- Abou-Chahine, F.; Preston, T. J.; Dunning, G. T.; Orr-Ewing, A. J.; Greetham, G. M.; Clark, I. P.; Towrie, M.; Reid, S. A.  
*Photoisomerization and Photoinduced Reactions in Liquid CCl4 and CHCl3*  
Journal of Physical Chemistry A, (117): 13388-13398 2013.
- Abraham, M. Y.; Wang, Y. Z.; Xie, Y. M.; Gilliard, R. J.; Wei, P. R.; Vaccaro, B. J.; Johnson, M. K.; Schaefer, H. F.; Schleyer, P. V.; Robinson, G. H.  
*Oxidation of Carbene-Stabilized Diarsenic: Diarsene Dications and Diarsenic Radical Cations*  
Journal of the American Chemical Society, (135): 2486-2488 2013.
- Abrahamo, O.; Machado, A. E. D.; Silva, F. F. S.; Madurro, J. M.; de Castro, C. M.; Sonoda, M. T.  
*Tyramine electropolymerization revisited by DFT and experimental study*  
Journal of Molecular Structure, (1037): 200-208 2013.
- Aceves-Hernandez, J. M.; Vazquez, I. N.; Hinojosa-Torres, J.; Carrillo, G. P.; Razo, G. A.; Ruvalcaba, R. M.  
*Sibutramine characterization and solubility, a theoretical study*  
Journal of Molecular Structure, (1038): 163-169 2013.
- Acosta-Silva, C.; Bertran, J.; Branchadell, V.; Oliva, A.  
*Quantum Mechanical Study on the Mechanism of Peptide Release in the Ribosome*  
Journal of Physical Chemistry B, (117): 3503-3515 2013.
- Adams, R. D.; Wong, Y. O.; Zhang, Q.  
*Studies of the Structures and Bonding of Gold-Bridged Dirhenium Carbonyl Cluster Complexes*  
Organometallics, (32): 7540-7546 2013.

- Adeniyi, A. A.; Ajibade, P. A.  
*Effects of bidentate coordination on the molecular properties rpta-C based complex using theoretical approach*  
Journal of Molecular Modeling, (19): 1325-1338 2013.
- Adeniyi, A. A.; Ajibade, P. A.  
*Insights into the Intramolecular Properties of eta 6-Arene-Ru-Based Anticancer Complexes Using Quantum Calculations*  
Journal of Chemistry, 2013.
- Adhikari, U.; Scheiner, S.  
*First Steps in Growth of a Polypeptide toward beta-Sheet Structure*  
Journal of Physical Chemistry B, (117): 11575-11583 2013.
- Adhikari, U.; Scheiner, S.  
*Magnitude and Mechanism of Charge Enhancement of CH center dot center dot O Hydrogen Bonds*  
Journal of Physical Chemistry A, (117): 10551-10562 2013.
- Adhikari, U.; Scheiner, S.  
*Preferred Configurations of Peptide-Peptide Interactions*  
Journal of Physical Chemistry A, (117): 489-496 2013.
- Afifi, M. S.; Farag, R. S.; Shaaban, I. A.; Wilson, L. D.; Zoghaib, W. M.; Mohamed, T. A.  
*Infrared and NMR spectra, tautomerism, vibrational assignment, normal coordinate analysis, and quantum mechanical calculations of 4-amino-5-pyrimidinecarbonitrile*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (111): 277-289 2013.
- Afonin, A. V.; Ushakov, I. A.; Pavlov, D. V.; Petrova, O. V.; Sobenina, L. N.; Mikhaleva, A. I.; Trofimov, B. A.  
*Structural studies of meso-CF3-3(5)-aryl(hetaryl)- and 3,5-diaryl(dihetaryl)-BODIPY dyes by H-1, C-13 and F-19 NMR spectroscopy and DFT calculations*  
Journal of Fluorine Chemistry, (145): 51-57 2013.
- Afonin, A. V.; Ushakov, I. A.; Pavlov, D. V.; Schmidt, E. Y.; Dvorko, M. Y.  
*Structural peculiarities of configurational isomers of 1-styrylpyrroles according to H-1, C-13 and N-15 NMR spectroscopy and density functional theory calculations: electronic and steric hindrance for planar structure*  
Magnetic Resonance in Chemistry, (51): 339-349 2013.
- Agarwal, P.; Choudhary, N.; Gupta, A.; Tandon, P.  
*Density functional theory studies on the structure, spectra (FT-IR, FT-Raman, and UV) and first order molecular hyperpolarizability of 2-hydroxy-3-methoxy-N-(2-chloro-benzyl)-benzaldehyde-imine: Comparison to experimental data*  
Vibrational Spectroscopy, (64): 134-147 2013.
- Agarwala, H.; Ehret, F.; Chowdhury, A. D.; Maji, S.; Mobin, S. M.; Kaim, W.; Lahiri, G. K.  
*Electronic structure and catalytic aspects of Ru(tpm)(bqdi)(Cl/H2O) (n), tpm = tris(1-pyrazolyl)-methane and bqdi = o-benzoquinonediimine*  
Dalton Transactions, (42): 3721-3734 2013.
- Ahmed, A. A.  
*Density functional study of the intramolecular proton transfer and conformations in hydroxyaminosilanethione*  
Journal of Molecular Structure, (1032): 5-11 2013.

- Aiswaryalakshmi, P.; Mani, D.; Arunan, E.  
*Fe as Hydrogen/Halogen Bond Acceptor in Square Pyramidal Fe(CO)<sub>5</sub>*  
Inorganic Chemistry, (52): 9153-9161 2013.
- Akbari, A.; Ahmadi, M.; Takjoo, R.; Heinemann, F. W.  
*X-ray structure and theoretical studies on a palladium(II) Schiff base complex*  
Journal of Coordination Chemistry, (66): 1866-1875 2013.
- Akhtari, K.; Hassanzadeh, K.; Fakhraei, B.; Fakhraei, N.; Hassanzadeh, H.; Zarei, S. A.  
*A density functional theory study of the reactivity descriptors and antioxidant behavior of Crocin*  
Computational and Theoretical Chemistry, (1013): 123-129 2013.
- Albertin, G.; Antoniutti, S.; Bonaldo, L.; Botter, A.; Castro, J.  
*Azo Complexes of Osmium(II): Preparation and Reactivity of Organic Azide and Hydrazine Derivatives*  
Inorganic Chemistry, (52): 2870-2879 2013.
- Albrecht, C.; Schneider, E.; Engeser, M.; Schnakenburg, G.; Espinosa, A.; Streubel, R.  
*Synthesis and DFT calculations of spirooxaphosphirane complexes*  
Dalton Transactions, (42): 8897-8906 2013.
- Alcaide, B.; Almendros, P.; del Campo, T. M.; Quiros, M. T.; Soriano, E.; Marco-Contelles, J. L.  
*Controlled Heterocyclization/Cross-Coupling Domino Reaction of beta,gamma-Allenols and alpha-Allenic Esters: Method and Mechanistic Insight for the Preparation of Functionalized Buta-1,3-dienyl Dihydropyrans*  
Chemistry-a European Journal, (19): 14233-14244 2013.
- Alekseev, N. V.  
*A quantum chemical study of alkoxy derivatives of three-coordinate aluminum*  
Journal of Structural Chemistry, (54): 484-491 2013.
- Alen, S.; Sajan, D.; Vijayan, N.; Chaitanya, K.; Nemeč, I.; Jothy, V. B.  
*Growth, electronic absorption and vibrational spectral analysis of semiorganic nonlinear optical material potassium acid phthalate: A scaled quantum mechanical force field study*  
Journal of Molecular Structure, (1040): 155-163 2013.
- Alexandrova, A. N.; Nechay, M. R.; Lydon, B. R.; Buchan, D. P.; Yeh, A. J.; Tai, M. H.; Kostrikin, I. P.; Gabrielyan, L.  
*The same in the bulk but different as clusters: X<sub>3</sub>Y<sub>3</sub> (X = B, Al, Ga; Y = P, As)*  
Chemical Physics Letters, (588): 37-42 2013.
- Alizadeh, D.; Jamshidi, Z.; Shayesteh, A.  
*Spin-orbit and relativistic all-electron potential energy curves for the ground and low-lying excited states of AgAu*  
Physical Chemistry Chemical Physics, (15): 18678-18687 2013.
- Al-Jibori, S. A.; Al-Nassiry, A. I. A.; Hogarth, G.; Salassa, L.  
*Platinum and palladium bis(diphenylphosphino) ferrocene (dppf) complexes with heterocyclic N-acetamide ligands: Synthesis and molecular structures of MCl(sac)(kappa(2)-dppf) (M = Pt, Pd, sac = saccharinate), PtCl(ata)(kappa(2)-dppf) and Pt(ata)(2)(kappa(2)-dppf) (ataH = N-(2-thiazolyl)acetamide)*  
Inorganica Chimica Acta, (398): 46-53 2013.
- Al-Jibori, S. A.; Dayaaf, N. A.; Mohammed, M. Y.; Merzweiler, K.; Wagner, C.; Hogarth, G.; Richmond, M. G.

- cis-trans Isomerism at Square-Planar MN<sub>2</sub>S<sub>2</sub> Centers (M = Pd, Pt): Crystal Structures of N-Phenyl-N-(2-thiazoyl)thiourea Complexes trans-Pd(S<sub>2</sub>N<sub>3</sub>C<sub>10</sub>H<sub>8</sub>)(<sub>2</sub>) and cis-Pt(S<sub>2</sub>N<sub>3</sub>C<sub>10</sub>H<sub>8</sub>)(<sub>2</sub>) and Density Functional Calculations*  
Journal of Chemical Crystallography, (43): 365-372 2013.
- Alkorta, I.; Elguero, J.; Del Bene, J. E.  
*Pnicogen Bonded Complexes of PO<sub>2</sub>X (X = F, Cl) with Nitrogen Bases*  
Journal of Physical Chemistry A, (117): 10497-10503 2013.
- Alkorta, I.; Elguero, J.; Del Bene, J. E.  
*Pnicogen-Bonded Cyclic Trimers (PH<sub>2</sub>X)(<sub>3</sub>) with X = F, Cl, OH, NC, CN, CH<sub>3</sub>, H, and BH<sub>2</sub>*  
Journal of Physical Chemistry A, (117): 4981-4987 2013.
- Alkorta, I.; Sanchez-Sanz, G.; Elguero, J.; Del Bene, J. E.  
*Exploring (NH<sub>2</sub>F)(<sub>2</sub>), H<sub>2</sub>FP:NFH<sub>2</sub>, and (PH<sub>2</sub>F)(<sub>2</sub>) Potential Surfaces: Hydrogen Bonds or Pnicogen Bonds?*  
Journal of Physical Chemistry A, (117): 183-191 2013.
- Allan, C. J.; Cooper, B. F. T.; Cowley, H. J.; Rawson, J. M.; Macdonald, C. L. B.  
*Non-Innocent Ligand Effects on Low-Oxidation-State Indium Complexes*  
Chemistry-a European Journal, (19): 14470-14483 2013.
- Alparone, A.  
*Electron correlation effects and density analysis of the first-order hyperpolarizability of neutral guanine tautomers*  
Journal of Molecular Modeling, (19): 3095-3102 2013.
- Alvarez-Ros, M. C.; Palafox, M. A.  
*Molecular structure of the nucleoside analogue inosine using DFT methods: Conformational analysis, crystal simulations and possible behaviour*  
Journal of Molecular Structure, (1047): 358-371 2013.
- Amalanathan, M.; Joe, I. H.; Rastogi, V. K.  
*Molecular structure and vibrational spectral investigation of charge transfer NLO crystal Naphthalene Picrate for THz application*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (108): 256-267 2013.
- Amalanathan, M.; Xavier, T. S.; Joe, I. H.; Rastogi, V. K.  
*Normal coordinate analysis and Nonlinear Optical Response of cross-conjugated system 4,4-Dimethyl Benzophenone*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (116): 574-583 2013.
- Amaro-Estrada, J. I.; Maron, L.; Ramirez-Solis, A.  
*Aqueous Solvation of Hg(OH)(<sub>2</sub>): Energetic and Dynamical Density Functional Theory Studies of the Hg(OH)(<sub>2</sub>)-(H<sub>2</sub>O) (n=1-24) Structures*  
Journal of Physical Chemistry A, (117): 9069-9075 2013.
- Ammar, H. Y.; Eid, K. M.  
*NO<sub>2</sub> Interaction with Au Atom Adsorbed on Perfect and Defective MgO(100) Surfaces: Density Functional Theory Calculations*  
Journal of Nanoscience and Nanotechnology, (13): 6660-6671 2013.
- An, S. J.; Yin, B.; Liu, P.; Li, X. N.; Li, C.; Li, J. L.; Shi, Z.

- Microwave-Assisted Cascade Cycloaddition for C-N Bond Formation: An Approach to the Construction of 1,4,5,6-Tetrahydropyrimidine and 2-Imidazoline Derivatives*  
Synthesis-Stuttgart, (45): 2525-2532 2013.
- An, X. L.; Zhuo, H. Y.; Wang, Y. Y.; Li, Q. Z.  
*Competition between hydrogen bonds and halogen bonds in complexes of formamidine and hypohalous acids*  
Journal of Molecular Modeling, (19): 4529-4535 2013.
- Anafcheh, M.; Ghafouri, R.; Naderi, F.  
*Electronic and Chemical Characterization of Aluminum-Nitrogen (AlN) Substituted Fullerenes: C58AlN to C24Al12N12*  
Journal of Cluster Science, (24): 327-339 2013.
- Anbazhagan, R.; Sankaran, K. R.  
*Syntheses, spectral characterization, single crystal X-ray diffraction and DFT computational studies of novel thiazole derivatives*  
Journal of Molecular Structure, (1050): 73-80 2013.
- Andrada, K. F. C.; Peisino, L. E.; Guney, M.; Dastan, A.; Pierini, A. B.  
*Nucleophilic substitution of bromonorborenes and derivatives by electron transfer reactions*  
Organic & Biomolecular Chemistry, (11): 955-965 2013.
- Andrade, L. A. F.; Silla, J. M.; Duarte, C. J.; Rittner, R.; Freitas, M. P.  
*The preferred all-gauche conformations in 3-fluoro-1,2-propanediol*  
Organic & Biomolecular Chemistry, (11): 6766-6771 2013.
- Andrejeva, A.; Gardner, A. M.; Graneek, J. B.; Plowright, R. J.; Breckenridge, W. H.; Wright, T. G.  
*Theoretical Study of M<sup>+</sup>-RG(2) (M<sup>+</sup> = Li, Na, Be, Mg; RG = He-Rn)*  
Journal of Physical Chemistry A, (117): 13578-13590 2013.
- Andrejic, M.; Mata, R. A.  
*Study of ligand effects in aurophilic interactions using local correlation methods*  
Physical Chemistry Chemical Physics, (15): 18115-18122 2013.
- Andrews, L.; Thanthiriwatte, K. S.; Wang, X. F.; Dixon, D. A.  
*Thorium Fluorides ThF, ThF<sub>2</sub>, ThF<sub>3</sub>, ThF<sub>4</sub>, ThF<sub>3</sub>(F-2), and ThF<sub>5</sub>- Characterized by Infrared Spectra in Solid Argon and Electronic Structure and Vibrational Frequency Calculations*  
Inorganic Chemistry, (52): 8228-8233 2013.
- Anglada, J. M.; Hoffman, G. J.; Slipchenko, L. V.; Costa, M. M.; Ruiz-Lopez, M. F.; Francisco, J. S.  
*Atmospheric Significance of Water Clusters and Ozone-Water Complexes*  
Journal of Physical Chemistry A, (117): 10381-10396 2013.
- Anju, R. S.; Roy, D. K.; Mondal, B.; Ramkumar, V.; Ghosh, S.  
*An Early-Late Transition Metal Hybrid Analogue of Hexaborane(12)*  
Organometallics, (32): 4618-4623 2013.
- Antony, S.; Bayse, C. A.  
*Density Functional Theory Study of the Attack of Ebselen on a Zinc-Finger Model*  
Inorganic Chemistry, (52): 13803-13805 2013.
- Anusha, C.; De, S.; Parameswaran, P.

- Ring contraction of six-membered metallabenzynes to five-membered metal-carbene complexes: a comparison with organic analogues*  
Dalton Transactions, (42): 14733-14741 2013.
- Arab, A.; Gobal, F.; Nahali, N.; Nahali, M.  
*Electronic and Structural Properties of Neutral, Anionic, and Cationic RhxCu<sub>4-x</sub>(x=0-4) Small Clusters: A DFT Study*  
Journal of Cluster Science, (24): 273-287 2013.
- Aragoni, M. C.; Arca, M.; Bencini, A.; Caltagirone, C.; Garau, A.; Isaia, F.; Light, M. E.; Lippolis, V.; Lodeiro, C.; Mameli, M.; Montis, R.; Mostallino, M. C.; Pintus, A.; Puccioni, S.  
*Zn<sup>2+</sup>/Cd<sup>2+</sup> optical discrimination by fluorescent chemosensors based on 8-hydroxyquinoline derivatives and sulfur-containing macrocyclic units*  
Dalton Transactions, (42): 14516-14530 2013.
- Ari, H.; Buyukmumcu, Z.; Ozpozan, T.; Ilhan, I. O.; Bahadir, O.  
*Vibrational and theoretical analysis of pentyl-4-benzoyl-1,2,4-dinitrophenyl-5-phenyl-1H-pyrazole-3-carboxylate*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (110): 193-204 2013.
- Arivazhagan, M.; Arunagiri, C.; Subashini, A.  
*Quantum chemical determination of molecular geometries and interpretation of FT-IR and FT-Raman spectra for 3,4-dinitrotoluene*  
Indian Journal of Pure & Applied Physics, (51): 191-201 2013.
- Arivazhagan, M.; Jeyavijayan, S.; Geethapriya, J.  
*Conformational stability, vibrational spectra, molecular structure, NBO and HOMO-LUMO analysis of 5-nitro-2-furaldehyde oxime based on DFT calculations*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (104): 14-25 2013.
- Arjunan, V.; Govindaraja, S. T.; Jayapraksh, A.; Mohan, S.  
*Structural, vibrational and nuclear magnetic resonance investigations of 4-bromoisoquinoline by experimental and theoretical DFT methods*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (107): 62-71 2013.
- Arjunan, V.; Govindaraja, S. T.; Subramanian, S.; Mohan, S.  
*Conformational analysis, spectroscopic and quantum chemical investigations of 2-bromo-3-nitroacetophenone*  
Journal of Molecular Structure, (1037): 73-84 2013.
- Arjunan, V.; Jayaprakash, A.; Carthigayan, K.; Periandy, S.; Mohan, S.  
*Conformational, structural, vibrational and quantum chemical analysis on 4-aminobenzohydrazide and 4-hydroxybenzohydrazide - A comparative study*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (108): 100-114 2013.
- Arjunan, V.; Jayaprakash, A.; Santhanam, R.; Marchewka, M. K.; Mohan, S.  
*Electronic structure simulations of 2,6-dimethyl-2,5-heptadien-4-one by FTIR, FT-Raman, NMR, UV-vis, NBO and density functional theory*  
Molecular Simulation, (39): 185-198 2013.
- Arjunan, V.; Kalaivani, M.; Marchewka, M. K.; Mohan, S.  
*Crystal structure, vibrational and DFT simulation studies of melaminium dihydrogen phosphite monohydrate*

- Journal of Molecular Structure, (1045): 160-170 2013.
- Arjunan, V.; Kalaivani, M.; Marchewka, M. K.; Mohan, S.  
*Structural and vibrational spectral investigations of melaminium maleate monohydrate by FTIR, FT-Raman and quantum chemical calculations*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (107): 90-101 2013.
- Arjunan, V.; Kalaivani, M.; Senthilkumari, S.; Mohan, S.  
*Vibrational, NMR and quantum chemical investigations of acetoacetanilide, 2-chloroacetoacetanilide and 2-methylacetoacetanilide*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (115): 154-174 2013.
- Arjunan, V.; Raj, A.; Mythili, C. V.; Mohan, S.  
*Vibrational, electronic and quantum chemical studies of 5-benzimidazole carboxylic acid*  
Journal of Molecular Structure, (1036): 326-340 2013.
- Arjunan, V.; Raj, A.; Santhanam, R.; Marchewka, M. K.; Mohan, S.  
*Structural, vibrational, electronic investigations and quantum chemical studies of 2-amino-4-methoxybenzothiazole*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (102): 327-340 2013.
- Arjunan, V.; Raj, A.; Subramanian, S.; Mohan, S.  
*Vibrational, electronic and quantum chemical studies of 1,2,4-benzenetricarboxylic-1,2-anhydride*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (110): 141-150 2013.
- Arjunan, V.; Sakiladevi, S.; Marchewka, M. K.; Mohan, S.  
*FTIR, FT-Raman, FT-NMR and quantum chemical investigations of 3-acetylcoumarin*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (109): 79-89 2013.
- Arjunan, V.; Santhanam, R.; Rani, T.; Rosi, H.; Mohan, S.  
*Conformational, vibrational, NMR and DFT studies of N-methylacetanilide*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (104): 182-196 2013.
- Arjunan, V.; Santhanam, R.; Sakiladevi, S.; Marchewka, M. K.; Mohan, S.  
*Synthesis and characterization of an anticoagulant 4-hydroxy-1-thiocoumarin by FTIR, FT-Raman, NMR, DFT, NBO and HOMO-LUMO analysis*  
Journal of Molecular Structure, (1037): 305-316 2013.
- Arjunan, V.; Santhanam, R.; Subramanian, S.; Mohan, S.  
*Primidone - An antiepileptic drug - characterisation by quantum chemical and spectroscopic (FTIR, FT-Raman, H-1, C-13 NMR and UV-Visible) investigations*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (109): 282-297 2013.
- Armakovic, S.; Armakovic, S. J.; Setrajcic, J. P.; Dzambas, L. D.  
*Specificities of boron disubstituted sumanenes*  
Journal of Molecular Modeling, (19): 1153-1166 2013.
- Arshadi, S.; Asghari, A.; Raheimi, H.; Abedini, S.  
*Influence of Pyrazine Ring Doping on the N-15 and B-11 NMR and Electronic Structure Parameters in Zigzag Boron Nitride Nanotube: A DFT Study*  
Journal of Chemistry, 2013.

Artem'ev, A. V.; Gusarova, N. K.; Bagryanskaya, I. Y.; Doronina, E. P.; Verkhoturova, S. I.; Sidorkin, V. F.; Trofimov, B. A.

*Alkali Metal Thioselenophosphinates, M SeSPR2 : One-Pot Multicomponent Synthesis, DFT Study, and Synthetic Application*

European Journal of Inorganic Chemistry: 415-426 2013.

Asghari, S.; Haghdadi, M.; Ahangar, S. M.; Ramezani, S.

*One-pot synthesis of N-substituted 2,4-thiazolidinediones and computational investigation of the products*  
Monatshefte für Chemie, (144): 337-343 2013.

Ashikari, Y.; Shimizu, A.; Nokami, T.; Yoshida, J.

*Halogen and Chalcogen Cation Pools Stabilized by DMSO. Versatile Reagents for Alkene Difunctionalization*

Journal of the American Chemical Society, (135): 16070-16073 2013.

Atkinson, S. J.; Robertson, H. E.; Holbling, M.; du Mont, W. W.; Mitrofan, C.; Hassler, K.; Masters, S. L.

*Do halogen and methyl substituents have electronic effects on the structures of simple disilanes? An experimental and theoretical study of the molecular structures of the series X3SiSiMe3 (X = H, F, Cl and Br)*  
Structural Chemistry, (24): 851-857 2013.

Audran, G.; Bremond, P.; Ibanou, M. B. B.; Marque, S. R. A.; Roubaud, V.; Siri, D.

*Chemically triggered C-ON bond homolysis in alkoxyamines: regioselectivity and chemoselectivity*  
Organic & Biomolecular Chemistry, (11): 7738-7750 2013.

Audran, G.; Bremond, P.; Marque, S. R. A.; Gaudel-Siri, A.; Siri, D.; Santelli, M.

*Theoretical modelling of the epoxidation of vinylallenes to give cyclopentenones*  
Tetrahedron Letters, (54): 6607-6610 2013.

Aviles-Moreno, J. R.; Quesada-Moreno, M. M.; Lopez-Gonzalez, J. J.; Martinez-Haya, B.

*Chiral Recognition of Amino Acid Enantiomers by a Crown Ether: Chiroptical IR-VCD Response and Computational Study*

Journal of Physical Chemistry B, (117): 9362-9370 2013.

Awual, M. R.; Ismael, M.; Yaita, T.; El-Safty, S. A.; Shiwaku, H.; Okamoto, Y.; Suzuki, S.

*Trace copper(II) ions detection and removal from water using novel ligand modified composite adsorbent*  
Chemical Engineering Journal, (222): 67-76 2013.

Aysina, J.; Maranzana, A.; Tonachini, G.; Tosi, P.; Ascenzi, D.

*Growth of polyphenyls via ion-molecule reactions: An experimental and theoretical mechanistic study*  
Journal of Chemical Physics, (138) 2013.

Azar, R. J.; Horn, P. R.; Sundstrom, E. J.; Head-Gordon, M.

*Useful lower limits to polarization contributions to intermolecular interactions using a minimal basis of localized orthogonal orbitals: Theory and analysis of the water dimer*  
Journal of Chemical Physics, (138) 2013.

Azizkarimi, S.; Omidyan, R.; Azimi, G.

*Electronically excited states of protonated phenol and para-substituted phenol*  
Chemical Physics Letters, (555): 19-25 2013.

Azofra, L. M.; Alkorta, I.; Toro-Labbe, A.; Elguero, J.

*Modeling the mechanism of glycosylation reactions between ethanol, 1,2-ethanediol and methoxymethanol*



- Physical Chemistry Chemical Physics, (15): 14026-14036 2013.
- Azofra, L. M.; Altarsha, M.; Ruiz-Lopez, M. F.; Ingrosso, F.  
*A theoretical investigation of the CO<sub>2</sub>-philicity of amides and carbamides*  
Theoretical Chemistry Accounts, (132) 2013.
- Baei, M. T.  
*Si-Doped B<sub>12</sub>N<sub>12</sub> Nanocage as an Adsorbent for Dissociation of N<sub>2</sub>O to N-2 Molecule*  
Heteroatom Chemistry, (24): 476-481 2013.
- Bagchi, S.; Mandal, D.; Ghosh, D.; Das, A. K.  
*Interaction Between Group IIb Divalent Transition-Metal Cations and 3-Mercaptopropionic Acid: A Computational and Topological Perspective*  
Journal of Physical Chemistry A, (117): 1601-1613 2013.
- Baggioli, A.; Meille, S. V.; Raos, G.; Po, R.; Brinkmann, M.; Famulari, A.  
*Intramolecular CH/interactions in alkylaromatics: Monomer conformations for poly(3-alkylthiophene) atomistic models*  
International Journal of Quantum Chemistry, (113): 2154-2162 2013.
- Bagheri, S.; Masoodi, H. R.; Mohammadi, M.; Zakarianezhad, M.; Makiabadi, B.  
*The influence of number of nitrogen atoms on the NMR data in aromatic azine center dot center dot center dot HF complexes*  
Chemical Physics Letters, (572): 26-31 2013.
- Bai, G.; Yi, H. B.; Li, H. J.; Xu, J. J.  
*Hydration characteristics of Ca<sup>2+</sup> and Mg<sup>2+</sup>: a density functional theory, polarized continuum model and molecular dynamics investigation*  
Molecular Physics, (111): 553-568 2013.
- Bai, X. B.; Li, Q. Z.; Li, R.; Cheng, J. B.; Li, W. Z.  
*Is a MH (M = Be and Mg) radical a better electron donor in halogen-hydride interaction?: A theoretical comparison with HMM*  
International Journal of Quantum Chemistry, (113): 1293-1298 2013.
- Balachandran, J.; Reddy, P.; Dunietz, B. D.; Gavini, V.  
*End-Group Influence on Frontier Molecular Orbital Reorganization and Thermoelectric Properties of Molecular Junctions*  
Journal of Physical Chemistry Letters, (4): 3825-3833 2013.
- Balachandran, V.; Karthick, T.; Perumal, S.; Nataraj, A.  
*Comparative theoretical studies on natural atomic orbitals, natural bond orbitals and simulated UV-visible spectra of N-(methyl)phthalimide and N-(2 bromoethyl)phthalimide*  
Indian Journal of Pure & Applied Physics, (51): 178-184 2013.
- Balachandran, V.; Nataraj, A.; Karthick, T.  
*Molecular structure, spectroscopic (FT-IR, FT-Raman) studies and first-order molecular hyperpolarizabilities, HOMO-LUMO, NBO analysis of 2-hydroxy-p-toluic acid*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (104): 114-129 2013.
- Balachandran, V.; Parimala, K.

- Molecular structures, FT-IR and FT-Raman spectra, NBO analysis, NLO properties, reactive sites and quantum chemical calculations of keto-enol tautomerism (2-amino-4-pyrimidinol and 2-amino-pyrimidine-4(1H)-one)*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (102): 30-51 2013.
- Balachandran, V.; Rajeswari, S.; Lalitha, S.  
*Vibrational spectra, NBO analysis, first order hyperpolarizabilities, thermodynamic functions and NMR chemical shielding anisotropy (CSA) parameters of 5-nitro-2-furoic acid by ab initio HF and DFT calculations*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (113): 268-280 2013.
- Balachandran, V.; Rajeswari, S.; Lalitha, S.  
*Vibrational spectral analysis, computation of thermodynamic functions for various temperatures and NBO analysis of 2,3,4,5-tetrachlorophenol using ab initio HF and DFT calculations*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (101): 356-369 2013.
- Balachandran, V.; Santhi, G.; Karpagam, V.  
*Spectroscopic (FT-IR and FT-Raman) studies, NBO, HOMO-LUMO, NMR analyses and thermodynamics functions of 5-bromo-2-methoxybenzaldehyde*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (106): 262-274 2013.
- Balachandran, V.; Santhi, G.; Karpagam, V.; Lakshmi, A.  
*Molecular structure, spectroscopic (FT-IR, FT-Raman), NBO and HOMO-LUMO analyses, computation of thermodynamic functions for various temperatures of 2, 6-dichloro-3-nitrobenzoic acid*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (110): 130-140 2013.
- Bandyopadhyay, R.; Nguyen, J. H.; Swidan, A.; Macdonald, C. L. B.  
*Water and Ammonia Complexes of Germanium(II) Dications*  
Angewandte Chemie-International Edition, (52): 3469-3472 2013.
- Banerjee, S.; Mukherjee, A. K.  
*Interactions of the aquated forms of the anticancer drug AMD443 with DNA purine bases: A detailed computational approach*  
Inorganica Chimica Acta, (400): 130-141 2013.
- Bankiewicz, B.; Palusiak, M.  
*The shape of the halogen atom-anisotropy of electron distribution and its dependence on basis set and method used*  
Structural Chemistry, (24): 1297-1306 2013.
- Baranac-Stojanovic, M.  
*Cyclic pi Electron De localization in Fluoroborazines*  
Journal of Physical Chemistry A, (117): 11540-11547 2013.
- Baranac-Stojanovic, M.; Stojanovic, M.  
*Substituent effects on cyclic electron delocalization in symmetric B- and N- trisubstituted borazine derivatives*  
Rsc Advances, (3): 24108-24117 2013.
- Barnett, C. B.; Naidoo, K. J.  
*PNP Diminishes Guanosine Glycosidic Bond Strength Through Restrictive Ring Pucker as a Precursor to Phosphorylation*  
Journal of Physical Chemistry B, (117): 6019-6026 2013.

- Barry, B. M.; Stein, B. W.; Larsen, C. A.; Wirtz, M. N.; Geiger, W. E.; Waterman, R.; Kemp, R. A.  
*Metal Complexes (M = Zn, Sn, and Pb) of 2-Phosphinobenzenethiolates: Insights into Ligand Folding and Hemilability*  
Inorganic Chemistry, (52): 9875-9884 2013.
- Bartlett, G. J.; Newberry, R. W.; VanVeller, B.; Raines, R. T.; Woolfson, D. N.  
*Interplay of Hydrogen Bonds and  $n \rightarrow \pi^*$  Interactions in Proteins*  
Journal of the American Chemical Society, (135): 18682-18688 2013.
- Basaric, N.; Doslic, N.; Ivkovic, J.; Wang, Y. H.; Veljkovic, J.; Mlinaric-Majerski, K.; Wan, P.  
*Excited State Intramolecular Proton Transfer (ESIPT) from Phenol to Carbon in Selected Phenyl naphthols and Naphthylphenols*  
Journal of Organic Chemistry, (78): 1811-1823 2013.
- Baschieri, A.; Sambri, L.; Gualandi, I.; Tonelli, D.; Monti, F.; Degli Esposti, A.; Armaroli, N.  
*Carbazole-terpyridine donor-acceptor luminophores*  
Rsc Advances, (3): 6507-6517 2013.
- Bashir, A.; Ajibewa, T.; Ogbazghi, F.; Alia, J. D.  
*Natural bond orbitals related to the  $pK_a$  of carboxyl acids and phenols*  
Abstracts of Papers of the American Chemical Society, (245) 2013.
- Bee, S.; Agarwal, P.; Gupta, A.; Tandon, P.  
*Use of vibrational spectroscopy to study 2-4-(N-dodecanoylamino)phenyl-5-(4-nitrophenyl)-1,3,4-oxadiazole: A combined theoretical and experimental approach*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (114): 236-255 2013.
- Belosevic, S.; Cendic, M.; Djukic, M.; Vasojevic, M.; Meetsma, A.; Matovic, Z. D.  
*Crystal structure, configurational and density functional theory analysis of nickel(II) complexes with pentadentate 1,3-pd3a-type ligands*  
Inorganica Chimica Acta, (399): 146-153 2013.
- Belyakov, A. V.; Baskakov, A. A.; Ivanov, A. D.; Garabadzhiu, A. V.; Arnason, I.  
*Conformational preferences of fluorocyclohexane and 1-fluoro-1-silacyclohexane molecules: ab initio study and NBO analysis*  
Structural Chemistry, (24): 763-768 2013.
- Ben Yaghlane, S.; Cotton, C. E.; Francisco, J. S.; Linguerrri, R.; Hochlaf, M.  
*Ab initio structural and spectroscopic study of HPS<sub>x</sub> and HSP<sub>x</sub> (x=0,+1,-1) in the gas phase*  
Journal of Chemical Physics, (139) 2013.
- Benedikt, U.; Schneider, W. B.; Auer, A. A.  
*Modelling electrified interfaces in quantum chemistry: constant charge vs. constant potential*  
Physical Chemistry Chemical Physics, (15): 2712-2724 2013.
- Benitez, J. I.; Flores, R.; Castro, M.  
*Theoretical study for the adsorption of CO on neutral and charged Pd-13 clusters*  
Canadian Journal of Chemistry-Revue Canadienne De Chimie, (91): 1033-1042 2013.
- Benson, M. T.; Harrup, M. K.; Gering, K. L.  
*Lithium binding in fluorinated phosphazene trimers*  
Computational and Theoretical Chemistry, (1005): 25-34 2013.

- Berger, G.  
*Using conceptual density functional theory to rationalize regioselectivity: A case study on the nucleophilic ring-opening of activated aziridines*  
Computational and Theoretical Chemistry, (1010): 11-18 2013.
- Berger, G.; Gelbcke, M.; Cauet, E.; Luhmer, M.; Neve, J.; Dufrasne, F.  
*Synthesis of N-15-labeled vicinal diamines through N-activated chiral aziridines: tools for the NMR study of platinum-based anticancer compounds*  
Tetrahedron Letters, (54): 545-548 2013.
- Berges, J.; Fourre, I.; Pilme, J.; Kozelka, J.  
*Quantum Chemical Topology Study of the Water-Platinum(II) Interaction*  
Inorganic Chemistry, (52): 1217-1227 2013.
- Bernhammer, J. C.; Frison, G.; Huynh, H. V.  
*Electronic Structure Trends in N-Heterocyclic Carbenes (NHCs) with Varying Number of Nitrogen Atoms and NHC-Transition-Metal Bond Properties*  
Chemistry-a European Journal, (19): 12892-12905 2013.
- Bhatia, S.; Malkhede, Y. J.; Bharatam, P. V.  
*Existence of dynamic tautomerism and divalent N(I) character in N-(pyridin-2-yl)thiazol-2-amine*  
Journal of Computational Chemistry, (34): 1577-1588 2013.
- Bi, F. Z.; Gao, J.; Wang, L. L.; Du, L. K.; Song, B.; Liu, C. B.  
*Polarization-enhanced bonding process of halogen bond, a theoretical study on F-H/F-X (X = F, Cl, Br, I) and ammonia*  
Chemical Physics, (426): 16-22 2013.
- Billes, F.; Hernanz, A.; Mikosch, H.; Bratu, I.  
*Structure and vibrational spectroscopy of the fenbufen-beta-cyclodextrin inclusion complex*  
Vibrational Spectroscopy, (69): 30-39 2013.
- Biswal, H. S.; Bhattacharyya, S.; Wategaonkar, S.  
*Molecular-Level Understanding of Ground- and Excited-State O-H center dot center dot center dot O Hydrogen Bonding Involving the Tyrosine Side Chain: A Combined High-Resolution Laser Spectroscopy and Quantum Chemistry Study*  
Chemphyschem, (14): 4165-4176 2013.
- Blanco, F.; Kelly, B.; Sanchez-Sanz, G.; Trujillo, C.; Alkorta, I.; Elguero, J.; Rozas, I.  
*Non-Covalent Interactions: Complexes of Guanidinium with DNA and RNA Nucleobases*  
Journal of Physical Chemistry B, (117): 11608-11616 2013.
- Bleiker, E.; Boer, M.; Kluijft, I.; Hartig, A.; Hahn, D.; Plukker, J.; Sijmons, R.; Hillegersberg, R.; Cats, A.; Ausems, M.  
*Multidisciplinary Care for CDH1 Carriers Opting for Prophylactic Gastrectomy*  
Psycho-Oncology, (22): 25-25 2013.
- Bochevarov, A. D.; Harder, E.; Hughes, T. F.; Greenwood, J. R.; Braden, D. A.; Philipp, D. M.; Rinaldo, D.; Halls, M. D.; Zhang, J.; Friesner, R. A.  
*Jaguar: A high-performance quantum chemistry software program with strengths in life and materials sciences*  
International Journal of Quantum Chemistry, (113): 2110-2142 2013.

- Bolgova, A. I.; Lugovik, K. I.; Subbotina, J. O.; Slepukhin, P. A.; Bakulev, V. A.; Belskaya, N. P.  
*Unexpected result for the acylation of arylhydrazonoethanethioamides*  
Tetrahedron, (69): 7423-7429 2013.
- Bomble, L.; Steinmann, S. N.; Perez-Peralta, N.; Merino, G.; Corminboeuf, C.  
*Bonding analysis of planar hypercoordinate atoms via the generalized BLW-LOL*  
Journal of Computational Chemistry, (34): 2242-2248 2013.
- Bontemps, S.; Devillard, M.; Mallet-Ladeira, S.; Bouhadir, G.; Miqueu, K.; Bourissou, D.  
*Phosphino-Boryl-Naphthalenes: Geometrically Enforced, Yet Lewis Acid Responsive P -> B Interactions*  
Inorganic Chemistry, (52): 4714-4720 2013.
- Boo, B. H.; Kim, J. H.  
*Fluorescence and Fluorescence Excitation Spectroscopy of 5,8-Dihydroxy-1,4-naphthoquinone. Analysis of the Electronic Spectra via the Time-Dependent DFT Calculation*  
Bulletin of the Korean Chemical Society, (34): 309-312 2013.
- Bouacha, S.; Nacereddine, A. K.; Djerourou, A.  
*A theoretical study of the mechanism, stereoselectivity and Lewis acid catalyst on the Diels-Alder cycloaddition between furan and activated alkenes*  
Tetrahedron Letters, (54): 4030-4033 2013.
- Braunschweig, H.; Damme, A.; Dewhurst, R. D.; Kramer, T.; Ostreicher, S.; Radacki, K.; Vargas, A.  
*Ditopic Ambiphilicity of an Anionic Dimetalloborylene Complex*  
Journal of the American Chemical Society, (135): 2313-2320 2013.
- Brea, O.; Yanez, M.; Mo, O.; Lamsabhi, A.  
*On the stability of (uracil)(2)-Cu (2+) complexes in the gas phase. Different pathways for the formation of (uracil-H)(uracil)-Cu (+) monocations*  
Organic & Biomolecular Chemistry, (11): 3862-3870 2013.
- Bretschneider, A.; Andrada, D. M.; Dechert, S.; Meyer, S.; Mata, R. A.; Meyer, F.  
*Preorganized Anion Traps for Exploiting Anion-pi Interactions: An Experimental and Computational Study*  
Chemistry-a European Journal, (19): 16988-17000 2013.
- Brizuela, A. B.; Raschi, A. B.; Castillo, M. V.; Leyton, P.; Romano, E.; Brandan, S. A.  
*Theoretical structural and vibrational properties of the artificial sweetener sucralose*  
Computational and Theoretical Chemistry, (1008): 52-60 2013.
- Broeckaert, L.; Frenking, G.; Geerlings, P.; De Proft, F.  
*Reactivity of Dicoordinated Stannylenes (Sn-0) versus Stannylenes (Sn-II): An Investigation Using DFT-Based Reactivity Indices*  
Chemphyschem, (14): 3233-3247 2013.
- Broeckaert, L.; Turek, J.; Olejnik, R.; Ruzicka, A.; Biesemans, M.; Geerlings, P.; Willem, R.; De Proft, F.  
*Combined NMR and DFT Study on the Complexation Behavior of Lappert's Tin(II) Amide*  
Organometallics, (32): 2121-2134 2013.
- Brovarets, O. O.; Zhurakivsky, R. O.; Hovorun, D. M.  
*DFT tautomerization of the long Aa (TM) A\* Watson-Crick base pair formed by the amino and imino tautomers of adenine: combined QM and QTAIM investigation*  
Journal of Molecular Modeling, (19): 4223-4237 2013.

Bruna, P.; Decken, A.; Greer, S.; Grein, F.; Jenkins, H. D. B.; Mueller, B.; Passmore, J.; Paulose, T. A. P.; Rautiainen, J. M.; Richardson, S.; Schriver, M. J.

*Synthesis of (TDAE)(O<sub>2</sub>SSO<sub>2</sub>)(s) and Discovery of (TDAE)(O<sub>2</sub>SSSSO<sub>2</sub>)(s) Containing the First Polythionite, O<sub>2</sub>SSSSO<sub>2</sub> (2-)*

Inorganic Chemistry, (52): 13651-13662 2013.

Bruna, P.; Decken, A.; Grein, F.; Passmore, J.; Rautiainen, J. M.; Richardson, S.; Whidden, T.

*Synthesis of N(CH<sub>3</sub>)(4) (2)O<sub>3</sub>SOSO<sub>2</sub>(s) and N(CH<sub>3</sub>)(4) (2) (O<sub>2</sub>SO)(2)SO<sub>2</sub> center dot SO<sub>2</sub>(s) Containing (SO<sub>4</sub>)(SO<sub>2</sub>)(x)(2-) x=1, 2, Members of a New Class of Sulfur Oxydianions*

Inorganic Chemistry, (52): 7193-7202 2013.

Buhl, M.; Knight, F. R.; Kristkova, A.; Malkin Ondik, I.; Malkina, O. L.; Randall, R. A. M.; Slawin, A. M. Z.; Woollins, J. D.

*Weak Te,Te Interactions through the Looking Glass of NMR SpinSpin Coupling*

Angewandte Chemie-International Edition, (52): 2495-2498 2013.

Buil, M. L.; Esteruelas, M. A.; Fernandez, I.; Izquierdo, S.; Onate, E.

*Cationic Dihydride Boryl and Dihydride Silyl Osmium(IV) NHC Complexes: A Marked Diagonal Relationship*

Organometallics, (32): 2744-2752 2013.

Bundhun, A.; Ramasami, P.; Murray, J. S.; Politzer, P.

*Trends in sigma-hole strengths and interactions of F3MX molecules (M = C, Si, Ge and X = F, Cl, Br, I)*

Journal of Molecular Modeling, (19): 2739-2746 2013.

Bussy, U.; Delaforge, M.; El-Bekkali, C.; Ferchaud-Roucher, V.; Krempf, M.; Tea, I.; Galland, N.; Jacquemin, D.; Boujtita, M.

*Acebutolol and alprenolol metabolism predictions: comparative study of electrochemical and cytochrome P450-catalyzed reactions using liquid chromatography coupled to high-resolution mass spectrometry*

Analytical and Bioanalytical Chemistry, (405): 6077-6085 2013.

Bussy, U.; Tea, I.; Ferchaud-Roucher, V.; Krempf, M.; Silvestre, V.; Galland, N.; Jacquemin, D.; Andresen-Bergstrom, M.; Jurva, U.; Boujtita, M.

*Voltammetry coupled to mass spectrometry in the presence of isotope O-18 labeled water for the prediction of oxidative transformation pathways of activated aromatic ethers: Acebutolol*

Analytica Chimica Acta, (762): 39-46 2013.

Cabeza, J. A.; Damonte, M.; Garcia-Alvarez, P.; Perez-Carreno, E.

*Reactivity of a (Bis-NHC)tricarbonylruthenium(0) Complex with Methyl Triflate and Methyl Iodide.*

*Formation of Methyl- and Acetyl ruthenium(II) Derivatives: Experimental Results and Mechanistic DFT Calculations*

Organometallics, (32): 4382-4390 2013.

Cabeza, J. A.; Fernandez-Colinas, J. M.; Garcia-Alvarez, P.; Perez-Carreno, E.; Pruneda, V.; Van der Maelen, J. F.

*Deprotonation of C-Alkyl Groups of Cationic Triruthenium Clusters Containing Cyclometalated C-Alkylpyrazinium Ligands: Experimental and Computational Studies*

Chemistry-a European Journal, (19): 9251-9260 2013.

Cabeza, J. A.; Garcia-Alvarez, P.; Perez-Carreno, E.; Pruneda, V.

*Synthesis and Reactivity of Cationic Triruthenium Clusters Derived from 2-Methyl- and 4-*

*Methylpyrimidines: From Conventional Cyclometalated Ligands to Novel Types of N-Heterocyclic Carbenes*

Chemistry-a European Journal, (19): 3426-3436 2013.

Calbo, J.; Arago, J.; Orti, E.

- Theoretical study of the benzoquinone-tetrathiafulvalene-benzoquinone triad in neutral and oxidized/reduced states*  
Theoretical Chemistry Accounts, (132) 2013.
- Campanelli, A. R.  
*Structural variation, pi-charge transfer, and transmission of electronic substituent effects in (E)-beta-substituted styrenes: a quantum chemical study*  
Structural Chemistry, (24): 859-866 2013.
- Campetella, M.; Gontrani, L.; Bodo, E.; Ceccacci, F.; Marincola, F. C.; Caminiti, R.  
*Conformational isomerisms and nano-aggregation in substituted alkylammonium nitrates ionic liquids: An x-ray and computational study of 2-methoxyethylammonium nitrate*  
Journal of Chemical Physics, (138) 2013.
- Cao, J.; Xu, C.; Fan, Y. X.; Fan, L. Y.; Zhang, X. H.; Hu, C. W.  
*Selective Production of Electrostatically-Bound Adducts of Alkyl Cations/Polyoxoanions by the Collision-Induced Fragmentations of Their Quaternary Ammonium Counterparts*  
Journal of the American Society for Mass Spectrometry, (24): 884-894 2013.
- Cao, L. L.; Sun, C. Z.; Sun, N.; Meng, L.; Chen, D. Z.  
*Theoretical mechanism studies on the electrocatalytic reduction of CO<sub>2</sub> to formate by water-stable iridium dihydride pincer complex*  
Dalton Transactions, (42): 5755-5763 2013.
- Cao, Q.; Berski, S.; Rasanen, M.; Latajka, Z.; Khriachtchev, L.  
*Spectroscopic and Computational Characterization of the HCO center dot center dot center dot H<sub>2</sub>O Complex*  
Journal of Physical Chemistry A, (117): 4385-4393 2013.
- Cao, Y.; Wang, D. W.; Liu, B.; Yao, G. J.; Fu, Y. T.; Li, X. J.; Bi, Z. G.  
*The structure and electronic property of the smallest C<sub>20</sub>-glycine and Gd-encapsulated C<sub>20</sub>-glycine derivatives with potentially biological activity*  
International Journal of Quantum Chemistry, (113): 1440-1446 2013.
- Cao, Z. F.; Chen, Q. B.; Lu, Y. X.; Liu, H. L.; Hu, Y.  
*Density functional theory study on the interaction between metalloporphyrins and NH<sub>3</sub>*  
International Journal of Quantum Chemistry, (113): 1137-1146 2013.
- Carboni, M.; Abney, C. W.; Liu, S. B.; Lin, W. B.  
*Highly porous and stable metal-organic frameworks for uranium extraction*  
Chemical Science, (4): 2396-2402 2013.
- Cardenas-Jiron, G. I.; Cortez-Santibanez, L.  
*A three-layer ONIOM model for the outside binding of cationic porphyrins and nucleotide pair DNA*  
Journal of Molecular Modeling, (19): 811-824 2013.
- Castellano, M.; Fortea-Perez, F. R.; Bentama, A.; Stiriba, S. E.; Julve, M.; Lloret, F.; De Munno, G.; Armentano, D.; Li, Y. L.; Ruiz-Garcia, R.; Cano, J.  
*Dicopper(II) Metallacyclophanes with Oligo(p-phenylene-ethynylene) Spacers: Experimental Foundations and Theoretical Predictions on Potential Molecular Magnetic Wires*  
Inorganic Chemistry, (52): 7645-7657 2013.
- Castro, M.; Flores, R.; Duncan, M. A.

- Theoretical Study of Nascent Solvation in Ni+(Benzene)(m), m=3 and 4, Clusters*  
Journal of Physical Chemistry A, (117): 12546-12559 2013.
- Causa, M.; D'Amore, M.; Garzillo, C.; Gentile, F.; Savin, A.  
*The Bond Analysis Techniques (ELF and Maximum Probability Domains) Application to a Family of Models Relevant to Bio-Inorganic Chemistry*  
Applications of Density Functional Theory to Biological and Bioinorganic Chemistry, (150): 119-141 2013.
- Cavattoni, T.; Del Giacco, T.; Lanzalunga, O.; Mazzonna, M.; Mencarelli, P.  
*Structural Effects on the C-S Bond Cleavage in Aryl tert-Butyl Sulfoxide Radical Cations*  
Journal of Organic Chemistry, (78): 4886-4894 2013.
- Celik, M. A.; Dash, C.; Adiraju, V. A. K.; Das, A.; Yousufuddin, M.; Frenking, G.; Dias, H. V. R.  
*End-On and Side-On pi-Acid Ligand Adducts of Gold(I): Carbonyl, Cyanide, Isocyanide, and Cyclooctyne Gold(I) Complexes Supported by N-Heterocyclic Carbenes and Phosphines*  
Inorganic Chemistry, (52): 729-742 2013.
- Celik, M. A.; Frenking, G.; Neumuller, B.; Petz, W.  
*Exploiting the Twofold Donor Ability of Carbodiphosphoranes: Theoretical Studies of (PPh3)(2)C -> EH2 (q) (E-q=Be, B+, C2+, N3+, O4+) and Synthesis of the Dication (Ph3P)(2)C = CH2 (2+)*  
Chempluschem, (78): 1024-1032 2013.
- Cesar, V.; Castro, L. C. M.; Dombay, T.; Sortais, J. B.; Darcel, C.; Labat, S.; Miqueu, K.; Sotiropoulos, J. M.; Brousses, R.; Lugan, N.; Lavigne, G.  
*(Cyclopentadienyl)iron(II) Complexes of N-Heterocyclic Carbenes Bearing a Malonate or Imidate Backbone: Synthesis, Structure, and Catalytic Potential in Hydrosilylation*  
Organometallics, (32): 4643-4655 2013.
- Chakraborty, A.; Chakraborty, S.; Ganguly, T.  
*Photoisomerization within a novel synthesized photoswitchable dyad: experimental and theoretical approaches*  
Indian Journal of Physics, (87): 1113-1120 2013.
- Chamundeeswari, S. P. V.; Samuel, E. J. J.; Sundaraganesan, N.  
*Structural, vibrational, electronic and NMR spectral analysis of 3-chloro-6-methoxypyridazine by DFT calculations*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (110): 36-45 2013.
- Chan, B.; Ball, G. E.  
*A Benchmark Ab Initio and DFT Study of the Structure and Binding of Methane in the sigma-Alkane Complex CpRe(CO)(2)(CH4)*  
Journal of Chemical Theory and Computation, (9): 2199-2208 2013.
- Chandra, A. K.; Zeegers-Huyskens, T.  
*Theoretical study of the cooperativity in substituted dimethyl ethers complexed with two water molecules. Red or blue shifts of the nu(CH) vibrations?*  
Chemical Physics, (410): 66-70 2013.
- Chapyshev, S. V.; Ushakov, E. N.; Chernyak, A. V.  
*N-15 NMR spectra and reactivity of 2,4,6-triazidopyridines, 2,4,6-triazidopyrimidine and 2,4,6-triazido-s-triazine*  
Magnetic Resonance in Chemistry, (51): 562-568 2013.



- Chaudret, R.; Parks, J. M.; Yang, W. T.  
*Pseudobond parameters for QM/MM studies involving nucleosides, nucleotides, and their analogs*  
Journal of Chemical Physics, (138) 2013.
- Che, X.; Gao, J.; Liu, Y. J.; Liu, C. B.  
*Metal vs. chalcogen competition in the catalytic mechanism of cysteine dioxygenase*  
Journal of Inorganic Biochemistry, (122): 1-7 2013.
- Chen, F.; Wang, C. Z.; Shi, W. Q.; Zhang, M.; Liu, C. M.; Zhao, Y. L.; Chai, Z. F.  
*Two new uranyl fluoride complexes with U-VI=O-alkali (Na, Cs) interactions: Experimental and theoretical studies*  
Crystengcomm, (15): 8041-8048 2013.
- Chen, H.; Kong, X. Y.; Zheng, W. J.; Yao, J. N.; Kandalam, A. K.; Jena, P.  
*Anomalous Property of Ag(BO<sub>2</sub>)<sub>2</sub> Hyperhalogen: Does Spin-Orbit Coupling Matter?*  
Chemphyschem, (14): 3303-3308 2013.
- Chen, J. L.; Chen, S. L.; Liu, Z. G.; Feng, H.; Xie, Y. M.; King, R. B.  
*Methylborabenzene ligands in binuclear iron carbonyl derivatives: High spin states and iron-iron multiple bonding*  
Journal of Organometallic Chemistry, (747): 106-112 2013.
- Chen, L. Z.; Zhang, L.; Ren, F. D.; Cao, D. L.; Ren, J.  
*Theoretical Studies on Intermolecular Hydrogen-bond Interactions between Hexamethylenetetramine and Nitric Acid*  
Chinese Journal of Structural Chemistry, (32): 7-16 2013.
- Chen, Q.; Zhai, H. J.; Li, S. D.; Wang, L. S.  
*On the structures and bonding in boron-gold alloy clusters: B<sub>6</sub>Aun- and B<sub>6</sub>Aun (n = 1-3)*  
Journal of Chemical Physics, (138) 2013.
- Chen, X.; Wang, Y. Y.; Liu, B.; Yin, B.; Liu, P.; Shi, Q. Z.  
*New two-dimensional Mn(II) metal-organic framework featured spin canting*  
Dalton Transactions, (42): 7092-7100 2013.
- Chen, X. S.; Lu, P. F.; Dong, Y. H.; Xie, J.  
*Theoretical Study of Calix 4 pyrrole Complexes with Halide and Ammonium Ions*  
Acta Physico-Chimica Sinica, (29): 2187-2197 2013.
- Chen, Y. M.; Kuang, X. Y.; Sheng, X. W.; Wang, H. Q.; Shao, P.; Zhong, M. M.  
*Investigation of Carbon Monoxide Adsorption on Cationic Gold-Palladium Clusters*  
Zeitschrift Fur Naturforschung Section a-a Journal of Physical Sciences, (68): 651-658 2013.
- Chen, Y. S.  
*Theoretical Study of Interactions between Halogen-Substituted s-Triazine and Halide Anions*  
Journal of Physical Chemistry A, (117): 8081-8090 2013.
- Chen, Z. H.; Mo, Y. R.  
*Electron Transfer in Electrophilic Aromatic Nitration and Nitrosation: Computational Evidence for the Marcus Inverted Region*  
Journal of Chemical Theory and Computation, (9): 4428-4435 2013.
- Chen, Z. Q.; Xue, Y.

*MECHANISMS FOR THE DECOMPOSITION OF HYDROXYL-RADICAL-INDUCED CYTOSINE HYDROPEROXIDES:  
A COMPUTATIONAL STUDY*

Journal of Theoretical & Computational Chemistry, (12) 2013.

Cheng, C.; Zhang, M.; Sheng, L.

*AB INITIO AND DFT STUDY OF NON-COVALENT INTERACTIONS BETWEEN RARE GAS ATOMS AND  
AROMATIC RINGS*

Journal of Theoretical & Computational Chemistry, (12) 2013.

Cheng, N.; Liu, Y. J.; Zhang, C. Q.; Liu, C. B.

*A theoretical study on the halogen bonding interactions of C<sub>6</sub>F<sub>5</sub>I with a series of group 10 metal  
monohalides*

Journal of Molecular Modeling, (19): 3821-3829 2013.

Chermhini, A. N.; Farrokhpour, H.; Teimouri, A.; Pourmoghaddas, F.

*Theoretical studies on tautomerism of imidazole-2-selenone*

Structural Chemistry, (24): 1215-1227 2013.

Chi, Y. J.; Yu, H. T.

*Intramolecular cyclization reaction mechanism and regioselectivities of unsubstituted and benzene-  
substituted 4-penteniminy radicals: A DFT investigation*

Computational and Theoretical Chemistry, (1005): 75-83 2013.

Chipanina, N. N.; Oznobikhina, L. P.; Ushakova, I. V.; Shainyan, B. A.

*Electronic structure and basicity of trifluoro-N-methyl-N-(2-phenylethenyl)methanesulfonamide*

Russian Journal of Organic Chemistry, (49): 999-1003 2013.

Chmielowska, A.; Lodowski, P.; Jaworska, M.

*Redox Potentials and Protonation of the A-Cluster from Acetyl-CoA Synthase. A Density Functional Theory  
Study*

Journal of Physical Chemistry A, (117): 12484-12496 2013.

Cho, D.; Ko, K. C.; Lee, J. Y.

*Catalytic Mechanism for the Ruthenium-Complex-Catalyzed Synthesis of Amides from Alcohols and  
Amines: A DFT Study*

Organometallics, (32): 4571-4576 2013.

Cho, H. G.

*Observation of Elusive CF<sub>2</sub>Cl center dot center dot center dot Cl in Matrix Infrared Spectra and Density  
Functional Calculations*

Bulletin of the Korean Chemical Society, (34): 3274-3278 2013.

Cho, H. G.; Andrews, L.

*Infrared Spectra of CH<sub>3</sub>-MX and CH<sub>2</sub>X-MH Prepared in Reactions of Laser-Ablated Gold, Platinum,  
Palladium, and Nickel Atoms with CH<sub>3</sub>Cl and CH<sub>3</sub>Br*

Organometallics, (32): 2753-2759 2013.

Cho, H. G.; Andrews, L.

*Infrared Spectra of Manganese Insertion, Vinyl, and Cyclic Complexes Prepared in Reactions of Laser-  
Ablated Mn Atoms with Methane, Ethane, Ethyl Chloride, and 1,2-Dichloroethane*

Organometallics, (32): 3458-3468 2013.

Cho, H. G.; Andrews, L.

- Matrix Infrared Spectra and Density Functional Calculations for New iso-Halomethanes: CHCl<sub>2</sub>-Cl, CHFCl-Cl, CFCI<sub>2</sub>-Cl, CHBr<sub>2</sub>-Br, and CBr<sub>3</sub>-Br in Solid Argon*  
Journal of Physical Chemistry A, (117): 6525-6535 2013.
- Choi, H.; Park, Y. C.; Lee, Y. S.; Baeck, K. K.  
*Density functional theory calculations for simple prototypes of perfluorocarbons: neutral and anionic c-C<sub>4</sub>F<sub>8</sub> and 2-C<sub>4</sub>F<sub>8</sub>*  
Journal of Fluorine Chemistry, (146): 46-52 2013.
- Choudhary, A.; Fry, C. G.; Kamer, K. J.; Raines, R. T.  
*An n → pi\* interaction reduces the electrophilicity of the acceptor carbonyl group*  
Chemical Communications, (49): 8166-8168 2013.
- Choudhary, N.; Bee, S.; Gupta, A.; Tandon, P.  
*Comparative vibrational spectroscopic studies, HOMO-LUMO and NBO analysis of N-(phenyl)-2,2-dichloroacetamide, N-(2-chloro phenyl)-2,2-dichloroacetamide and N-(4-chloro phenyl)-2,2-dichloroacetamide based on density functional theory*  
Computational and Theoretical Chemistry, (1016): 8-21 2013.
- Chu, G. M.; Fernandez, I.; Sierra, M. A.  
*Synthesis, Structure, and Electronic Properties of Extended pi-Conjugated Group 6 Fischer Alkoxy-Bis(carbene) Complexes*  
Chemistry-a European Journal, (19): 5899-5908 2013.
- Church, J.; Pezeshki, S.; Davis, C.; Lin, H.  
*Charge Transfer and Polarization for Chloride Ions Bound in CIC Transport Proteins: Natural Bond Orbital and Energy Decomposition Analyses*  
Journal of Physical Chemistry B, (117): 16029-16043 2013.
- Clark, T.  
*sigma-Holes*  
Wiley Interdisciplinary Reviews-Computational Molecular Science, (3): 13-20 2013.
- Cocinero, E. J.; Lesarri, A.; Ecija, P.; Cimas, A.; Davis, B. G.; Basterretxea, F. J.; Fernandez, J. A.; Castano, F.  
*Free Fructose Is Conformationally Locked*  
Journal of the American Chemical Society, (135): 2845-2852 2013.
- Comba, P.; Martin, B.; Sanyal, A.  
*An efficient fluctuating charge model for transition metal complexes*  
Journal of Computational Chemistry, (34): 1598-1608 2013.
- Compaan, K. R.; Agarwal, J.; Dye, B. E.; Yamaguchi, Y.; Schaefer, H. F.  
*TOWARD DETECTION OF AICH<sub>2</sub> AND AICH<sub>2</sub><sup>+</sup> IN THE INTERSTELLAR MEDIUM*  
Astrophysical Journal, (778) 2013.
- Conde, A.; Vilella, L.; Balcells, D.; Diaz-Requejo, M. M.; Lledos, A.; Perez, P. J.  
*Introducing Copper as Catalyst for Oxidative Alkane Dehydrogenation*  
Journal of the American Chemical Society, (135): 3887-3896 2013.
- Contreras, M.; Osorio, E.; Ferraro, F.; Puga, G.; Donald, K. J.; Harrison, J. G.; Merino, G.; Tiznado, W.  
*Isomerization Energy Decomposition Analysis for Highly Ionic Systems: Case Study of Starlike E5Li<sub>7</sub><sup>+</sup> Clusters*  
Chemistry-a European Journal, (19): 2305-2310 2013.

- Cooper, D. L.; Ponec, R.  
*Bond formation in diatomic transition metal hydrides: Insights from the analysis of domain-averaged fermi holes*  
International Journal of Quantum Chemistry, (113): 102-111 2013.
- Cordaro, M.; Risitano, F.; Scala, A.; Rescifina, A.; Chiacchio, U.; Grassi, G.  
*Self-Catalyzed Mannich-Type Reaction of Enolizable Cyclic 1,3-Dicarbonyls to Acyclic Nitrones: An Entry to Functionalized beta-Enamino Diones*  
Journal of Organic Chemistry, (78): 3972-3979 2013.
- Corma, A.; Concepcion, P.; Boronat, M.; Sabater, M. J.; Navas, J.; Yacaman, M. J.; Larios, E.; Posadas, A.; Lopez-Quintela, M. A.; Buceta, D.; Mendoza, E.; Guilera, G.; Mayoral, A.  
*Exceptional oxidation activity with size-controlled supported gold clusters of low atomicity*  
Nature Chemistry, (5): 775-781 2013.
- Cormanich, R. A.; Ducati, L. C.; Tormena, C. F.; Rittner, R.  
*A theoretical and experimental 1H NMR spectroscopy study of the stereoelectronic interactions that rule the conformational energies of alanine and valine methyl ester*  
Journal of Physical Organic Chemistry, (26): 849-857 2013.
- Costa, A. C.; Ondar, G. F.; Versiane, O.; Ramos, J. M.; Santos, T. G.; Martin, A. A.; Raniero, L.; Bussi, G. G. A.; Soto, C. A. T.  
*DFT: B3LYP/6-311G (d, p) vibrational analysis of bis-(diethyldithiocarbamate)zinc(II) and natural bond orbitals*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (105): 251-258 2013.
- Costa, S. N.; Sales, F. A. M.; Freire, V. N.; Maia, F. F.; Caetano, E. W. S.; Ladeira, L. O.; Albuquerque, E. L.; Fulco, U. L.  
*L-Serine Anhydrous Crystals: Structural, Electronic, and Optical Properties by First-Principles Calculations, and Optical Absorption Measurement*  
Crystal Growth & Design, (13): 2793-2802 2013.
- Cotton, C. E.; Francisco, J. S.; Mitrushchenkov, A. O.  
*Structural and spectroscopic study of the linear proton-bound complex of PN with HNP+*  
Journal of Chemical Physics, (138) 2013.
- Cozzolino, A. F.; Elder, P. J. W.; Lee, L. M.; Vargas-Baca, I.  
*The role of the Lewis acid-base properties in the supramolecular association of 1,2,5-chalcogenadiazoles*  
Canadian Journal of Chemistry-Revue Canadienne De Chimie, (91): 338-347 2013.
- Crespo-Otero, R.; Bravo-Rodriguez, K.; Roy, S.; Benighaus, T.; Thiel, W.; Sander, W.; Sanchez-Garcia, E.  
*Interactions of Aromatic Radicals with Water*  
Chemphyschem, (14): 805-811 2013.
- Cui, G. F.; Liu, S. F.; Zhao, J.; Holby, E. F.; Li, Q.; Wu, G.  
*AuSn20 Eutectic Electrodeposition through Alternative Complexing of Pyrophosphoric Acid: Insights from Electrochemical and DFT Methods*  
Journal of Physical Chemistry C, (117): 21228-21233 2013.
- Cui, L. L.; Zhou, D. H.; Li, M. M.  
*Photophysical Properties of a Red-Shift Cu(II) Ratiometric Fluorescent Chemosensor*  
Acta Physico-Chimica Sinica, (29): 745-753 2013.

- Cullinane, J.; Jolleys, A.; Mair, F. S.  
*Thalophilic interactions and TI-aryl pi-interactions are competitive with cation-cation repulsion: LTI2L (2+) dications as salts of weakly co-ordinating anions*  
Dalton Transactions, (42): 11971-11975 2013.
- Dabbagh, H. A.; Zamani, M.; Fakhraee, S.  
*The nature of resonance and hyperconjugation for cyclic beta-silyl substituted carbocations: NBO, NRT, EDA, and NMR studies*  
Research on Chemical Intermediates, (39): 2011-2033 2013.
- Dakkouri, M.; Typke, V.  
*A theoretical investigation of the structure of 2-nitropyridine-N-oxide and the dependency of the NO<sub>2</sub> torsional motion on the applied wavefunction and basis set*  
Structural Chemistry, (24): 1627-1653 2013.
- Dalinger, I. L.; Khakimov, D. V.; Shkineva, T. K.; Vatsadze, I. A.; Popova, G. P.; Pivina, T. S.; Shevelev, S. A.  
*Quantum-chemical study of the reactivity of di- and trinitropyrazoles*  
Chemistry of Heterocyclic Compounds, (48): 1646-1651 2013.
- Danovich, D.; Shaik, S.; Rzepa, H. S.; Hoffmann, R.  
*A Response to the Critical Comments on "One Molecule, Two Atoms, Three Views, Four Bonds?"*  
Angewandte Chemie-International Edition, (52): 5926-5928 2013.
- Davalos, J. Z.; Gonzalez, J.; Guerrero, A.; Hnyk, D.; Holub, J.; Oliva, J. M.  
*Anionic Oligomerization of Li-2 B12H12 and Li CB11H12 : An Experimental and Computational Study*  
Journal of Physical Chemistry C, (117): 1495-1501 2013.
- Davila, Y. A.; Sancho, M. I.; Almandoz, M. C.; Blanco, S. E.  
*Solvent Effects on the Dissociation Constants of Hydroxyflavones in Organic-Water Mixtures. Determination of the Thermodynamic pK(a) Values by UV-Visible Spectroscopy and DFT Calculations*  
Journal of Chemical and Engineering Data, (58): 1706-1716 2013.
- Davis, A. P.; Fry, A. J.  
*Selective Oxidation of an Electronically Unsymmetrical Distyrylbenzene at Either of Two Sites*  
Journal of the Electrochemical Society, (160): G3091-G3096 2013.
- de Almeida, K. J.; Ramalho, T. C.; Neto, J. L.; Santiago, R. T.; Felicissimo, V. C.; Duarte, H. A.  
*Methane Dehydrogenation by Niobium Ions: A First-Principles Study of the Gas-Phase Catalytic Reactions*  
Organometallics, (32): 989-999 2013.
- De Haeck, J.; Tai, T. B.; Bhattacharyya, S.; Le, H. T.; Janssens, E.; Nguyen, M. T.; Lievens, P.  
*Structures and ionization energies of small lithium doped germanium clusters*  
Physical Chemistry Chemical Physics, (15): 5151-5162 2013.
- De, S.; Parameswaran, P.  
*Neutral tricoordinated beryllium(0) compounds - isostructural to BH<sub>3</sub> but isoelectronic to NH<sub>3</sub>*  
Dalton Transactions, (42): 4650-4656 2013.
- de Silva, P.; Korchowiec, J.; Ram, J. S. N.; Wesolowski, T. A.  
*Extracting Information about Chemical Bonding from Molecular Electron Densities via Single Exponential Decay Detector (SEDD)*  
Chimia, (67): 253-256 2013.

- De Vleeschouwer, F.; Chanldsjijev, A.; Yang, W. T.; Geerlings, P.; De Proft, F.  
*Pushing the Boundaries of Intrinsically Stable Radicals: Inverse Design Using the Thiadiazinyl Radical as a Template*  
Journal of Organic Chemistry, (78): 3151-3158 2013.
- Del Bene, J. E.; Akorta, I.; Elguero, J.  
*Characterizing Complexes with Pnicogen Bonds Involving  $sp(2)$  Hybridized Phosphorus Atoms:  $(H_2C=PX)_2$  with  $X = F, Cl, OH, CN, NC, CCH, H, CH_3,$  and  $BH_2$*   
Journal of Physical Chemistry A, (117): 6893-6903 2013.
- Del Bene, J. E.; Alkorta, I.; Elguero, J.  
*Properties of Complexes  $H_2C=(X)P:PXH_2$ , for  $X = F, Cl, OH, CN, NC, CCH, H, CH_3,$  and  $BH_2$ : P center dot center dot center dot P Pnicogen Bonding at sigma-Holes and pi-Holes*  
Journal of Physical Chemistry A, (117): 11592-11604 2013.
- Del Bene, J. E.; Alkorta, I.; Sanchez-Sanz, G.; Elguero, J.  
*Phosphorus As a Simultaneous Electron-Pair Acceptor in Intermolecular P center dot center dot center dot N Pnicogen Bonds and Electron-Pair Donor to Lewis Acids*  
Journal of Physical Chemistry A, (117): 3133-3141 2013.
- Deng, J. M.; Li, Q. S.; Xie, Y. M.; King, R. B.  
*Binuclear pentafluorocyclopentadienyl metal carbonyls of iron, cobalt, and nickel: Effect of fluorine substitution*  
Journal of Fluorine Chemistry, (154): 23-29 2013.
- Deng, J. M.; Li, Q. S.; Xie, Y. M.; King, R. B.; Schaefer, H. F.  
*Binuclear hexafluorocyclopentadiene iron carbonyls: bis(dihapto) versus trihapto-monohapto bonding in iron-iron bonded structures*  
New Journal of Chemistry, (37): 2902-2910 2013.
- Determan, J. J.; Wilson, A. K.  
*Bonding properties of selenium-carbon complexes: Computational modeling of  $H_3CSeH, H_2CSe, HOCSeH, H_2CSeO, SeC$  and  $H_2CSeOH$*   
Computational and Theoretical Chemistry, (1017): 41-47 2013.
- Devipriya, B.; Kumaradhas, P.  
*Charge density distribution and the electrostatic moments of CTPB in the active site of p300 enzyme: A DFT and charge density study*  
Journal of Theoretical Biology, (335): 119-129 2013.
- Devipriya, B.; Kumaradhas, P.  
*Molecular flexibility and the electrostatic moments of curcumin and its derivatives in the active site of p300: A theoretical charge density study*  
Chemico-Biological Interactions, (204): 153-165 2013.
- Dhaka, K.; Trivedi, R.; Bandyopadhyay, D.  
*Electronic structure and stabilities of Ni-doped germanium nanoclusters: a density functional modeling study*  
Journal of Molecular Modeling, (19): 1473-1488 2013.
- Dhaked, D. K.; Bharatam, P. V.  
*Nitro reversible arrow aci-nitro tautomerism and E/Z isomeric preferences of nitroethenediamine derivatives: a quantum chemical study*

- Rsc Advances, (3): 25268-25277 2013.
- Dhas, D. A.; Joe, I. H.; Roy, S. D. D.; Balachandran, S.  
*DFT computation and experimental analysis of vibrational and electronic spectra of phenoxy acetic acid herbicides*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (108): 89-99 2013.
- Di Palma, T. M.; Bende, A.  
*Vacuum ultraviolet photoionization and ab initio Investigations of methyl tert-butyl ether (MTBE) clusters and MTBE-water clusters*  
Chemical Physics Letters, (561): 18-23 2013.
- Die, D.; Zheng, B. X.; Wang, H.; Du, Q.  
*Geometries, stabilities, and magnetic properties of AunTi (n=1-9) clusters: A density functional study*  
Computational and Theoretical Chemistry, (1025): 67-73 2013.
- Dieckmann, A.; Richers, M. T.; Platonova, A. Y.; Zhang, C.; Seidel, D.; Houk, K. N.  
*Metal-Free alpha-Amination of Secondary Amines: Computational and Experimental Evidence for Azaquinone Methide and Azomethine Ylide Intermediates*  
Journal of Organic Chemistry, (78): 4132-4144 2013.
- Ding, W. L.; Wang, D. M.; Geng, Z. Y.; Zhao, X. L.; Xu, W. B.  
*Density functional theory characterization and verification of high-performance indoline dyes with D-A-pi-A architecture for dye-sensitized solar cells*  
Dyes and Pigments, (98): 125-135 2013.
- Ding, W. L.; Wang, D. M.; Geng, Z. Y.; Zhao, X. L.; Yan, Y. F.  
*Molecular Engineering of Indoline-Based D-A-pi-A Organic Sensitizers toward High Efficiency Performance from First-Principles Calculations*  
Journal of Physical Chemistry C, (117): 17382-17398 2013.
- Dixit, N.; Zalis, S.; Maiti, B.; Mishra, L.  
*Reversible and pH dependent photophysical properties of mixed-ligand Ru(II) complexes containing 2,2'-bipyridine and nitrosobarbiturate: Experimental and theoretical approach*  
Inorganica Chimica Acta, (404): 123-130 2013.
- Dobretsov, G.; Polyak, B.; Smolina, N.; Babushkina, T.; Syreishchikova, T.; Klimova, T.; Sverbil, V.; Peregudov, A.; Gryzunov, Y.; Sarkisov, O.  
*Interaction of a fluorescent probe, CAPIDAN, with human serum albumin*  
Journal of Photochemistry and Photobiology a-Chemistry, (251): 134-140 2013.
- Doi, H.; Aida, M.  
*Hydration of Adamantane Skeleton: Water Assembling around Amantadine and Halo-substituted Adamantanes*  
Chemistry Letters, (42): 292-294 2013.
- Domingo, L. R.; Perez, P.  
*Global and local reactivity indices for electrophilic/nucleophilic free radicals*  
Organic & Biomolecular Chemistry, (11): 4350-4358 2013.
- Domingo, L. R.; Perez, P.; Ortega, D. E.  
*Why Do Five-Membered Heterocyclic Compounds Sometimes Not Participate in Polar Diels-Alder Reactions?*

- Journal of Organic Chemistry, (78): 2462-2471 2013.
- Domingo, L. R.; Perez, P.; Saez, J. A.  
*Understanding C-C bond formation in polar reactions. An ELF analysis of the Friedel-Crafts reaction between indoles and nitroolefins*  
Rsc Advances, (3): 7520-7528 2013.
- Domingo, L. R.; Perez, P.; Saez, J. A.  
*Understanding the local reactivity in polar organic reactions through electrophilic and nucleophilic Parr functions*  
Rsc Advances, (3): 1486-1494 2013.
- Domingo, L. R.; Perez, P.; Saez, J. A.  
*Understanding the regioselectivity in hetero Diels-Alder reactions. An ELF analysis of the reaction between nitrosoethylene and 1-vinylpyrrolidine*  
Tetrahedron, (69): 107-114 2013.
- Domingo, L. R.; Saez, J. A.; Joule, J. A.; Rhyman, L.; Ramasami, P.  
*A DFT Study of the 3+2 versus 4+2 Cycloaddition Reactions of 1,5,6-Trimethylpyrazinium-3-olate with Methyl Methacrylate*  
Journal of Organic Chemistry, (78): 1621-1629 2013.
- Dudev, T.; Lim, C.  
*Importance of Metal Hydration on the Selectivity of Mg<sup>2+</sup> versus Ca<sup>2+</sup> in Magnesium Ion Channels*  
Journal of the American Chemical Society, (135): 17200-17208 2013.
- Durlak, P.; Mierzwicki, K.; Latajka, Z.  
*Investigations of the Very Short Hydrogen Bond in the Crystal of Nitromalonamide via Car-Parrinello and Path Integral Molecular Dynamics*  
Journal of Physical Chemistry B, (117): 5430-5440 2013.
- Dutta, B.; De, R.; Chowdhury, J.  
*Ab initio and DFT study to understand the physics behind the conformational barriers of isobutyl cyanide molecule*  
Indian Journal of Physics, (87): 855-863 2013.
- Dyminska, L.; Weglinski, Z.; Gagor, A.; Hanuza, J.  
*Structural and Vibrational Properties of Imidazo 4,5-c pyridine, a Structural Unit in Natural Products*  
Journal of Natural Products, (76): 1637-1646 2013.
- Dzambaski, Z.; Markovic, R.; Kleinpeter, E.; Baranac-Stojanovic, M.  
*2-Alkylidene-4-oxothiazolidine S-oxides: synthesis and stereochemistry*  
Tetrahedron, (69): 6436-6447 2013.
- Ebrahimi, A.; Habibi-Khorassani, M.; Akher, F. B.; Farrokhzadeh, A.; Karimi, P.  
*Caffeine as base analogue of adenine or guanine: A theoretical study*  
Journal of Molecular Graphics and Modelling, (42): 81-91 2013.
- Ebrahimi, A.; Habibi-Khorassani, M.; Shahraki, A.  
*The Radical Cationic Repair Pathway of Cyclobutane Pyrimidine Dimer: The Effect of Sugar-Phosphate Backbone*  
Photochemistry and Photobiology, (89): 74-82 2013.



- Echegaray, E.; Cardenas, C.; Rabi, S.; Rabi, N.; Lee, S.; Zadeh, F. H.; Toro-Labbe, A.; Anderson, J. S. M.; Ayers, P. W.  
*In pursuit of negative Fukui functions: examples where the highest occupied molecular orbital fails to dominate the chemical reactivity*  
Journal of Molecular Modeling, (19): 2779-2783 2013.
- Edwin, B.; Joe, I. H.  
*FT-Raman, FT-IR and UV-visible spectral investigations and ab initio computations of anti-epileptic drug: Vigabatrin*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (114): 633-641 2013.
- Edwin, B.; Joe, I. H.  
*Vibrational spectral analysis of anti-neurodegenerative drug Levodopa: A DFT study*  
Journal of Molecular Structure, (1034): 119-127 2013.
- Eich, A.; Schluter, S.; Schnakenburg, G.; Beck, J.  
*(Sb7Te8)(5+) - A Double Cube Shaped Polycationic Cluster*  
Zeitschrift fur Anorganische und Allgemeine Chemie, (639): 375-383 2013.
- El-Hellani, A.; Monot, J.; Guillot, R.; Bour, C.; Gandon, V.  
*Molecular versus Ionic Structures in Adducts of GaX3 with Monodentate Carbon-Based Ligands*  
Inorganic Chemistry, (52): 506-514 2013.
- Elroby, S. A. K.; Ahmed, A. A.; Hilal, R. H.  
*Conformational preference and mechanism of decarboxylation of levodopa. A quantum dynamics/quantum mechanics study*  
International Journal of Quantum Chemistry, (113): 1966-1974 2013.
- Elroby, S. A. K.; Aziz, S. G.; Hilal, R.  
*Electronic structure and decomposition reaction mechanism of cyclopropanone, phenylcyclopropanone and their sulfur analogues: a theoretical study*  
Journal of Molecular Modeling, (19): 1339-1353 2013.
- Emamian, S.; Tayyari, S. F.  
*Theoretical study of intramolecular hydrogen bonding in the halo derivatives of 1-amino-3-imino-prop-1-ene*  
Journal of Chemical Sciences, (125): 939-948 2013.
- Eshtiagh-Hosseini, H.; Chahkandi, M.; Housaindokht, M. R.; Mirzaei, M.  
*Bromide oxidation mechanism by vanadium bromoperoxidase functional models with new tripodal amine ligands: A comprehensive theoretical calculations study*  
Polyhedron, (60): 93-101 2013.
- Eshtiagh-Hosseini, H.; Mirzaei, M.; Biabani, M.; Lippolis, V.; Chahkandi, M.; Bazzicalupi, C.  
*Insight into the connecting roles of interaction synthons and water clusters within different transition metal coordination compounds of pyridine-2,5-dicarboxylic acid: experimental and theoretical studies*  
Crystengcomm, (15): 6752-6768 2013.
- Esfarili, M. D.; Behzadi, H.  
*Investigation into the nature of interactions in aspirin-water clusters including SAPT, AIM and NBO theories*  
Molecular Simulation, (39): 629-639 2013.
- Esterhuysen, C.; Frenking, G.

- Complexation behavior of two-coordinated carbon compounds containing fluorenyl ligands*  
Dalton Transactions, (42): 13349-13356 2013.
- Fan, X. Y.; Xu, L. Z.; Liu, L. X.; Yang, M. H.; Zeng, Q.; Yang, M. L.  
*Polarization response of methane encapsulated in water cages*  
Computational and Theoretical Chemistry, (1013): 52-56 2013.
- Fang, G. Y.; Ma, J.  
*Rapid atomic layer deposition of silica nanolaminates: synergistic catalysis of Lewis/Bronsted acid sites and interfacial interactions*  
Nanoscale, (5): 11856-11869 2013.
- Fang, Y.; Wang, L.; Ni, L.; Yao, J.  
*Hydrothermal Synthesis, Characterization and Natural Bond Orbital(NBO) Analysis of a Binuclear Lead(II) Complex with Cinnamic Acid and Medpq Ligands*  
Chinese Journal of Inorganic Chemistry, (29): 1551-1556 2013.
- Farmanzadeh, D.; Ashtiani, Z.  
*MANIPULATING PERFORMANCE OF A MOLECULAR WIRE WITH CHEMICAL MODIFICATION AND EXTERNAL ELECTRIC FIELD*  
Journal of Theoretical & Computational Chemistry, (12) 2013.
- Farmanzadeh, D.; Ghazanfary, S.  
*The effect of electric field on the interaction of glycine with (6,0) single-walled boron nitride nanotubes*  
Journal of the Serbian Chemical Society, (78): 75-83 2013.
- Farmanzadeh, D.; Soltanabadi, A.; Yeganegi, S.  
*DFT Study of the Geometrical and Electronic Structures of Geminal Dicationic Ionic Liquids 1,3-Bis 3-methylimidazolium-1-yl hexane Halides*  
Journal of the Chinese Chemical Society, (60): 551-558 2013.
- Farras, P.; Vinas, C.; Teixidor, F.  
*Preferential chlorination vertices in cobaltabisdicarbollide anions. Substitution rate correlation with site charges computed by the two atoms natural population analysis method (2a-NPA)*  
Journal of Organometallic Chemistry, (747): 119-125 2013.
- Favaro, D. C.; Contreras, R. H.; Tormena, C. F.  
*The electronic origin of unusually large (n)J(FN) coupling constants in some fluoroximes*  
Magnetic Resonance in Chemistry, (51): 334-338 2013.
- Faza, O. N.; Lopez, C. S.; Fernandez, I.  
*Noyori Hydrogenation: Aromaticity, Synchronicity, and Activation Strain Analysis*  
Journal of Organic Chemistry, (78): 5669-5676 2013.
- Fazaeli, R.; Solimannejad, M.; Seif, A.  
*Analysis of torsional barrier height of HSNO as the simplest S-nitrosothiol*  
Journal of Chemical Sciences, (125): 913-917 2013.
- Fedushkin, I. L.; Markina, O. V.; Lukoyanov, A. N.; Morozov, A. G.; Baranov, E. V.; Maslov, M. O.; Ketkov, S. Y.  
*Boron complexes of redox-active diimine ligand*  
Dalton Transactions, (42): 7952-7961 2013.

Feigl, A.; Chiorescu, I.; Deller, K.; Heidsieck, S. U. H.; Buchner, M. R.; Karttunen, V.; Bockholt, A.; Genest, A.; Rosch, N.; Rieger, B.

*Metal-Free Polymerization of Phenylsilane: Tris(pentafluorophenyl)borane-Catalyzed Synthesis of Branched Polysilanes at Elevated Temperatures*  
Chemistry-a European Journal, (19): 12526-12536 2013.

Fernandez, D.; Ortega-Castro, J.; Frau, J.

*Human farnesyl pyrophosphate synthase inhibition by nitrogen bisphosphonates: a 3D-QSAR study*  
Journal of Computer-Aided Molecular Design, (27): 739-754 2013.

Fernandez, L. E.; Gomez, A. A.; Totaro, R. M.; Coronel, A. C.; Varetta, E. L.

*Experimental and theoretical vibrational study of methylene bis(thiocyanate), CH<sub>2</sub>(SCN)<sub>2</sub>. A comparison with thiocyanogen, (SCN)<sub>2</sub>*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (110): 233-240 2013.

Ferrando-Soria, J.; Castellano, M.; Ruiz-Garcia, R.; Cano, J.; Julve, M.; Lloret, F.; Ruiz-Perez, C.; Pasan, J.; Canadillas-Delgado, L.; Armentano, D.; Journaux, Y.; Pardo, E.

*Dicopper(II) Metallacyclophanes with Electroswitchable Polymethyl-Substituted para-Phenylene Spacers*  
Chemistry-a European Journal, (19): 12124-12137 2013.

Ferraro, F.; Paez-Hernandez, D.; Murillo-Lopez, J. A.; Munoz-Castro, A.; Arratia-Perez, R.

*Antenna Effect by Organometallic Chromophores in Bimetallic d-f Complexes*  
Journal of Physical Chemistry A, (117): 7847-7854 2013.

Ferreira, A. S. D.; Carvalho, M.; Galvao, A. M.; Veiros, L. F.

*Tuning structure and properties of Pd and Pt camphor derived complexes*  
Inorganica Chimica Acta, (395): 169-175 2013.

Ferro-Costas, D.; Vila, A.; Mosquera, R. A.

*Anomeric Effect in Halogenated Methanols: A Quantum Theory of Atoms in Molecules Study*  
Journal of Physical Chemistry A, (117): 1641-1650 2013.

Ferullo, R. M.; Granados, A.; Lanterna, A.; Guida, J. A.; Piro, O. E.; Castellano, E. E.; Dennehy, M.

*Thiosaccharine disulfide: Synthesis, crystal structure, spectroscopic characterization and theoretical study*  
Journal of Molecular Structure, (1032): 48-55 2013.

Filippou, A. C.; Ghana, P.; Chakraborty, U.; Schnakenburg, G.

*Manganese-Tin Triple Bonds: A New Synthetic Route to the Manganese Stannylidyne Complex Cation trans- H(dmpe)<sub>2</sub>Mn Sn(C<sub>6</sub>H<sub>3</sub>-2,6-Mes<sub>2</sub>) (+) (dmpe = Me<sub>2</sub>PCH<sub>2</sub>CH<sub>2</sub>PMe<sub>2</sub>, Mes=2,4,6-Trimethylphenyl)*  
Journal of the American Chemical Society, (135): 11525-11528 2013.

Filippov, O. A.; Belkova, N. V.; Epstein, L. M.; Shubina, E. S.

*Chemistry of boron hydrides orchestrated by dihydrogen bonds*  
Journal of Organometallic Chemistry, (747): 30-42 2013.

Filippov, O. A.; Kirikina, V. A.; Belkova, N. V.; Stoccoro, S.; Zucca, A.; Babakhina, G. M.; Epstein, L. M.; Shubina, E. S.

*First Example of Hydrogen Bonding to Platinum Hydride*  
Zeitschrift Fur Physikalische Chemie-International Journal of Research in Physical Chemistry & Chemical Physics, (227): 869-880 2013.

Fitzsimmons, A.; Klobukowski, M.

*Basis set effects in simple compounds of heavy rare gases*  
Canadian Journal of Chemistry-Revue Canadienne De Chimie, (91): 894-901 2013.

- Fitzsimmons, A.; Klobukowski, M.  
*Structure and stability of organic molecules containing heavy rare gas atoms*  
Theoretical Chemistry Accounts, (132) 2013.
- Flores, J. C.; Lacour, M. A.; Sallenave, X.; Serein-Spirau, F.; Lere-Porte, J. P.; Moreau, J. J. E.; Miqueu, K.; Sotiropoulos, J. M.; Flot, D.  
*Comprehensive Analysis of Fragment Orbital Interactions to Build Highly -Conjugated Thienylene-Substituted Phenylene Oligomers*  
Chemistry-a European Journal, (19): 7532-7546 2013.
- Ford, T. A.  
*The Vibrational Spectra of the Boron Halides and Their Molecular Complexes. Part 14. Ab Initio Studies of the Boron Trifluoride-Nitrous Acid Complex*  
South African Journal of Chemistry-Suid-Afrikaanse Tydskrif Vir Chemie, (66): 221-230 2013.
- Fornies, J.; Fortuno, C.; Ibanez, S.; Martin, A.; Mastrorilli, P.; Gallo, V.; Tshipis, A.  
*Synthesis and Reactivity of the Unsaturated Trinuclear Phosphanido Complex (C6F5)(2)Pt(mu-PPH2)(2)Pt(mu-PPH2)(2)Pt(PPH3)*  
Inorganic Chemistry, (52): 1942-1953 2013.
- Forster, D.; Nickolaus, J.; Nieger, M.; Benko, Z.; Ehlers, A. W.; Gudat, D.  
*Donor-Free Phosphenium-Metal(0)-Halides with Unsymmetrically Bridging Phosphenium Ligands*  
Inorganic Chemistry, (52): 7699-7708 2013.
- Forte, G.; Fortuna, C. G.; Salerno, L.; Modica, M. N.; Siracusa, M. A.; Cardile, V.; Romeo, G.; Bulbarelli, A.; Lonati, E.; Pittala, V.  
*Antitumor properties of substituted (alpha E)-alpha-(1H-indol-3-ylmethylene)benzeneacetic acids or amides*  
Bioorganic & Medicinal Chemistry, (21): 5233-5245 2013.
- Fraind, A. M.; Sini, G.; Risko, C.; Ryzhkov, L. R.; Bredas, J. L.; Tovar, J. D.  
*Charge Delocalization through Benzene, Naphthalene, and Anthracene Bridges in pi-Conjugated Oligomers: An Experimental and Quantum Chemical Study*  
Journal of Physical Chemistry B, (117): 6304-6317 2013.
- Frank, A.; Berkefeld, A.; Drexler, M.; Moller, H. M.; Exner, T. E.  
*Small changes-Huge influences: NMR chemical shifts of Ni(II) complexes with polar substrates*  
International Journal of Quantum Chemistry, (113): 1787-1793 2013.
- Frean, S. M.; Palafox, M. A.; Rastogi, V. K.  
*Effect of the microhydration on the tautomerism in the anticarcinogenic drug 5-fluorouracil and relationships with other 5-haloderivatives*  
Journal of Molecular Structure, (1054): 32-45 2013.
- Freeman, F.; Adesina, I. T.; Le La, J.; Lee, J. Y.; Poplawski, A. A.  
*Conformers of Cysteine and Cysteine Sulfenic Acid and Mechanisms of the Reaction of Cysteine Sulfenic Acid with 5,5-Dimethyl-1,3-cyclohexanedione (Dimedone)*  
Journal of Physical Chemistry B, (117): 16000-16012 2013.
- Freindorf, M.; Sexton, T.; Kraka, E.; Cremer, D.  
*The mechanism of the cycloaddition reaction of 1,3-dipole molecules with acetylene: an investigation with the unified reaction valley approach*

- Theoretical Chemistry Accounts, (133) 2013.
- Freitas, M. P.  
*The anomeric effect on the basis of natural bond orbital analysis*  
Organic & Biomolecular Chemistry, (11): 2885-2890 2013.
- Fressigne, C.; Lhermet, R.; Girard, A. L.; Durandetti, M.; Maddaluno, J.  
*Influence of the Acetylenic Substituent on the Intramolecular Carbolithiation of Alkynes: A DFT Theoretical Study*  
Journal of Organic Chemistry, (78): 9659-9669 2013.
- Fretz, S. J.; Hadad, C. M.; Hart, D. J.; Vyas, S.; Yang, D. X.  
*Birch Reductive Alkylation of Methyl m-(Hydroxymethyl)benzoate Derivatives and the Behavior of o- and p-(Hydroxymethyl)benzoates under Reductive Alkylation Conditions*  
Journal of Organic Chemistry, (78): 83-92 2013.
- Fry, A.  
*Computational studies of ion pairing. 9. The "steric" effect of tetraalkylammonium ions with electrochemically generated anions is not steric*  
Electrochemistry Communications, (35): 88-90 2013.
- Fry, A. J.  
*Computational Studies of Ion Pairing. 8. Ion Pairing of Tetraalkylammonium Ions to Nitrosobenzene and Benzaldehyde Redox Species. A General Binding Motif for the Interaction of Tetraalkylammonium Ions with Benzenoid Species*  
Journal of Organic Chemistry, (78): 5476-5481 2013.
- Fu, Y. W.; Chen, M. J.  
*Theoretical Investigation on the Electronic Properties of Alternating Donor-acceptor Conjugated Oligomers and the Effect of D-A Ratio on Electronic Properties*  
Chemical Journal of Chinese Universities-Chinese, (34): 447-454 2013.
- Fu, Y. W.; Shen, W.; Chen, M. J.  
*THEORETICAL DESIGN OF THE ELECTRONIC STRUCTURES AND CONDUCTION PROPERTIES OF CONJUGATED DONOR-ACCEPTOR COPOLYMERS*  
Acta Polymerica Sinica: 870-877 2013.
- Futamura, R.; Jorge, M.; Gomes, J. R. B.  
*Structures and energetics of organosilanes in the gaseous phase: a computational study*  
Theoretical Chemistry Accounts, (132) 2013.
- Gabr, R. K.; Hatakeyama, T.; Takenaka, K.; Takizawa, S.; Okada, Y.; Nakamura, M.; Sasai, H.  
*DFT Study of a 5-endo-trig-Type Cyclization of 3-Alkenoic Acids by Using Pd-Spiro-bis(isoxazoline) as Catalyst: Importance of the Rigid Spiro Framework for Both Selectivity and Reactivity*  
Chemistry-a European Journal, (19): 9518-9525 2013.
- Gajewy, J.; Gawronski, J.; Kwit, M.  
*Mechanism and Enantioselectivity of Zinc(diamine)(diol) -Catalyzed Asymmetric Hydrosilylation of Ketones: DFT, NMR and ECD Studies*  
European Journal of Organic Chemistry: 307-318 2013.
- Galan, J. F.; Tang, C. N.; Chakrabarty, S.; Liu, Z. W.; Moyna, G.; Pophristic, V.

- Conformational preferences of furan- and thiophene-based arylamides: a combined computational and experimental study*  
Physical Chemistry Chemical Physics, (15): 11883-11892 2013.
- Galeev, T. R.; Dunnington, B. D.; Schmidt, J. R.; Boldyrev, A. I.  
*Solid state adaptive natural density partitioning: a tool for deciphering multi-center bonding in periodic systems*  
Physical Chemistry Chemical Physics, (15): 5022-5029 2013.
- Galimberti, D.; Milani, A.; Castiglioni, C.  
*Infrared intensities and charge mobility in hydrogen bonded complexes*  
Journal of Chemical Physics, (139) 2013.
- Galvao, T. L. P.; Rocha, I. M.; da Silva, M.; da Silva, M.  
*From 2-Hydroxypyridine to 4(3H)-Pyrimidinone: Computational Study on the Control of the Tautomeric Equilibrium*  
Journal of Physical Chemistry A, (117): 12668-12674 2013.
- Galvao, T. L. P.; Rocha, I. M.; da Silva, M.; da Silva, M.  
*Is Uracil Aromatic? The Enthalpies of Hydrogenation in the Gaseous and Crystalline Phases, and in Aqueous Solution, as Tools to Obtain an Answer*  
Journal of Physical Chemistry A, (117): 5826-5836 2013.
- Gandhi, T.; Rajkumar, S.; Prathyusha, V.; Priyakumar, U. D.  
*Synthesis and Reactivity Studies of Dicationic Dihydrogen Complexes Bearing Sulfur-Donor Ligands: A Combined Experimental and Computational Study*  
European Journal of Inorganic Chemistry: 1434-1443 2013.
- Gangarapu, S.; Marcelis, A. T. M.; Zuilhof, H.  
*Carbamate Stabilities of Sterically Hindered Amines from Quantum Chemical Methods: Relevance for CO<sub>2</sub> Capture*  
Chemphyschem, (14): 3936-3943 2013.
- Ganguly, A.; Paul, B. K.; Ghosh, S.; Guchhait, N.  
*A computational acumen into the relative applicability of geometrical and quantum chemical criteria in assessing intramolecular hydrogen bonding (IMHB) interaction: 5-Halosalicylic acids as representative examples*  
Computational and Theoretical Chemistry, (1018): 102-114 2013.
- Gao, M.; Yang, X.; Cheng, J. B.; Li, Q. Z.; Li, W. Z.; Loffredo, R. E.  
*Interplay between Metal center dot center dot center dot pi Interactions and Hydrogen Bonds: Some Unusual Synergetic Effects of Coinage Metals and Substituents*  
Chemphyschem, (14): 3341-3347 2013.
- Gao, W.; Jiao, J. Q.; Feng, H. J.; Xuan, X. P.; Chen, L. P.  
*From clusters to liquid: what are the preferred ways for benzene and pyrrole to interact?*  
Theoretical Chemistry Accounts, (132) 2013.
- Gao, W.; Jiao, J. Q.; Feng, H. J.; Xuan, X. P.; Chen, L. P.  
*Natures of benzene-water and pyrrole-water interactions in the forms of sigma and pi types: theoretical studies from clusters to liquid mixture*  
Journal of Molecular Modeling, (19): 1273-1283 2013.

- Garcia-Ricard, O. J.; Meza-Morales, P.; Silva-Martinez, J. C.; Curet-Arana, M. C.; Hogan, J. A.; Hernandez-Maldonado, A. J.  
*Carbon dioxide storage and sustained delivery by Cu-2(pzdc)(2)L L = dipyridyl-based ligand pillared-layer porous coordination networks*  
Microporous and Mesoporous Materials, (177): 54-58 2013.
- Gautam, S.; Dharamvir, K.; Goel, N.  
*CO2 adsorption and activation over medium sized Cu-n (n=7, 13 and 19) clusters: A density functional study*  
Computational and Theoretical Chemistry, (1009): 8-16 2013.
- Georg, H. C.; Fileti, E. E.; Malaspina, T.  
*Ab initio study of weakly bound halogen complexes: RXa <-PH3*  
Journal of Molecular Modeling, (19): 329-336 2013.
- Georgieva, I.; Trendafilova, N.; Dodoff, N. I.  
*Effect of the metal center dot center dot center dot metal interactions on the absorption properties of Pt(II) and Pd(II) complexes of glyoxilic acid oxime in solution and solid state: Theoretical and experimental study*  
Journal of Photochemistry and Photobiology a-Chemistry, (267): 35-48 2013.
- Gerasimova, T. P.; Katsyuba, S. A.  
*Bipyridine and phenanthroline IR-spectral bands as indicators of metal spin state in hexacoordinated complexes of Fe(II), Ni(II) and Co(II)*  
Dalton Transactions, (42): 1787-1797 2013.
- Geri, J. B.; Pernicone, N. C.; York, J. T.  
*Comparing the impact of different supporting ligands on copper(I)-ethylene interactions*  
Polyhedron, (52): 207-215 2013.
- Ghailane, T.; Balkhmima, R. A.; Ghailane, R.; Souizi, A.; Touir, R.; Touhami, M. E.; Marakchi, K.; Komiha, N.  
*Experimental and theoretical studies for mild steel corrosion inhibition in 1 M HCl by two new benzothiazine derivatives*  
Corrosion Science, (76): 317-324 2013.
- Ghatee, M. H.; Pakdel, L.  
*Pyridine adsorption on small Nin-cluster (n=2,3,4): A study of geometry and electronic structure*  
International Journal of Quantum Chemistry, (113): 1549-1555 2013.
- Ghiasi, R.  
*Theoretical study of structure, bonding, and aromaticity of borazyne and B-substituted borazines*  
Russian Journal of Physical Chemistry A, (87): 2231-2238 2013.
- Ghiasi, R.; Amini, E.  
*Theoretical Investigations on Electronics Structure and Chemical Bonding on Iridathiabenzene and Iridaoxabenzene*  
Russian Journal of Physical Chemistry A, (87): 1684-1691 2013.
- Ghiasi, R.; Mehrabani, M. M.  
*MOLECULAR STRUCTURE, NATURAL BOND ORBITAL, SUBSTITUENT EFFECT AND CHEMICAL REACTIVITY ANALYSIS OF TERMINAL BORYLENE RUTHENIUM COMPLEXES: Ru(PH3)(2)HCl(BC6H4X)*  
Journal of Theoretical & Computational Chemistry, (12) 2013.

- Gholivand, K.; Dorosti, N.  
*Some new compounds with P(E)NHC(O) (E = lone pair, O, S) linkage: synthesis, spectroscopic, crystal structures, theoretical studies, and antimicrobial evaluation*  
Monatshefte für Chemie, (144): 1417-1425 2013.
- Gholivand, K.; Valmoozi, A. A. E.; Mahzouni, H. R.  
*Structural and electronic aspects of hydrogen bonding in two polymorphs of butylene-N,N'-bis(O,O'-diarylphosphoramidate)*  
Acta Crystallographica Section B-Structural Science, (69): 55-61 2013.
- Gholivand, K.; Valmoozi, A. A. E.; Mahzouni, H. R.; Ghadimi, S.; Rahimi, R.  
*Molecular Docking and QSAR Studies: Noncovalent Interaction between Acephate Analogous and the Receptor Site of Human Acetylcholinesterase*  
Journal of Agricultural and Food Chemistry, (61): 6776-6785 2013.
- Ghosh, D.; Sen, K.; Bagchi, S.; Das, A. K.  
*The nature of lead-sulfur interaction in Pb-II(S<sub>2</sub>COEt)<sub>n</sub> (2-n) (n=1,2,3,4) complexes: topological exploration and formation analysis*  
New Journal of Chemistry, (37): 1408-1416 2013.
- Ghosh, S.; Hogarth, G.; Hollingsworth, N.; Holt, K. B.; Richards, I.; Richmond, M. G.; Sanchez, B. E.; Unwin, D.  
*Models of the iron-only hydrogenase: a comparison of chelate and bridge isomers of Fe-2(CO)(4){Ph<sub>2</sub>PN(R)PPh<sub>2</sub>}(μ-pdt) as proton-reduction catalysts*  
Dalton Transactions, (42): 6775-6792 2013.
- Ghosh, S.; Schauble, E. A.; Couloume, G. L.; Blum, J. D.; Bergquist, B. A.  
*Estimation of nuclear volume dependent fractionation of mercury isotopes in equilibrium liquid-vapor evaporation experiments*  
Chemical Geology, (336): 5-12 2013.
- Gidron, O.; Diskin-Posner, Y.; Bendikov, M.  
*High Charge Delocalization and Conjugation in Oligofuran Molecular Wires*  
Chemistry-a European Journal, (19): 13140-13150 2013.
- Gil, D. M.; Piro, O. E.; Echeverria, G. A.; Tuttolomondo, M. E.; Ben Altabef, A.  
*Layered crystal structure, conformational and vibrational properties of 2,2,2-trichloroethoxysulfonamide: An experimental and theoretical study*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (116): 122-131 2013.
- Gilli, G.; Bertolasi, V.; Gilli, P.  
*Solid-State N-H center dot center dot center dot O/O-H center dot center dot center dot N Tautomerism in Resonance-Assisted 1-(Arylazo)-2-Naphthols and Its Through-Space π\* ← π Perturbation in TCNQ Cocrystals. A Variable-Temperature X-ray Crystal Study*  
Crystal Growth & Design, (13): 3308-3320 2013.
- Giricheva, N. I.; Girichev, G. V.; Dakkouri, M.; Ivanov, S. N.; Petrov, V. M.; Petrova, V. N.  
*Molecular structure and barriers to internal rotation of alpha-naphthalenesulfonyl chloride: a study by gas-phase electron diffraction and quantum chemical calculations*  
Structural Chemistry, (24): 819-826 2013.
- Giricheva, N. I.; Girichev, G. V.; Fedorov, M. S.; Ivanov, S. N.  
*Substituent effect on geometric and electronic structure of benzenesulfonic acid: gas-phase electron diffraction and quantum chemical studies of 4-CH<sub>3</sub>C<sub>6</sub>H<sub>4</sub>SO<sub>3</sub>H and 3-NO<sub>2</sub>C<sub>6</sub>H<sub>4</sub>SO<sub>3</sub>H molecules*



- Structural Chemistry, (24): 807-818 2013.
- Giricheva, N. I.; Petrov, V. M.; Oberhammer, H.; Petrova, V. N.; Dakkouri, M.; Ivanov, S. N.; Girichev, G. V.  
*Interrelation of nonequivalent C-C bonds of naphthalene frame and spatial orientation of substituents: Beta-naphthalene sulfonyl fluoride and beta-naphthalene sulfonyl chloride*  
Journal of Molecular Structure, (1042): 66-72 2013.
- Glendening, E. D.; Landis, C. R.; Weinhold, F.  
*NBO 6.0: Natural bond orbital analysis program*  
Journal of Computational Chemistry, (34): 1429-1437 2013.
- Glendening, E. D.; Landis, C. R.; Weinhold, F.  
*NBO 6.0: Natural bond orbital analysis program (vol 34, pg 1429, 2013)*  
Journal of Computational Chemistry, (34): 2134-2134 2013.
- Gnanasambandan, T.; Gunasekaran, S.; Seshadri, S.  
*Molecular structure analysis and spectroscopic characterization of carbimazole with experimental (FT-IR, FT-Raman and UV-Vis) techniques and quantum chemical calculations*  
Journal of Molecular Structure, (1052): 38-49 2013.
- Gnanasambandan, T.; Gunasekaran, S.; Seshadri, S.  
*The spectroscopic (FTIR, FT-Raman and UV-Vis spectra), DFT and normal coordinate computations of m-nitromethylbenzoate*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (112): 52-61 2013.
- Gobinath, E.; Xavier, R. J.  
*Quantum chemical calculations, vibrational studies, HOMO-LUMO and NBO/NLMO analysis of 2-bromo-5-nitrothiazole*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (104): 394-402 2013.
- Gobinath, E.; Xavier, R. J.  
*Spectroscopic investigations, quantum chemical calculations, HOMO-LUMO and NBO/NLMO analysis of 4-pyridinecarbohydrazide*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (115): 815-822 2013.
- Gogoi, U.; Guha, A. K.; Phukan, A. K.  
*Tracing the Route to Ammonia: A Theoretical Study on the Possible Pathways for Dinitrogen Reduction with Tripodal Iron Complexes*  
Chemistry-a European Journal, (19): 11077-11089 2013.
- Gohee, P.; Abdallah, H. H.; Archibong, E. F.; Ramasami, P.  
*First principles gas phase study of the structures, energetics and spectroscopic parameters of aluminium antimonide, Al<sub>x</sub>Sb<sub>y</sub> (x + y=3, 5), clusters*  
European Physical Journal D, (67) 2013.
- Golchoubian, H.; Rezaee, E.; Farmanzadeh, D.  
*Investigation of keto-enol tautomerism in tetraketonate ligands*  
Structural Chemistry, (24): 481-489 2013.
- Gold, B.; Dudley, G. B.; Alabugin, I. V.  
*Moderating Strain without Sacrificing Reactivity: Design of Fast and Tunable Noncatalyzed Alkyne-Azide Cycloadditions via Stereoelectronically Controlled Transition State Stabilization*  
Journal of the American Chemical Society, (135): 1558-1569 2013.

- Gomez, H.; Lluch, J. M.; Masgrau, L.  
*Substrate-Assisted and Nucleophilically Assisted Catalysis in Bovine alpha 1,3-Galactosyltransferase. Mechanistic Implications for Retaining Glycosyltransferases*  
Journal of the American Chemical Society, (135): 7053-7063 2013.
- Goncalves, G.; Tomaz, I.; Correia, I.; Veiros, L. F.; Castro, M.; Avecilla, F.; Palacio, L.; Maestro, M.; Kiss, T.; Jakusch, T.; Garcia, M. H. V.; Pessoa, J. C.  
*A novel (VO)-O-IV-pyrimidinone complex: synthesis, solution speciation and human serum protein binding*  
Dalton Transactions, (42): 11841-11861 2013.
- Gong, S. D.; Wu, Y.; Li, Q. S.; Xie, Y. M.; King, R. B.  
*Comparison of the difluoromethylene and carbonyl ligands in binuclear iron complexes*  
Journal of Fluorine Chemistry, (151): 12-19 2013.
- Gong, Y.; Hu, H. S.; Rao, L. F.; Li, J.; Gibson, J. K.  
*Experimental and Theoretical Studies on the Fragmentation of Gas-Phase Uranyl-, Neptunyl-, and Plutonyl-Diglycolamide Complexes*  
Journal of Physical Chemistry A, (117): 10544-10550 2013.
- Gorelsky, S. I.  
*Origins of regioselectivity of the palladium-catalyzed (aromatic)C-H bond metalation-deprotonation*  
Coordination Chemistry Reviews, (257): 153-164 2013.
- Gorske, B. C.; Nelson, R. C.; Bowden, Z. S.; Kufe, T. A.; Childs, A. M.  
*"Bridged" n ->pi\* Interactions Can Stabilize Peptoid Helices*  
Journal of Organic Chemistry, (78): 11172-11183 2013.
- Govender, P. P.; Navizet, I.; Perry, C. B.; Marques, H. M.  
*DFT Studies of Trans and Cis Influences in the Homolysis of the Co-C Bond in Models of the Alkylcobalamins*  
Journal of Physical Chemistry A, (117): 3057-3068 2013.
- Grabowski, S. J.  
*Cooperativity of hydrogen and halogen bond interactions*  
Theoretical Chemistry Accounts, (132) 2013.
- Grabowski, S. J.  
*Dihydrogen bond and X-H center dot center dot center dot sigma interaction as sub-classes of hydrogen bond*  
Journal of Physical Organic Chemistry, (26): 452-459 2013.
- Grabowski, S. J.  
*Hydrogen and halogen bonds are ruled by the same mechanisms*  
Physical Chemistry Chemical Physics, (15): 7249-7259 2013.
- Grabowski, S. J.  
*Non-covalent interactions - QTAIM and NBO analysis*  
Journal of Molecular Modeling, (19): 4713-4721 2013.
- Grabowski, S. J.  
*sigma-Hole Bond Versus Hydrogen Bond: From Tetravalent to Pentavalent N, P, and As Atoms*  
Chemistry-a European Journal, (19): 14600-14611 2013.

- Grabowski, S. J.; Alkorta, I.; Elguero, J.  
*Complexes between Dihydrogen and Amine, Phosphine, and Arsine Derivatives. Hydrogen Bond versus Pnictogen Interaction*  
Journal of Physical Chemistry A, (117): 3243-3251 2013.
- Graton, J.; Besseau, F.; Brossard, A. M.; Charpentier, E.; Deroche, A.; Le Questel, J. Y.  
*Hydrogen-Bond Acidity of OH Groups in Various Molecular Environments (Phenols, Alcohols, Steroid Derivatives, and Amino Acids Structures): Experimental Measurements and Density Functional Theory Calculations*  
Journal of Physical Chemistry A, (117): 13184-13193 2013.
- Gregson, M.; Lu, E.; McMaster, J.; Lewis, W.; Blake, A. J.; Liddle, S. T.  
*A Cerium(IV)-Carbon Multiple Bond*  
Angewandte Chemie-International Edition, (52): 13016-13019 2013.
- Grocka, I.; Latos-Grazynski, L.; Stepień, M.  
*Ruthenocenoporphyrinoids: Conformation Determines Macrocyclic  $\pi$  Conjugation Transmitted Across a d-Electron Metallocene*  
Angewandte Chemie-International Edition, (52): 1044-1048 2013.
- Groenewold, G. S.; Delmore, J. E.; Benson, M. T.; Tsuda, T.; Hagiwara, R.  
*Fluorohydrogenate Cluster Ions in the Gas Phase: Electrospray Ionization Mass Spectrometry of the 1-Ethyl-3-methylimidazolium(+) F(HF)(2.3)(-) Ionic Liquid*  
Journal of Physical Chemistry A, (117): 14191-14199 2013.
- Groom, L. R.; Schwarz, A. D.; Nova, A.; Clot, E.; Mountford, P.  
*Synthesis and Reactions of a Cyclopentadienyl-Amidinate Titanium tert-Butoxyimido Compound*  
Organometallics, (32): 7520-7539 2013.
- Gu, P.; Lu, R. Q.; Wang, S. T.; Lu, Y. K.; Liu, D.  
*The comparative study on interactions between ionic liquid and CO<sub>2</sub>/SO<sub>2</sub> by a hybrid density functional approach in the gas phase*  
Computational and Theoretical Chemistry, (1020): 22-31 2013.
- Guha, A. K.; Gogoi, U.; Phukan, A. K.  
*Revisiting the Reactivity of Different Carbon Bases: A Theoretical Study*  
International Journal of Quantum Chemistry, (113): 2471-2477 2013.
- Guidara, S.; Feki, H.; Abid, Y.  
*Vibrational spectral studies and non-linear optical properties of L-leucine L-leucinium picrate: A Density Functional Theory approach*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (115): 437-444 2013.
- Guillaume, S. M.; Annunziata, L.; del Rosal, I.; Iftner, C.; Maron, L.; Roesky, P. W.; Schmid, M.  
*Ring-opening polymerization of racemic beta-butyrolactone promoted by rare earth trisborohydride complexes towards a PHB-diol: an experimental and DFT study*  
Polymer Chemistry, (4): 3077-3087 2013.
- Gunasekaran, S.; Rajalakshmi, K.; Kumaresan, S.  
*Study of molecular structure and assignments of fundamental modes of 2-ethylpyridine-4-carbothioamide by density functional methods*  
Indian Journal of Physics, (87): 723-732 2013.

- Gunasekaran, S.; Rajalakshmi, K.; Kumaresan, S.  
*Vibrational analysis, electronic structure and nonlinear optical properties of Levofloxacin by density functional theory*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (112): 351-363 2013.
- Gunay, N.; Pir, H.; Avci, D.; Atalay, Y.  
*NLO and NBO Analysis of Sarcosine-Maleic Acid by Using HF and B3LYP Calculations*  
Journal of Chemistry, 2013.
- Gunbas, G.; Sheppard, W. L.; Fettinger, J. C.; Olmstead, M. M.; Mascal, M.  
*Extreme Oxatriquinanes: Structural Characterization of alpha-Oxyoxonium Species with Extraordinarily Long Carbon-Oxygen Bonds*  
Journal of the American Chemical Society, (135): 8173-8176 2013.
- Guo, J. F.; Shi, W. J.; Ren, F. D.; Cao, D. L.; Zhang, Y. S.  
*A B3LYP and MP2(full) theoretical investigation into the cooperativity effect between dihydrogen-bonding and H-Ma (TM)  $\sigma$  (TM)  $\pi$  (TM)  $\pi$  (M = Li, Na, K) interactions among HF, MH with the  $\pi$ -electron donor C<sub>2</sub>H<sub>2</sub>, C<sub>2</sub>H<sub>4</sub> or C<sub>6</sub>H<sub>6</sub>*  
Journal of Molecular Modeling, (19): 3153-3163 2013.
- Guo, L. F.; Huang, Z. G.; Shen, T. T.; Ma, L. L.; Niu, X. Q.  
*Theoretical Study on the Hydrogen Bonding Interactions in Complexes of 5-Hydroxytryptamine with Water*  
Chinese Journal of Chemistry, (31): 1079-1086 2013.
- Gupta, K.; Giri, S.; Chattaraj, P. K.  
*Charge-based DFT descriptors for Diels-Alder reactions*  
Journal of Physical Organic Chemistry, (26): 187-193 2013.
- Gushchin, P. V.; Kuznetsov, M. L.; Haukka, M.; Kukushkin, V. Y.  
*Recognition of a Novel Type X=N-Hal center dot center dot center dot Hal (X = C, S, P; Hal = F, Cl, Br, I)*  
*Halogen Bonding*  
Journal of Physical Chemistry A, (117): 2827-2834 2013.
- Gutsev, G. L.; Weatherford, C. A.; Jena, P.; Johnson, E.; Ramachandran, B. R.  
*Competition between surface chemisorption and cage formation in Fe<sub>12</sub>O<sub>12</sub> clusters*  
Chemical Physics Letters, (556): 211-216 2013.
- Gutsev, G. L.; Weatherford, C. W.; Belay, K. G.; Ramachandran, B. R.; Jena, P.  
*An all-electron density functional theory study of the structure and properties of the neutral and singly charged M-12 and M-13 clusters: M = Sc-Zn*  
Journal of Chemical Physics, (138) 2013.
- Guzzetti, K. A.; Brizuela, A. B.; Romano, E.; Brandan, S. A.  
*Structural and vibrational study on zwitterions of L-threonine in aqueous phase using the FT-Raman and SCRF calculations*  
Journal of Molecular Structure, (1045): 171-179 2013.
- Gyepes, R.; Pacigova, S.; Tatiersky, J.; Sivak, M.  
*Anion- $\pi$ , lone pair- $\pi$  and  $\pi$ - $\pi$  interactions in VO(O-2)(+) complexes with one dipicolinato(2-)-N,O,O ligand and bearing picolinamidium, nicotinamidium or phenanthrolium as counterions*  
Journal of Molecular Structure, (1041): 113-121 2013.
- Ha, T. J.; Sonar, P.; Dodabalapur, A.

- Charge transport study of high mobility polymer thin-film transistors based on thiophene substituted diketopyrrolopyrrole copolymers*  
Physical Chemistry Chemical Physics, (15): 9735-9741 2013.
- Haberhauert, G.; Gleiter, R.  
*Interplay between 1,3-Butadien-1,4-diyl and 2-Buten-1,4-dicarbene Derivatives: The Quest for Nucleophilic Carbenes*  
Journal of the American Chemical Society, (135): 8022-8030 2013.
- Haghdadi, M.  
*DFT molecular orbital calculations and natural bond orbital analysis of 1,2,7-thiadiazepane conformers*  
Monatshefte für Chemie, (144): 1653-1661 2013.
- Hailmann, M.; Herkert, L.; Himmelspach, A.; Finze, M.  
*Difunctionalized {closo-1-CB11} Clusters: 1-and 2-Amino-12-ethynylcarba-closo-dodecaborates*  
Chemistry-a European Journal, (19): 15745-15758 2013.
- Hameed, S. A.; Alrouby, S. K.; Hilal, R.  
*Design of molecular switching and signaling based on proton transfer in 2-hydroxy Schiff bases: a computational study*  
Journal of Molecular Modeling, (19): 559-569 2013.
- Han, G. Z.; Ding, Y. L.; Qian, P.; Zhang, C.; Song, W.  
*Theoretical investigation of gas phase ethanol(water)<sub>n</sub> (n=15) clusters and comparison with gas phase pure water clusters (water)<sub>n</sub> (n=26)*  
International Journal of Quantum Chemistry, (113): 1511-1521 2013.
- Han, J.; Dai, X.; Cheng, C.; Xin, M. S.; Wang, Z. G.; Huai, P.; Zhang, R. Q.  
*Strong Adsorption Between Uranium Dicarbide and Graphene Surface Induced by f Electrons*  
Journal of Physical Chemistry C, (117): 26849-26857 2013.
- Hansmann, M. M.; Rominger, F.; Hashmi, A. S. K.  
*Gold-allenylidenes - an experimental and theoretical study*  
Chemical Science, (4): 1552-1559 2013.
- Hapka, M.; Klos, J.; Korona, T.; Chalasinski, G.  
*Theoretical Studies of Potential Energy Surface and Bound States of the Strongly Bound He(S-1)-BeO ((1)Sigma(+)) Complex*  
Journal of Physical Chemistry A, (117): 6657-6663 2013.
- Harb, C.; Kravtsov, P.; Choudhuri, M.; Sirianni, E. R.; Yap, G. P. A.; Lever, A. B. P.; Crutchley, R. J.  
*Phenylcyanamidoruthenium Scorpionate Complexes*  
Inorganic Chemistry, (52): 1621-1630 2013.
- Harinipriya, S.; Sudha, V.; Sangaranarayanan, M. V.; Malar, E. J. P.  
*Adsorption of Enantiomers on Metal Surfaces: Application to D- and L-Alanine on Cu, Ni and Zn Electrodes*  
Journal of the Electrochemical Society, (160): G102-G110 2013.
- Harrison, D. J.; Gorelsky, S. I.; Lee, G. M.; Korobkov, I.; Baker, R. T.  
*Cobalt Fluorocarbene Complexes*  
Organometallics, (32): 12-15 2013.
- Hasanayn, F.; Baroudi, A.; Bengali, A. A.; Goldman, A. S.

- Hydrogenation of Dimethyl Carbonate to Methanol by trans- Ru(H)(2)(PNN)(CO) Catalysts: DFT Evidence for Ion-Pair-Mediated Metathesis Paths for C-OMe Bond Cleavage*  
Organometallics, (32): 6969-6985 2013.
- Hayes, C. J.; Simpkins, N. S.  
*Bridgehead enolate or bridgehead organolithium? DFT calculations provide insights into a difficult bridgehead substitution reaction in the synthesis of the polycyclic polyprenylated acylphloroglucinol (PPAP) nemorosone*  
Organic & Biomolecular Chemistry, (11): 8458-8462 2013.
- He, D. S.; Ma, M.  
*Quantum chemical study of extraction characteristics of kinetic synergist OT in liquid membrane using HPMBP as carrier*  
Separation and Purification Technology, (107): 289-296 2013.
- He, H. Y.; Zhang, S. J.; Liu, X. M.; Wang, J. Q.; Yao, X. Q.; Zhang, X. P.  
*Structures and hydrogen bonds of biodegradable naphthenate ionic liquids*  
Fluid Phase Equilibria, (360): 169-179 2013.
- He, X. D.; Sun, C. Z.; Sun, N.; Chen, D. Z.  
*Computational study on the mechanism of non-catalyzed and catalyzed bromolactonization*  
Computational and Theoretical Chemistry, (1024): 45-51 2013.
- Heiden, Z. M.; Chen, S. T.; Mock, M. T.; Dougherty, W. G.; Kassel, W. S.; Rousseau, R.; Bullock, R. M.  
*Protonation of Ferrous Dinitrogen Complexes Containing a Diphosphine Ligand with a Pendent Amine*  
Inorganic Chemistry, (52): 4026-4039 2013.
- Hellmann, G.; Hack, A.; Thiemermann, E.; Luche, O.; Raabe, G.; Gais, H. J.  
*Chiral Fluorinated alpha-Sulfonyl Carbanions: Enantioselective Synthesis and Electrophilic Capture, Racemization Dynamics, and Structure*  
Chemistry-a European Journal, (19): 3869-3897 2013.
- Hengesbach, F.; Jin, X.; Hepp, A.; Wibbeling, B.; Wurthwein, E. U.; Uhl, W.  
*Activation of Isocyanates and Carbon Dioxide by a Monomeric Aluminium Hydrazide as an Active Lewis Pair*  
Chemistry-a European Journal, (19): 13901-13909 2013.
- Hepperle, S. S.; Wang, Y. A.  
*Comprehensive Computational Study of Decamethylzincocene Formation. 1. Reaction of ZnR<sub>2</sub> Reagents with Decamethylzincocene*  
Journal of Physical Chemistry A, (117): 4657-4663 2013.
- Hering, C.; Rothe, J.; Schulz, A.; Villinger, A.  
*Structure and Bonding of Novel Acyclic Bisaminoarsenium Cations*  
Inorganic Chemistry, (52): 7781-7790 2013.
- Hering, C.; Schulz, A.; Villinger, A.  
*On the Synthesis and Reactivity of Highly Labile Pseudohalogen Phosphenium Ions*  
Inorganic Chemistry, (52): 5214-5225 2013.
- Heverly-Coulson, G. S.; Boyd, R. J.; Mo, O.; Yanez, M.  
*Revealing Unexpected Mechanisms for Nucleophilic Attack on SS and SeSe Bridges*  
Chemistry-a European Journal, (19): 3629-3638 2013.

- Hey, J.; Andrada, D. M.; Michel, R.; Mata, R. A.; Stalke, D.  
*Strong Intermolecular Interactions Shaping a Small Piano-Stool Complex*  
Angewandte Chemie-International Edition, (52): 10365-10369 2013.
- Hicks, J.; Hadlington, T. J.; Schenk, C.; Li, J. Y.; Jones, C.  
*Utilizing Steric Bulk to Stabilize Molybdenum Aminogermolyne and Aminogermylene Complexes*  
Organometallics, (32): 323-329 2013.
- Higashibayashi, S.; Onogi, S.; Srivastava, H. K.; Sastry, G. N.; Wu, Y. T.; Sakurai, H.  
*Stereoelectronic Effect of Curved Aromatic Structures: Favoring the Unexpected endo Conformation of Benzylic-Substituted Sumanene*  
Angewandte Chemie-International Edition, (52): 7314-7316 2013.
- Higelin, A.; Keller, S.; Gohringer, C.; Jones, C.; Krossing, I.  
*Unusual Tilted Carbene Coordination in Carbene Complexes of Gallium(I) and Indium(I)*  
Angewandte Chemie-International Edition, (52): 4941-4944 2013.
- Hilal, R.; Hassan, W. M. I.; Alyoubi, A.; Aziz, S. G.; Elroby, S. A. K.  
*Intermolecular interaction in the benzene-Ar-n and benzene dimer van der Waals complexes: DFT analysis of the charge distribution and electric response properties*  
Indian Journal of Chemistry Section a-Inorganic Bio-Inorganic Physical Theoretical & Analytical Chemistry, (52): 19-27 2013.
- Hill, J. G.; Hu, X. J.  
*Theoretical Insights into the Nature of Halogen Bonding in Prereactive Complexes*  
Chemistry-a European Journal, (19): 3620-3628 2013.
- Hnyk, D.; Holub, J.; Ruzicka, A.; Padelkova, Z.; Buhl, M.  
*Expanding the structural chemistry of the weakly coordinating closo-carborane CB<sub>11</sub>H<sub>12</sub> (-): its monoiodo derivatives with and without C (5v) symmetry*  
Structural Chemistry, (24): 927-932 2013.
- Ho, M.; Navarrete-Lopez, A. M.; Zicovich-Wilson, C. M.; Ramirez-Solis, A.  
*Electronic Charge Density Analysis of Li-Doped Polyacetylene: Molecular vs Periodic Descriptions and Nature of Li-to-Chain Bonding*  
Journal of Physical Chemistry B, (117): 725-730 2013.
- Hoffend, C.; Diefenbach, M.; Januszewski, E.; Bolte, M.; Lerner, H. W.; Holthausen, M. C.; Wagner, M.  
*Effects of boron doping on the structural and optoelectronic properties of 9,10-diarylanthracenes*  
Dalton Transactions, (42): 13826-13837 2013.
- Hoffmann, A.; Herres-Pawlis, S.  
*Dissection of Different Donor Abilities Within Bis(pyrazolyl)pyridinylmethane Transition Metal Complexes*  
Zeitschrift für Anorganische und Allgemeine Chemie, (639): 1426-1432 2013.
- Hong, K.; Kim, J.; Kim, T. K.  
*Theoretical Investigation of the Reaction of Ce<sup>+</sup> with Water in the Gas Phase: Density Functional Theory Calculations*  
Bulletin of the Korean Chemical Society, (34): 1551-1554 2013.
- Hong, Y. J.; Tantillo, D. J.

- C-H center dot center dot center dot pi interactions as modulators of carbocation structure - implications for terpene biosynthesis*  
Chemical Science, (4): 2512-2518 2013.
- Hoppe, H. A.; Kazmierczak, K.; Romano, E.; Brandan, S. A.  
*A structural and vibrational study on the first condensed borosulfate K-5 B(SO<sub>4</sub>)(4) by using the FTIR-Raman spectra and DFT calculations*  
Journal of Molecular Structure, (1037): 294-300 2013.
- Horbatenko, Y.; Vyboishchikov, S. F.  
*Si center dot center dot center dot H Interligand Interactions in Cobalt(V) and Iridium(V) Bis(silyl)bis(hydride) Complexes*  
Chempluschem, (78): 1073-1081 2013.
- Horn, P. R.; Sundstrom, E. J.; Baker, T. A.; Head-Gordon, M.  
*Unrestricted absolutely localized molecular orbitals for energy decomposition analysis: Theory and applications to intermolecular interactions involving radicals*  
Journal of Chemical Physics, (138) 2013.
- Hou, R. B.; Tang, Z. X.; Fan, Y. J.; Yi, X. H.; Wang, B. B.; Sun, Y. L.  
*Radicals Created from the Reactions of 2'-Deoxyadenosine-5'-monophosphate with Hydroxyl Radical*  
Acta Physico-Chimica Sinica, (29): 1937-1944 2013.
- Housaindokht, M. R.; Sargolzaei, M.; Bozorgmehr, M. R.  
*Ab initio study of ion replacement in Spinach plastocyanin protein*  
Bulgarian Chemical Communications, (45): 201-206 2013.
- Hratchian, H. P.; Kraka, E.  
*Improved Predictor-Corrector Integrators For Evaluating Reaction Path Curvature*  
Journal of Chemical Theory and Computation, (9): 1481-1488 2013.
- Hu, H. X.; Du, L.; Li, X. C.; Zhao, H. X.; Zhang, X. H.; Shi, S. M.; Li, H. L.; Tang, X. Y.; Yang, J.  
*Experimental, Quantum Chemical and Molecular Dynamics Studies of Imidazoline Molecules Against the Corrosion of Steel and Quantitative Structure-Activity Relationship Analysis Using the Support Vector Machine (SVM) Method*  
International Journal of Electrochemical Science, (8): 11228-11247 2013.
- Hu, W.; Li, J.; Deng, S. W.; Huang, J. Y.; Le, X. Y.; Zheng, W. X.  
*Computational mechanistic study on oxidative esterification of alcohols to esters catalyzed by palladium complex*  
Journal of Organometallic Chemistry, (740): 10-16 2013.
- Huang, H. S.; Zhang, T. L.; Zhang, S. T.; Zhang, J. G.; Wu, X. F.; Xu, J. H.  
*Theoretical Study of the Structure, Mechanism of Detonation Initiation and Stability of Transition Metal Carbohydrazide Nitrates*  
Chinese Journal of Structural Chemistry, (32): 1491-1496 2013.
- Huber, S. M.; Scanlon, J. D.; Jimenez-Izal, E.; Ugalde, J. M.; Infante, I.  
*On the directionality of halogen bonding*  
Physical Chemistry Chemical Physics, (15): 10350-10357 2013.
- Hurtado, M.; Monte, M.; Lamsabhi, A. M.; Yanez, M.; Mo, O.; Salpin, J. Y.



- Modeling Interactions between an Amino Acid and a Metal Dication: Cysteine-Calcium(II) Reactions in the Gas Phase*  
Chempluschem, (78): 1124-1133 2013.
- Huynh, H. V.; Frison, G.  
*Electronic Structural Trends in Divalent Carbon Compounds*  
Journal of Organic Chemistry, (78): 328-338 2013.
- Hyodo, K.; Kondo, M.; Funahashi, Y.; Nakamura, S.  
*Catalytic Enantioselective Decarboxylative Cyanoalkylation of Imines by Using Palladium Pincer Complexes with C-2-Symmetric Chiral Bis(imidazoline)s*  
Chemistry-a European Journal, (19): 4128-4134 2013.
- Ignatyev, I. S.; Montejo, M.; Gonzalez, J. J. L.  
*An assessment of DFT methods for predicting the thermochemistry of ion-molecule reactions of group 14 elements (Si, Ge, Sn)*  
Journal of Molecular Modeling, (19): 5439-5444 2013.
- Ignatyev, I. S.; Montejo, M.; Ortega, P. G. R.; Gonzalez, J. J. L.  
*Quantum chemical study of silanediols as metal binding groups for metalloprotease inhibitors*  
Journal of Molecular Modeling, (19): 1819-1834 2013.
- Ildiz, G. O.; Nunes, C. M.; Fausto, R.  
*Matrix Isolation Infrared Spectra and Photochemistry of Hydantoin*  
Journal of Physical Chemistry A, (117): 726-734 2013.
- Ilieva, S.; Nalbantova, D.; Hadjieva, B.; Galabov, B.  
*Aminolysis of Phenyl N-Phenylcarbamate via an Isocyanate Intermediate: Theory and Experiment*  
Journal of Organic Chemistry, (78): 6440-6449 2013.
- Imamura, Y.; Suzuki, J.; Nakai, H.  
*Kinetic Energy Decomposition Scheme Based on Information Theory*  
Journal of Computational Chemistry, (34): 2787-2795 2013.
- Ionescu, C. M.; Geidl, S.; Varekova, R. S.; Koca, J.  
*Rapid Calculation of Accurate Atomic Charges for Proteins via the Electronegativity Equalization Method*  
Journal of Chemical Information and Modeling, (53): 2548-2558 2013.
- Isaia, F.; Aragoni, M. C.; Arca, M.; Caltagirone, C.; Demartin, F.; Garau, A.; Lippolis, V.  
*Gold oxidative dissolution by (thioamide)-I-2 adducts*  
Dalton Transactions, (42): 492-498 2013.
- Isegawa, M.; Wang, B.; Truhlar, D. G.  
*Electrostatically Embedded Molecular Tailoring Approach and Validation for Peptides*  
Journal of Chemical Theory and Computation, (9): 1381-1393 2013.
- Ito, F.  
*Infrared studies of the CH3I-H2O complex and large CH3I clusters in Ar matrices*  
Journal of Molecular Structure, (1035): 54-60 2013.
- Itoh, Y.; Yamanaka, M.; Mikami, K.  
*Theoretical Study on the Regioselectivity of Baeyer-Villiger Reaction of alpha-Me-, -F-, -CF3-Cyclohexanones*

- Journal of Organic Chemistry, (78): 146-153 2013.
- Ivanov, S. N.; Giricheva, N. I.; Fedorov, M. S.; Men'shikova, I. A.; Nurkevich, T. V.; Tarasova, E. G.  
*Electronic effects of the functional groups in ortho-Nitrobenzenesulfonic acids on the results of NBO analysis*  
Russian Journal of Physical Chemistry A, (87): 608-614 2013.
- Ivanova, A.; Romanova, J.; Tadjer, A.; Baumgarten, M.  
*Magnetostructural Correlation for Rational Design of Mn(II) Hybrid-Spin Complexes*  
Journal of Physical Chemistry A, (117): 670-678 2013.
- Ivanova, B. B.; Spitteller, M.  
*Optical and nonlinear optical properties of new Schiff's bases: experimental versus theoretical study of inclusion interactions*  
Journal of Inclusion Phenomena and Macrocyclic Chemistry, (75): 211-221 2013.
- Iwamoto, J.; Matsumoto, Y.; Honma, K.  
*Solvated structures of pyrrole-acetonitrile binary clusters studied by infrared cavity ringdown spectroscopy*  
Chemical Physics, (419): 184-192 2013.
- Iwasa, T.; Nakajima, A.  
*Geometric, electronic, and optical properties of a boron-doped aluminum cluster of B<sub>2</sub>Al<sub>21</sub>⁻: A density functional theory study*  
Chemical Physics Letters, (582): 100-104 2013.
- Izadyar, M.  
*N-Phenyl-1-methyl-6-methylenecyclohexa-2,4-dienylmethanimine retro cheletropic-ene reaction, a theoretical kinetic study*  
Progress in Reaction Kinetics and Mechanism, (38): 408-416 2013.
- Izadyar, M.; Gholizadeh, M.; Khavani, M.; Housaindokht, M. R.  
*Quantum Chemistry Aspects of the Solvent Effects on 3,4-Dimethyl-2,5-dihydrothiophen-1,1-dioxide Pyrolysis Reaction*  
Journal of Physical Chemistry A, (117): 2427-2433 2013.
- Jackson, T. A.; Gutman, C. T.; Maliekal, J.; Miller, A. F.; Brunold, T. C.  
*Geometric and Electronic Structures of Manganese-Substituted Iron Superoxide Dismutase*  
Inorganic Chemistry, (52): 3356-3367 2013.
- Jackson, V. E.; Gutowski, K. E.; Dixon, D. A.  
*Density Functional Theory Study of the Complexation of the Uranyl Dication with Anionic Phosphate Ligands with and without Water Molecules*  
Journal of Physical Chemistry A, (117): 8939-8957 2013.
- Jafari, H.; Danaee, I.; Eskandari, H.; RashvandAvei, M.  
*Electrochemical and Theoretical Studies of Adsorption and Corrosion Inhibition of N,N'-Bis(2-hydroxyethoxyacetophenone)-2,2-dimethyl-1,2-propanediimine on Low Carbon Steel (API 5L Grade B) in Acidic Solution*  
Industrial & Engineering Chemistry Research, (52): 6617-6632 2013.
- Jahani, P. M.; Nowroozi, A.  
*Conformational analysis, tautomeric preference, intramolecular hydrogen bonding, and solvent effect on dinitrosamine: A quantum chemical study*

- International Journal of Quantum Chemistry, (113): 1026-1033 2013.
- Jameh-Bozorgchi, S.; Nori-Shargh, D.; Mousavi, S. N.; Rezaei, A.  
*Hybrid-DFT Study and NBO Interpretation of the Configurational Behavior of 2-Halotetrahydrothiopyran S-Oxides*  
Phosphorus Sulfur and Silicon and the Related Elements, (188): 839-849 2013.
- Jamshidi, Z.; Eskandari, K.; Azami, S. M.  
*Nature of closed- and open-shell interactions between noble metals and rare gas atoms*  
International Journal of Quantum Chemistry, (113): 1981-1991 2013.
- Jamshidi, Z.; Farhangian, H.; Tehrani, Z. A.  
*Glucose interaction with Au, Ag, and Cu clusters: Theoretical investigation*  
International Journal of Quantum Chemistry, (113): 1062-1070 2013.
- Janaki, A.; Balachandran, V.; Lakshmi, A.  
*alpha-Bromo-p-tolunitrile: Conformational stability, vibrational spectroscopic studies, NBO analysis and thermodynamic functions based on density functional theory*  
Journal of Molecular Structure, (1042): 15-24 2013.
- Janes, T.; Rawson, J. M.; Song, D. T.  
*Syntheses and structures of Li, Fe, and Mo derivatives of N,N'-bis(2,6-diisopropylphenyl)-o-phenylenediamine*  
Dalton Transactions, (42): 10640-10648 2013.
- Jarvis, A. G.; Sehnal, P. E.; Bajwa, S. E.; Whitwood, A. C.; Zhang, X. B.; Cheung, M. S.; Lin, Z. Y.; Fairlamb, I. J. S.  
*A Remarkable cis- and trans-Spanning Dibenzylidene Acetone Diphosphine Chelating Ligand (dbaphos)*  
Chemistry-a European Journal, (19): 6034-6043 2013.
- Javan, A. J.; Javan, M. J.; Tehrani, Z. A.  
*Theoretical Investigation on Antioxidant Activity of Bromophenols from the Marine Red Alga Rhodomela confervoides: H-Atom vs Electron Transfer Mechanism*  
Journal of Agricultural and Food Chemistry, (61): 1534-1541 2013.
- Jayabharathi, J.; Thanikachalam, V.; Jayamoorthy, K.  
*Optical properties of 1,2-diaryl benzimidazole derivatives - A combined experimental and theoretical studies*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (115): 74-78 2013.
- Jayarathna, N. B.; Pardue, D. B.; Ray, S.; Yousufuddin, M.; Thakur, K. G.; Cundari, T. R.; Dias, H. V. R.  
*Silver(I) complexes of tris(pyrazolyl)borate ligands bearing six trifluoromethyl and three additional electron-withdrawing substituents*  
Dalton Transactions, (42): 15399-15410 2013.
- Jesus, A. J. L.; Redinha, J. S.  
*Molecular insight into the amine-water interaction: A combined vibrational, energetic and NBO/NEDA study*  
Computational and Theoretical Chemistry, (1023): 74-82 2013.
- Ji, K. G.; Nelson, J.; Zhang, L. M.  
*Gold-catalyzed regioselective oxidation of propargylic carboxylates: a reliable access to alpha-carboxy-alpha,beta-unsaturated ketones/aldehydes*  
Beilstein Journal of Organic Chemistry, (9): 1925-1930 2013.

- Ji, W. Y.; Xia, X. L.; Ren, X. H.; Wang, F.; Wang, H. J.; Diao, K. S.  
*The non-covalent bindings of CF<sub>2</sub>Cl<sub>2</sub> with NO and SO<sub>2</sub>*  
Structural Chemistry, (24): 49-54 2013.
- Jia, C.; Wang, W. L.; Zhang, T. L.; Gao, L. J.; Fu, F.; Wang, D. J.  
*Impact of Water Molecules on the Isomerization of CH<sub>3</sub>S(OH)CH<sub>2</sub> to CH<sub>3</sub>S(O)CH<sub>3</sub>: A Computational Investigation*  
Chinese Journal of Chemistry, (31): 1341-1347 2013.
- Jia, J. F.; Wu, H. S.; Chen, Z. H.; Mo, Y. R.  
*Elucidation of the Forces Governing the Stereochemistry of Biphenyl*  
European Journal of Organic Chemistry: 611-616 2013.
- Jiang, L. Z.; Orimoto, Y.; Aoki, Y.  
*Stereoelectronic effects in Menshutkin-type S(N)<sub>2</sub> reactions: theoretical study based on through-space/bond orbital interaction analysis*  
Journal of Physical Organic Chemistry, (26): 885-891 2013.
- Jin, B.; Jin, Q.  
*Probing the multiple (delta- and pi-) aromaticity of Hf<sub>3</sub>F<sub>3</sub> (-) anion, Hf<sub>3</sub>F<sub>3</sub>X<sub>2</sub> (+) (X = Li, Na, and K), and Hf<sub>3</sub>F<sub>3</sub>Y (+) (Y = Be and Mg) clusters*  
Computational and Theoretical Chemistry, (1013): 130-135 2013.
- Jin, J. L.; Li, H. B.; Lu, T.; Duan, Y. A.; Geng, Y.; Wu, Y.; Su, Z. M.  
*Density functional studies on photophysical properties and chemical reactivities of the triarylboranes: effect of the constraint of planarity*  
Journal of Molecular Modeling, (19): 3437-3446 2013.
- Jin, L. X.; Wang, W. L.; Hu, D. D.; Min, S. T.  
*Effects of Protonation and C5 Methylation on the Electrophilic Addition Reaction of Cytosine: A Computational Study*  
Journal of Physical Chemistry B, (117): 3-12 2013.
- Jin, P.; Nagase, S.  
*Density functional theory study of fullerene-carbene Lewis acid-base adducts: critical role of dispersion interactions*  
Rsc Advances, (3): 10177-10180 2013.
- Jin, R. F.; Zhang, J. P.  
*Photophysical Properties of Derivatives of 2-(2-Hydroxyphen-yl)-1,3,4-oxadiazole: A Theoretical Study*  
Journal of Physical Chemistry A, (117): 8285-8292 2013.
- Jina, R. F.; Tang, S. S.  
*Theoretical study on optical and electronic properties of bipolar molecules with 1,8-naphthalimide and triphenylamine moieties as organic light-emitting materials*  
Journal of Molecular Graphics and Modelling, (42): 120-128 2013.
- Jissy, A. K.; Meena, S. K.; Datta, A.  
*Reactivity of germanones: far removed from ketones - a computational study*  
Rsc Advances, (3): 24321-24327 2013.
- Jodaian, V.; Mirzaei, M.; Arca, M.; Aragoni, M. C.; Lippolis, V.; Tavakoli, E.; Langeroodi, N. S.

- First example of a 1:1 vanadium(IV)-citrate complex featuring the 2,2'-bipyridine co-ligand: Synthesis, X-ray crystal structure and DFT calculations*  
Inorganica Chimica Acta, (400): 107-114 2013.
- John, A.; Modak, S.; Madasu, M.; Katari, M.; Ghosh, P.  
*Palladium complexes of the N-fused heterocycle derived abnormal N-heterocyclic carbenes for the much-preferred Cu-free and the amine-free Sonogashira coupling in air*  
Polyhedron, (64): 20-29 2013.
- Jornet, D.; Castillo, M. A.; Sabater, M. C.; Domingo, L. R.; Tormos, R.; Miranda, M. A.  
*Xanthone-photosensitized detoxification of the veterinary anthelmintic fenbendazole*  
Journal of Photochemistry and Photobiology a-Chemistry, (264): 34-40 2013.
- Jose, D.; Nijamudheen, A.; Datta, A.  
*Tip enhanced Raman spectroscopy (TERS) as a probe for the buckling distortion in silicene*  
Physical Chemistry Chemical Physics, (15): 8700-8704 2013.
- Joseph, L.; Sajan, D.; Chaitanya, K.; Devarajegowda, H. C.; Isac, J.  
*Density functional theory study, FT-IR and FT-Raman spectra and SQM force field calculation for vibrational analysis of 1, 3-Bis (hydroxymethyl) benzimidazolin-2-one*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (114): 432-440 2013.
- Joseph, L.; Sajan, D.; Shettigar, V.; Chaitanya, K.; Misra, N.; Sundius, T.; Nemeč, I.  
*Synthesis, crystal growth, thermal studies and scaled quantum chemical studies of structural and vibrational spectra of the highly efficient organic NLO crystal: 1-(4-Aminophenyl)-3-(3,4-dimethoxyphenyl)-prop-2-en-1-one*  
Materials Chemistry and Physics, (141): 248-262 2013.
- Joshi, B. D.; Srivastava, A.; Gupta, V.; Tandon, P.; Jain, S.  
*Spectroscopic and quantum chemical study of an alkaloid aristolochic acid I*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (116): 258-269 2013.
- Joshi, B. D.; Srivastava, A.; Honorato, S. B.; Tandon, P.; Pessoa, O. D. L.; Fachine, P. B. A.; Ayala, A. P.  
*Study of molecular structure, vibrational, electronic and NMR spectra of oncocalyxone A using DFT and quantum chemical calculations*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (113): 367-377 2013.
- Jothi, M.; Selvaraju, K.; Kumaradhas, P.  
*Exploring the Effect of External Electric Field on Octane Dithiolate Molecular Nanowire: A Quantum Chemical and Charge Density Study*  
Journal of Computational and Theoretical Nanoscience, (10): 789-797 2013.
- Ju, M. G.; Liang, W. Z.  
*Computational Insight on the Working Principles of Zinc Porphyrin Dye-Sensitized Solar Cells*  
Journal of Physical Chemistry C, (117): 14899-14911 2013.
- Junold, K.; Baus, J. A.; Burschka, C.; Vent-Schmidt, T.; Riedel, S.; Tacke, R.  
*Five-Coordinate Silicon(II) Compounds with Si-M Bonds (M = Cr, Mo, W, Fe): Bis N,N'-diisopropylbenzamidinato(-) silicon(II) as a Ligand in Transition-Metal Complexes*  
Inorganic Chemistry, (52): 11593-11599 2013.
- Jurca, T.; Korobkov, I.; Gorelsky, S. I.; Richeson, D. S.  
*Noncovalent Interactions of Metal Cations and Arenes Probed with Thallium(I) Complexes*

- Inorganic Chemistry, (52): 5749-5756 2013.
- Kakkar, R.; Bhandari, M.  
*Theoretical investigation of the alloxan-dialuric acid redox cycle*  
International Journal of Quantum Chemistry, (113): 2060-2069 2013.
- Kalume, A.; George, L.; Cunningham, N.; Reid, S. A.  
*Concerted and sequential pathways of proton-coupled electron transfer in hydrogen halide elimination*  
Chemical Physics Letters, (556): 35-38 2013.
- Kannan, V.; Thirupugalmani, K.; Brahadeeswaran, S.  
*Studies on vibrational, NMR spectra and quantum chemical calculations of N-Succinopyridine: An organic nonlinear optical material*  
Journal of Molecular Structure, (1049): 268-279 2013.
- Kapovsky, M.; Dares, C.; Dodsworth, E. S.; Begum, R. A.; Raco, V.; Lever, A. B. P.  
*Proton-Induced Disproportionation of a Ruthenium Noninnocent Ligand Complex Yielding a Strong Oxidant and a Strong Reductant*  
Inorganic Chemistry, (52): 169-181 2013.
- Karabacak, M.; Sinha, L.; Prasad, O.; Asiri, A. M.; Cinar, M.  
*An experimental and theoretical investigation of Acenaphthene-5-boronic acid: Conformational study, NBO and NLO analysis, molecular structure and FT-IR, FT-Raman, NMR and UV spectra*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (115): 753-766 2013.
- Karafiloglou, P.; Kyriakidou, K.  
*Unpaired electrons at the second-order reduced density matrix level: Covalent bonding, and coulomb and fermi correlations in closed shell systems*  
International Journal of Quantum Chemistry, (113): 1775-1786 2013.
- Karakaya, M.; Uchun, F.; Tokatli, A.  
*Density Functional Theory Study on Conformers of Benzoylcholine Chloride*  
Journal of Spectroscopy, 2013.
- Karakaya, M.; Ucu, F.  
*Quantum Chemical Computational Study on Chlorocholine Chloride and Bromocholine Bromide*  
Asian Journal of Chemistry, (25): 4869-4877 2013.
- Karnan, M.; Balachandran, V.; Murugan, M.  
*FT-IR, Raman and DFT study of 5-chloro-4-nitro-o-toluidine and NBO analysis with other halogen (Br, F) substitution*  
Journal of Molecular Structure, (1039): 197-206 2013.
- Karnan, M.; Balachandran, V.; Murugan, M.; Murali, M. K.; Nataraj, A.  
*Vibrational (FT-IR and FT-Raman) spectra, NBO, HOMO-LUMO, Molecular electrostatic potential surface and computational analysis of 4-(trifluoromethyl)benzylbromide*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (116): 84-95 2013.
- Karpinska, G.; Dobrowolski, J. C.  
*On constitutional isomers and tautomers of oxadiazolones and their mono- and disulfur analogues (C<sub>2</sub>H<sub>2</sub>N<sub>2</sub>XY; X, Y = S, O)*  
Computational and Theoretical Chemistry, (1005): 35-44 2013.

- Karthick, T.; Balachandran, V.; Perumal, S.; Lakshmi, A.  
*Rotational isomers, spectroscopic (FT-IR, FT-Raman) studies and quantum chemical calculations on 2,4,6-tris(dimethylaminomethyl) phenol*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (113): 52-66 2013.
- Karthick, T.; Balachandran, V.; Perumal, S.; Nataraj, A.  
*Vibrational (FT-IR and FT-Raman) spectra and quantum chemical studies on the molecular orbital calculations, chemical reactivity and thermodynamic parameters of 2-chloro-5-(trifluoromethyl) aniline*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (107): 72-81 2013.
- Karunakaran, C.; Jayabharathi, J.; Perumal, M. V.; Thanikachalam, V.; Thakur, P. K.  
*Electronic properties of phenanthrimidazoles as hole transport materials in organic light emitting devices and in photoelectron transfer to ZnO nanoparticles*  
Journal of Physical Organic Chemistry, (26): 386-406 2013.
- Karunakaran, V.; Balachandran, V.  
*Experimental and computational study on molecular structure, natural bond orbital and natural hybrid orbital analysis of non-linear optical material trans-3-(o-hydroxyphenyl-1-phenyl)-2-propen-1-one*  
Journal of Molecular Structure, (1053): 66-78 2013.
- Kasapbasi, E. E.; Whangbo, M. H.  
*On the nature of the photochemical reaction of polypyridyl Ru(II) complexes leading to sunlight-to-chemical energy conversion: density functional analysis*  
Rsc Advances, (3): 9414-9418 2013.
- Kasetti, Y.; Bharatam, P. V.  
*Pharmacophoric features of drugs with guanlyurea moiety: an electronic structure analysis*  
Journal of Molecular Modeling, (19): 1865-1874 2013.
- Kassaee, M. Z.; Zandi, H.; Rad, H. A.; Ghambarian, M.  
*Reaching for cyclacenes and short nanotubes through Si substitutions as studied by DFT calculations*  
Monatshefte fur Chemie, (144): 1783-1786 2013.
- Kaur, B.; Bhattacharya, S. N.; Henry, D. J.  
*Interpreting the near-infrared reflectance of a series of perylene pigments*  
Dyes and Pigments, (99): 502-511 2013.
- Kaur, D.; Aulakh, D.; Sharma, R.; Singh, H.  
*A computational investigation into the nature of hydrogen bonds involving divalent sulfur*  
Journal of Sulfur Chemistry, (34): 512-526 2013.
- Kaur, D.; Khanna, S.; Aulakh, D.  
*The explicit interactions of five-membered saturated heterocyclics containing one and two heteroatoms with single water molecule*  
Structural Chemistry, (24): 357-367 2013.
- Ke, I. S.; Gabbai, F. P.  
*Cu-3( $\mu(2)$ -Cl)(3) and Ag-3( $\mu(2)$ -Cl)(3) Complexes Supported by Tetradentate Trisphosphinostibine and -bismuthine Ligands: Structural Evidence for Triply Bridging Heavy Pnictines*  
Australian Journal of Chemistry, (66): 1281-1287 2013.
- Ke, I. S.; Gabbai, F. P.  
 *$\sigma$ -Donor/Acceptor-Confused Ligands: The Case of a Chlorostibine*

- Inorganic Chemistry, (52): 7145-7151 2013.
- Kebede, M. A.; Varner, M. E.; Scharko, N. K.; Gerber, R. B.; Raff, J. D.  
*Photooxidation of Ammonia on TiO<sub>2</sub> as a Source of NO and NO<sub>2</sub> under Atmospheric Conditions*  
Journal of the American Chemical Society, (135): 8606-8615 2013.
- Keiko, N. A.; Aksamentova, T. N.; Chipanina, N. N.; Verochkina, E. A.; Vchislo, N. V.  
*2-Alkoxy- and 2-alkylthio-2-alkenals in the reactions of electrophilic and nucleophilic addition. DFT study and NBO analysis*  
Tetrahedron, (69): 2022-2032 2013.
- Khaliullin, R. Z.; Kuhne, T. D.  
*Microscopic properties of liquid water from combined ab initio molecular dynamics and energy decomposition studies*  
Physical Chemistry Chemical Physics, (15): 15746-15766 2013.
- Kheirjou, S.; Mehrpajouh, S.; Fattahi, A.  
*DRASTIC INFLUENCE OF BORON ATOM ON THE ACIDITY OF ALCOHOL IN BOTH GAS PHASE AND SOLUTION PHASE, A DFT STUDY*  
Journal of Theoretical & Computational Chemistry, (12) 2013.
- Khenkin, A. M.; Efremenko, I.; Martin, J. M. L.; Neumann, R.  
*Polyoxometalate-Catalyzed Insertion of Oxygen from O<sub>2</sub> into Tin-Alkyl Bonds*  
Journal of the American Chemical Society, (135): 19304-19310 2013.
- Khodabandeh, M. H.; Reisi, H.; Davari, M. D.; Zare, K.; Zahedi, M.; Ohanessian, G.  
*Interaction Modes and Absolute Affinities of -Amino Acids for Mn<sup>2+</sup>: A Comprehensive Picture*  
Chemphyschem, (14): 1733-1745 2013.
- Khorassani, S. M. H.; Maghsoodlou, M. T.; Ghasempour, H.; Zakarianezhad, M.; Nassiri, M.; Ghahghaie, Z.  
*AIM analysis, synthetic, kinetic and mechanistic investigations of the reaction between triphenylphosphine and dialkyl acetylenedicarboxylate in the presence of 3-methoxythiophenol*  
Journal of Chemical Sciences, (125): 387-399 2013.
- Kia, M.; Golzar, M.; Mahjoub, K.; Soltani, A.  
*A first-principles study of functionalized clusters and carbon nanotubes or fullerenes with 5-Aminolevulinic acid as vehicles for drug delivery*  
Superlattices and Microstructures, (62): 251-259 2013.
- Kidwell, N. M.; Reilly, N. J.; Nebgen, B.; Mehta-Hurt, D. N.; Hoehn, R. D.; Kokkin, D. L.; McCarthy, M. C.; Slipchenko, L. V.; Zwiernik, T. S.  
*Jet-Cooled Spectroscopy of the alpha-Methylbenzyl Radical: Probing the State-Dependent Effects of Methyl Rocking Against a Radical Site*  
Journal of Physical Chemistry A, (117): 13465-13480 2013.
- Kim, J.; Hong, K.; Kim, H. K.; Lee, Y. S.; Kim, T. K.  
*Strong Spin-Orbit Coupling Facilitates C-H Activation in the Reactions of Os<sup>+</sup> with CH<sub>3</sub>F: Theoretical Investigations*  
Journal of Chemical Theory and Computation, (9): 1087-1092 2013.
- Kim, K. C.; Yu, D. C.; Snurr, R. Q.  
*Computational Screening of Functional Groups for Ammonia Capture in Metal-Organic Frameworks*  
Langmuir, (29): 1446-1456 2013.



- Kimura, T.; Suzuki, T.; Takata, K.; Soga, A.; Nomoto, Y.; Kamiyama, T.; Nakai, Y.; Matsui, H.; Fujisawa, M.  
*Excess enthalpies of binary mixtures of butylamines plus propanols at 298.15 K*  
Journal of Thermal Analysis and Calorimetry, (113): 1467-1474 2013.
- Kirby, A. J.; Medeiros, M.; Mora, J. R.; Oliveira, P. S. M.; Amer, A.; Williams, N. H.; Nome, F.  
*Intramolecular General Base Catalysis in the Hydrolysis of a Phosphate Diester. Computational Guidance to a Choice of Mechanism*  
Journal of Organic Chemistry, (78): 1343-1353 2013.
- Knippenberg, S.; Hajgato, B.  
*The cage fragmentation of doubly ionized norbornane: A Born-Oppenheimer molecular dynamics study*  
Chemical Physics Letters, (584): 24-29 2013.
- Knizia, G.  
*Intrinsic Atomic Orbitals: An Unbiased Bridge between Quantum Theory and Chemical Concepts*  
Journal of Chemical Theory and Computation, (9): 4834-4843 2013.
- Knurr, B. J.; Weber, J. M.  
*Solvent-Mediated Reduction of Carbon Dioxide in Anionic Complexes with Silver Atoms*  
Journal of Physical Chemistry A, (117): 10764-10771 2013.
- Kong, X. Y.; Deng, X. J.; Xu, H. G.; Yang, Z.; Xu, X. L.; Zheng, W. J.  
*Photoelectron spectroscopy and density functional calculations of Ag<sub>n</sub>Si<sub>n</sub> (n=3-12) clusters*  
Journal of Chemical Physics, (138) 2013.
- Koppel, I. A.; Burk, P.; Kasemets, K.; Koppel, I.  
*Relativistic effects on acidities and basicities of Bronsted acids and bases containing gold*  
Physical Chemistry Chemical Physics, (15): 17971-17975 2013.
- Koput, J.  
*Ab initio potential energy surface and vibration-rotation energy levels of lithium monohydroxide*  
Journal of Chemical Physics, (138) 2013.
- Kotena, Z. M.; Behjatmanesh-Ardakani, R.; Hashim, R.; Achari, V. M.  
*Hydrogen bonds in galactopyranoside and glucopyranoside: a density functional theory study*  
Journal of Molecular Modeling, (19): 589-599 2013.
- Kovacs, A.; Konings, R. J. M.; Varga, Z.; Szieberth, D.  
*Structure and Other Molecular Properties of Actinide Trichlorides AnCl<sub>3</sub> (An = Th-Cm)*  
Journal of Physical Chemistry A, (117): 11357-11363 2013.
- Kraka, E.; Freindorf, M.; Cremer, D.  
*Chiral Discrimination by Vibrational Spectroscopy Utilizing Local Modes*  
Chirality, (25): 185-196 2013.
- Kramer, C.; Bereau, T.; Spinn, A.; Liedl, K. R.; Gedeck, P.; Meuwly, M.  
*Deriving Static Atomic Multipoles from the Electrostatic Potential*  
Journal of Chemical Information and Modeling, (53): 3410-3417 2013.
- Krishnakumar, V.; Murugeswari, K.; Surumbarkuzhali, N.  
*Molecular structure, intramolecular hydrogen bonding and vibrational spectral investigation of 2-fluoro benzamide - A DFT approach*

- Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (114): 410-420 2013.
- Krishnamoorthy, B. S.; Kahlal, S.; Ghosh, S.; Halet, J. F.  
*Electronic, geometrical, and thermochemical studies on group-14 element-diruthenaborane cluster compounds: a theoretical investigation*  
Theoretical Chemistry Accounts, (132) 2013.
- Krishnan, V. S.; SampathKrishnan, S.; Muthu, S.; Renuga, S.  
*Experimental and computational study on molecular structure and vibrational analysis of 4,5-Bis(hydroxymethyl)-2-methylpyridin-3-ol by normal coordinate treatment*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (115): 191-201 2013.
- Ksenafontov, D. N.; Moiseeva, N. F.; Rykov, A. N.; Shishkov, I. F.; Oberhammer, H.  
*Molecular structure of carphedon as studied by gas electron diffraction and quantum chemical calculations*  
Structural Chemistry, (24): 171-179 2013.
- Kumar, A.; Katari, M.; Ghosh, P.  
*Understanding the lability of a trans bound pyridine ligand in a saturated six-membered N-heterocyclic carbene based (NHC)PdCl<sub>2</sub>(pyridine) type complex: A case study*  
Polyhedron, (52): 524-529 2013.
- Kuprat, M.; Schulz, A.; Villinger, A.  
*Arsa-Diazonium Salts With an Arsenic-Nitrogen Triple Bond*  
Angewandte Chemie-International Edition, (52): 7126-7130 2013.
- Kusama, H.; Funaki, T.; Sayama, K.  
*Theoretical study of cyclometalated Ru(II) dyes: Implications on the open-circuit voltage of dye-sensitized solar cells*  
Journal of Photochemistry and Photobiology a-Chemistry, (272): 80-89 2013.
- Kuznetsov, V. V.; Seregin, V. V.; Laptev, A. A.; Khakimov, D. V.; Pivina, T. S.; Simakova, A. P.; Vedenyapina, M. D.; Vedenyapin, A. A.; Makhova, N. N.  
*Kinetic and quantum chemical studies of the mechanism of formation of 1,2-dialkyldiaziridines*  
Russian Chemical Bulletin, (61): 1121-1127 2013.
- Lai, C. H.  
*A comparison of diamino- and diamidocarbenes toward dimerization*  
Journal of Molecular Modeling, (19): 4387-4394 2013.
- Lai, C. H.  
*Computational comparison of the kinetic stabilities of diamino- and diamidocarbenes in the 1,2-H shift reaction*  
Journal of Molecular Modeling, (19): 2935-2944 2013.
- Lai, C. H.  
*A theoretical study on the hydrogen adducts of diamidocarbenes and diaminocarbenes*  
Journal of Molecular Modeling, (19): 5523-5532 2013.
- Lai, Y. S.; Chen, S. S.  
*Adsorption of Organophosphate Pesticides with Humic Fraction-Immobilized Silica Gel in Hexane*  
Journal of Chemical and Engineering Data, (58): 2290-2301 2013.

- Lakshmi, A.; Balachandran, V.  
*Rotational isomers, NBO and spectral analyses of N-(2-hydroxyethyl) phthalimide based on quantum chemical calculations*  
Journal of Molecular Structure, (1033): 40-50 2013.
- Landis, C. R.; Weinhold, F.  
*3c/4e (sigma)over-cap-Type Long-Bonding: A Novel Transitional Motif toward the Metallic De localization Limit*  
Inorganic Chemistry, (52): 5154-5166 2013.
- Langseth, E.; Scheuermann, M. L.; Balcells, D.; Kaminsky, W.; Goldberg, K. I.; Eisenstein, O.; Heyn, R. H.; Tilset, M.  
*Generation and Structural Characterization of a Gold(III) Alkene Complex*  
Angewandte Chemie-International Edition, (52): 1660-1663 2013.
- Lastra-Barreira, B.; Diez, J.; Crochet, P.; Fernandez, I.  
*Functionalized arene- ruthenium( II) complexes: dangling vs. tethering side chain*  
Dalton Transactions, (42): 5412-5420 2013.
- Lathiotakis, N. N.  
*Correlation measures as benchmarks in reduced density matrix functional theory*  
International Journal of Quantum Chemistry, (113): 762-765 2013.
- Lau, E. Y.; Wong, S. E.; Baker, S. E.; Bearinger, J. P.; Koziol, L.; Valdez, C. A.; Satcher, J. H.; Aines, R. D.; Lightstone, F. C.  
*Comparison and Analysis of Zinc and Cobalt-Based Systems as Catalytic Entities for the Hydration of Carbon Dioxide*  
Plos One, (8) 2013.
- Lawson, D. B.; Spaulding, S.  
*Non-fused polyaromatic hydrocarbons: interactions of aromatic and antiaromatic rings through a CC bond*  
Structural Chemistry, (24): 223-232 2013.
- Lee, L. P.; Cole, D. J.; Payne, M. C.; Skylaris, C. K.  
*Natural bond orbital analysis in the ONETEP code: Applications to large protein systems*  
Journal of Computational Chemistry, (34): 429-444 2013.
- Lee, M. E.; Kang, M. S.; Choi, K. H.  
*A Density Functional Theory Study of Additives in Electrolytes of a Dye Sensitized Solar Cell*  
Bulletin of the Korean Chemical Society, (34): 2491-2494 2013.
- Lefevre, G. P.; Baillie, R. A.; Fabulyak, D.; Legzdins, P.  
*Insights into the Intermolecular C-H Activations of Hydrocarbons Initiated by Cp\*W(NO)(eta(3)-allyl)(CH<sub>2</sub>CMe<sub>3</sub>) Complexes*  
Organometallics, (32): 5561-5572 2013.
- Lein, M.; Harrison, J. A.; Nielson, A. J.  
*Identification of non-classical C-H center dot center dot center dot M interactions in early and late transition metal complexes containing the CH(ArO)(3) ligand*  
Dalton Transactions, (42): 10939-10951 2013.
- Lestard, M. E. D.; Diaz, S. B.; Puiatti, M.; Echeverria, G. A.; Piro, O. E.; Pierini, A. B.; Ben Altabef, A.; Tuttolomondo, M. E.

- Vibrational and Structural Behavior of L-Cysteine Ethyl Ester Hydrochloride in the Solid State and in Aqueous Solution*  
Journal of Physical Chemistry A, (117): 14243-14252 2013.
- Lestard, M. E. D.; Picot, R. A. C.; Tuttolomondo, M. E.; Ben Altabef, A.  
*Trimethylsilyl trichloroacetate vibrational, structural and electronic properties and their comparison with related acetates*  
Vibrational Spectroscopy, (65): 124-131 2013.
- Lewin, V.; Rivollier, J.; Coudert, S.; Buisson, D. A.; Baumann, D.; Rousseau, B.; Legrand, F. X.; Kourilova, H.; Berthault, P.; Dognon, J. P.; Heck, M. P.; Huber, G.  
*Synthesis of Cucurbit 6 uril Derivatives and Insights into Their Solubility in Water*  
European Journal of Organic Chemistry: 3857-3865 2013.
- Leyton, P.; Paipa, C.; Berrios, A.; Zarate, A.; Castillo, M. V.; Brandan, S. A.  
*Structural study and characterization of the dipeptide 2- 5-amino-5-oxo-2-(phenylmethoxycarbonylamino) pentanoyl amino acetic acid by vibrational spectroscopy and DFT calculations*  
Journal of Molecular Structure, (1031): 110-118 2013.
- Li, B. H.; Shi, W. J.; Ren, F. D.  
*A B3LYP and MP2 theoretical investigation on the cooperativity effect between the X-H center dot center dot center dot H-M (X = F, Cl, Br; M = Li, Na, K) dihydrogen-bonding and H-M center dot center dot center dot pi interactions involving C6H6*  
Computational and Theoretical Chemistry, (1020): 81-90 2013.
- Li, D. Z.; Dong, C. C.; Zhang, S. G.  
*(B3O3H3)(n)M (+)(n=1, 2; M = Cu, Ag, Au): a new class of metal-cation complexes*  
Journal of Molecular Modeling, (19): 3219-3224 2013.
- Li, H. D.; Feng, H.; Sun, W. G.; King, R. B.; Schaefer, H. F.  
*Extreme Metal Carbonyl Back Bonding in Cyclopentadienylthorium Carbonyls Generates Bridging C2O2 Ligands by Carbonyl Coupling*  
Inorganic Chemistry, (52): 6893-6904 2013.
- Li, H. D.; Feng, H.; Sun, W. G.; Xie, Y. M.; King, R. B.; Schaefer, H. F.  
*Alkyne Dichotomy: Splitting of Bis(dialkylamino)acetylenes, Dimethoxyacetylene, Bis(methylthio)acetylene, and Their Heavier Congeners To Give Carbyne Ligands in Iron Carbonyl Derivatives*  
Organometallics, (32): 88-94 2013.
- Li, H. F.; Winget, P.; Risko, C.; Sears, J. S.; Bredas, J. L.  
*Tuning the electronic and photophysical properties of heteroleptic iridium(III) phosphorescent emitters through ancillary ligand substitution: a theoretical perspective*  
Physical Chemistry Chemical Physics, (15): 6293-6302 2013.
- Li, H. Y.; Lu, Y. X.; Wu, W. H.; Liu, Y. T.; Peng, C. J.; Liu, H. L.; Zhu, W. L.  
*Noncovalent interactions in halogenated ionic liquids: theoretical study and crystallographic implications*  
Physical Chemistry Chemical Physics, (15): 4405-4414 2013.
- Li, J.; Xu, W. L.; Hu, J.; Ling, M.; Yao, J. H.  
*Hydrolysis Reaction Mechanism of 2,4-Dichlorophenoxy Acetic Acid Metabolism*  
Acta Physico-Chimica Sinica, (29): 1923-1930 2013.
- Li, L. C.; Bai, K. K.; Cai, W. F.

- Theoretical Investigation on Interaction between Guanine and Luteolin*  
Chinese Journal of Chemical Physics, (26): 533-540 2013.
- Li, M. J.; Liu, W. X.; Peng, C. R.; Ren, Q. H.; Lu, W. C.; Deng, W.  
*A DFT study on reaction of eupatilin with hydroxyl radical in solution*  
International Journal of Quantum Chemistry, (113): 966-974 2013.
- Li, P.; Wang, W. H.; Bi, S. W.; Sun, H. T.  
*Theoretical studies on the interaction mechanisms between tetrachloro-p-benzoquinone and hydrogen peroxide*  
Structural Chemistry, (24): 1253-1264 2013.
- Li, P.; Wang, W. H.; Sun, H. T.; Bi, S. W.  
*A DFT study on the electron affinity of tetrachloro-p-benzoquinone: Toward to understanding its electron-accepting ability in solution*  
Computational and Theoretical Chemistry, (1006): 127-132 2013.
- Li, Q. Z.; Liu, W. M.; Li, R.; Li, W. Z.; Cheng, J. B.; Gong, B. A.  
*Influence of insertion of a noble gas atom on halogen bonding in H<sub>2</sub>O center dot center dot center dot XCCNgF and H<sub>3</sub>N center dot center dot center dot XCCNgF (X = Cl and Br; Ng = Ar, Kr, and Xe) complexes*  
Structural Chemistry, (24): 25-31 2013.
- Li, R.; Wang, Y. T.; Chen, C. L.  
*COMPUTATIONAL MODELING STUDY ON METABOLISM MECHANISM OF OSELTAMIVIR*  
Journal of Theoretical & Computational Chemistry, (12) 2013.
- Li, S.; Zhou, L.; Su, Y. C.; Han, B.; Deng, F.  
*C-13 and N-15 spectral editing inside histidine imidazole ring through solid-state NMR spectroscopy*  
Solid State Nuclear Magnetic Resonance, (54): 13-17 2013.
- Li, S. C.; Li, Y.; Wu, D.; Li, Z. R.  
*Density functional study of structural and electronic properties of small binary Be (n) Cu (m) (n plus m=2 similar to 7) clusters*  
Journal of Molecular Modeling, (19): 3065-3075 2013.
- Li, W.  
*Linear scaling explicitly correlated MP2-F12 and ONIOM methods for the long-range interactions of the nanoscale clusters in methanol aqueous solutions*  
Journal of Chemical Physics, (138) 2013.
- Li, W. Y.; Huang, D. F.; Lv, Y. J.  
*Theoretical study on the mechanism and stereochemistry of the cinchona-thiourea organocatalytic hydrophosphonylation of an alpha-ketoester*  
Organic & Biomolecular Chemistry, (11): 7497-7506 2013.
- Li, W. Y.; Su, Z. S.; Hu, C. W.  
*Mechanism of Ketone Allylation with Allylboronates as Catalyzed by Zinc Compounds: A DFT Study*  
Chemistry-a European Journal, (19): 124-134 2013.
- Li, X. H.; Hao, X. P.; Zhang, X. Z.; Yang, X. D.  
*Natural Bond Orbital (NBO) Population Study of Some Para-Substituted N-Methyl-N-nitrosobenzenesulfonamide Biological Molecules in MeCN Solution*  
Journal of Solution Chemistry, (42): 263-271 2013.

- Li, X. H.; Ju, X. H.  
*Density functional theory study on (Mg(BH<sub>4</sub>))(n) (n=1-4) clusters as a material for hydrogen storage*  
Computational and Theoretical Chemistry, (1025): 46-51 2013.
- Li, X. H.; Zhang, R. Z.; Zhang, X. Z.  
*N-NO<sub>2</sub> bond dissociation energies in acetonitrile: An assessment of contemporary computational methods*  
Journal of Molecular Graphics and Modelling, (43): 66-71 2013.
- Li, X. H.; Zhang, R. Z.; Zhang, X. Z.  
*Theoretical investigation on the geometric, spectroscopic, nonlinear optical parameter, and frontier molecular orbital of 1,3-bis(4-methoxyphenyl)prop-2-en-1-one by DFT/ab initio calculations*  
Canadian Journal of Chemistry-Revue Canadienne De Chimie, (91): 1225-1232 2013.
- Li, X. H.; Zhang, R. Z.; Zhang, X. Z.  
*Theoretical studies on vibrational spectra, thermodynamic properties, and detonation properties for 1,2,4,5-tetrazine derivatives*  
Canadian Journal of Chemistry-Revue Canadienne De Chimie, (91): 662-670 2013.
- Li, X. N.; Li, C.; Yin, B.; Li, C.; Liu, P.; Li, J. L.; Shi, Z.  
*DDQ-Induced Dehydrogenation of Heterocycles for CC Double Bond Formation: Synthesis of 2-Thiazoles and 2-Oxazoles*  
Chemistry-an Asian Journal, (8): 1408-1411 2013.
- Li, X. Y.; Yang, Z. Y.; Xu, J. X.  
*Comprehensive Theoretical Investigation on the Regioselectivity in the Nucleophilic Ring Opening of Epoxides*  
Current Organic Synthesis, (10): 169-177 2013.
- Li, X. Y.; Zhang, D. W.  
*Noble gas-coinage metal interactions of (AuRn<sup>+</sup>)(n) (n=1-3) series: ab initio calculations*  
European Physical Journal D, (67) 2013.
- Li, Y.; Lin, Z. Y.  
*Theoretical Studies of Ring-Opening Reactions of Phenylcyclobutabenzenol and Its Reactions with Alkynes Catalyzed by Rhodium Complexes*  
Journal of Organic Chemistry, (78): 11357-11365 2013.
- Li, Y.; Mondal, K. C.; Roesky, H. W.; Zhu, H. P.; Stollberg, P.; Herbst-Irmer, R.; Stalke, D.; Andrada, D. M.  
*Acyclic Germylones: Congeners of Allenes with a Central Germanium Atom*  
Journal of the American Chemical Society, (135): 12422-12428 2013.
- Li, Y.; Wu, H. Q.; Xu, H. L.; Sun, S. L.; Su, Z. M.  
*The symmetric and asymmetric thiophene-fused benzocarborane: structures and first hyperpolarizabilities*  
Journal of Molecular Modeling, (19): 3741-3747 2013.
- Li, Y.; Zhang, J. A.; Wang, Y. B.; Pan, M.; Su, C. Y.  
*Crystal structures, DFT calculations and biological activities of three mercury complexes from a pentadentate thioether ligand*  
Inorganic Chemistry Communications, (34): 4-7 2013.
- Li, Y. N.; Wang, S. G.; Wang, T.; Gao, R.; Geng, C. Y.; Li, Y. W.; Wang, J. G.; Jiao, H. J.  
*Energies and Spin States of FeS<sub>0</sub><sup>-</sup>, FeS<sub>20</sub><sup>-</sup>, Fe<sub>2</sub>S<sub>20</sub><sup>-</sup>, Fe<sub>3</sub>S<sub>40</sub><sup>-</sup>, and Fe<sub>4</sub>S<sub>40</sub><sup>-</sup> Clusters*

- Chemphyschem, (14): 1182-1189 2013.
- Li, Y. W.; Zhang, S. H.; Wang, Q.; Jena, P.  
*Structure and properties of Mn<sub>4</sub>Cl<sub>9</sub>: An antiferromagnetic binary hyperhalogen*  
Journal of Chemical Physics, (138) 2013.
- Li, Z. S.; Zhao, X.; Zou, L. Y.; Ren, A. M.  
*SOThe Dynamics Simulation and Quantum Calculation Investigation About Luminescence Mechanism of Coelenteramide*  
Photochemistry and Photobiology, (89): 849-855 2013.
- Li, Z. S.; Zou, L. Y.; Min, C. G.; Ren, A. M.  
*The effect of micro-environment on luminescence of aequorin: The role of amino acids and explicit water molecules on spectroscopic properties of coelenteramide*  
Journal of Photochemistry and Photobiology B-Biology, (127): 94-99 2013.
- Li, Z. W.; Wu, W. S.; Du, Z. Y.; Hao, X. Y.  
*Structure and interaction between the BMIM Ala alanine anion and the 1-butyl-3-methylimidazolium cation in ion pairs*  
Journal of Structural Chemistry, (54): 676-683 2013.
- Liang, J. X.; Wang, Y. B.; Geng, Z. Y.; Li, G. H.; Wei, Y. J.  
*Substituent effects on the compounds (CXX<sub>2</sub> center dot-)X-1 (X-1, X-2 = H, F, Cl, Br, I) from theoretical investigation*  
Structural Chemistry, (24): 455-461 2013.
- Liang, J. X.; Wang, Y. B.; Geng, Z. Y.; Wang, Y. Z.; Wang, Y. C.  
*Gas-phase reaction of the isobutenyl anion with N<sub>2</sub>O from ab initio calculations*  
Journal of Structural Chemistry, (54): 292-300 2013.
- Liang, J. X.; Wang, Y. B.; Hasi, Q. M. G.; Geng, Z. Y.  
*CCl<sub>4</sub> Activation Mechanisms by Gas-Phase CHBr center dot- and CBr<sub>2</sub> center dot-: A Comparative Study*  
Bulletin of the Korean Chemical Society, (34): 426-432 2013.
- Liang, J. X.; Wang, Y. B.; Zhang, Q.; Li, Y.; Geng, Z. Y.; Wang, X. H.  
*DFT study on the reactions of ClO-/BrO- with RCl (R = CH<sub>3</sub>, C<sub>2</sub>H<sub>5</sub>, and C<sub>3</sub>H<sub>7</sub>) in gas phase*  
Journal of Molecular Modeling, (19): 1739-1750 2013.
- Licini, G.; Zonta, C.  
*Revisiting the Hammett Parameter for the Determination of Philicity: Nucleophilic Substitution with Inverse Charge Interaction*  
Angewandte Chemie-International Edition, (52): 2911-2914 2013.
- Lima, J. M. M.; Silva, V. H. C.; Camargo, L.; de Oliveira, H. C. B.; Camargo, A. J.  
*Theoretical investigation on ruthenium tetraazaporphyrin as potential nitric oxide carrier in biological systems*  
Journal of Molecular Modeling, (19): 1727-1737 2013.
- Lin, C. H.; Nesterov, V. N.; Richmond, M. G.  
*2- (Diphenylphosphino)methyl -6-methylpyridine (PN) coordination chemistry at triosmium clusters: Regiospecific ligand activation and DFT evaluation of the isomeric Os-3(CO)(10)(PN) clusters*  
Journal of Organometallic Chemistry, (744): 24-34 2013.

- Lin, H.; Zhu, S. G.; Li, H. Z.; Peng, X. H.  
*Structure and detonation performance of a novel HMX/LLM-105 cocrystal explosive*  
Journal of Physical Organic Chemistry, (26): 898-907 2013.
- Lin, H.; Zhu, S. G.; Li, H. Z.; Peng, X. H.  
*Synthesis, characterization, AIM and NBO analysis of HMX/DMI cocrystal explosive*  
Journal of Molecular Structure, (1048): 339-348 2013.
- Lin, H.; Zhu, S. G.; Zhang, L.; Peng, X. H.; Chen, P. Y.; Li, H. Z.  
*Intermolecular interactions, thermodynamic properties, crystal structure, and detonation performance of HMX/NTO cocrystal explosive*  
International Journal of Quantum Chemistry, (113): 1591-1599 2013.
- Lin, T. P.; Gabbai, F. P.  
*Tellurium Ions as sigma-Acceptor Ligands*  
Angewandte Chemie-International Edition, (52): 3864-3868 2013.
- Liu, C. G.  
*Quantum chemical studies on a series of transition metal carbon dioxide complexes: Metal-carbon bonding and electronic structures*  
Molecular Physics, (111): 257-265 2013.
- Liu, F. L.; Mi, L.; Jiang, Y. F.  
*Heterofullerenes C<sub>48</sub>N<sub>12</sub> and C<sub>48</sub>B<sub>12</sub> with Rare T-h Symmetry: a DFT Study*  
Chinese Journal of Structural Chemistry, (32): 839-846 2013.
- Liu, H. X.; Man, R. L.; Wang, Z. X.; Yi, P. G.; Zeng, J. X.  
*COOPERATIVITY BETWEEN HYDROGEN BOND AND HALOGEN BOND IN HBr center dot center dot center dot BrX center dot center dot center dot HBr (X = F, Cl, Br)*  
Journal of Theoretical & Computational Chemistry, (12) 2013.
- Liu, J. H.; Xia, X. L.; Li, Y.; Wang, H. J.; Li, Z. Y.  
*Theoretical study on the interaction of glutathione with group IA (Li<sup>+</sup>, Na<sup>+</sup>, K<sup>+</sup>), IIA (Be<sup>2+</sup>, Mg<sup>2+</sup>, Ca<sup>2+</sup>), and IIIA (Al<sup>3+</sup>) metal cations*  
Structural Chemistry, (24): 251-261 2013.
- Liu, J. L.; Zheng, M.; Zhang, C. C.; Xu, D. G.  
*"Amide Resonance" in the Catalysis of 1,2-alpha-L-Fucosidase from Bifidobacterium bifidum*  
Journal of Physical Chemistry B, (117): 10080-10092 2013.
- Liu, J. X.; Zhang, X. G.  
*Investigation on NO<sub>x</sub> adsorption in M'-MAPO-5 (M = Si, Ti; M' = Ag, Cu) by density functional theory calculation*  
Applied Surface Science, (265): 274-280 2013.
- Liu, S.; Li, S. S.; Liu, D. J.; Wang, C. S.  
*Site Preferences of Adenine Hydrogen Bonding to Peptide Amides*  
Acta Physico-Chimica Sinica, (29): 2551-2557 2013.
- Liu, X.; Ito, H.; Torikai, E.  
*Exchange-Correlation Interaction and AO-Hybridization of Alkali-Metal Atomic Clusters*  
Journal of Physical Chemistry A, (117): 9099-9107 2013.



- Liu, X. F.; Cheng, J. B.; Li, Q. Z.; Li, W. Z.  
*Competition of hydrogen, halogen, and pnictogen bonds in the complexes of HArF with XH<sub>2</sub>P (X = F, Cl, and Br)*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (101): 172-177 2013.
- Liu, X. F.; Li, Q. Z.; Cheng, J. B.; Li, W. Z.  
*Influence of cooperativity on the frequency shift of the Ar-H stretch vibration in HArF complexes*  
Molecular Physics, (111): 497-504 2013.
- Liu, Y.; Ganguly, R.; Huynh, H. V.; Leongt, W. K.  
*Palladium-Osmium Heterometallic Clusters Containing N-Heterocyclic Carbene Ligands*  
Organometallics, (32): 7559-7563 2013.
- Liu, Y. T.; Wang, X.; Liu, X. Y.; Li, X. P.; Ji, Y. Q.  
*Theoretical Studies on Structure, Isomerization, and Stability of Si, O, S*  
Chemical Research in Chinese Universities, (29): 351-354 2013.
- Liu, Y. Y.; Geng, Z. Y.; Wang, Y. C.; Liu, J. L.; Hou, X. F.  
*DFT studies for activation of C-H bond in methane by gas-phase Rh-n(+) (n=1-3)*  
Computational and Theoretical Chemistry, (1015): 52-63 2013.
- Lizarraga, E.; Romano, E.; Raschi, A. B.; Leyton, P.; Paipa, C.; Catalan, C. A. N.; Brandan, S. A.  
*A structural and vibrational study of dehydrofukinone combining FTIR, FTRaman, UV-visible and NMR spectroscopies with DFT calculations*  
Journal of Molecular Structure, (1048): 331-338 2013.
- Lo, R.; Bhattacharya, A.; Ganguly, B.  
*Probing the selective salt rejection behavior of thin film composite membranes: A DFT study*  
Journal of Membrane Science, (436): 90-96 2013.
- Lobayan, R. M.; Bentz, E. N.; Jubert, A. H.; Pomilio, A. B.  
*Charge delocalization in Z-isomers of (4  $\alpha$  -> 6 '' , 2  $\alpha$  -> O -> 1 '')-phenylflavans with R = H, OH and OCH<sub>3</sub>. Effects on bond dissociation enthalpies and ionization potentials*  
Computational and Theoretical Chemistry, (1006): 37-46 2013.
- Lobayan, R. M.; Schmit, M. C. P.; Jubert, A. H.; Vitale, A.  
*Aqueous solvent effects on the conformational space of tryptamine. Structural and electronic analysis*  
Journal of Molecular Modeling, (19): 1109-1123 2013.
- Loerbroks, C.; Rinaldi, R.; Thiel, W.  
*The Electronic Nature of the 1,4-beta-Glycosidic Bond and Its Chemical Environment: DFT Insights into Cellulose Chemistry*  
Chemistry-a European Journal, (19): 16282-16294 2013.
- Long, S.; Panunzio, M.; Qin, W. L.; Bongini, A.; Monari, M.  
*Efficient Aldol-Type Reaction of O-Protected -Hydroxy Aldehydes and N-Trimethylsilyl Ketene Imines: Synthesis of ,-Dihydroxy-Nitriles*  
European Journal of Organic Chemistry, (2013): 5127-5142 2013.
- Lopatin, S. I.; Panin, A. I.; Shugurov, S. M.  
*Stability and structures of gaseous In<sub>2</sub>MoO<sub>4</sub>, In<sub>2</sub>WO<sub>4</sub> and In<sub>2</sub>W<sub>2</sub>O<sub>7</sub>*  
Dalton Transactions, (42): 8339-8346 2013.

- Lopatin, S. I.; Panin, A. I.; Shugurov, S. M.  
*Thermodynamic properties and structure of gaseous BMoO4*  
Dalton Transactions, (42): 1210-1214 2013.
- Lopchuk, J. M.; Hughes, R. P.; Gribble, G. W.  
*What Controls Regiochemistry in 1,3-Dipolar Cycloadditions of Munchnones with Nitrostyrenes?*  
Organic Letters, (15): 5218-5221 2013.
- Lopez, A. H. D.; Caramori, G. F.; Coimbra, D. F.; Parreira, R. L. T.; da Silva, E. H.  
*The Two Faces of Hydrogen-Bond Strength on Triple AAA-DDD Arrays*  
Chemphyschem, (14): 3994-4001 2013.
- Lopez, S. A.; Munk, M. E.; Houk, K. N.  
*Mechanisms and Transition States of 1,3-Dipolar Cycloadditions of Phenyl Azide with Enamines: A Computational Analysis*  
Journal of Organic Chemistry, (78): 1576-1582 2013.
- Lu, B.; Li, Y. X.; Wang, Y. L.; Aue, D. H.; Luo, Y. D.; Zhang, L. M.  
*3,3-Signitropic Rearrangement versus Carbene Formation in Gold-Catalyzed Transformations of Alkynyl Aryl Sulfoxides: Mechanistic Studies and Expanded Reaction Scope*  
Journal of the American Chemical Society, (135): 8512-8524 2013.
- Lu, N.; Wang, H. T.  
*Theoretical mechanism studies on the competitive CO-induced N-N bond cleavage of N2O with N-O bond cleavage mediated by (eta(5)-C5Me5)Mo N(Pr-i)C(Me)N(Pr-i) (CO)(2)*  
Dalton Transactions, (42): 13931-13939 2013.
- Lu, N.; Wang, H. T.  
*Theoretical study of enantiomeric and geometric control in chiral guanidine-catalyzed asymmetric 1,4-addition of 5H-oxazol-4-ones*  
International Journal of Quantum Chemistry, (113): 2267-2276 2013.
- Lu, N.; Wang, H. T.; Wang, Y. P.  
*Theoretical Mechanism Studies on the Enantioselectivity of aza-MBH-type Reaction of Nitroalkene to N-tosylimine Catalyzed by Thiourea-tertiary Amine*  
Bulletin of the Korean Chemical Society, (34): 3591-3596 2013.
- Lu, R. Q.; Gu, P.; Liu, D.; Lu, Y. K.; Wang, S. T.  
*The nature of interactions between N-butylpyridinium tetrafluoroborate and thiophenic compounds: A theoretical investigation*  
Comptes Rendus Chimie, (16): 1118-1126 2013.
- Lu, R. Q.; Lin, J.; Qu, Z. Q.  
*Theoretical study on interactions between thiophene/dibenzothiophene/cyclohexane/toluene and 1-methyl-3-octylimidazolium tetrafluoroborate*  
Structural Chemistry, (24): 507-515 2013.
- Lu, R. Q.; Liu, D.; Lu, Y. K.; Lin, J.  
*Electronic and topological properties of interactions between imidazolium-based ionic liquids and thiophenic compounds: a theoretical investigation*  
Journal of the Iranian Chemical Society, (10): 733-744 2013.
- Lu, R. Q.; Liu, D.; Wang, S. T.; Lu, Y. K.

*Theoretical Study on Interactions between N-Butylpyridinium Nitrate and Thiophenic Compounds*  
Bulletin of the Korean Chemical Society, (34): 1814-1822 2013.

Lu, R. Q.; Qu, Z. Q.; Lin, J.

*Comparative study of interactions between thiophene\pyridine\benzene\heptane and 1-butyl-3-methylimidazolium trifluoromethanesulfonate by density functional theory*  
Journal of Molecular Liquids, (180): 207-214 2013.

Lu, T.; Chen, F. W.

*Bond Order Analysis Based on the Laplacian of Electron Density in Fuzzy Overlap Space*  
Journal of Physical Chemistry A, (117): 3100-3108 2013.

Lund, H.; Oeckler, O.; Schroder, T.; Schulz, A.; Villinger, A.

*Mercury Azides and the Azide of Millon's Base*  
Angewandte Chemie-International Edition, (52): 10900-10904 2013.

Luo, J.; Hu, J. W.; Zhuang, Y.; Wei, X. H.; Huang, X. F.

*Theoretical study on the radical anions and reductive dechlorination of selected polychlorinated dibenzo-p-dioxins*  
Chemosphere, (91): 765-770 2013.

Lupan, A.; King, R. B.

*Comparison of hypoelectronic deltahedral dirhenaboranes having eight to twelve vertices with their rhenium analogues: Examples of polyhedral surface metal-metal multiple bonds*  
Polyhedron, (60): 151-157 2013.

Lupan, A.; King, R. B.

*Dimetallaboranes with Polyhedral Surface Metal-Metal Multiple Bonds: Deltahedral Dirhenaboranes with Pentalenedirhenium Vertices*  
Organometallics, (32): 4002-4008 2013.

Lupan, A.; King, R. B.

*Hypoelectronic diruthenaboranes and diosmaboranes having eight to twelve vertices: capped isocloso and bicapped closo structures*  
New Journal of Chemistry, (37): 2528-2536 2013.

Lupan, A.; King, R. B.

*Metal-metal interactions in deltahedral dirhoda- and diiridadicarbaboranes*  
Inorganica Chimica Acta, (397): 83-87 2013.

Lyhs, B.; Blaser, D.; Wolper, C.; Schulz, S.; Haack, R.; Jansen, G.

*Synthesis and Structure of Base-Stabilized Germanium(II) Diazide IPrGe(N-3)(2)*  
Inorganic Chemistry, (52): 7236-7241 2013.

Ma, L. L.; Huang, Z. G.; Niu, X. Q.; Shen, T. T.; Guo, L. F.

*A theoretical study on the hydrogen bonding interactions in HXeCCH center dot center dot center dot Y (Y = H<sub>2</sub>O and HF) complexes*  
Computational and Theoretical Chemistry, (1017): 14-21 2013.

Ma, X. G.; Wang, F.

*Gamma-ray spectra of methane in the positron-electron annihilation process*  
Radiation Physics and Chemistry, (85): 59-63 2013.

- Maass, C.; Andrada, D. M.; Mata, R. A.; Herbst-Irmer, R.; Stalke, D.  
*Effects of Metal Coordination on the pi-System of the 2,5-Bis-{{pyrrolidino}-methyl}-pyrrole Pincer Ligand*  
Inorganic Chemistry, (52): 9539-9548 2013.
- MacGowan, S. A.; Senge, M. O.  
*Computational Quantification of the Physicochemical Effects of Heme Distortion: Redox Control in the Reaction Center Cytochrome Subunit of Blastochloris viridis*  
Inorganic Chemistry, (52): 1228-1237 2013.
- Machura, B.; Wolff, M.; Palion, J.; Benoist, E.  
*Synthesis, spectroscopic characterization and X-ray crystal structures of mononuclear and binuclear oxidorhenium(V) complexes containing indazolyl moieties*  
Inorganica Chimica Acta, (404): 144-154 2013.
- Mackeprang, K.; Schroder, S. D.; Kjaergaard, H. G.  
*Weak intramolecular OH center dot center dot center dot pi hydrogen bonding in methallyl- and allyl-carbinol*  
Chemical Physics Letters, (582): 31-37 2013.
- MacLeod, M. K.; Michl, J.  
*Five Stereoinactive Orbitals on Silicon: Charge and Spin Localization in the n-Si4Me10-center dot Radical Anion by Trigonal Bipyramidalization*  
Journal of Physical Chemistry Letters, (4): 1649-1653 2013.
- Maekawa, H.; Sul, S.; Ge, N. H.  
*Vibrational correlation between conjugated carbonyl and diazo modes studied by single- and dual-frequency two-dimensional infrared spectroscopy*  
Chemical Physics, (422): 22-30 2013.
- MahdaviFar, Z.; Abbasi, N.; Shakerzadeh, E.  
*A comparative theoretical study of CO2 sensing using inorganic AlN, BN and SiC single walled nanotubes*  
Sensors and Actuators B-Chemical, (185): 512-522 2013.
- Maihom, T.; Wannakao, S.; Boekfa, B.; Limtrakul, J.  
*Density functional study of the activity of gold-supported ZSM-5 zeolites for nitrous oxide decomposition*  
Chemical Physics Letters, (556): 217-224 2013.
- Maihom, T.; Wannakao, S.; Boekfa, B.; Limtrakul, J.  
*Production of Formic Acid via Hydrogenation of CO2 over a Copper-Alkoxide-Functionalized MOF: A Mechanistic Study*  
Journal of Physical Chemistry C, (117): 17650-17658 2013.
- Mairychova, B.; Svoboda, T.; Stepnicka, P.; Ruzicka, A.; Havenith, R. W. A.; Alonso, M.; De Proft, F.; Jambor, R.; Dostal, L.  
*Synthesis and Structural Characterization of Heteroboroxines with MB2O3 Core (M = Sb, Bi, Sn)*  
Inorganic Chemistry, (52): 1424-1431 2013.
- Majumder, M.; Manogaran, S.  
*Redundant internal coordinates, compliance constants and non-bonded interactions - some new insights*  
Journal of Chemical Sciences, (125): 9-15 2013.
- Makiabadi, B.; Zakarianejad, M.; Bagheri, S.; Masoodi, H. R.; Aghaie, R. S.

*Intermolecular Interactions in Uracil-Nitrous Acid Complexes: Structures, Binding Energy, Topological Properties, and Nuclear Magnetic Resonance Study*  
International Journal of Quantum Chemistry, (113): 2361-2371 2013.

Malenov, D. P.; Janjic, G. V.; Veljkovic, D. Z.; Zaric, S. D.  
*Mutual influence of parallel, CH/O, OH/pi and lone pair/pi interactions in water/benzene/water system*  
Computational and Theoretical Chemistry, (1018): 59-65 2013.

Mammino, L.  
*Investigation of the antioxidant properties of hyperjovinol A through its Cu(II) coordination ability*  
Journal of Molecular Modeling, (19): 2127-2142 2013.

Manchineella, S.; Prathyusha, V.; Priyakumar, U. D.; Govindaraju, T.  
*Solvent-Induced Helical Assembly and Reversible Chiroptical Switching of Chiral Cyclic-Dipeptide-Functionalized Naphthalenediimides*  
Chemistry-a European Journal, (19): 16615-16624 2013.

Mancini, A.; Aragoni, M. C.; Bingham, A. L.; Castellano, C.; Coles, S. L.; Demartin, F.; Hursthouse, M. B.; Isaia, F.; Lippolis, V.; Maninchedda, G.; Pintus, A.; Arca, M.  
*Reactivity of Fluoro-Substituted Bis(thiocarbonyl) Donors with Diiodine: An XRD, FT-Raman, and DFT Investigation*  
Chemistry-an Asian Journal, (8): 3071-3078 2013.

Mancini, A.; Aragoni, M. C.; Bricklebank, N.; Castellano, C.; Demartin, F.; Isaia, F.; Lippolis, V.; Pintus, A.; Arca, M.  
*Formation of T-Shaped versus Charge-Transfer Molecular Adducts in the Reactions Between Bis(thiocarbonyl) Donors and Br-2 and I-2*  
Chemistry-an Asian Journal, (8): 639-647 2013.

Mancini, P. M. E.; Della Rosa, C. D.; Ormachea, C. M.; Kneeteman, M. N.; Domingo, L. R.  
*Experimental and theoretical studies on polar Diels-Alder reactions of 1-nitronaphthalene developed in ionic liquids*  
Rsc Advances, (3): 13825-13834 2013.

Mansour, A. M.  
*Coordination behavior of sulfamethazine drug towards Ru(III) and Pt(II) ions: Synthesis, spectral, DFT, magnetic, electrochemical and biological activity studies*  
Inorganica Chimica Acta, (394): 436-445 2013.

Mansour, A. M.  
*Experimental and quantum chemical studies of sulfamethazine complexes with Ni(II) and Cu(II) ions*  
Journal of Coordination Chemistry, (66): 1118-1128 2013.

Mansour, A. M.  
*Molecular structure and spectroscopic properties of novel manganese(II) complex with sulfamethazine drug*  
Journal of Molecular Structure, (1035): 114-123 2013.

Mansour, A. M.; Ghani, N. T. A.  
*Hydrogen-bond effect, spectroscopic and molecular structure investigation of sulfamethazine Schiff-base: Experimental and quantum chemical calculations*  
Journal of Molecular Structure, (1040): 226-237 2013.

Mansour, A. M.; Hassaneen, H. M.; Mohammed, Y. S.; Ghani, N. T. A.

- Single crystal, spectral, computational studies and in vitro cytotoxicity of 2-chloro-3-formylpyrido 2,1-a isoquinoline-1-carbonitrile derivative*  
Journal of Molecular Structure, (1045): 180-190 2013.
- Manzetti, S.; Lu, T.  
*The geometry and electronic structure of Aristolochic acid: possible implications for a frozen resonance*  
Journal of Physical Organic Chemistry, (26): 473-483 2013.
- Mao, J. X.; Lee, A. S.; Kitchin, J. R.; Nulwala, H. B.; Luebke, D. R.; Damodaran, K.  
*Interactions in 1-ethyl-3-methyl imidazolium tetracyanoborate ion pair: Spectroscopic and density functional study*  
Journal of Molecular Structure, (1038): 12-18 2013.
- Marek, A.; Pepin, R.; Peng, B.; Laszlo, K. J.; Bush, M. F.; Turecek, F.  
*Electron Transfer Dissociation of Photolabeled Peptides. Backbone Cleavages Compete with Diazirine Ring Rearrangements*  
Journal of the American Society for Mass Spectrometry, (24): 1641-1653 2013.
- Markovic, J. M. D.; Markovic, Z. S.; Krstic, J. B.; Milenkovic, D.; Lucic, B.; Amic, D.  
*Interpretation of the IR and Raman spectra of morin by density functional theory and comparative analysis*  
Vibrational Spectroscopy, (64): 1-9 2013.
- Markovic, S.; Markovic, V.; Joksovic, M. D.; Todorovic, N.; Joksovic, L.; Divjakovic, V.; Trifunovic, S.  
*Debromination of endo-(+)-3-Bromocamphor with Primary Amines*  
Journal of the Brazilian Chemical Society, (24): 1099-+ 2013.
- Markovic, Z.; Amic, D.; Milenkovic, D.; Dimitric-Markovic, J. M.; Markovic, S.  
*Examination of the chemical behavior of the quercetin radical cation towards some bases*  
Physical Chemistry Chemical Physics, (15): 7370-7378 2013.
- Markovic, Z.; Dorovic, J.; Dekic, M.; Radulovic, M.; Markovic, S.; Ilic, M.  
*DFT study of free radical scavenging activity of erodiol*  
Chemical Papers, (67): 1453-1461 2013.
- Markovic, Z.; Milenkovic, D.; Dorovic, J.; Markovic, J. M. D.; Lucic, B.; Amic, D.  
*A DFT and PM6 study of free radical scavenging activity of ellagic acid*  
Monatshefte fur Chemie, (144): 803-812 2013.
- Markovic, Z. S.; Manojlovic, N. T.; Jeremic, S. R.; Zivic, M.  
*HPLC, UV-vis and NMR spectroscopic and DFT characterization of purpurin isolated from Rubia tinctorum L*  
Hemijaska Industrija, (67): 77-88 2013.
- Martinez, L.; Gancheff, J. S.; Hahn, F. E.; Burrow, R. A.; Gonzalez, R.; Kremer, C.; Chiozzone, R.  
*Nickel(II) complexes with methyl(2-pyridyl)ketone oxime: Synthesis, crystal structures and DFT calculations*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (105): 439-445 2013.
- Martiniano, H.; Cabral, B. J. C.  
*Structure and electronic properties of a strong dipolar liquid: Born-Oppenheimer molecular dynamics of liquid hydrogen cyanide*  
Chemical Physics Letters, (555): 119-124 2013.
- Martin-Rodriguez, M.; Castello, L. M.; Najera, C.; Sansano, J. M.; Larranaga, O.; de Cozar, A.; Cossio, F. P.

- Synthetic scope and DFT analysis of the chiral binap-gold(I) complex-catalyzed 1,3-dipolar cycloaddition of azlactones with alkenes*  
Beilstein Journal of Organic Chemistry, (9): 2422-2433 2013.
- Masoodi, H. R.; Bagheri, S.; Mohammadi, M.; Zakarianezhad, M.; Makiabadi, B.  
*The influence of cation- $\pi$  and anion- $\pi$  interactions on some NMR data of s-triazine center dot center dot center dot HF hydrogen bonding: A theoretical study*  
Chemical Physics Letters, (588): 31-36 2013.
- Matsumoto, Y.; Iwamoto, J.; Honma, K.  
*Cyclic structure of pyrrole-acetone binary clusters: Comparative study of the N-H center dot center dot center dot O=C hydrogen bond*  
Chemical Physics Letters, (578): 43-48 2013.
- Mazurek, A.; Dobrowolski, J. C.  
*The sEDA(=) and pEDA(=) descriptors of the double bonded substituent effect*  
Organic & Biomolecular Chemistry, (11): 2997-3013 2013.
- McGovern, G. P.; Zhu, D.; Aquino, A. J. A.; Vidovic, D.; Findlater, M.  
*Synthesis and Characterization of Terpyridine-Supported Boron Cations: Evidence for Pentacoordination at Boron*  
Inorganic Chemistry, (52): 13865-13868 2013.
- McKee, W. C.; Wu, J. I.; Rzepa, H. S.; Schleyer, P. V.  
*A Huckel Theory Perspective on Mobius Aromaticity*  
Organic Letters, (15): 3432-3435 2013.
- McKinnon, S. D. J.; Patrick, B. O.; Lever, A. B. P.; Hicks, R. G.  
*Binuclear Ruthenium Complexes of a Neutral Radical Bridging Ligand. A New "Spin" on Mixed Valency*  
Inorganic Chemistry, (52): 8053-8066 2013.
- Meenakshisundaram, S. P.; Karthikeyan, B.; Muthu, K.; Sebastian, S.  
*Molecular structure, spectroscopic (FT-IR, FT-Raman, UV-vis), NBO, thermochemistry analysis of bis(thiourea)zinc(II) chloride crystals*  
Molecular Simulation, (39): 584-595 2013.
- Melissen, S.; Tognetti, V.; Dupas, G.; Jouanneau, J.; Le, G.; Joubert, L.  
*A DFT study of the AlCl<sub>3</sub>-catalyzed Friedel-Crafts acylation of phenyl aromatic compounds*  
Journal of Molecular Modeling, (19): 4947-4958 2013.
- Meng, Q. X.; Li, M.  
*Nickel/zinc-catalyzed decarbonylative addition of anhydrides to alkynes: A DFT study*  
Journal of Molecular Modeling, (19): 4545-4554 2013.
- Meng, Q. X.; Wang, F.; Li, M.  
*Theoretical investigation of Co(0)-catalyzed intramolecular hydroacylation of 4-pentenal*  
Journal of Molecular Modeling, (19): 2225-2234 2013.
- Meng, S. C.; Li, W.; Yin, X. L.; Xie, J. M.  
*A comprehensive theoretical study of the hydrogen bonding interactions and microscopic solvation structures of a pyridyl-urea-based hydrogelator in aqueous solution*  
Computational and Theoretical Chemistry, (1006): 76-84 2013.

- Metzker, G.; Stefaneli, E. V.; Pereira, J. C. M.; Lima, F. D. A.; da Silva, S. C.; Franco, D. W.  
*Nitric oxide and nitroxyl formation in the reduction of trans-tetraamminenitrosyltriethylphosphiteruthenium(II) ion*  
Inorganica Chimica Acta, (394): 765-769 2013.
- Meyer, C.; Neue, B.; Schepmann, D.; Yanagisawa, S.; Yamaguchi, J.; Wurthwein, E. U.; Itami, K.; Wunsch, B.  
*Improvement of sigma(1) receptor affinity by late-stage C-H-bond arylation of spirocyclic lactones*  
Bioorganic & Medicinal Chemistry, (21): 1844-1856 2013.
- Miao, C. Q.; Lu, H. G.; Li, S. D.  
*Covalent Bonding in Au(BO)(2)(-) and Au(BS)(2)(-)*  
Journal of Cluster Science, (24): 233-241 2013.
- Micciarelli, M.; Altucci, C.; Della Ventura, B.; Velotta, R.; Tosa, V.; Perez, A. B. G.; Rodriguez, M. P.; de Lera, A. R.; Bende, A.  
*Low-lying excited-states of 5-benzyluracil*  
Physical Chemistry Chemical Physics, (15): 7161-7173 2013.
- Mieda, S.; Aida, M.  
*Macrodipole Moment of Polypeptides in beta-Sheet and Its Prediction from Dipole Moments of Amino Acid Residues as Building Blocks: Alanine and Glycine in beta-Strand*  
Chemistry Letters, (42): 473-475 2013.
- Mihaly, T.; Bette, M.; Mihaly, B.; Schmidt, J.; Schmidt, H.; Steinborn, D.  
*Synthesis, structure and characterization of adenine-based aminocarbene complexes of platinum(II)*  
Journal of Organometallic Chemistry, (739): 57-62 2013.
- Min, C. G.; Li, Z. S.; Ren, A. M.; Zou, L. Y.; Guo, J. F.; Goddard, J. D.  
*The fluorescent properties of coelenteramide, a substrate of aequorin and obelin*  
Journal of Photochemistry and Photobiology a-Chemistry, (251): 182-188 2013.
- Mindich, A. L.; Bokach, N. A.; Kuznetsov, M. L.; Starova, G. L.; Zhdanov, A. P.; Zhizhin, K. Y.; Miltsov, S. A.; Kuznetsov, N. T.; Kukushkin, V. Y.  
*Borylated Tetrazoles from Cycloaddition of Azide Anions to Nitrilium Derivatives of closo-Decaborate Clusters*  
Organometallics, (32): 6576-6586 2013.
- Miranda, R.; Valencia-Vazquez, O.; Maya-Vega, C. A.; Nicolas-Vazquez, I.; Vargas-Rodriguez, Y. M.; Morales-Serna, J. A.; Garcia-Rios, E.; Salmon, M.  
*Synthesis of Cyclooveratrylene Macrocycles and Benzyl Oligomers Catalysed by Bentonite under Microwave/Infrared and Solvent-Free Conditions*  
Molecules, (18): 12820-12844 2013.
- Miranda-Rojas, S.; Munoz-Castro, A.; Arratia-Perez, R.; Mendizabal, F.  
*Theoretical insights into the adsorption of neutral, radical and anionic thiophenols on gold(111)*  
Physical Chemistry Chemical Physics, (15): 20363-20370 2013.
- Miroló, L.; Schmidt, T.; Eckhardt, S.; Meuwly, M.; Fromm, K. M.  
*pH-Dependent Coordination of AgI Ions by Histidine: Experiment, Theory, and a Model for SilE*  
Chemistry-a European Journal, (19): 1754-1761 2013.
- Mishra, R.; Srivastava, A.; Sharma, A.; Tandon, P.; Baraldi, C.; Gamberini, M. C.



- Structural, electronic, thermodynamical and charge transfer properties of Chloramphenicol Palmitate using vibrational spectroscopy and DFT calculations*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (101): 335-342 2013.
- Mishra, S.; Tandon, P.; Eravuchira, P. J.; El-Abassy, R. M.; Materny, A.  
*Vibrational spectroscopy and density functional theory analysis of 3-O-caffeoylquinic acid*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (104): 358-367 2013.
- Misra, R.; Maity, D. K.; Bhattacharyya, S. P.  
*Deciphering the role of multiple hydrogen bonding sites on the microsolvation of 3-(phenylamino)-2-cyclohexen-1-one with water in the excited states*  
Chemical Physics, (425): 148-155 2013.
- Mitra, P.; Chakraborty, B.; Bhattacharyya, D.; Basu, S.  
*Excimer of 9-Aminoacridine Hydrochloride Hydrate in Confined Medium: An Integrated Experimental and Theoretical Study*  
Journal of Physical Chemistry A, (117): 1428-1438 2013.
- Mo, O.; Lamsabhi, A.; Yanez, M.; Heverly-Coulson, G. S.; Boyd, R. J.  
*Dramatic Substituent Effects on the Mechanisms of Nucleophilic Attack on Se-S Bridges*  
Journal of Computational Chemistry, (34): 2537-2547 2013.
- Mo, O.; Yanez, M.; Alkorta, I.; Elguero, J.  
*Enhancing and modulating the intrinsic acidity of imidazole and pyrazole through beryllium bonds*  
Journal of Molecular Modeling, (19): 4139-4145 2013.
- Moghadam, A. J.; Omidyan, R.; Mirkhani, V.; Azimi, G.  
*Theoretical Investigation of Excited State Proton Transfer Process in the N-Salicylidene-2-bromoethylamine*  
Journal of Physical Chemistry A, (117): 718-725 2013.
- Moghaddam, H. M.; Jelodar, M. D.  
*Ab initio investigation on electronic properties of the adenine molecule contacted with gold electrodes: effects of an external electric field*  
Indian Journal of Physics, (87): 99-105 2013.
- Moghanian, H.; Mobinikhaledi, A.; Monjezi, R.  
*Synthesis, spectroscopy (vibrational, NMR and UV-vis) studies, HOMO-LUMO and NBO analysis of 8-formyl-7-hydroxy-4-methylcoumarin by ab initio calculations*  
Journal of Molecular Structure, (1052): 135-145 2013.
- Mollania, F.; Raissi, H.  
*MOLECULAR STRUCTURE, VIBRATIONAL ASSIGNMENTS, CONFORMATIONAL STABILITY, GROUND AND EXCITED STATE HYDROGEN-BONDING ANALYSIS OF 2-NITROSO VINYL AMINE*  
Journal of Theoretical & Computational Chemistry, (12) 2013.
- Molon, M.; Gemel, C.; Seidel, R. W.; Jerabek, P.; Frenking, G.; Fischer, R. A.  
*The Organozinc Rich Compounds Cp\*M(ZnR)(5) (M = Fe, Ru; R = Cp\*, Me, Cl, Br)*  
Inorganic Chemistry, (52): 7152-7160 2013.
- Momeni, M. R.; Rivard, E.; Brown, A.  
*Carbene-Bound Borane and Silane Adducts: A Comprehensive DFT Study on Their Stability and Propensity for Hydride-Mediated Ring Expansion*  
Organometallics, (32): 6201-6208 2013.

- Monajjemi, M.  
*Non bonded interaction between BnNn (stator) and BN(-,0,+ )B (rotor) systems: A quantum rotation in IR region*  
Chemical Physics, (425): 29-45 2013.
- Monajjemi, M.; Hosseini, M. S.; Molaamin, F.  
*Theoretical Study of Boron Nitride Nanotubes with Armchair Forms*  
Fullerenes Nanotubes and Carbon Nanostructures, (21): 381-393 2013.
- Montalbano, F.; Cal, P.; Carvalho, M.; Goncalves, L. M.; Lucas, S. D.; Guedes, R. C.; Veiros, L. F.; Moreira, R.; Gois, P. M. R.  
*Discovery of new heterocycles with activity against human neutrophil elastase based on a boron promoted one-pot assembly reaction*  
Organic & Biomolecular Chemistry, (11): 4465-4472 2013.
- Montero-Campillo, M. M.; Lamsabhi, A.; Mo, O.; Yanez, M.  
*Modulating weak intramolecular interactions through the formation of beryllium bonds: complexes between squaric acid and BeH<sub>2</sub>*  
Journal of Molecular Modeling, (19): 2759-2766 2013.
- Montero-Campillo, M. M.; Lamsabhi, A. M.; Mo, O.; Yanez, M.  
*UV/Vis Spectra of Subporphyrazines and Subphthalocyanines with Aluminum and Gallium: A Time-Dependent DFT Study*  
Chemphyschem, (14): 915-922 2013.
- Mora, J. R.; Perez, C. D.; Maldonado, A.; Lorono, M.; Cordova, T.; Chuchani, G.  
*Theoretical study on thermal decomposition kinetics of allyl formates in the gas phase*  
Computational and Theoretical Chemistry, (1019): 48-54 2013.
- Morales-Bayuelo, A.  
*Understanding the electronic reorganization in the thermal isomerization reaction of trans-3,4-dimethylcyclobutene. Origins of outward Pseudodiradical {2n+2} torquoselectivity*  
International Journal of Quantum Chemistry, (113): 1534-1543 2013.
- Morales-Meza, S.; Sanchez-Castro, M. E.; Sanchez, M.  
*Penta- and heteropentadienyl ligands coordinated to beryllium*  
Journal of Molecular Modeling, (19): 5153-5158 2013.
- Moreno, D.; Martinez-Guajardo, G.; Diaz-Celaya, A.; Mercero, J. M.; de Coss, R.; Perez-Peralta, N.; Merino, G.  
*Re-examination of the C<sub>6</sub>Li<sub>6</sub> Structure: To Be, or not To Be Symmetric*  
Chemistry-a European Journal, (19): 12668-12672 2013.
- Moret, M. E.; Zhang, L. M.; Peters, J. C.  
*A Polar Copper-Boron One-Electron sigma-Bond*  
Journal of the American Chemical Society, (135): 3792-3795 2013.
- Morgan, K. M.; Ellis, J. A.; Lee, J.; Fulton, A.; Wilson, S. L.; Dupart, P. S.; Dastoori, R.  
*Thermochemical Studies of Epoxides and Related Compounds*  
Journal of Organic Chemistry, (78): 4303-4311 2013.
- Mueller, L. J.; Dunn, M. F.

- NMR Crystallography of Enzyme Active Sites: Probing Chemically Detailed, Three-Dimensional Structure in Tryptophan Synthase*  
Accounts of Chemical Research, (46): 2008-2017 2013.
- Mukherjee, V.; Singh, N. P.; Yadav, R. A.  
*Theoretical DFT study on spectroscopic signature and molecular dynamics of neurotransmitter and effect of hydrogen removal*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (107): 46-54 2013.
- Murugavelu, M.; Imran, P. K. M.; Sankaran, K. R.; Nagarajan, S.  
*Self-assembly and photophysical properties of a minuscule tailed perylene bisimide*  
Materials Science in Semiconductor Processing, (16): 461-466 2013.
- Musio, R.; Sciacovelli, O.  
*S-33 NMR spectroscopy. 4. Substituent effects on the S-33 nuclear quadrupole coupling constants and electric field gradient in 3-and 4-substituted benzenesulphonates studied by DFT calculations in vacuo and in aqueous solution*  
Journal of Molecular Structure, (1051): 115-123 2013.
- Muthu, S.; Maheswari, J. U.; Srinivasan, S.; Paulraj, E. I.  
*Spectroscopic studies, potential energy surface and molecular orbital calculations of pramipexole*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (115): 64-73 2013.
- Muthu, S.; Paulraj, E. I.  
*Molecular structure and spectroscopic characterization of ethyl 4-aminobenzoate with experimental techniques and DFT quantum chemical calculations*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (112): 169-181 2013.
- Muthu, S.; Paulraj, E. I.  
*Spectroscopic and molecular structure (monomeric and dimeric structure) investigation of 2- (2-hydroxyphenyl) carbonyloxy benzoic acid by DFT method: A combined experimental and theoretical study*  
Journal of Molecular Structure, (1038): 145-162 2013.
- Muthu, S.; Porchelvi, E. E.  
*Experimental spectroscopic (FTIR, FT-Raman, FT-NMR, UV-Visible) and DFT studies of 1-ethyl-1,4-dihydro-7-methyl-4oxo-1,8 naphthyridine-3-carboxylic acids*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (116): 220-235 2013.
- Muthu, S.; Porchelvi, E. E.  
*FTIR, FT-RAMAN, NMR, spectra, normal co-ordinate analysis, NBO, NLO and DFT calculation of N,N-diethyl-4-methylpiperazine-1-carboxamide molecule*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (115): 275-286 2013.
- Muthu, S.; Prasath, M.  
*Quantum chemical studies, vibrational analysis, molecular structure, first order hyper polarizability, NBO and HOMO-LUMO analysis of 3-hydroxybenzaldehyde and its cation*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (115): 789-799 2013.
- Muthu, S.; Prasath, M.; Balaji, R. A.  
*Experimental and theoretical investigations of spectroscopic properties of 8-chloro-1-methyl-6-phenyl-4H-1,2,4 triazolo 4,3-a 1,4 benzodiazepine*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (106): 129-145 2013.

- Muthu, S.; Renuga, S.  
*Vibrational and spectroscopic investigation on the structure of 5H-dibenzo b,f azipine-5-carboxamide*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (114): 1-10 2013.
- Muya, J. T.; Lijnen, E.; Nguyen, M. T.; Ceulemans, A.  
*The Boron Conundrum: Which Principles Underlie the Formation of Large Hollow Boron Cages?*  
Chemphyschem, (14): 346-363 2013.
- Nakamura, T.; Miyazaki, M.; Ishiuchi, S.; Weiler, M.; Schmies, M.; Dopfer, O.; Fujii, M.  
*IR Spectroscopy of the 4-AminobenzonitrileAr Cluster in the S0, S1 Neutral and D0 Cationic States*  
Chemphyschem, (14): 741-745 2013.
- Nakazawa, T.; Kaji, Y.  
*Structural, bonding, and magnetic properties of Fen-xSix (n, x <= 6) clusters: Theoretical investigation based on density functional theory*  
Computational Materials Science, (68): 350-360 2013.
- Nam, K.  
*Acceleration of Semiempirical Quantum Mechanical Calculations by Extended Lagrangian Molecular Dynamics Approach*  
Journal of Chemical Theory and Computation, (9): 3393-3403 2013.
- Naseem, S.; Laurent, A. D.; Carroll, E. C.; Vengris, M.; Kumauchi, M.; Hoff, W. D.; Krylov, A. I.; Larsen, D. S.  
*Photo-isomerization upshifts the pK(a) of the Photoactive Yellow Protein chromophore to contribute to photocycle propagation*  
Journal of Photochemistry and Photobiology a-Chemistry, (270): 43-52 2013.
- Naseh, M.; Sedaghat, T.; Tarassoli, A.; Shakerzadeh, E.  
*DFT studies of ONO Schiff bases, their anions and diorganotin(IV) complexes: Tautomerism, NBO and AIM analysis*  
Computational and Theoretical Chemistry, (1005): 53-57 2013.
- Nataraj, A.; Balachandran, V.; Karthick, T.  
*Molecular orbital studies (hardness, chemical potential, electrophilicity, and first electron excitation), vibrational investigation and theoretical NBO analysis of 2-hydroxy-5-bromobenzaldehyde by density functional method*  
Journal of Molecular Structure, (1031): 221-233 2013.
- Nataraj, A.; Balachandran, V.; Karthick, T.  
*Molecular structure, vibrational spectra, first hyperpolarizability and HOMO-LUMO analysis of p-acetylbenzotrile using quantum chemical calculation*  
Journal of Molecular Structure, (1038): 134-144 2013.
- Naumkin, F. Y.  
*Shape and property alteration of small silver clusters via doping by carbon: CAgn (n <= 6)*  
Computational and Theoretical Chemistry, (1021): 191-196 2013.
- Naumkin, F. Y.; Fisher, K.  
*Small metal-organic molecular sandwiches: Versatile units for induced structure manipulation*  
Chemical Physics Letters, (590): 52-57 2013.
- Ndambuki, S.; Ziegler, T.

- An analysis of unsupported triple and quadruple metal-metal bonds between two homonuclear group 6 transition elements based on the combined natural orbitals for chemical valence and extended transition state method*  
International Journal of Quantum Chemistry, (113): 753-761 2013.
- Neela, Y. I.; Mahadevi, A. S.; Sastry, G. N.  
*Analyzing coordination preferences of Mg<sup>2+</sup> complexes: insights from computational and database study*  
Structural Chemistry, (24): 637-650 2013.
- Neela, Y. I.; Mahadevi, A. S.; Sastry, G. N.  
*First principles study and database analyses of structural preferences for sodium ion (Na<sup>+</sup>) solvation and coordination*  
Structural Chemistry, (24): 67-79 2013.
- Nemeth, B.; Guegan, J. P.; Veszpremi, T.; Guillemin, J. C.  
*Trimethylaluminum and Borane Complexes of Primary Amines*  
Inorganic Chemistry, (52): 346-354 2013.
- Neuvonen, K.; Neuvonen, H.; Koch, A.; Kleinpeter, E.  
*Nature of the steric Omega(S), E-R and E-S ' substituent constants. Comparison with the aid of NBO and STERIC analysis*  
Computational and Theoretical Chemistry, (1015): 34-43 2013.
- Newberry, R. W.; Raines, R. T.  
*n ->pi(star) interactions in poly(lactic acid) suggest a role in protein folding*  
Chemical Communications, (49): 7699-7701 2013.
- Newberry, R. W.; VanVeller, B.; Guzei, I. A.; Raines, R. T.  
*n ->pi\* Interactions of Amides and Thioamides: Implications for Protein Stability*  
Journal of the American Chemical Society, (135): 7843-7846 2013.
- Nguyen, T. A. N.; Frenking, G.  
*Structure and bonding of tetrylone complexes (CO)(4)W{E(PPh3)(2)} (E = C-Pb)*  
Molecular Physics, (111): 2640-2646 2013.
- Nicolas-Vazquez, I.; Perez-Caballero, G.; Jimenez, A. G.; Rangel, G. G.; Ruvalcaba, R. M.  
*A novel azocompound, 2-(4-phenylazoaniline)-4-phenylphenol: Spectroscopic and quantum-chemical approach*  
International Journal of Quantum Chemistry, (113): 1107-1115 2013.
- Nijamudheen, A.; Datta, A.  
*Mechanism for C-I Bond Dissociation in Iodoethane, Iodobenzene, and Iodoethene for the C-C Cross Coupling Reactions over Gold Clusters*  
Journal of Physical Chemistry C, (117): 21433-21440 2013.
- Niu, X. Q.; Huang, Z. G.; Ma, L. L.; Shen, T. T.; Guo, L. F.  
*Density functional theory, natural bond orbital and quantum theory of atoms in molecule analyses on the hydrogen bonding interactions in tryptophan-water complexes*  
Journal of Chemical Sciences, (125): 949-958 2013.
- Nizovtsev, A. S.  
*Activation of C-H bond in methane by Pd atom from the bonding evolution theory perspective*  
Journal of Computational Chemistry, (34): 1917-1924 2013.

- Nori-Shargh, D.; Mousavi, S. N.; Boggs, J. E.  
*Pseudo Jahn-Teller Effect and Natural Bond Orbital Analysis of Structural Properties of Tetrahydridometallenes M<sub>2</sub>H<sub>4</sub>, (M = Si, Ge, and Sn)*  
 Journal of Physical Chemistry A, (117): 1621-1631 2013.
- Nori-Shargh, D.; Yahyaei, H.; Mousavi, S. N.; Maasoomi, A.; Kayi, H.  
*Natural bond orbital, nuclear magnetic resonance analysis and hybrid-density functional theory study of sigma-aromaticity in Al<sub>2</sub>F<sub>6</sub>, Al<sub>2</sub>Cl<sub>6</sub>, Al<sub>2</sub>Br<sub>6</sub> and Al<sub>2</sub>I<sub>6</sub>*  
 Journal of Molecular Modeling, (19): 2549-2557 2013.
- Novikov, A. S.; Dement'ev, A. I.; Medvedev, Y. N.  
*Theoretical study of the reactivity of Rh(II) and Rh(III) Bis(isonitrile) complexes in cycloaddition reactions with nitrones*  
 Russian Journal of Inorganic Chemistry, (58): 320-330 2013.
- Novikov, A. S.; Kuznetsov, M. L.; Pombeiro, A. J. L.  
*Theory of the Formation and Decomposition of N-Heterocyclic Aminoxy-carbenes through Metal-Assisted 2+3 -Dipolar Cycloaddition/Retro-Cycloaddition*  
 Chemistry-a European Journal, (19): 2874-2888 2013.
- Novikov, A. S.; Kuznetsov, M. L.; Pombeiro, A. J. L.; Bokach, N. A.; Shul'pin, G. B.  
*Generation of HO center dot Radical from Hydrogen Peroxide Catalyzed by Aqua Complexes of the Group III Metals M(H<sub>2</sub>O)(n) (3+) (M = Ga, In, Sc, Y, or La): A Theoretical Study*  
 Acs Catalysis, (3): 1195-1208 2013.
- Oda, A.; Torigoe, H.; Itadani, A.; Ohkubo, T.; Yumura, T.; Kobayashi, H.; Kuroda, Y.  
*Mechanism of CH<sub>4</sub> Activation on a Monomeric Zn<sup>2+</sup>-Ion Exchanged in MFI-Type Zeolite with a Specific Al Arrangement: Similarity to the Activation Site for H<sub>2</sub>*  
 Journal of Physical Chemistry C, (117): 19525-19534 2013.
- Odoh, S. O.; Govind, N.; Schreckenbach, G.; de Jong, W. A.  
*Cation-Cation Interactions in (UO<sub>2</sub>)<sub>2</sub>(OH)<sub>n</sub> (4-n) Complexes*  
 Inorganic Chemistry, (52): 11269-11279 2013.
- Oftadeh, M.; Kabiri, A.  
*Charge Transfer in Some Complexes of Crown Ether and of Thiocrown Ether with Dihalogens: DFT Study*  
 Acta Chimica Slovenica, (60): 790-796 2013.
- Oftadeh, M.; Moghadary, M.; Solimannejad, M.; Semnani, A.  
*A Study of Donor-Acceptor in the Charge Transfer Molecular Complexes of Some Thiocrown Ethers with Dihalogen Molecules by DFT Method*  
 Acta Chimica Slovenica, (60): 95-104 2013.
- Oftadeh, M.; Selahvarzi, S.; Keshavarz, M. H.  
*Intermolecular Interactions between TNAZ and H<sub>2</sub>O: a DFT Study*  
 Central European Journal of Energetic Materials, (10): 289-300 2013.
- Ogawa, T.; Kajita, Y.; Wasada-Tsutsui, Y.; Wasada, H.; Masuda, H.  
*Preparation, Characterization, and Reactivity of Dinitrogen Molybdenum Complexes with Bis(diphenylphosphino)amine Derivative Ligands that Form a Unique 4-Membered P-N-P Chelate Ring*  
 Inorganic Chemistry, (52): 182-195 2013.

- Okamura, T.; Nakagawa, J.  
*Contribution of Intramolecular NH center dot center dot center dot O Hydrogen Bonds to Magnesium-Carboxylate Bonds*  
Inorganic Chemistry, (52): 10812-10824 2013.
- Okur, H. I.; Kherb, J.; Cremer, P. S.  
*Cations Bind Only Weakly to Amides in Aqueous Solutions*  
Journal of the American Chemical Society, (135): 5062-5067 2013.
- Oliaey, A. R.; Boshra, A.  
*DFT study of Fe@B36N36 (n+) (n=2, 3) endohedral nanocages: Chemical reactivity, NBO analysis and thermochemistry*  
Physica E-Low-Dimensional Systems & Nanostructures, (52): 136-143 2013.
- Oliva, J. M.; Rue, J.; Hnyk, D.; Kennedy, J. D.; Rosenfeld, V. R.  
*Borane Polyhedra as Building Blocks for Unknown but Potentially Isolatable New Molecules - Extensions based on Computations of the Known B18H22 Isomers*  
Croatica Chemica Acta, (86): 485-494 2013.
- Olivato, P. R.; Cerqueira, C. R.; Contieri, B.; Santos, J. M. M.; Zukerman-Schpector, J.  
*Conformational preferences for some 3,3-bis (4 '-substituted phenylsulfanyl) 1-methyl-2-piperidinones through spectroscopic and theoretical studies*  
Journal of Sulfur Chemistry, (34): 617-626 2013.
- Omelchenko, I. V.; Shishkin, O. V.; Gorb, L.; Hill, F. C.; Leszczynski, J.  
*Substituent effects and aromaticity of six-membered heterocycles*  
Structural Chemistry, (24): 725-733 2013.
- Oparina, L. A.; Artem'ev, A. V.; Vysotskaya, O. V.; Kolyvanov, N. A.; Bagryanskaya, I. Y.; Doronina, E. P.; Gusarova, N. K.  
*Three-component reaction between secondary phosphine sulfides, elemental selenium and vinyl ethers: the first examples of Markovnikov addition of thioselenophosphinic acids to double bond*  
Tetrahedron, (69): 6185-6195 2013.
- Ormazabal-Toledo, R.; Contreras, R.; Campodonico, P. R.  
*Reactivity Indices Profile: A Companion Tool of the Potential Energy Surface for the Analysis of Reaction Mechanisms. Nucleophilic Aromatic Substitution Reactions as Test Case*  
Journal of Organic Chemistry, (78): 1091-1097 2013.
- Ormazabal-Toledo, R.; Contreras, R.; Tapia, R. A.; Campodonico, P. R.  
*Specific nucleophile-electrophile interactions in nucleophilic aromatic substitutions*  
Organic & Biomolecular Chemistry, (11): 2302-2309 2013.
- Ormazabal-Toledo, R.; Santos, J. G.; Rios, P.; Castro, E. A.; Campodonico, P. R.; Contreras, R.  
*Hydrogen Bond Contribution to Preferential Solvation in S<sub>N</sub>Ar Reactions*  
Journal of Physical Chemistry B, (117): 5908-5915 2013.
- Ortega, M.; Montejo, M.; Gonzalez, J. J. L.  
*Stabilizing factors of the molecular structure in silicon-based peptidomimetics in gas-phase and water solution. Assessment of the correlation between different descriptors of hydrogen bond strength*  
Journal of Molecular Modeling, (19): 4293-4304 2013.
- Osman, O. I.; Elroby, S. A. K.; Hilal, R. H.; Aziz, S. G.

- Theoretical characterization of gas-phase thermolysis products of ethane-1,2-diol, 2-chloroethanol and 2-fluoroethanol*  
Molecular Physics, (111): 643-659 2013.
- Osorio, E.; Vasquez, A.; Florez, E.; Mondragon, F.; Donald, K. J.; Tiznado, W.  
*Theoretical design of stable small aluminium-magnesium binary clusters*  
Physical Chemistry Chemical Physics, (15): 2222-2229 2013.
- Ostojic, B. D.; Mistic, S.; Dordevic, D. S.  
*A theoretical study of conformational flexibility, magnetic properties, and polarizabilities of trimethylnaphthalenes*  
International Journal of Quantum Chemistry, (113): 1890-1898 2013.
- Ostrowski, W.; Sniecikowska, L.; Hoffmann, M.; Franski, R.  
*Demethoxycurcumin-Metal Complexes: Fragmentation and Comparison with Curcumin-Metal Complexes, as Studied by ESI-MS/MS*  
Journal of Spectroscopy, 2013.
- Ota, K.; Koyasu, K.; Ohshimo, K.; Misaizu, F.  
*Structures of cobalt oxide cluster cations studied by ion mobility mass spectrometry*  
Chemical Physics Letters, (588): 63-67 2013.
- Otaki, H.; Ando, K.  
*Atoms-in-molecules analysis of the effect of intermolecular interactions on dielectric properties in hydrogen-bonded material 5-bromo-9-hydroxyphenalenone*  
International Journal of Quantum Chemistry, (113): 386-392 2013.
- Oyedepo, G. A.; Peterson, C.; Schoendorff, G.; Wilson, A. K.  
*Spectroscopic properties of Ar-x-Zn and Ar-x-Ag+ (x=1,2) van der Waals complexes*  
Journal of Chemical Physics, (138) 2013.
- Oziminski, W. P.  
*Stability and aromaticity of tautomers and kinetics of proton transfer in 6-methylpentafulvene and its exo-substituted derivatives: a computational study*  
Structural Chemistry, (24): 981-991 2013.
- Oziminski, W. P.  
*Theoretical study on the solvent influence on 1,2,3-triazole tautomeric equilibrium. A comparison of incremental microsolvation and continuum solvation model approaches*  
Tetrahedron, (69): 3197-3205 2013.
- Oziminski, W. P.; Krygowski, T. M.  
*Comparative studies on CH center dot center dot center dot F- hydrogen bond formation in benzene and exocyclically substituted pentafulvene derivatives*  
Journal of Physical Organic Chemistry, (26): 575-582 2013.
- Oziminski, W. P.; Palusiak, M.; Dominikowska, J.; Krygowski, T. M.; Havenith, R. W. A.; Gibson, C. M.; Fowler, P. W.  
*Capturing the elusive aromaticity of bicalicene*  
Physical Chemistry Chemical Physics, (15): 3286-3293 2013.
- Ozkanlar, A.; Samuels, A.; Clark, A. E.  
*Modulation of hydride formation energies in transition metal doped Mg by alteration of spin state*  
Chemical Physics Letters, (560): 10-14 2013.



- Oztopcu, O.; Holzacker, C.; Puchberger, M.; Weil, M.; Mereiter, K.; Veiros, L. F.; Kirchner, K.  
*Synthesis and Characterization of Hydrido Carbonyl Molybdenum and Tungsten PNP Pincer Complexes*  
Organometallics, (32): 3042-3052 2013.
- Paduani, C.; Jena, P.  
*Role of Ti-based catalysts in the dehydrogenation mechanism of magnesium borohydride: A cluster approach*  
International Journal of Hydrogen Energy, (38): 2357-2362 2013.
- Pal, S.; Kundu, T. K.  
*Pentagonal dodecahedron methane hydrate cage and methanol system - An ab initio study*  
Journal of Chemical Sciences, (125): 379-385 2013.
- Palafox, M. A.; Iza, N.  
*Structure-activity relationships of the antiviral D4T and seven 4'-substituted derivatives using MP2 and DFT methods*  
Structural Chemistry, (24): 967-980 2013.
- Palafox, M. A.; Jothy, V. B.; Singhal, S.; Joe, I. H.; Kumar, S.; Rastogi, V. K.  
*FT-IR, FT-Raman spectra and other molecular properties of 3,5-dichlorobenzonitrile: A DFT study*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (116): 509-517 2013.
- Palafox, M. A.; Rastogi, V. K.; Kumar, S.; Joe, H.  
*The biomolecule of 5-bromocytosine: FT-IR and FT-Raman spectra and DFT calculations. Identification of the tautomers in the isolated state and simulation the spectra in the solid state*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (111): 104-122 2013.
- Pan, B. F.; Evers-McGregor, D. A.; Bezpalko, M. W.; Foxman, B. M.; Thomas, C. M.  
*Multimetallc Complexes Featuring a Bridging N-heterocyclic Phosphido/Phosphenium Ligand: Synthesis, Structure, and Theoretical Investigation*  
Inorganic Chemistry, (52): 9583-9589 2013.
- Pan, X. L.; Zhou, Y. X.; Liu, W.; Liu, J. Y.; Dong, H.  
*Stereoelectronic Control of Cleavage of Dioxolane Five-membered Ring on Carbohydrates*  
Chemical Research in Chinese Universities, (29): 551-555 2013.
- Pan, Y.; Zhu, W. H.; Xiao, H. M.  
*Theoretical studies on the structures, heats of formation, energetic properties and pyrolysis mechanisms of nitrogen-rich difurazano 3,4-b:3',4'-e piperazine derivatives and their analogues*  
Structural Chemistry, (24): 1071-1087 2013.
- Pandey, G.; Pal, S.; Laha, R.  
*Direct Benzylic CH Activation for CO Bond Formation by Photoredox Catalysis*  
Angewandte Chemie-International Edition, (52): 5146-5149 2013.
- Pandey, K. K.  
*Nature of M-(eta(2)-H-SiR2) bonds in chromium, molybdenum and tungsten complexes (eta(5)-C5H5)(dmpe)M(eta(2)-H-SiR2) and (eta(5)-C5H5)(CO)(2)M(eta(2)-H-SiMe2) : A theoretical study*  
Polyhedron, (55): 241-248 2013.
- Panek, J. J.; Filarowski, A.; Jezierska-Mazzarello, A.

- Impact of proton transfer phenomena on the electronic structure of model Schiff bases: An AIM/NBO/ELF study*  
Journal of Chemical Physics, (139) 2013.
- Pangh, A.; Zahedi, E.  
*Theoretical study of proton transfer in ammonia-hydrogen halides in the presence of methanol*  
Research on Chemical Intermediates, (39): 3303-3317 2013.
- Papp, T.; Kollar, L.; Kegl, T.  
*Employment of quantum chemical descriptors for Hammett constants: Revision Suggested for the acetoxy substituent*  
Chemical Physics Letters, (588): 51-56 2013.
- Parameswari, A. R.; Kumaradhas, P.  
*Exploring the conformation, charge density distribution and the electrostatic properties of galanthamine molecule in the active site of AChE using DFT and AIM theory*  
International Journal of Quantum Chemistry, (113): 1200-1208 2013.
- Parimala, K.; Balachandran, V.  
*Structural study, NCA, FT-Raman spectral investigations, NBO analysis and thermodynamic properties of 2',4'-difluoroacetophenone by HF and DFT calculations*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (110): 269-284 2013.
- Pasteka, L. F.; Rajskey, T.; Urban, M.  
*Toward Understanding the Bonding Character in Complexes of Coinage Metals with Lone-Pair Ligands. CCSD(T) and DFT Computations*  
Journal of Physical Chemistry A, (117): 4472-4485 2013.
- Patel, R. N.; Patel, D. K.; Sondhiya, V. P.; Shukla, K. K.; Singh, Y.; Kumar, A.  
*Synthesis, crystal structure and superoxide dismutase activity of two new bis(mu-acetato/mu-nitrato) bridged copper(II) complexes with N<sup>-</sup>-phenyl(pyridin-2-yl)methylidene benzohydrazone*  
Inorganica Chimica Acta, (405): 209-217 2013.
- Paul, B. K.; Guchhait, N.  
*Geometrical criteria versus quantum chemical criteria for assessment of intramolecular hydrogen bond (IMHB) interaction: A computational comparison into the effect of chlorine substitution on IMHB of salicylic acid in its lowest energy ground state conformer*  
Chemical Physics, (412): 58-67 2013.
- Paul, B. K.; Guchhait, N.  
*Looking at the Green Fluorescent Protein (GFP) chromophore from a different perspective: A computational insight*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (103): 295-303 2013.
- Paul, B. K.; Guchhait, N.  
*A quantum chemical computational insight into the intramolecular hydrogen bond interaction in an antibacterial drug molecule-2-acetylindan-1,3-dione*  
Computational and Theoretical Chemistry, (1012): 20-26 2013.
- Paul, S.; Goswami, T.; Misra, A.; Chattaraj, P. K.  
*Concurrent loss of aromaticity and onset of superexchange in Mg<sub>3</sub>Na<sub>2</sub> with an increasing Na-Mg-3 distance*  
Theoretical Chemistry Accounts, (132) 2013.

- Pavlin, M.; Mavri, J.; Repic, M.; Vianello, R.  
*Quantum-chemical approach to determining the high potency of clorgyline as an irreversible acetylenic monoamine oxidase inhibitor*  
Journal of Neural Transmission, (120): 875-882 2013.
- Payaka, A.; Yotmanee, P.; Tongraar, A.  
*Characteristics of the "Hypercoordination" of hydroxide (OH-) in water: A comparative study of HF/MM and B3LYP/MM MD simulations*  
Journal of Molecular Liquids, (188): 89-95 2013.
- Peerannawar, S. R.; Gejji, S. P.  
*Structure and spectral characteristics of diquat-cucurbituril complexes from density functional theory*  
Journal of Molecular Modeling, (19): 5113-5127 2013.
- Pei, K. M.; Cui, Z. H.; Chen, W. G.  
*An adduct of Cl-substituted benzotriazole and hydroxy benzophenone as a novel UVA/UVB absorber: Theory-guided design, synthesis, and calculations*  
Journal of Molecular Structure, (1032): 100-104 2013.
- Pelzer, A. W.; Jellinek, J.; Jackson, K. A.  
*H-2 Reactions on Palladium Clusters*  
Journal of Physical Chemistry A, (117): 10407-10415 2013.
- Peng, A. P.; Zhang, X. H.; Li, Q. S.; King, R. B.; Schaefer, H. F.  
*Coaxial versus perpendicular structures for a range of binuclear cyclopentadienylpalladium derivatives*  
New Journal of Chemistry, (37): 775-783 2013.
- Perez-Cruz, F.; Villamena, F. A.; Zapata-Torres, G.; Das, A.; Headley, C. A.; Quezada, E.; Lopez-Alarcon, C.; Olea-Azar, C.  
*Selected hydroxycoumarins as antioxidants in cells: physicochemical and reactive oxygen species scavenging studies*  
Journal of Physical Organic Chemistry, (26): 773-783 2013.
- Peyghan, A. A.; Baei, M. T.; Hashemian, S.; Torabi, P.  
*Adsorption of CO molecule on AlN nanotubes by parallel electric field*  
Journal of Molecular Modeling, (19): 859-870 2013.
- Phukan, A. K.; Guha, A. K.; Sarmah, S.  
*Ligand Properties of Boron-Substituted Five-, Six-, and Seven-Membered Heterocyclic Carbenes: A Theoretical Study*  
Organometallics, (32): 3238-3248 2013.
- Phukan, A. K.; Guha, A. K.; Sarmah, S.; Dewhurst, R. D.  
*Electronic and Ligand Properties of Annulated Normal and Abnormal (Mesoionic) N-Heterocyclic Carbenes: A Theoretical Study*  
Journal of Organic Chemistry, (78): 11032-11039 2013.
- Pichierri, F.  
*DFT study of caesium ion complexation by cucurbit n urils (n=5-7)*  
Dalton Transactions, (42): 6083-6091 2013.
- Piekos, L.; Mitoraj, M. P.

- Theoretical description of dihydrogen/hydride and trihydride molybdocene complexes: An insight from static and molecular dynamics simulations*  
Journal of Computational Chemistry, (34): 294-304 2013.
- Pir, H.; Gunay, N.; Tamer, O.; Avci, D.; Atalay, Y.  
*Theoretical investigation of 5-(2-Acetoxyethyl)-6-methylpyrimidin-2, 4-dione: Conformational study, NBO and NLO analysis, molecular structure and NMR spectra*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (112): 331-342 2013.
- Pir, H.; Gunay, N.; Tamer, O.; Avci, D.; Tarcan, E.; Atalay, Y.  
*Quantum chemical computational studies on bis-thiourea zinc acetate*  
Materials Science-Poland, (31): 357-371 2013.
- Pizzirani, D.; Pagliuca, C.; Realini, N.; Branduardi, D.; Bottegoni, G.; Mor, M.; Bertozzi, F.; Scarpelli, R.; Piomelli, D.; Bandiera, T.  
*Discovery of a New Class of Highly Potent Inhibitors of Acid Ceramidase: Synthesis and Structure-Activity Relationship (SAR)*  
Journal of Medicinal Chemistry, (56): 3518-3530 2013.
- Platts, J. A.; Hill, J. G.; Riley, K. E.; Rezac, J.; Hobza, P.  
*Basis Set Dependence of Interaction Energies Computed Using Composite Post-MP2 Methods*  
Journal of Chemical Theory and Computation, (9): 330-337 2013.
- Polenz, I.; Schmidt, F. G.; Friedrich, J.; Tchernook, I.; Spange, S.  
*Radical Polymerization of MMA Co-initiated by 2-Phenyloxazoline*  
Macromolecular Chemistry and Physics, (214): 1473-1483 2013.
- Polestshuk, P. M.  
*Ad hoc methods for accurate determination of Bader's atomic boundary*  
Journal of Chemical Physics, (139) 2013.
- Politzer, P.; Murray, J. S.; Clark, T.  
*Halogen bonding and other sigma-hole interactions: a perspective*  
Physical Chemistry Chemical Physics, (15): 11178-11189 2013.
- Pollock, J. B.; Cook, T. R.; Schneider, G. L.; Stang, P. J.  
*Multi-Component Coordination-Driven Self-Assembly: Construction of Alkyl-Based Structures and Molecular Modelling*  
Chemistry-an Asian Journal, (8): 2423-2429 2013.
- Popov, I. A.; Boldyrev, A. I.  
*Computational probing of all-boron  $Li_2nB_2nH_{2n+2}$  polyenes*  
Computational and Theoretical Chemistry, (1004): 5-11 2013.
- Popov, I. A.; Li, Y. F.; Chen, Z. F.; Boldyrev, A. I.  
*"Benzation" of graphene upon addition of monovalent chemical species*  
Physical Chemistry Chemical Physics, (15): 6842-6848 2013.
- Popov, I. A.; Piazza, Z. A.; Li, W. L.; Wang, L. S.; Boldyrev, A. I.  
*A combined photoelectron spectroscopy and ab initio study of the quasi-planar B-24(-) cluster*  
Journal of Chemical Physics, (139) 2013.
- Popov, I. A.; Popov, V. F.; Bozhenko, K. V.; Cernusak, I.; Boldyrev, A. I.

- Structural changes in the series of boron-carbon mixed clusters C<sub>x</sub>B<sub>10-x</sub> (x=3-10) upon substitution of boron by carbon*  
Journal of Chemical Physics, (139) 2013.
- Pourayoubi, M.; Izadyar, M.; Elahi, B.; Parvez, M.  
*Combination of X-ray crystallography and theoretical study to evaluate the effect of N-H center dot center dot center dot O=P versus N-H center dot center dot center dot O=C hydrogen bonds on the N-H stretching frequencies*  
Journal of Molecular Structure, (1034): 354-362 2013.
- Powers, D. C.; Ritter, T.  
*A Transition State Analogue for the Oxidation of Binuclear Palladium(II) to Binuclear Palladium(III) Complexes*  
Organometallics, (32): 2042-2045 2013.
- Prabavathi, N.; Nilufer, A.; Krishnakumar, V.  
*Spectroscopic (FT-IR, FT-Raman, UV and NMR) investigation, conformational stability, NLO properties, HOMO-LUMO and NBO analysis of hydroxyquinoline derivatives by density functional theory calculations*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (114): 449-474 2013.
- Prabavathi, N.; Nilufer, A.; Krishnakumar, V.  
*Vibrational spectroscopic (FT-IR and FT-Raman) studies, natural bond orbital analysis and molecular electrostatic potential surface of Isoxanthopterin*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (114): 101-113 2013.
- Prestianni, A.; Ferrante, F.; Simakova, O. A.; Duca, D.; Murzin, D. Y.  
*Oxygen-Assisted Hydroxymatairesinol Dehydrogenation: A Selective Secondary-Alcohol Oxidation over a Gold Catalyst*  
Chemistry-a European Journal, (19): 4577-4585 2013.
- Priya, M. S.; Rani, N. U.; James, C.  
*Molecular modeling and spectral comparison for the change in methyl position of nitrophenol compounds 2-methyl-4-nitrophenol and 3-methyl-4-nitrophenol: A density functional theoretical study*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (107): 188-195 2013.
- Qin, P. H.; Zhang, W.; Lu, W. C.  
*Theoretical study of hydrated Ca<sup>2+</sup>-amino acids (glycine, threonine and phenylalanine) clusters*  
Computational and Theoretical Chemistry, (1021): 164-170 2013.
- Qin, Z. B.; Cong, R.; Wu, X.; Liu, Z. L.; Xie, H.; Tang, Z. C.; Jiang, L.; Fan, H. J.  
*Photoelectron velocity-map imaging spectroscopic and theoretical study on the reactivity of the gold atom toward CH<sub>3</sub>SH, CH<sub>3</sub>OH, and H<sub>2</sub>O*  
Journal of Chemical Physics, (139) 2013.
- Qiu, Y. X.; Wan, M. D.; Chen, X. Y.; Wang, S. G.  
*Reaction Mechanisms of Ethylene Hydrogenation Catalyzed by Gold(I) Complexes*  
Acta Physico-Chimica Sinica, (29): 279-286 2013.
- Qu, Z. W.; Zhu, H.  
*Toward Reversible Dihydrogen Activation by Borole Compounds*  
Journal of Physical Chemistry C, (117): 11989-11993 2013.
- Queen, M. S.; Towey, B. D.; Murray, K. A.; Veldkamp, B. S.; Byker, H. J.; Szilagy, R. K.

- Electronic structure of Ni(II)S-4 complexes from S K-edge X-ray absorption spectroscopy*  
Coordination Chemistry Reviews, (257): 564-578 2013.
- Quesada-Moreno, M. M.; Azofra, L. M.; Aviles-Moreno, J. R.; Alkorta, I.; Elguero, J.; Lopez-Gonzalez, J. J.  
*Conformational Preference and Chiroptical Response of Carbohydrates D-Ribose and 2-Deoxy-D-ribose in Aqueous and Solid Phases*  
Journal of Physical Chemistry B, (117): 14599-14614 2013.
- Rabanal-Leon, W. A.; Arratia-Perez, R.  
*RELATIVISTIC-DFT STUDY OF THE ELECTRONIC STRUCTURE, BONDING AND ENERGETIC OF THE ReF8 (-) AND UF8 (2-) IONS*  
Journal of the Chilean Chemical Society, (58): 2020-2024 2013.
- Rachelin, Y. P.; Nair, L. P.; James, C.  
*Electronic structure investigations and spectroscopic studies on the herbicidal molecule 4-Nitro phenyl-phenylether*  
Journal of Molecular Structure, (1036): 56-62 2013.
- Racz, A.; Varadi, A.; Mazak, K.; Kokosi, J.; Noszal, B.  
*Synthetic and quantum chemical study on the regioselective addition of amines to methyl maleamate*  
Journal of Molecular Modeling, (19): 3683-3694 2013.
- Rahm, M.; Christe, K. O.  
*Quantifying the Nature of Lone Pair Domains*  
Chemphyschem, (14): 3714-3725 2013.
- Rai, S.; Singh, H.  
*Electronic structure theory based study of proline interacting with gold nano clusters*  
Journal of Molecular Modeling, (19): 4099-4109 2013.
- Raissi, H.; Farzad, F.; Eslamdoost, S.; Mollania, F.  
*CONFORMATIONAL PROPERTIES AND INTRAMOLECULAR HYDROGEN BONDING OF 3-AMINO-PROPENESELENAL: AN AB INITIO AND DENSITY FUNCTIONAL THEORY STUDIES*  
Journal of Theoretical & Computational Chemistry, (12) 2013.
- Raissi, H.; Farzad, F.; Farsi, H.  
*THEORETICAL INVESTIGATION OF SUBSTITUTION EFFECT ON THE PROTON TRANSFER MECHANISM IN 3-MERCAPTO-PROPENETHIAL*  
Journal of Theoretical & Computational Chemistry, (12) 2013.
- Raissi, H.; Khanmohammadi, A.; Yoosefian, M.; Mollania, F.  
*Ab initio and DFT studies on 1-(thionitrosomethylene) hydrazine: conformers, energies, and intramolecular hydrogen-bond strength*  
Structural Chemistry, (24): 1121-1133 2013.
- Rajamani, T.; Muthu, S.  
*Electronic absorption, vibrational spectra, non-linear optical properties, NBO analysis and thermodynamic properties of 9- (2-hydroxyethoxy) methyl guanine molecule by density functional method*  
Solid State Sciences, (16): 90-101 2013.
- Rajamani, T.; Muthu, S.  
*Vibrational spectra, first order hyperpolarizability, NBO, Fukui function and HOMO-LUMO analysis of 2- 4-(1,3-benzodioxol-5-ylmethyl)-1-piperazinyl pyrimidine*

- Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (115): 654-666 2013.
- Rajamani, T.; Muthu, S.; Karabacak, M.  
*Electronic absorption, vibrational spectra, nonlinear optical properties, NBO analysis and thermodynamic properties of N-(4-nitro-2-phenoxyphenyl) methanesulfonamide molecule by ab initio HF and density functional methods*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (108): 186-196 2013.
- Ramachandran, G.; Muthu, S.; Maheswari, J. U.  
*Density functional theory and Ab initio studies of vibrational spectroscopic (FT-IR, FT-Raman and UV) first order hyperpolarizabilities, NBO, HOMO-LUMO and TD-DFT analysis of the 1,2-Dihydropyrazolo (4,3-E) Pyrimidin-4-one*  
Solid State Sciences, (16): 45-52 2013.
- Ramachandran, G.; Muthu, S.; Renuga, S.  
*Quantum mechanical study of the structure and spectroscopic (FT-IR, FT-Raman), first-order hyperpolarizability, NBO and HOMO-LUMO analysis of S-S-2 methylamino-l-phenyl propan-1-ol*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (107): 386-398 2013.
- Ramanathan, N.; Sankaran, K.  
*Phosphoryl chloride-methanol adducts: Matrix isolation infrared and DFT studies*  
Journal of Molecular Structure, (1054): 331-338 2013.
- Rao, H. B.; Wang, Y. Y.; Zeng, X. Y.; Xue, Y.; Li, Z. R.  
*Theoretical study on the aminolysis of p-substituted phenyl acetates with dimeric ammonia in vacuo and acetonitrile*  
Computational and Theoretical Chemistry, (1008): 8-14 2013.
- Rasekh, M. F.  
*THEORETICAL INVESTIGATION ON THE STRUCTURE AND PROPERTIES OF ALUMAZINE center dot center dot center dot M COMPLEXES (M=Li+, Na+, K+, Be2+, Mg2+, AND Ca2+)*  
Journal of Theoretical & Computational Chemistry, (12) 2013.
- Rastogi, V. K.; Palafox, M. A.; Tomar, R.; Singh, U.  
*2-Amino-3,5-dichlorobenzonitrile: DFT calculations in the monomer and dimer forms, FT-IR and FT-Raman spectra, molecular geometry, atomic charges and thermodynamical parameters*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (110): 458-470 2013.
- Rau, N. J.; Welles, E. A.; Wenthold, P. G.  
*Anionic Substituent Control of the Electronic Structure of Aromatic Nitrenes*  
Journal of the American Chemical Society, (135): 683-690 2013.
- Ray, D.; Dalapati, S.; Guchhait, N.  
*Spectral properties of a simple azine Schiff base and its sensing ability towards protic environment through hydrogen bonding interaction*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (115): 219-226 2013.
- Ray, M. J.; Randall, R. A. M.; Arachchige, K. S. A.; Slawin, A. M. Z.; Buhl, M.; Lebl, T.; Kilian, P.  
*Synthetic, Structural, NMR, and Computational Study of a Geminally Bis(peri-substituted) Tridentate Phosphine and Its Chalcogenides and Transition-Metal Complexes*  
Inorganic Chemistry, (52): 4346-4359 2013.
- Reddy, K.; Rosa, I. M. L.; Doriguetto, A. C.; Bastos, E. L.; Silva, L. F.

- Iodine-Catalyzed Prins Cyclization of Homoallylic Alcohols and Aldehydes*  
Molecules, (18): 11100-11130 2013.
- Reddy, K. H. K.; Jemmis, E. D.  
*Stabilization of diborane(4) by transition metal fragments and a novel metal to pi Dewar-Chatt-Duncanson model of back donation*  
Dalton Transactions, (42): 10633-10639 2013.
- Reimann, S.; Sharif, M.; Wittler, K.; Knopke, L. R.; Surkus, A. E.; Roth, C.; Ludwig, R.; Langer, P.  
*3-Pyrenylacrylates: Synthetic, Photophysical, Theoretical and Electrochemical Investigations*  
Zeitschrift Fur Naturforschung Section B-a Journal of Chemical Sciences, (68): 367-377 2013.
- Ren, Y.; Wei, X. G.; Ren, S. J.; Lau, K. C.; Wong, N. B.; Li, W. K.  
*The alpha-Effect Exhibited in Gas-Phase S(N)2@N and S(N)2@C Reactions*  
Journal of Computational Chemistry, (34): 1997-2005 2013.
- Revunova, K.; Gorelsky, S. I.; Lemaire, M. T.  
*Synthesis and coordination chemistry of a potential precursor to a triarylamminium radical cation ditopic ligand*  
Polyhedron, (52): 1118-1125 2013.
- Rhyman, L.; Ramasami, P.; Joule, J. A.; Domingo, L. R.  
*A density functional theory study of the regio- and stereoselectivity of the 1,3-dipolar cycloaddition of C-methyl substituted pyrazinium-3-olates with methyl acrylate and methyl methacrylate*  
Computational and Theoretical Chemistry, (1025): 58-66 2013.
- Rhyman, L.; Ramasami, P.; Joule, J. A.; Saez, J. A.; Domingo, L. R.  
*Understanding the formation of 3+2 and 2+4 cycloadducts in the Lewis acid catalysed reaction between methyl glyoxylate oxime and cyclopentadiene: a theoretical study*  
Rsc Advances, (3): 447-457 2013.
- Rigby, J.; Izgorodina, E. I.  
*Assessment of atomic partial charge schemes for polarisation and charge transfer effects in ionic liquids*  
Physical Chemistry Chemical Physics, (15): 1632-1646 2013.
- Rinderspacher, B. C.  
*Electro-optic and spectroscopic properties of push-pull-chromophores with non-aromatic pi-bridges*  
Chemical Physics Letters, (585): 21-26 2013.
- Rios, N.; Varela, J.; Birriel, E.; Gonzalez, M.; Cerecetto, H.; Merlino, A.; Porcal, W.  
*Identification of novel benzimidazole derivatives as anti-Trypanosoma cruzi agents: solid-phase synthesis, structure-activity relationships and molecular docking studies*  
Future Medicinal Chemistry, (5): 1719-1732 2013.
- Robledo, M.; Martin, F.; Alcamí, M.; Diaz-Tendero, S.  
*Exohedral interaction in cationic lithium metallofullerenes*  
Theoretical Chemistry Accounts, (132) 2013.
- Roffe, G. W.; Cox, H.  
*Computational Study of the Coordination of Methane to First Row Transition Metal Dication Complexes*  
Journal of Physical Chemistry A, (117): 3017-3024 2013.
- Rogachev, A. Y.; Hoffmann, R.



- Hypervalent Compounds as Ligands: I-3-Anion Adducts with Transition Metal Pentacarbonyls*  
Inorganic Chemistry, (52): 7161-7171 2013.
- Rogachev, A. Y.; Hoffmann, R.  
*Iodine (I-2) as a Janus-Faced Ligand in Organometallics*  
Journal of the American Chemical Society, (135): 3262-3275 2013.
- Rokob, T. A.; Bako, I.; Stirling, A.; Hamza, A.; Papai, I.  
*Reactivity Models of Hydrogen Activation by Frustrated Lewis Pairs: Synergistic Electron Transfers or Polarization by Electric Field?*  
Journal of the American Chemical Society, (135): 4425-4437 2013.
- Roldan, M. L.; Ledesma, A. E.; Raschi, A. B.; Castillo, M. V.; Romano, E.; Brandan, S. A.  
*A new experimental and theoretical investigation on the structures of aminoethyl phosphonic acid in aqueous medium based on the vibrational spectra and DFT calculations*  
Journal of Molecular Structure, (1041): 73-81 2013.
- Romano, E.; Brizuela, A. B.; Guzzetti, K. A.; Brandan, S. A.  
*An experimental and theoretical study on the hydration in aqueous medium of the antihypertensive agent tolazoline hydrochloride*  
Journal of Molecular Structure, (1037): 393-401 2013.
- Romano, E.; Davies, L. E.; Brandan, S. A.  
*Structural and vibrational studies and molecular force field of zinc difluoromethanesulfinate*  
Journal of Molecular Structure, (1044): 144-151 2013.
- Romano, E.; Ladetto, M. F.; Brandan, S. A.  
*Structural and vibrational studies of the potential anticancer agent, 5-difluoromethyl-1,3,4-thiadiazole-2-amino by DFT calculations*  
Computational and Theoretical Chemistry, (1011): 57-64 2013.
- Rong, Y.; Al-Harbi, A.; Krieger, B.; Parkin, G.  
*Structural Characterization of 2-Imidazolones: Comparison with their Heavier Chalcogen Counterparts*  
Inorganic Chemistry, (52): 7172-7182 2013.
- Roohi, H.; Bagheri, S.  
*Effect of axial strain on structural and electronic properties of zig-zag type of boron nitride nanotube (BNNT): a quantum chemical study*  
Structural Chemistry, (24): 409-420 2013.
- Roohi, H.; Jahantab, M.  
*Adsorption of parent nitrosamine on the nanocrystalline M-ZSM-5 zeolite: A density functional study*  
Journal of Chemical Sciences, (125): 1607-1618 2013.
- Roohi, H.; Khyrkah, S.  
*Ion-pairs formed in Mim(+) N(CN)(2)(-) ionic liquid: Structures, binding energies, NMR SSCCs, volumetric, thermodynamic and topological properties*  
Journal of Molecular Liquids, (177): 119-128 2013.
- Roohi, H.; Roshan, K.; Nokhastean, R.  
*Can the substituent in the para position of anilide ion influence the N-center dot center dot center dot H-F - > N-H center dot center dot center dot F- switching: a quantum chemical study*  
Structural Chemistry, (24): 1319-1330 2013.

- Rosenstengel, K.; Schulz, A.; Villinger, A.  
*Solid State Structure of Bi(N-3)(3), Bi(N-3)(3)center dot Solvates and the Structural Dynamics in the Bi(N-3)(6) (3-) Anion*  
Inorganic Chemistry, (52): 6110-6126 2013.
- Rosli, A. N.; Abu Bakar, M. A.; Manan, N. S. A.; Woi, P. M.; Lee, V. S.; Zain, S. M.; Ahmad, M. R.; Alias, Y.  
*G3 Assisted Rational Design of Chemical Sensor Array Using Carbonitrile Neutral Receptors*  
Sensors, (13): 13835-13860 2013.
- Rosokha, S. V.; Stern, C. L.; Ritzert, J. T.  
*Experimental and Computational Probes of the Nature of Halogen Bonding: Complexes of Bromine-Containing Molecules with Bromide Anions*  
Chemistry-a European Journal, (19): 8774-8788 2013.
- Roy, G.; Jayaram, P. N.; Mugesh, G.  
*Inhibition of Lactoperoxidase-Catalyzed Oxidation by Imidazole-Based Thiones and Selones: A Mechanistic Study*  
Chemistry-an Asian Journal, (8): 1910-1921 2013.
- Roy, L. E.; Bridges, N. J.; Martin, L. R.  
*Theoretical insights into covalency driven f element separations*  
Dalton Transactions, (42): 2636-2642 2013.
- Rozas, I.; Sanchez-Sanz, G.; Alkorta, I.; Elguero, J.  
*Solvent effects on guanidinium-anion interactions and the problem of guanidinium Y-aromaticity*  
Journal of Physical Organic Chemistry, (26): 378-385 2013.
- Ruiz-Blanco, Y. B.; Alves, M. J.; Rodriguez-Borges, J. E.; Molina, R.  
*STUDY BASED ON ELECTRONIC DESCRIPTORS OF THE DIASTEREOSELECTIVE AZA-DIELS-ALDER CYCLOADDITION OF (1R)-10-(N, N-DIETHYLSULFAMOYL)ISOBORNYL 2H-AZIRINE-3-CARBOXYLATE TO E,E-1,4-DIACETOXY-1,3-BUTADIENE*  
Journal of the Chilean Chemical Society, (58): 2243-2247 2013.
- Rusakov, Y. Y.; Krivdin, L. B.  
*Modern quantum chemical methods for calculating spin-spin coupling constants: theoretical basic and structural applications in chemistry*  
Russian Chemical Reviews, (82): 90-121 2013.
- Rzepa, H. S.  
*Chemical datuments as scientific enablers*  
Journal of Cheminformatics, (5) 2013.
- Rzepa, H. S.  
*A Computational Evaluation of the Evidence for the Synthesis of 1,3-Dimethylcyclobutadiene in the Solid State and Aqueous Solution*  
Chemistry-a European Journal, (19): 4932-4937 2013.
- Sadchikova, E. V.; Bakulev, V. A.; Subbotina, J. O.; Privalova, D. L.; Dehaen, W.; Van Hecke, K.; Robeyns, K.; Van Meervelt, L.; Mokrushin, V. S.  
*Synthesis and structure of new imidazo- and pyrazolo 5,1-d 1,2,3,5 thiaziazines based on the reaction of diazoazoles with acyl isothiocyanates controlled by S center dot center dot center dot O interaction*  
Tetrahedron, (69): 6987-6992 2013.

- Saed, B.; Omidyan, R.  
*Electronically Excited States of Protonated Aromatic Hydrocarbons: Phenanthrene and Pyrene*  
Journal of Physical Chemistry A, (117): 2499-2507 2013.
- Saeedi, M.; Anafcheh, M.; Ghafouri, R.; Hadipour, N. L.  
*A computational investigation of the electronic properties of Octahedral Al (n) N (n) and Al (n) P (n) cages (n=12, 16, 28, 36, and 48)*  
Structural Chemistry, (24): 681-689 2013.
- Safonova, L. P.; Kiselev, M. G.; Fedorova, I. V.  
*Complexes of sulfuric acid with N,N-dimethylformamide: An ab initio investigation*  
Pure and Applied Chemistry, (85): 225-236 2013.
- Saha, S.; Dinadayalane, T. C.; Leszczynska, D.; Leszczynski, J.  
*DFT-based reactivity study of (5,5) armchair boron nitride nanotube (BNNT)*  
Chemical Physics Letters, (565): 69-73 2013.
- Sahu, C.; Pakhira, S.; Sen, K.; Das, A. K.  
*A Computational Study of Detoxification of Lewisite Warfare Agents by British Anti-lewisite: Catalytic Effects of Water and Ammonia on Reaction Mechanism and Kinetics*  
Journal of Physical Chemistry A, (117): 3496-3506 2013.
- Sahu, C.; Sen, K.; Pakhira, S.; Mondal, B.; Das, A. K.  
*Binding affinity of substituted ureido-benzenesulfonamide ligands to the carbonic anhydrase receptor: A theoretical study of enzyme inhibition*  
Journal of Computational Chemistry, (34): 1907-1916 2013.
- Saini, P.; Bhasin, P.; Bansal, R. K.  
*Reinvestigation of homoaromaticity of cyclohepta-1,3,5-triene*  
Computational and Theoretical Chemistry, (1017): 72-77 2013.
- Saito, M.; Fujita, M.; Kanatomi, Y.; Ishimura, K.  
*Debromination of 1,2-Bis(phenylseleno)benzene Dibromide*  
Bulletin of the Chemical Society of Japan, (86): 990-992 2013.
- Sajan, D.; Chaitanya, K.; Safakath, K.; Philip, R.; Suthan, T.; Rajesh, N. P.  
*Three-photon absorption and vibrational spectroscopic study of 2-methylamino-5-chlorobenzophenone*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (106): 253-261 2013.
- Sajan, D.; Devi, T. U.; Safakath, K.; Philip, R.; Nemec, I.; Karabacak, M.  
*Ultrafast optical nonlinearity, electronic absorption, vibrational spectra and solvent effect studies of ninhydrin*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (109): 331-343 2013.
- Sajan, D.; Vijayan, N.; Safakath, K.; Philip, R.; Karabacak, M.  
*Multi-photon absorption effect and intra-molecular charge transfer of donor-pi-acceptor chromophore ethyl p-amino benzoate*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (108): 197-210 2013.
- Sajith, P. K.; Suresh, C. H.  
*Trans and Cis Influences in Hypervalent Iodine(III) Complexes: A DFT Study*  
Inorganic Chemistry, (52): 6046-6054 2013.

- Sakata, K.; Fujimoto, H.  
*Quantum Chemical Study of B(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub>-Catalyzed Hydrosilylation of Carbonyl Group*  
Journal of Organic Chemistry, (78): 12505-12512 2013.
- Sakata, K.; Fujimoto, H.  
*Quantum Chemical Study of Diels-Alder Reactions Catalyzed by Lewis Acid Activated Oxazaborolidines*  
Journal of Organic Chemistry, (78): 3095-3103 2013.
- Sakota, K.; Harada, S.; Sekiya, H.  
*Infrared spectroscopy of hydrated N-(2-phenylethyl)acetamide clusters: The electron-redistribution within the solute weakens local hydrogen bond*  
Chemical Physics, (419): 138-144 2013.
- Salahub, D. R.; de la Lande, A.; Goursot, A.; Zhang, R.; Zhang, Y.  
*Recent Progress in Density Functional Methodology for Biomolecular Modeling*  
Applications of Density Functional Theory to Biological and Bioinorganic Chemistry, (150): 1-64 2013.
- Saleem, H.; Subashchandrabose, S.; Erdogdu, Y.; Thanikachalam, V.; Jayabharathi, J.  
*FT-IR, FT-Raman spectral and conformational studies on (E)-2-(2-hydroxybenzylidenamino)-3-(1H-indol-3yl) propionic acid*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (101): 91-99 2013.
- Saloni, J.; Walker, K.; Hill, G.  
*Theoretical Investigation on Monomer and Solvent Selection for Molecular Imprinting of Nitrocompounds*  
Journal of Physical Chemistry A, (117): 1531-1534 2013.
- Salzner, U.  
*Quantitatively Correct UV-vis Spectrum of Ferrocene with TDB3LYP*  
Journal of Chemical Theory and Computation, (9): 4064-4073 2013.
- Samdal, S.; Mollendal, H.; Guillemin, J. C.  
*Microwave Spectrum and Conformational Properties of 4-Isocyano-1-butyne (HC CCH<sub>2</sub>CH<sub>2</sub>N C)*  
Journal of Physical Chemistry A, (117): 10304-10310 2013.
- Samolia, M.; Kumar, T. J. D.  
*A first-principles study of hydrogen interaction and saturation on ScAl<sub>3</sub>*  
Journal of Alloys and Compounds, (552): 457-462 2013.
- San Juan, R. R.; Allan, C. J.; Iqbal, M.; Eichhorn, S. H.; Macdonald, C. L. B.; Carmichael, T. B.  
*New Dihexadecyldithiophosphate SAMs on Gold Provide Insight into the Unusual Dependence of Adsorbate Chelation on Substrate Morphology in SAMs of Dialkyldithiophosphinic Acids*  
Journal of the American Chemical Society, (135): 15784-15793 2013.
- Sanchez-Eleuterio, A.; Sandoval-Lira, J.; Garcia-Sanchez, J.; Monterrosas-Perez, L.; Hernandez-Perez, J. M.; Quintero, L.; Sartillo-Piscil, F.  
*beta-Oxygen Effect in the Barton-McCombie Deoxygenation Reaction: Further Experimental and Theoretical Findings*  
Journal of Organic Chemistry, (78): 9127-9136 2013.
- Sanchez-Sanz, G.; Alkorta, I.; Trujillo, C.; Elguero, J.  
*Intramolecular Pnicogen Interactions in PHF(CH<sub>2</sub>)<sub>n</sub>PHF (n=26) Systems*  
Chemphyschem, (14): 1656-1665 2013.

- Sanchez-Sanz, G.; Trujillo, C.; Rozas, I.; Elguero, J.  
*A theoretical study on the aromaticity of benzene and related derivatives incorporating a C-C C-C fragment*  
Tetrahedron, (69): 7333-7344 2013.
- Sanchez-Sanz, G.; Trujillo, C.; Solimannejad, M.; Alkorta, I.; Elguero, J.  
*Orthogonal interactions between nitril derivatives and electron donors: pnictogen bonds*  
Physical Chemistry Chemical Physics, (15): 14310-14318 2013.
- Sandhiya, L.; Kolandaivel, P.; Senthilkumar, K.  
*Depletion of atmospheric ozone by nitrogen dioxide: a bifurcated reaction pathway*  
Theoretical Chemistry Accounts, (132) 2013.
- Sandoval, C. A. F.; Hernandez, R. I. C.; Basurto, J. C.; Conde, H. I. B.; Martinez, I. I. P.; Garcia, J. N. F.; Torres, B. N.; Ferrara, J. G. T.  
*Synthesis and theoretic calculations of benzoxazoles and docking studies of their interactions with triosephosphate isomerase*  
Medicinal Chemistry Research, (22): 2768-2777 2013.
- Sangeetha, V.; Govindarajan, M.; Kanagathara, N.; Marchewka, M. K.; Drozd, M.; Anbalagan, G.  
*Vibrational, DFT, and thermal analysis of 2,4,6-triamino-1,3,5-triazin-1-ium 3-(prop-2-enoyloxy) propanoate acrylic acid monosolvate monohydrate*  
Journal of Molecular Structure, (1054): 307-320 2013.
- Santos-Carballal, D.; Suardiaz, R.; Crespo-Otero, R.; Gonzalez, L.; Perez, C. S.  
*Conformational and NMR study of some furan derivatives by DFT methods*  
Journal of Molecular Modeling, (19): 4591-4601 2013.
- Sanz, D.; Claramunt, R. M.; Mathey, F.; Alkorta, I.; Sanchez-Sanz, G.; Elguero, J.  
*Intermolecular spin-spin coupling constants between P-31 atoms*  
Comptes Rendus Chimie, (16): 937-944 2013.
- Saputro, A. G.; Kasai, H.; Asazawa, K.; Kishi, H.; Tanaka, H.  
*Comparative Study on the Catalytic Activity of the TM-N-2 Active Sites (TM = Mn, Fe, Co, Ni) in the Oxygen Reduction Reaction: Density Functional Theory Study*  
Journal of the Physical Society of Japan, (82) 2013.
- Sarma, B. K.  
*Redox regulation of protein tyrosine phosphatase 1B (PTP1B): Importance of steric and electronic effects on the unusual cyclization of the sulfenic acid intermediate to a sulfenyl amide*  
Journal of Molecular Structure, (1048): 410-419 2013.
- Sarmah, S.; Guha, A. K.; Phukan, A. K.  
*Donor-Acceptor Complexes of Normal and Abnormal N-Heterocyclic Carbenes with Group 13 (B, Al, Ga) Elements: A Combined DFT and Atoms-in-Molecules Study*  
European Journal of Inorganic Chemistry: 3233-3239 2013.
- Sarmah, S.; Guha, A. K.; Phukan, A. K.; Kumar, A.; Gadre, S. R.  
*Stabilization of Si(0) and Ge(0) compounds by different silylenes and germlyenes: a density functional and molecular electrostatic study*  
Dalton Transactions, (42): 13200-13209 2013.
- Sarojini, K.; Krishnan, H.; Kanakam, C. C.; Muthu, S.

*Synthesis, structural, spectroscopic studies, NBO analysis, NLO and HOMO-LUMO of 4-methyl-N-(3-nitrophenyl)benzene sulfonamide with experimental and theoretical approaches*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (108): 159-170 2013.

Sathyanarayananmoorthi, V.; Karunathan, R.; Kannappan, V.

*Molecular Modeling and Spectroscopic Studies of Benzothiazole*  
Journal of Chemistry, 2013.

Sato, T.; Hirose, Y.; Yoshioka, D.; Shimojo, T.; Oi, S.

*1,2,4-Triazol-3-ylidenes with an N-2,4-Dinitrophenyl Substituent as Strongly pi-Accepting N-Heterocyclic Carbenes*  
Chemistry-a European Journal, (19): 15710-15718 2013.

Sattler, W.; Ruccolo, S.; Parkin, G.

*Synthesis, Structure, and Reactivity of a Terminal Organozinc Fluoride Compound: Hydrogen Bonding, Halogen Bonding, and Donor-Acceptor Interactions*  
Journal of the American Chemical Society, (135): 18714-18717 2013.

Schaefer, J.; Himmel, D.; Krossing, I.

*Au(2-C2H4)3 + Al(ORF)4 a Stable Homoleptic (Ethene)gold Complex*  
European Journal of Inorganic Chemistry: 2712-2717 2013.

Schaper, L. A.; Wei, X. H.; Altmann, P. J.; Ofele, K.; Pothig, A.; Drees, M.; Mink, J.; Herdtweck, E.; Bechlars, B.; Herrmann, W. A.; Kuhn, F. E.

*Synthesis and Comparison of Transition Metal Complexes of Abnormal and Normal Tetrazolylienes: A Neglected Ligand Species*  
Inorganic Chemistry, (52): 7031-7044 2013.

Schneider, W. B.; Benedikt, U.; Auer, A. A.

*Interaction of Platinum Nanoparticles with Graphitic Carbon Structures: A Computational Study*  
Chemphyschem, (14): 2984-2989 2013.

Schoeller, W. W.; Frey, G. D.

*On the acceptor properties of a Al-Nacnac carbene analogue, a density functional investigation*  
Journal of Organometallic Chemistry, (744): 172-177 2013.

Schulz, A.; Villinger, A.; Westenkirchner, A.

*Synthesis of 1,3-Dichloro-cyclo-1,3-diphosphadiazanes from Silylated Amino(dichloro)phosphanes*  
Inorganic Chemistry, (52): 11457-11468 2013.

Schulz, S.; Kuczkowski, A.; Blaser, D.; Wolper, C.; Jansen, G.; Haack, R.

*Solid-State Structures of Trialkylbismuthines BiR3 (R = Me, i-Pr)*  
Organometallics, (32): 5445-5450 2013.

Sebastian, S.; Sylvestre, S.; Jayarajan, D.; Amalanathan, M.; Oudayakumar, K.; Gnanapoongothai, T.; Jayavarthan, T.

*Molecular structure, Normal Coordinate Analysis, harmonic vibrational frequencies, Natural Bond Orbital, TD-DFT calculations and biological activity analysis of antioxidant drug 7-hydroxycoumarin*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (101): 370-381 2013.

Sebastian, S.; Sylvestre, S.; Oudayakumar, K.; Jayavarthan, T.; Karthikeyan, B.; Sundaraganesan, N.

*Molecular structure, vibrational spectra and first-order hyperpolarisability analysis of 2-amino-6-nitrobenzothiazole by DFT method*

Molecular Simulation, (39): 1052-1064 2013.

Sebastian, S.; Sylvestre, S.; Sundaraganesan, N.; Amalanathan, M.; Ayyapan, S.; Oudayakumar, K.; Karthikeyan, B.  
*Vibrational spectra, molecular structure, natural bond orbital, first order hyperpolarizability, TD-DFT and thermodynamic analysis of 4-amino-3-hydroxy-1-naphthalenesulfonic acid by DFT approach*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (107): 167-178 2013.

Sedghamiz, E.; Halfinezhad, Z.; Shiroudi, A.; Zahedi, E.  
*Influence of NO<sub>2</sub> attachment on the nuclear magnetic shielding tensors of N and B nuclei in C<sub>30</sub>B<sub>15</sub>N<sub>15</sub> heterofullerene: a DFT study*  
Research on Chemical Intermediates, (39): 3843-3857 2013.

Seif, A.; Bagherzadeh, R.; Goodarzi, M.; Azizi, K.  
*Ab initio study of 1:1 complexes of nitrogen trifluoride with nitrous oxide and carbon dioxide in vacuo*  
Journal of Chemical Sciences, (125): 1277-1284 2013.

Seif, A.; Ebrahimi, S.; Vessally, E.; Goodarzi, M.  
*Comparative study on the stabilities and properties of heterodimers containing the intermolecular interactions of CF<sub>2</sub>Cl<sub>2</sub> with the isoelectronic and isostructure species of N<sub>2</sub>O and CO<sub>2</sub>*  
Structural Chemistry, (24): 1737-1745 2013.

Semenov, S. G.; Bedrina, M. E.  
*A quantum chemical study of silsesquioxanes: H<sub>8</sub>Si<sub>8</sub>O<sub>12</sub>, Me<sub>8</sub>Si<sub>8</sub>O<sub>12</sub>, H@Me<sub>8</sub>Si<sub>8</sub>O<sub>12</sub>, He@Me<sub>8</sub>Si<sub>8</sub>O (12+), and He@Me<sub>8</sub>Si<sub>8</sub>O<sub>12</sub>*  
Journal of Structural Chemistry, (54): 159-163 2013.

Sen, K.; Ghosh, D.; Pakhira, S.; Banu, T.; Das, A. K.  
*Structure, stability, and dissociation of small ionic silicon oxide clusters SiO<sub>n</sub>+(n=3, 4) : Insight from density functional and topological exploration*  
Journal of Chemical Physics, (139) 2013.

Sen, T. K.; Sau, S. C.; Mukherjee, A.; Hota, P. K.; Mandal, S. K.; Maity, B.; Koley, D.  
*Abnormal N-heterocyclic carbene main group organometallic chemistry: a debut to the homogeneous catalysis*  
Dalton Transactions, (42): 14253-14260 2013.

Senthilkumar, L.; Umadevi, P.; Nithya, K. N. S.; Kolandaivel, P.  
*Density functional theory investigation of cocaine water complexes*  
Journal of Molecular Modeling, (19): 3411-3425 2013.

Serafin, L. M.; Law, M. M.; van Mourik, T.  
*Computational Studies of Bridging Structures and Isomerism in Substituted Disilynes*  
Journal of Chemical Theory and Computation, (9): 2697-2705 2013.

Seridi, L.; Boufelfel, A.  
*Wagonin hosted @ beta-cyclodextrin: Structural, electronic and nuclear studies*  
Journal of Molecular Liquids, (188): 13-21 2013.

Seridi, S.; Seridi, A.; Berredjem, M.; Kadri, M.  
*Host-guest interaction between 3,4-dihydroisoquinoline-2(1H)-sulfonamide and beta-cyclodextrin: Spectroscopic and molecular modeling studies*  
Journal of Molecular Structure, (1052): 8-16 2013.

- Sevillano, J. J. G.; Calero, S.; Ania, C. O.; Parra, J. B.; Kapteijn, F.; Gascon, J.; Hamad, S.  
*Toward a Transferable Set of Charges to Model Zeolitic Imidazolate Frameworks: Combined Experimental-Theoretical Research*  
Journal of Physical Chemistry C, (117): 466-471 2013.
- Sevincek, R.; Karabiyik, H.; Karabiyik, H.  
*Changes in ligating abilities of the singlet and triplet states of normal, abnormal and remote N-heterocyclic carbenes depending on their aromaticities*  
Journal of Molecular Modeling, (19): 5327-5341 2013.
- Shaaban, I. A.; Mohamed, T. A.; Zoghaib, W. M.; Wilson, L. D.; Farag, R. S.; Afifi, M. S.; Badr, Y. A.  
*Tautomerism, Raman, infrared and ultraviolet-visible spectra, vibrational assignments, MP2 and B3LYP calculations of dienol 3,4-dihydroxypyridine, keto-enol 3-hydroxypyridin-4-one and keto-enol dimer*  
Journal of Molecular Structure, (1043): 52-67 2013.
- Shahangi, F.; Chermahini, A. N.; Dabbagh, H. A.; Teimouri, A.; Farrokhpour, H.  
*Enantiomeric separation of D- and L-lactic acid enantiomers by use of nanotubular cyclicpeptides: A DFT study*  
Computational and Theoretical Chemistry, (1020): 163-169 2013.
- Shahraki, M.; Habibi-Khorassani, S. M.; Ebrahimi, A.; Maghsoodlou, M.; Ghalandarzehi, Y.  
*Intramolecular hydrogen bonding in chemoselective synthesized 2-substituted pyrrole stable phosphorus ylide: GIAO, AIM, and NBO approaches*  
Structural Chemistry, (24): 623-635 2013.
- Shaik, S.; Rzepa, H. S.; Hoffmann, R.  
*One Molecule, Two Atoms, Three Views, Four Bonds?*  
Angewandte Chemie-International Edition, (52): 3020-3033 2013.
- Shainyan, B. A.; Chipanina, N. N.; Oznobikhina, L. P.; Chernysheva, G. N.; Rozentsveig, I. B.  
*Hydrogen-bonded complexes of sulfonamides and thioamides with DMF: FT-IR and DFT study, NBO analysis*  
Journal of Physical Organic Chemistry, (26): 335-344 2013.
- Shainyan, B. A.; Chipanina, N. N.; Oznobikhina, L. P.; Danilevich, Y. S.  
*The structure and proton affinity of N-benzyl-N-(allenyl)trifluoromethanesulfonamide: FT-IR, DFT and ab initio study, NBO analysis*  
Journal of Physical Organic Chemistry, (26): 653-658 2013.
- Shaira, A.; Reddy, D.; Jaganyi, D.  
*A kinetic and mechanistic study into the substitution behaviour of platinum(II) polypyridyl complexes with a series of azole ligands*  
Dalton Transactions, (42): 8426-8436 2013.
- Shakourian-Fard, M.; Fattahi, A.  
*INFLUENCE OF CATION-HETEROATOM (Li+, Na+, AND K+) INTERACTION ON THE STRUCTURAL AND THERMOCHEMICAL PROPERTIES OF 2'-DEOXYTHYMIDINE NUCLEOSIDE: QTAIM AND NBO ANALYZES*  
Journal of Theoretical & Computational Chemistry, (12) 2013.
- Sharada, S. M.; Zimmerman, P. M.; Bell, A. T.; Head-Gordon, M.  
*Insights into the Kinetics of Cracking and Dehydrogenation Reactions of Light Alkanes in H-MFI*  
Journal of Physical Chemistry C, (117): 12600-12611 2013.



- She, M. Y.; Xiao, D. W.; Yin, B.; Yang, Z.; Liu, P.; Li, J. L.; Shi, Z.  
*An efficiently cobalt-catalyzed carbonylative approach to phenylacetic acid derivatives*  
Tetrahedron, (69): 7264-7268 2013.
- Sheela, N. R.; Sampathkrishnan, S.; Kumar, M. T.; Muthu, S.  
*Quantum mechanical study of the structure and spectroscopic, first order hyperpolarizability, Fukui function, NBO, normal coordinate analysis of Phenyl-N-(4-Methyl Phenyl) Nitroene*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (112): 62-77 2013.
- Sheela, N. R.; Sampathkrishnan, S.; Kumar, M. T.; Muthu, S.  
*Synthesis, spectroscopic (FT-IR, FT-Raman, C-13, H-1, UV) study, first order hyperpolarizability, NBO analysis, HOMO and LUMO analysis of 2(2-Hydroxyphenyl)-N-(4-Methylphenyl) Nitroene*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (109): 272-281 2013.
- Shehab, O. R.; Mansour, A. M.  
*Charge transfer complexes of 2-arylaminoethyl-1H-benzimidazole with 2,3-dichloro-5,6-dicyano-1,4-benzoquinone: Experimental and DFT studies*  
Journal of Molecular Structure, (1047): 121-135 2013.
- Shen, J.; Wang, H. J.; Xia, Y. M.  
*A DFT study of hydrogen bond interactions between oxidative 2'-deoxyadenosine nucleotides and RNA nucleotides*  
Structural Chemistry, (24): 559-571 2013.
- Shen, Y. L.; Meng, Q. S.; Huang, S. Y.; Gong, J. L.; Ma, X. B.  
*DFT investigations for the reaction mechanism of dimethyl carbonate synthesis on Pd(II)/beta zeolites*  
Physical Chemistry Chemical Physics, (15): 13116-13127 2013.
- Sheng, W. H.; Wang, M.; Lein, M.; Jiang, L. B.; Wei, W. X.; Wang, J. Y.  
*Mechanism of Copper(I)-Catalyzed Allylic Alkylation of Phosphorothioate Esters: Influence of the Leaving Group on alpha Regioselectivity*  
Chemistry-a European Journal, (19): 14126-14142 2013.
- Shi, J. H.; Su, Y. H.; Jiang, W.  
*Enantioseparation and Chiral Recognition of alpha-Cyclohexylmandelic Acid and Methyl alpha-Cyclohexylmandelate on Hydroxypropyl-beta-Cyclodextrin as Chiral Selector: HPLC and Molecular Modeling*  
Journal of Chromatographic Science, (51): 8-16 2013.
- Shieh, M.; Chu, Y. Y.; Chi, H. H.; Chen, H. S.; Hsing, K. J.; Huang, C. Y.  
*Reactions of Iron Acyl Chalcogenide Clusters with Electrophiles: Reactivity Comparison and Theoretical Calculations*  
Journal of the Chinese Chemical Society, (60): 725-734 2013.
- Shieh, M.; Huang, C. Y.; Lee, C. J.; Hsing, K. J.; Li, Y. W.; Chu, Y. Y.; Jhu, W. T.  
*Controlled synthesis of copper halide-incorporated triiron carbonyl sulfide clusters: Synthesis, electrochemistry, and computational studies*  
Polyhedron, (52): 879-889 2013.
- Shigemoto, I.; Kawakami, T.; Okumura, M.  
*A quantum chemical study on polymerization catalysts for polyesters: Catalytic performance of chelated complexes of titanium*  
Polymer, (54): 3297-3305 2013.

- Shil, S.; Paul, S.; Misra, A.  
*Charge-Transfer-Induced Magnetism in Mixed-Stack Complexes*  
Journal of Physical Chemistry C, (117): 2016-2023 2013.
- Shimasaki, T.; Nakayasu, K.; Shibata, M.; Yamaguchi, T.  
*Theoretical Studies on Structures and Electronic State of Alkyl-Substituted Ethyl Cations*  
Journal of Chemistry, 2013.
- Shiroudi, A.; Zahedi, E.  
*DFT Study of the Mechanism and Regioselectivity of 1,3-Pentadiene with Methyl Acrylate Using Theoretical Approaches*  
Chinese Journal of Structural Chemistry, (32): 243-251 2013.
- Shiroudi, A.; Zahedi, E.  
*Isomerisation reactions of alpha-methyl allyl acetate, trifluoroacetate : theoretical study*  
Progress in Reaction Kinetics and Mechanism, (38): 249-265 2013.
- Shishkina, S. V.; Slabko, A. I.; Berski, S.; Latajka, Z.; Shishkin, O. V.  
*Tuning of character of the N-O bond in HONO from covalent to protocovalent by different types of intramolecular interactions*  
Journal of Chemical Physics, (139) 2013.
- Shishkina, S. V.; Slabko, A. I.; Shishkin, O. V.  
*Conjugation vs hyperconjugation in molecular structure of acrolein*  
Chemical Physics Letters, (556): 18-22 2013.
- Shukla, M.; Saha, S.  
*Relationship between stabilization energy and thermophysical properties of different imidazolium ionic liquids: DFT studies*  
Computational and Theoretical Chemistry, (1015): 27-33 2013.
- Sicilia, V.; Borja, P.; Casas, J. M.; Fuertes, S.; Martin, A.  
*Selective synthesis of new half-lantern benzoquinolate platinum complexes. DFT and photophysical studies on the platinum (II,II) derivative*  
Journal of Organometallic Chemistry, (731): 10-17 2013.
- Siddiqui, S. A.; Bouarissa, N.  
*First principle study of the interaction of elemental Hg with small neutral, anionic and cationic Pd-n (n=1-6) clusters*  
Operator id LLP Date (MM/DD/YY)-1-2014 Week#3 Start Time9.30 End Time S. No.Accn #Item RangeJob NameTotal Items Start TimeEnd TimeTotal time(in mins)AT and break timeQuery item  
Journal of Chemical Sciences, (125): 1629-1637 2013.
- Siddiqui, S. A.; Bouarissa, N.; Rasheed, T.; Al-Assiri, M. S.  
*Quantum chemical study of the interaction of elemental Hg with small neutral, anionic and cationic Au-n (n=1-6) clusters*  
Materials Research Bulletin, (48): 995-1002 2013.
- Sidorkin, V. F.; Doronina, E. P.; Belogolova, E. F.  
*A New Approach to the Design of Neutral 10-C-5 Trigonal-Bipyramidal Carbon Compounds: A "-Electron Cap" Effect*  
Chemistry-a European Journal, (19): 10302-10311 2013.

- Sieh, D.; Burger, P.  
*Si-H Activation in an Iridium Nitrido Complex-A Mechanistic and Theoretical Study*  
Journal of the American Chemical Society, (135): 3971-3982 2013.
- Sigolaev, Y. F.; Semenov, S. G.; Belyakov, A. V.  
*Quantum-Chemical Study of Silacyclohexanes C<sub>5</sub>H<sub>10</sub>SiHCN, C<sub>5</sub>H<sub>10</sub>SiH(t-Bu), C<sub>5</sub>H<sub>10</sub>Si(t-Bu)CN, and C<sub>5</sub>H<sub>10</sub>SiHF*  
Russian Journal of General Chemistry, (83): 932-937 2013.
- Silla, J. M.; Cormanich, R. A.; Rittner, R.; Freitas, M. P.  
*Conformational analysis and intramolecular interactions in monosubstituted phenylboranes and phenylboronic acids*  
Beilstein Journal of Organic Chemistry, (9): 1127-1134 2013.
- Silla, J. M.; Duarte, C. J.; Rittner, R.; Freitas, M. P.  
*Conformational analysis of 6-fluorosalicyclic acid*  
Rsc Advances, (3): 25765-25768 2013.
- Singh, B. G.; Thomas, E.; Sawant, S. N.; Takahashi, K.; Dedachi, K.; Iwaoka, M.; Priyadarsini, K. I.  
*Radical Cations of Aromatic Selenium Compounds: Role of Se center dot center dot center dot X Nonbonding Interactions*  
Journal of Physical Chemistry A, (117): 9259-9265 2013.
- Singh, H. J.; Mukherjee, U.  
*A computational approach to design energetic ionic liquids*  
Journal of Molecular Modeling, (19): 2317-2327 2013.
- Singh, R. N.; Kumar, A.; Rawat, P.; Srivastava, A.  
*Synthesis, spectroscopic and structural evaluation of ethyl 2-cyano-3-{5-(4-nitro-benzoyl)-hydrazonomethyl-1H-pyrrol-2-yl}-acrylate using experimental and theoretical approaches*  
Journal of Molecular Structure, (1049): 419-428 2013.
- Singh, R. N.; Kumar, A.; Rawat, P.; Tiwari, R. K.; Singh, A. K.  
*Studies on molecular structure, spectral analysis, chemical reactivity and first hyperpolarizability of a newly synthesized 1,9-bis(4-isonicotinoyl)-hydrazonomethyl-5-phenyl-dipyrromethane using experimental and theoretical approaches*  
Journal of Molecular Structure, (1052): 67-75 2013.
- Singh, R. N.; Kumar, A.; Tiwari, R. K.; Rawat, P.  
*Study of spectroscopic, reactivity and NLO properties of synthesized dipyrromethane containing cyanovinylhydrazide using experimental and theoretical approaches*  
Journal of Molecular Structure, (1048): 448-459 2013.
- Singh, R. N.; Kumar, A.; Tiwari, R. K.; Rawat, P.  
*Synthesis, molecular structure, hydrogen-bonding, NBO and chemical reactivity analysis of a novel 1,9-bis(2-cyano-2-ethoxycarbonylvinyl)-5-(4-hydroxyphenyl)-dipyrromethane: A combined experimental and theoretical (DFT and QTAIM) approach*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (113): 378-385 2013.
- Singh, R. N.; Kumar, A.; Tiwari, R. K.; Rawat, P.  
*Synthesis, molecular structure, multiple interactions and chemical reactivity analysis of a novel ethyl 2-cyano-3-5-(hydrazinoxyalyl-hydrazonomethyl)-1H-pyrrol-2-yl-acrylate and its dimer: A combined experimental and theoretical (DFT and QTAIM) approach*

- Journal of Molecular Structure, (1037): 420-430 2013.
- Singla, N.; Bhadram, V. S.; Narayana, C.; Chowdhury, P.  
*White Light Generation by Carbonyl Based Indole Derivatives Due to Proton Transfer: An Efficient Fluorescence Sensor*  
Journal of Physical Chemistry A, (117): 2738-2752 2013.
- Singla, N.; Chowdhury, P.  
*Density functional investigation of photo induced Intramolecular Proton Transfer (IPT) in Indole-7-carboxaldehyde and its experimental verification*  
Journal of Molecular Structure, (1045): 72-80 2013.
- Singla, N.; Kumar, R.; Pathak, A.; Chowdhury, P.  
*Excited state behavior of Pyrrole 2-carboxyldehyde: Theoretical and experimental study*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (112): 125-131 2013.
- Singla, P.; Singhal, S.; Goel, N.  
*Theoretical study on adsorption and dissociation of NO<sub>2</sub> molecules on BNNT surface*  
Applied Surface Science, (283): 881-887 2013.
- Sinha, L.; Karabacak, M.; Narayan, V.; Cinar, M.; Prasad, O.  
*Molecular structure, electronic properties, NLO, NBO analysis and spectroscopic characterization of Gabapentin with experimental (FT-IR and FT-Raman) techniques and quantum chemical calculations*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (109): 298-307 2013.
- Siwatch, R. K.; Yadav, D.; Mukherjee, G.; Rajaraman, G.; Nagendran, S.  
*Digermylene Oxide Complexes: Facile Synthesis and Reactivity*  
Inorganic Chemistry, (52): 13384-13391 2013.
- Siwek, A.; Staczek, P.; Wujec, M.; Bielawski, K.; Bielawska, A.; Paneth, P.  
*Cytotoxic effect and molecular docking of 4-ethoxycarbonylmethyl-1-(piperidin-4-ylcarbonyl)-thiosemicarbazide-a novel topoisomerase II inhibitor*  
Journal of Molecular Modeling, (19): 1319-1324 2013.
- Smith, J. M.; Alahmadi, Y. J.; Rowley, C. N.  
*Range-Separated DFT Functionals are Necessary to Model Thio-Michael Additions*  
Journal of Chemical Theory and Computation, (9): 4860-4865 2013.
- Snieszek, M.; Stecko, S.; Panfil, I.; Furman, B.; Urbanczyk-Lipkowska, Z.; Chmielewski, M.  
*Thermal and Sc(OTf)<sub>3</sub> catalyzed 1,3-dipolar cycloaddition of open-chain nitrones to alpha,beta-unsaturated lactones: combined experimental and computational studies*  
Tetrahedron-Asymmetry, (24): 89-103 2013.
- Soliman, S. M.  
*Molecular structure, spectroscopic properties, NLO and NBO analysis of 3,4-Lutidine and Ag(3,4-Lutidine)<sub>2</sub>NO<sub>3</sub> complex*  
Journal of Molecular Structure, (1048): 308-320 2013.
- Soliman, S. M.; Albering, J.; Abu-Youssef, M. A. M.  
*Low temperature X-ray molecular structure, tautomerism and spectral properties of 2,3-dihydroxyquinoxaline*  
Journal of Molecular Structure, (1053): 48-60 2013.

- Solimannejad, M.; Gharabaghi, M.; Alkorta, I.  
*Ab initio study of water clustering in the presence of a methyl radical*  
Structural Chemistry, (24): 491-497 2013.
- Solimannejad, M.; Gholipour, A.  
*Revealing substituent effects on the concerted interaction of pnictogen, chalcogen, and halogen bonds in substituted s-triazine ring*  
Structural Chemistry, (24): 1705-1711 2013.
- Solimannejad, M.; Malekani, M.  
*Substituent Effects on the Cooperativity of Halogen Bonding*  
Journal of Physical Chemistry A, (117): 5551-5557 2013.
- Solimannejad, M.; Nassirinia, N.; Amani, S.  
*A computational study of 1:1 and 1:2 complexes of nitril halides (O<sub>2</sub>NX) with HCN and HNC*  
Structural Chemistry, (24): 651-659 2013.
- Song, G. L.; Li, Z. H.; Fan, K. N.  
*Extended Energy Divide-and-Conquer Method Based on Charge Conservation*  
Journal of Chemical Theory and Computation, (9): 1992-1999 2013.
- Song, I. K.; Kang, Y. K.  
*Conformational preferences of taurine in the gas phase and in water*  
Computational and Theoretical Chemistry, (1025): 8-15 2013.
- Song, K. H.; Wang, X.; Qian, P.; Zhang, C.; Zhang, Q.  
*Theoretical study of interaction of formamide with kaolinite*  
Computational and Theoretical Chemistry, (1020): 72-80 2013.
- Song, Q. X.; Ding, Z. D.; Liu, J. H.; Li, Y.; Wang, H. J.  
*Theoretical study on the binding mechanism between N<sup>6</sup>-methyladenine and natural DNA bases*  
Journal of Molecular Modeling, (19): 1089-1098 2013.
- Song, Q. X.; Qiu, Z. M.; Wang, H. J.; Xia, Y. M.; Shen, J.; Zhang, Y.  
*The effect of methylation on the hydrogen-bonding and stacking interaction of nucleic acid bases*  
Structural Chemistry, (24): 55-65 2013.
- Soto, C. A. T.; Costa, A. C.; Ramos, J. M.; Versiane, O.; Ondar, G. F.; Ferreira, G. B.; Favero, P. P.; Rangel, J. L.; Raniero, L.; Costa, G. B.; Bussi, G. G. A.; Martin, A. A.  
*Surface enhanced Raman scattering, electronic spectrum and Mulliken charge distribution in the normal modes of bis(diethyldithiocarbamate)zinc(II) complex*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (110): 443-449 2013.
- Soto, C. A. T.; Costa, A. C.; Ramos, J. M.; Vieira, L. S.; Rost, N. C. V.; Versiane, O.; Rangel, J. L.; Mondragon, M. A.; Raniero, L.; Martin, A. A.  
*Surface enhanced Raman scattering, electronic spectrum, natural bond orbital, and mulliken charge distribution in the normal modes of diethyldithiocarbamate copper (II) complex, Cu(DDTC)<sub>2</sub>*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (116): 546-555 2013.
- Soto, C. A. T.; Ramos, J. M.; Costa, A. C.; Vieira, L. S.; Rangel, J. L.; Raniero, L.; Favero, P. P.; Lemma, T.; Ondar, G. F.; Versiane, O.; Martin, A. A.  
*Surface enhancement Raman scattering of tautomeric thiobarbituric acid. Natural bond orbitals and B3LYP/6-311+G (d, p) assignments of the Fourier Infrared and Fourier Raman Spectra*

- Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (114): 475-485 2013.
- Soto-Delgado, J.; Saez, J. A.; Tapia, R. A.; Domingo, L. R.  
*Theoretical study on the molecular mechanism of the 5+2 vs. 4+2 cyclization mediated by Lewis acid in the quinone system*  
Organic & Biomolecular Chemistry, (11): 8357-8365 2013.
- Sousa, C. C. S.; Matos, M. A. R.; Santos, L.; Morais, V. M. F.  
*Energetics of 2-and 3-coumaranone isomers: A combined calorimetric and computational study*  
Journal of Chemical Thermodynamics, (67): 210-216 2013.
- Sousa, C. C. S.; Morais, V. M. F.; Matos, M. A. R.  
*Experimental and computational thermochemistry of 6,7-dihydro-4(5H)-benzofuranone*  
Journal of Chemical Thermodynamics, (56): 83-88 2013.
- Sozen-Aktas, P.; Del Rosal, I.; Manoury, E.; Demirhan, F.; Lledos, A.; Poli, R.  
*Speciation of Cp\*2M2O5 in Polar and Donor Solvents*  
Chemistry-a European Journal, (19): 3969-3985 2013.
- Sparta, M.; Valdez, C. E.; Alexandrova, A. N.  
*Metal-Dependent Activity of Fe and Ni Acireductone Dioxygenases: How Two Electrons Reroute the Catalytic Pathway*  
Journal of Molecular Biology, (425): 3007-3018 2013.
- Spata, V. A.; Matsika, S.  
*Bonded Excimer Formation in pi-Stacked 9-Methyladenine Dimers*  
Journal of Physical Chemistry A, (117): 8718-8728 2013.
- Spisak, S. N.; Sumner, N. J.; Zabula, A. V.; Filatov, A. S.; Rogachev, A. Y.; Petrukhina, M. A.  
*Tuning Binding of Rubidium Ions to Planar and Curved Negatively Charged pi Surfaces*  
Organometallics, (32): 3773-3779 2013.
- Sridevi, C.; Velraj, G.  
*Structural, vibrational, electronic, NMR, NLO and reactivity analyses of (3Z)-3-(2-oxo-2-phenylethylidene)-1,3-dihydro-2H-indol-2-one (OPEDI) by ab initio HF and DFT calculations*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (107): 334-346 2013.
- Srivastava, A.; Mishra, R.; Tandon, P.; Bansal, A. K.  
*FT-Raman, FT-IR, UV spectroscopic, NBO and DFT quantum chemical study on the molecular structure, vibrational and electronic transitions of clopidogrel hydrogen sulfate form 1: A comparison to form 2*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (104): 409-418 2013.
- Stachowicz, A.; Korchowiec, J.  
*Bond detectors for molecular dynamics simulations, Part I: Hydrogen bonds*  
Journal of Computational Chemistry, (34): 2261-2269 2013.
- Stange, P.; Fumino, K.; Ludwig, R.  
*Ion Speciation of Protic Ionic Liquids in Water: Transition from Contact to Solvent-Separated Ion Pairs*  
Angewandte Chemie-International Edition, (52): 2990-2994 2013.
- Steglenko, D. V.; Navrotskii, M. B.; Orlinson, B. S.; Novakov, I. A.; Gerasimov, E. N.  
*DFT study of the effect of carbitol on the mechanism of aminolysis of 6-methyl-2-(methylsulfanyl)pyrimidin-4(3H)-one*

- Russian Journal of Organic Chemistry, (49): 1042-1046 2013.
- Steudel, R.; Steudel, Y.  
*Polysulfide Chemistry in Sodium Sulfur Batteries and Related Systems A Computational Study by G3X(MP2) and PCM Calculations*  
Chemistry-a European Journal, (19): 3162-3176 2013.
- Stosser, R.; Herrmann, W.  
*Isotope Effects in ESR Spectroscopy*  
Molecules, (18): 6679-6722 2013.
- Su, J.; Dau, P. D.; Qiu, Y. H.; Liu, H. T.; Xu, C. F.; Huang, D. L.; Wang, L. S.; Li, J.  
*Probing the Electronic Structure and Chemical Bonding in Tricoordinate Uranyl Complexes  $UO_2X_3^-$  ( $X = F, Cl, Br, I$ ): Competition between Coulomb Repulsion and U-X Bonding*  
Inorganic Chemistry, (52): 6617-6626 2013.
- Su, J.; Dau, P. D.; Xu, C. F.; Huang, D. L.; Liu, H. T.; Wei, F.; Wang, L. S.; Li, J.  
*A Joint Photoelectron Spectroscopy and Theoretical Study on the Electronic Structure of  $UCl_5^-$  and  $UCl_5$*   
Chemistry-an Asian Journal, (8): 2489-2496 2013.
- Su, M. D.; Chuang, C. C.  
*Theory predicts triplet ground-state carbene containing the N-heterocyclic carbenic unit*  
Theoretical Chemistry Accounts, (132) 2013.
- Su, Z.; Kim, C. K.  
*DFT investigation of C-H bond activation of malononitrile in the presence of amines*  
New Journal of Chemistry, (37): 3920-3927 2013.
- Su, Z.; Lee, H. W.; Kim, C. K.  
*Asymmetric 1,4-Michael Addition Reactions Catalyzed by a Cinchona Alkaloid Derived Primary Amine: A Theoretical Investigation of the Reaction Mechanism and Enantioselectivity*  
European Journal of Organic Chemistry: 1706-1715 2013.
- Su, Z. S.; Li, W. Y.; Wang, J.; Hu, C. W.; Feng, X. M.  
*A Theoretical Investigation on the Strecker Reaction Catalyzed by a Ti-IV-Complex Catalyst Generated from a Cinchona Alkaloid, Achiral Substituted 2,2'-Biphenol, and Tetraisopropyl Titanate*  
Chemistry-a European Journal, (19): 1637-1646 2013.
- Suardiaz, R.; Masgrau, L.; Lluch, J. M.; Gonzalez-Lafont, A.  
*An Insight into the Regiospecificity of Linoleic Acid Peroxidation Catalyzed by Mammalian 15-Lipoxygenases*  
Journal of Physical Chemistry B, (117): 3747-3754 2013.
- Suardiaz, R.; Masgrau, L.; Lluch, J. M.; Gonzalez-Lafont, A.  
*On the Regio- and Stereospecificity of Arachidonic Acid Peroxidation Catalyzed by Mammalian 15-Lipoxygenases: A Combined Molecular Dynamics and QM/MM Study*  
Chemphyschem, (14): 3777-3787 2013.
- Subashchandrabose, S.; Meganathan, C.; Erdogdu, Y.; Saleem, H.; Jajkumar, C.; Latha, P.  
*Vibrational and conformational analysis on-N-1-N-2-bis((pyridine-4-yl)methylene) benzene-1,2-diamine*  
Journal of Molecular Structure, (1042): 37-44 2013.
- Sudha, S.; Sundaraganesan, N.; Vanchinathan, K.; Muthu, K.; Meenakshisundaram, S. P.

- Spectroscopic (FTIR, FT-Raman, NMR and UV) and molecular structure investigations of 1,5-diphenylpenta-2,4-dien-1-one: a combined experimental and theoretical approach*  
Molecular Simulation, (39): 330-349 2013.
- Sultana, N.; Fabian, W. M. F.  
*A computational study of base-catalyzed reactions of cyclic 1,2-diones: cyclobutane-1,2-dione*  
Beilstein Journal of Organic Chemistry, (9): 594-601 2013.
- Sun, B. L.; McKee, M. L.  
*Computational Study of the Initial Stage of Diborane Pyrolysis*  
Inorganic Chemistry, (52): 5962-5969 2013.
- Sun, C. L.; Jiang, X. N.; Wang, C. S.  
*Cooperative enhancement of water binding to antiparallel -sheet models: Analysis by ab initio calculations*  
International Journal of Quantum Chemistry, (113): 1453-1460 2013.
- Sun, C. L.; Li, J.; Geng, H. W.; Li, H.; Ai, Y.; Wang, Q.; Pan, S. L.; Zhang, H. L.  
*Understanding the Unconventional Effects of Halogenation on the Luminescent Properties of Oligo(Phenylene Vinylene) Molecules*  
Chemistry-an Asian Journal, (8): 3091-3100 2013.
- Sun, H.; Chu, H. Y.; Fu, T.; Shen, H. J.; Li, G. H.  
*Theoretical Elucidation of the Origin for Assembly of the DAP12 Dimer with Only One NKG2C in the Lipid Membrane*  
Journal of Physical Chemistry B, (117): 4789-4797 2013.
- Sun, W. M.; Li, Y.; Wu, D.; Li, Z. R.  
*Designing Aromatic Superatoms*  
Journal of Physical Chemistry C, (117): 24618-24624 2013.
- Sun, W. M.; Wu, D.; Li, Y.; Li, Z. R.  
*Substituent Effects on the Structural Features and Nonlinear Optical Properties of the Organic Alkalide Li+(calix 4 pyrrole)Li*  
Chemphyschem, (14): 408-416 2013.
- Sun, X. T.; Che, X.; Jun, G.; Feng, D. C.; Liu, C. B.  
*Theoretical investigation of the mechanism of forming a silicic bis-heterocyclic compound between dichlorosilylenesilylene Cl<sub>2</sub>Si=Si: and ethylene*  
Progress in Reaction Kinetics and Mechanism, (38): 183-190 2013.
- Sun, Y. X.; Liu, Z. W.; Song, R. J.; Yu, C.; Hao, Q. L.; Xu, L. X.  
*Synthesis, structure, vibrational spectral, nonlinear optical and electron-behavioral studies of N-(5-chloro-2-hydroxyphenyl)-(3-hydroxyphenyl)-methalimine*  
Optical Materials, (35): 2519-2526 2013.
- Sun, Y. X.; Liu, Z. W.; Yu, C.; Huang, C. L.; Hao, Q. L.; Xu, L. X.  
*Synthesis, structural, vibrational spectral, nonlinear optical, electron transfer studies of N-(5-chloro-2-hydroxyphenyl)-(3-bromo-6-oxocyclohexa-2,4-dienylidene)met hylamine*  
Organic Electronics, (14): 1538-1550 2013.
- Sun, Z.; Schaefer, H. F.; Xie, Y. M.; Liu, Y. D.; Zhong, R. G.  
*Does the metal-metal sextuple bond exist in the bimetallic sandwich compounds Cr-2(C<sub>6</sub>H<sub>6</sub>)(2), Mo-2(C<sub>6</sub>H<sub>6</sub>)(2), and W-2(C<sub>6</sub>H<sub>6</sub>)(2)?*



- Molecular Physics, (111): 2523-2535 2013.
- Sung, C. Y.; Al Hashimi, S.; McCormick, A.; Cococcioni, M.; Tsapatsis, M.  
*A DFT study on multivalent cation-exchanged Y zeolites as potential selective adsorbent for H<sub>2</sub>S*  
Microporous and Mesoporous Materials, (172): 7-12 2013.
- Suntsova, M. A.; Marochkin, I.; Dorofeeva, O. V.  
*Structure and energetic properties of 1,5-dinitrobiuret*  
Structural Chemistry, (24): 745-750 2013.
- Suponitsky, K. Y.; Masunov, A. E.  
*Supramolecular step in design of nonlinear optical materials: Effect of pi ... pi stacking aggregation on hyperpolarizability*  
Journal of Chemical Physics, (139) 2013.
- Suresh, D. M.; Amalanathan, M.; Sebastian, S.; Sajan, D.; Joe, I. H.; Jothy, V. B.; Nemeč, I.  
*Vibrational spectral investigation and natural bond orbital analysis of pharmaceutical compound 7-Amino-2,4-dimethylquinolinium formate - DFT approach*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (115): 595-602 2013.
- Suresh, D. M.; Sajan, D.; Diao, Y. P.; Nemeč, I.; Joe, I. H.; Jothy, V. B.  
*Structural conformations and density functional study on the intramolecular charge transfer based on vibrational spectra of 2,4-dihydroxy-N'-(4-methoxybenzylidene)benzohydrazide*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (110): 157-168 2013.
- Sutradhar, D.; Zeegers-Huyskens, T.; Chandra, A. K.  
*Strong Hyperconjugative Interactions in Isolated and Water Complexes of Desflurane: A Theoretical Investigation*  
Journal of Physical Chemistry A, (117): 8545-8554 2013.
- Sutradhar, D.; Zeegers-Huyskens, T.; Chandra, A. K.  
*A theoretical investigation on the conformation and the interaction of CHF<sub>2</sub>OCHF<sub>2</sub> (desflurane II) with one water molecule*  
Journal of Molecular Modeling, (19): 5045-5052 2013.
- Szatkowski, L.; Dybala-Defratyka, A.  
*A computational study on enzymatically driven oxidative coupling of chlorophenols: An indirect dehalogenation reaction*  
Chemosphere, (91): 258-264 2013.
- Szatylowicz, H.; Krygowski, T. M.; Guerra, C. F.; Bickelhaupt, F. M.  
*Complexes of 4-substituted phenolates with HF and HCN: Energy decomposition and electronic structure analyses of hydrogen bonding*  
Journal of Computational Chemistry, (34): 696-705 2013.
- Szczepanik, D.; Mrozek, J.  
*Minimal set of molecule-adapted atomic orbitals from maximum overlap criterion*  
Journal of Mathematical Chemistry, (51): 2687-2698 2013.
- Szczepanik, D.; Mrozek, J.  
*On quadratic bond-order decomposition within molecular orbital space*  
Journal of Mathematical Chemistry, (51): 1619-1633 2013.

- Szczepanik, D.; Mrozek, J.  
*On several alternatives for Lowdin orthogonalization*  
Computational and Theoretical Chemistry, (1008): 15-19 2013.
- Szczepanik, D.; Mrozek, J.  
*Stationarity of electron distribution in ground-state molecular systems*  
Journal of Mathematical Chemistry, (51): 1388-1396 2013.
- Szlachcic, P.; Seidler, T.; Stadnicka, K.  
*Structural and theoretical study on the 1:2 addition complex of 1,2,4,5-bis{8',11'-dithia 4.3.3 propella(3',4')}benzene with I-2*  
Journal of Molecular Structure, (1033): 162-170 2013.
- Szymczak, J. J.; Hofmann, F. D.; Meuwly, M.  
*Structure and dynamics of solvent shells around photoexcited metal complexes*  
Physical Chemistry Chemical Physics, (15): 6268-6277 2013.
- Tachikawa, H.; Iyama, T.; Kawabata, H.  
*Interaction of Hydroxyl OH Radical with Graphene Surface: A Density Functional Theory Study*  
Japanese Journal of Applied Physics, (52) 2013.
- Tai, C. K.; Hsieh, W. Y.; Yeh, P. L.; Chiu, H. L.; Wang, B. C.  
*Photo-physical Properties of N-methyl-3,4-fulleropyrrolidine and Its Derivatives: A DFT and TD-DFT Investigation*  
Journal of the Chinese Chemical Society, (60): 251-260 2013.
- Tainter, C. J.; Ni, Y.; Shi, L.; Skinner, J. L.  
*Hydrogen Bonding and OH-Stretch Spectroscopy in Water: Hexamer (Cage), Liquid Surface, Liquid, and Ice*  
Journal of Physical Chemistry Letters, (4): 12-17 2013.
- Takagi, A.; Ikawa, T.; Kurita, Y.; Saito, K.; Azechi, K.; Egi, M.; Itoh, Y.; Tokiwa, H.; Kita, Y.; Akai, S.  
*Generation of 3-borylbenzynes, their regioselective Diels-Alder reactions, and theoretical analysis*  
Tetrahedron, (69): 4338-4352 2013.
- Takjoo, R.; Centore, R.  
*Synthesis, X-ray structure, spectroscopic properties and DFT studies of some dithiocarbazate complexes of nickel(II)*  
Journal of Molecular Structure, (1031): 180-185 2013.
- Takjoo, R.; Mague, J. T.; Akbari, A.; Ahmadi, M.  
*Synthesis, spectral, DFT and X-ray study of a cis-MoO<sub>2</sub> complex with a new isothiosemicarbazone ligand*  
Journal of Coordination Chemistry, (66): 1854-1865 2013.
- Talipov, M. R.; Khomyakov, D. G.; Xian, M.; Timerghazin, Q. K.  
*Computational design of S-nitrosothiol "Click" reactions*  
Journal of Computational Chemistry, (34): 1527-1530 2013.
- Talipov, M. R.; Timerghazin, Q. K.  
*Protein Control of S-Nitrosothiol Reactivity: Interplay of Antagonistic Resonance Structures*  
Journal of Physical Chemistry B, (117): 1827-1837 2013.
- Talipov, M. R.; Timerghazin, Q. K.; Rathore, R.

- Controlling the Structure of Reactive Intermediates via Incipient Covalent Bonding with the Counterions: Coexistence of Two Distinct Forms of the C<sub>6</sub>F<sub>6</sub> Cation Radical in a Single Crystal*  
Journal of Physical Chemistry C, (117): 23568-23574 2013.
- Tanak, H.; Marchewka, M. K.; Drozd, M.  
*Molecular structure and vibrational spectra of Bis(melaminium) terephthalate dihydrate: A DFT computational study*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (105): 156-164 2013.
- Tanaka, N.; Yamagishi, S.; Nishikiori, H.  
*Computational study of the reaction between chloroacetone and OH radical*  
Computational and Theoretical Chemistry, (1020): 108-112 2013.
- Tanase, T.; Hatada, S.; Mochizuki, A.; Nakamae, K.; Kure, B.; Nakajima, T.  
*Flexible, linear, tetranuclear palladium complexes supported by tetraphosphine ligands with electron-withdrawing groups*  
Dalton Transactions, (42): 15941-15952 2013.
- Tang, H. R.; Wu, C.  
*Reactivity of Azole Anions with CO<sub>2</sub> from the DFT Perspective*  
Chemsuschem, (6): 1050-1056 2013.
- Tantawy, W.; Hashem, A.; Yousif, N.; Flefel, E.  
*The water-boryl radical as a proton-coupled electron transfer reagent for carbon dioxide, formic acid, and formaldehyde - Theoretical approach*  
Canadian Journal of Chemistry-Revue Canadienne De Chimie, (91): 155-168 2013.
- Tao, S.; Yu, L. J.; Pang, R.; Huang, Y. F.; Wu, D. Y.; Tian, Z. Q.  
*Binding Interaction and Raman Spectra of rho-pi Conjugated Molecules Containing CH<sub>2</sub>/NH<sub>2</sub> Groups Adsorbed on Silver Surfaces: A DFT Study of Wagging Modes*  
Journal of Physical Chemistry C, (117): 18891-18903 2013.
- Tao, S.; Yu, L. J.; Wu, D. Y.; Tian, Z. Q.  
*Raman Spectra of Amino Wagging Vibrational Modes in p-pi-Conjugated Molecules*  
Acta Physico-Chimica Sinica, (29): 1609-1617 2013.
- Tarade, T.; Vrcek, V.  
*Reactivity of amines with hypochlorous acid: Computational study of steric, electronic, and medium effects*  
International Journal of Quantum Chemistry, (113): 881-890 2013.
- Taxak, N.; Kalra, S.; Bharatam, P. V.  
*Mechanism-Based Inactivation of Cytochromes by Furan Epoxide: Unraveling the Molecular Mechanism*  
Inorganic Chemistry, (52): 13496-13508 2013.
- Taxak, N.; Patel, B.; Bharatam, P. V.  
*Carbene Generation by Cytochromes and Electronic Structure of Heme-Iron-Porphyrin-Carbene Complex: A Quantum Chemical Study*  
Inorganic Chemistry, (52): 5097-5109 2013.
- Tayyari, S. F.; Holakoei, S.; Mandizadeh, S. J.  
*Conformational analysis and vibrational assignment of bis-gem-diol of hexafluoroacetylacetone*  
Journal of Molecular Structure, (1041): 190-199 2013.

- Tehrani, Z. A.; Fattahi, A.  
*Comparison of gas phase intrinsic properties of cytosine and thymine nucleobases with their O-alkyl adducts: different hydrogen bonding preferences for thymine versus O-alkyl thymine*  
Journal of Molecular Modeling, (19): 2993-3005 2013.
- Tehrani, Z. A.; Fattahi, A.  
*Conformational aspects of glutathione tripeptide: electron density topological & natural bond orbital analyses*  
Structural Chemistry, (24): 147-158 2013.
- Tehrani, Z. A.; Jamshidi, Z.; Farhangian, H.  
*Do coinage metal anions interact with substituted benzene derivatives?*  
Journal of Molecular Modeling, (19): 4763-4772 2013.
- Tehrani, Z. A.; Shakourian-Fard, M.; Fattahi, A.  
*Computational investigation of thermochemical properties of non-natural C-nucleobases: different hydrogen-bonding preferences for non-natural Watson-Crick base pairs*  
Structural Chemistry, (24): 1015-1025 2013.
- Tentscher, P. R.; Arey, J. S.  
*On the Nature of Interactions of Radicals with Polar Molecules*  
Journal of Physical Chemistry A, (117): 12560-12568 2013.
- Tentscher, P. R.; Eustis, S. N.; McNeill, K.; Arey, J. S.  
*Aqueous Oxidation of Sulfonamide Antibiotics: Aromatic Nucleophilic Substitution of an Aniline Radical Cation*  
Chemistry-a European Journal, (19): 11216-11223 2013.
- Teodoro, T. Q.; Haiduke, R. L. A.  
*Atomic charge and atomic dipole fluxes during stretching displacements in small molecules*  
Computational and Theoretical Chemistry, (1005): 58-67 2013.
- Tian, W. K.; Miao, Q.; Li, Q. Z.; Li, W. Z.; Cheng, J. B.  
*Superalkali Li3M (M = Cl, Br, I) as a Lewis base in halogen bonding: A heavier halogen is a stronger Lewis base than a lighter halogen*  
Computational and Theoretical Chemistry, (1012): 41-46 2013.
- Timerghazin, Q. K.; Talipov, M. R.  
*Unprecedented External Electric Field Effects on S-Nitrosothiols: Possible Mechanism of Biological Regulation?*  
Journal of Physical Chemistry Letters, (4): 1034-1038 2013.
- Timoshenko, V. M.; Kaminska, E. I.; Rozhenko, A. B.; Vlasenko, Y. G.; Chernega, A. N.; Shermolovich, Y. G.  
*Molecular and electronic structure of triethylammonium salt of N- (1-acetyl-2-oxopropyl)(phenyl)-(4)-sulfanylidene ethanesulfonamide*  
Journal of Sulfur Chemistry, (34): 421-431 2013.
- Tiwari, R. K.; Kumar, A.; Rawat, P.; Singh, R. N.  
*Molecular structure, hydrogen-bonding, chemical reactivity and first hyperpolarizability analysis of a new synthesized 1,9-bis(2-cyano-2-ethoxycarbonylviny1)-5-(2-nitrophenyl)-dipyrromethane: Experimental and theoretical (DFT and QTAIM) approach*  
Journal of Molecular Structure, (1052): 165-176 2013.

- Tiwari, R. K.; Kumar, A.; Rawat, P.; Singh, R. N.  
*Synthesis, molecular structure, hydrogen-bonding and chemical reactivity analysis of 1,9-bis(2-cyano-2-ethoxycarbonylvinyl)-5-(2-chlorophenyl)-dipyrromethane : A combined experimental and theoretical approach*  
Journal of Molecular Structure, (1047): 169-178 2013.
- Tofan, D.; Temprado, M.; Majumdar, S.; Hoff, C. D.; Cummins, C. C.  
*Functionalization Reactions Characteristic of a Robust Bicyclic Diphosphane Framework*  
Inorganic Chemistry, (52): 8851-8864 2013.
- Tokatli, A.; Akyurekli, S.  
*Aromatic character of fluorinated pyridines*  
Structural Chemistry, (24): 445-454 2013.
- Tong, J.; Li, Y.; Wu, D.; Wu, Z. J.  
*Theoretical study of substitution effect in superalkali OM3 (M = Li, Na, K)*  
Chemical Physics Letters, (575): 27-31 2013.
- Tong, J.; Wu, D.; Li, Y.; Wang, Y.; Wu, Z. J.  
*Superalkali character of alkali-monocyclic (pseudo)oxocarbon clusters*  
Dalton Transactions, (42): 9982-9989 2013.
- Tong, J.; Wu, Z. J.; Li, Y.; Wu, D.  
*Prediction and characterization of novel polynuclear superalkali cations*  
Dalton Transactions, (42): 577-584 2013.
- Tong, M. Q.; Yin, Z. F.; Wang, Y.; Chen, G. J.  
*Dehydrogenation mechanisms of ammonia borane catalyzed by Pd atoms adsorbed on an MgO(100) surface*  
International Journal of Hydrogen Energy, (38): 15285-15294 2013.
- Torabifard, H.; Fattahi, A.  
*DFT study on Thiotepa and Tepa interactions with their DNA receptor*  
Structural Chemistry, (24): 1-11 2013.
- Tousek, J.; Straka, M.; Sklenar, V.; Marek, R.  
*Origin of the Conformational Modulation of the C-13 NMR Chemical Shift of Methoxy Groups in Aromatic Natural Compounds*  
Journal of Physical Chemistry A, (117): 661-669 2013.
- Trifunovic, S. R.; Miletic, V. D.; Jevtic, V. V.; Meetsma, A.; Matovic, Z. D.  
*Nickel(II) in chelate N2O2 environment. DFT approach and in-depth molecular orbital and configurational analysis*  
Dalton Transactions, (42): 13357-13368 2013.
- Troche-Pesqueira, E.; Perez-Juste, I.; Navarro-Vazquez, A.; Cid, M. M.  
*A beta-cyclodextrin-resveratrol inclusion complex and the role of geometrical and electronic effects on its electronic induced circular dichroism*  
Rsc Advances, (3): 10242-10250 2013.
- Tsipis, A.; Gkarpounis, D.  
*Probing the electronic structure, magnetotropy, and absorption spectra of benzene trapped by lanthanide monoxides, C6H6 center dot center dot center dot LnO, using DFT methods*

International Journal of Quantum Chemistry, (113): 694-708 2013.

Tsipis, A. C.; Gkekas, G. N.

*The molecular, electronic, bonding, and photophysical features of the (c-Pt-3)Tl(c-Pt-3) (+) inorganic metallocenes*

Dalton Transactions, (42): 8307-8316 2013.

Tsipis, A. C.; Gkekas, G. N.

*Shedding light on the bonding, photophysical and magnetotropic properties of triangular Pt-3 complexes and their "open-face" TlPt3 half-sandwiches*

Dalton Transactions, (42): 2201-2212 2013.

Tsipis, A. C.; Stalikas, A. V.

*Face-to-Face Stacks of Trinuclear Gold(I) Trihalides with Benzene, Hexafluorobenzene, and Borazine: Impact of Aromaticity on Stacking Interactions*

Inorganic Chemistry, (52): 1047-1060 2013.

Tsvion, E.; Rasanen, M.; Gerber, R. B.

*Destabilization of noble-gas hydrides by a water environment: calculations for HXeOH@(H<sub>2</sub>O)(n), HXeOXeH@(H<sub>2</sub>O)(n), HXeBr@(H<sub>2</sub>O)(n), HXeCCH@(H<sub>2</sub>O)(n)*

Physical Chemistry Chemical Physics, (15): 12610-12616 2013.

Tsuge, M.; Berski, S.; Rasanen, M.; Latajka, Z.; Khriachtchev, L.

*Experimental and computational study of the HXeI center dot center dot center dot HY complexes (Y = Br and I)*

Journal of Chemical Physics, (138) 2013.

Tsuge, M.; Lignell, A.; Rasanen, M.; Khriachtchev, L.

*Environmental effects on noble-gas hydrides: HXeBr, HXeCCH, and HXeH in noble-gas and molecular matrices*

Journal of Chemical Physics, (139) 2013.

Tsuji, Y.; Koga, J.; Yoshizawa, K.

*Asymmetric Diarylethene as a Dual-Functional Device Combining Switch and Diode*

Bulletin of the Chemical Society of Japan, (86): 947-954 2013.

Turecek, F.; Moss, C. L.; Pikalov, I.; Pepin, R.; Gulyuz, K.; Polfer, N. C.; Bush, M. F.; Brown, J.; Williams, J.; Richardson, K.

*Gas-phase structures of phosphopeptide ions: A difficult case*

International Journal of Mass Spectrometry, (354): 249-256 2013.

Tyaglivy, A. S.; Steglenko, D. V.; Gulevskaya, A. V.

*Reaction of 3-Alkynylquinoxaline-2-carbonitriles with Sodium Azide: an Experimental and Theoretical Study*

Chemistry of Heterocyclic Compounds, (49): 1255-1263 2013.

Ucar, I.; Tamer, O.; Sariboga, B.; Buyukgungor, O.

*Three novel dipicolinate complexes with the pyridine-2,6-dimethanol - A combined structural, spectroscopic, antimicrobial and computational study*

Solid State Sciences, (15): 7-16 2013.

Umadevi, V.; Senthilkumar, L.; Kolandaivel, P.

*Theoretical investigations on the hydrogen bonding of nitrile isomers with H<sub>2</sub>O, HF, NH<sub>3</sub> and H<sub>2</sub>S*

Molecular Simulation, (39): 908-921 2013.

- Uzunova, E. L.; Mikosch, H.  
*Cation site preference in zeolite clinoptilolite: A density functional study*  
Microporous and Mesoporous Materials, (177): 113-119 2013.
- Uzunova, E. L.; Mikosch, H.; St Nikolov, G.  
*Density functional study of copper-exchanged zeolites and related microporous materials: Adsorption of nitrosyls*  
International Journal of Quantum Chemistry, (113): 723-728 2013.
- Vafaezadeh, M.; Dizicheh, Z. B.; Hashemi, M. M.  
*Mesoporous silica-functionalized dual Bronsted acidic ionic liquid as an efficient catalyst for thioacetalization of carbonyl compounds in water*  
Catalysis Communications, (40): 96-100 2013.
- Vaganek, A.; Rimarcik, J.; Ilcin, M.; Skorna, P.; Lukes, V.; Klein, E.  
*Homolytic N-H bond cleavage in anilines: Energetics and substituent effect*  
Computational and Theoretical Chemistry, (1014): 60-67 2013.
- Vahdani, S.; Sarem, M.; Hadizadeh, F.  
*Quantum Chemistry Based Quantitative Structure-Activity Relationship Prediction Setting for Toxicity of 4-Imidazolyl-1,4-Dihydropyridines as Calcium Channel Blockers*  
Asian Journal of Chemistry, (25): 2663-2667 2013.
- Van Damme, N.; Lough, A. J.; Gorelsky, S. I.; Lemaire, M. T.  
*Molecular and Electronic Structures of Complexes Containing 1-(2-pyridylazo)-2-phenanthrol (PAPL): Revisiting a Redox-Active Ligand*  
Inorganic Chemistry, (52): 13021-13028 2013.
- van der Westhuizen, B.; Swarts, P. J.; van Jaarsveld, L. M.; Liles, D. C.; Siegert, U.; Swarts, J. C.; Fernandez, I.; Bezuidenhout, D. I.  
*Substituent Effects on the Electrochemical, Spectroscopic, and Structural Properties of Fischer Mono- and Biscarbene Complexes of Chromium(0)*  
Inorganic Chemistry, (52): 6674-6684 2013.
- Varbanov, H. P.; Jakupec, M. A.; Roller, A.; Jensen, F.; Galanski, M.; Keppler, B. K.  
*Theoretical Investigations and Density Functional Theory Based Quantitative Structure-Activity Relationships Model for Novel Cytotoxic Platinum(IV) Complexes*  
Journal of Medicinal Chemistry, (56): 330-344 2013.
- Varekova, R. S.; Geidl, S.; Ionescu, C. M.; Skrehota, O.; Bouchal, T.; Sehnal, D.; Abagyan, R.; Koca, J.  
*Predicting pK(a) values from EEM atomic charges*  
Journal of Cheminformatics, (5) 2013.
- Varga, Z.; Hargittai, M.  
*Group 14 structural variations: perhalo derivatives of the "dimetallenes": dicarbenes, disilenes, digermenes, distannenes, and diplumbenes*  
Structural Chemistry, (24): 837-850 2013.
- Varshavskii, Y. S.; Cherkasova, T. G.; Gal'ding, M. R.; Gindin, V. A.; Podkorytov, I. S.; Sizova, O. V.; Smirnov, S. N.; Nikol'skii, A. B.  
*Direct C-13-P-31 coupling constant of coordinated triphenylphosphine as a characteristic of electron-withdrawing power of the metal center*

- Russian Journal of General Chemistry, (83): 567-569 2013.
- Vaz, P. D.; Nolasco, M. M.; Ribeiro-Claro, P. J. A.  
*Intermolecular C-H center dot center dot center dot O interactions in cyclopentanone: An inelastic neutron scattering study*  
Chemical Physics, (427): 117-123 2013.
- Vedha, S. A.; Solomon, R. V.; Venuvanalingam, P.  
*On the Nature of Hypercoordination in Dihalogenated Perhalocyclohexasilanes*  
Journal of Physical Chemistry A, (117): 3529-3538 2013.
- Vektariene, A.  
*Insights into the Mechanism of the Benzoannelated Thieno 3,2-b furan Halogenation. Importance of HOMO-HOMO Interaction*  
Journal of Physical Chemistry A, (117): 8449-8458 2013.
- Vergote, T.; Nahra, F.; Peeters, D.; Riant, O.; Leyssens, T.  
*NHC-copper(I) bifluoride complexes: "Auto-activating" catalysts*  
Journal of Organometallic Chemistry, (730): 95-103 2013.
- Verma, P.; Xu, X. F.; Truhlar, D. G.  
*Adsorption on Fe-MOF-74 for C1-C3 Hydrocarbon Separation*  
Journal of Physical Chemistry C, (117): 12648-12660 2013.
- Viana, R. B.; Santos, E. D. A.; Valencia, L. J.; Cavalcante, R. M.; Costa, E. B.; Moreno-Fuquen, R.; da Silva, A. B. F.  
*4-Hydroxy-2,5-dimethylphenyl-benzophenone: Conformational stability, FT-IR and Raman investigation*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (102): 386-392 2013.
- Vieuxmaire, O. P. J.; Piau, R. E.; Alary, F.; Heully, J. L.; Sutra, P.; Igau, A.; Boggio-Pasqua, M.  
*Theoretical Investigation of Phosphinidene Oxide Polypyridine Ruthenium(II) Complexes: Toward the Design of a New Class of Photochromic Compounds*  
Journal of Physical Chemistry A, (117): 12821-12830 2013.
- Vikas; Kaur, G.  
*Global reaction route mapping of isomerization pathways of exotic C6H molecular species*  
Journal of Chemical Physics, (139) 2013.
- Vogt, M.; Rivada-Whealaghan, O.; Iron, M. A.; Leitus, G.; Diskin-Posner, Y.; Shimon, L. J. W.; Ben-David, Y.; Milstein, D.  
*Anionic Nickel(II) Complexes with Doubly Deprotonated PNP Pincer-Type Ligands and Their Reactivity toward CO<sub>2</sub>*  
Organometallics, (32): 300-308 2013.
- Vrana, J.; Jambor, R.; Ruzicka, A.; Lycka, A.; De Proft, F.; Dostal, L.  
*N -> As intramolecularly coordinated organoarsenic(III) chalcogenides: Isolation of terminal As-S and As-Se bonds*  
Journal of Organometallic Chemistry, (723): 10-14 2013.
- Vuorinen, S.; Lahcini, M.; Hatanpaa, T.; Sundberg, M.; Leskela, M.; Repo, T.  
*Bismuth(III) Alkoxide Catalysts for Ring-Opening Polymerization of Lactides and epsilon-Caprolactone*  
Macromolecular Chemistry and Physics, (214): 707-715 2013.
- Wagner, M.; Deaky, V.; Dietz, C.; Martincova, J.; Mahieu, B.; Jambor, R.; Herres-Pawlis, S.; Jurkschat, K.



*Insights into the Intramolecular Donor Stabilisation of Organostannylenes Palladium and Platinum Complexes: Syntheses, Structures and DFT Calculations*  
Chemistry-a European Journal, (19): 6695-6708 2013.

Wagner, M.; Henn, M.; Dietz, C.; Schurmann, M.; Prosenc, M. H.; Jurkschat, K.  
*Chromium Pentacarbonyl-Substituted Organotin(II) Cation Stabilized by p-Dimethylaminopyridine or Triphenylphosphane Oxide*  
Organometallics, (32): 2406-2415 2013.

Waidmann, C. R.; Pierpont, A. W.; Batista, E. R.; Gordon, J. C.; Martin, R. L.; Silks, L. A.; West, R. M.; Wu, R. L.  
*Functional group dependence of the acid catalyzed ring opening of biomass derived furan rings: an experimental and theoretical study*  
Catalysis Science & Technology, (3): 106-115 2013.

Wallevik, S. O.; Bjornsson, R.; Kvaran, A.; Jonsdottir, S.; Arnason, I.; Belyakov, A. V.; Kern, T.; Hassler, K.  
*Conformational Properties of 1-Halogenated-1-Silacyclohexanes, C<sub>5</sub>H<sub>10</sub>SiHX (X = Cl, Br, I): Gas Electron Diffraction, Low-Temperature NMR, Temperature-Dependent Raman Spectroscopy, and Quantum-Chemical Calculations*  
Organometallics, (32): 6996-7005 2013.

Wang, B.; Truhlar, D. G.  
*Tuned and Balanced Redistributed Charge Scheme for Combined Quantum Mechanical and Molecular Mechanical (QM/MM) Methods and Fragment Methods: Tuning Based on the CM5 Charge Model*  
Journal of Chemical Theory and Computation, (9): 1036-1042 2013.

Wang, B. J.; Cao, Z. X.  
*Sequential covalent bonding activation and general base catalysis: insight into N-heterocyclic carbene catalyzed formylation of N-H bonds using carbon dioxide and silane*  
Rsc Advances, (3): 14007-14015 2013.

Wang, C. S.; Liu, P.; Yu, N.  
*Site-Preference of Uracil and Thymine Hydrogen Bonding to Quercetin*  
Acta Physico-Chimica Sinica, (29): 1173-1182 2013.

Wang, C. W.; Chen, Z. H.; Wu, W.; Mo, Y. R.  
*How the Generalized Anomeric Effect Influences the Conformational Preference*  
Chemistry-a European Journal, (19): 1436-1444 2013.

Wang, C. Z.; Lan, J. H.; Zhao, Y. L.; Chai, Z. F.; Wei, Y. Z.; Shi, W. Q.  
*Density Functional Theory Studies of UO<sub>2</sub><sup>2+</sup> and NpO<sub>2</sub><sup>2+</sup> Complexes with Carbamoylmethylphosphine Oxide Ligands*  
Inorganic Chemistry, (52): 196-203 2013.

Wang, C. Z.; Shi, W. Q.; Lan, J. H.; Zhao, Y. L.; Wei, Y. Z.; Chai, Z. F.  
*Complexation Behavior of Eu(III) and Am(III) with CMPO and Ph<sub>2</sub>CMPO Ligands: Insights from Density Functional Theory*  
Inorganic Chemistry, (52): 10904-10911 2013.

Wang, F.; Liu, H.; Gong, X. D.  
*A theoretical study on the structure and hygroscopicity of ammonium dinitramide*  
Structural Chemistry, (24): 1537-1543 2013.

Wang, H.; Wang, H. Y.; Sun, Z. H.; King, R. B.

- A monotonic increase of formal metal-metal bond orders from one to five upon loss of carbonyl groups from binuclear benzene chromium carbonyls*  
Chemical Physics, (421): 49-56 2013.
- Wang, J.; Zhang, M. Y.; Zou, H. Y.; Yu, H. L.; Wang, W. Y.; Song, H. J.; Li, X. Q.; Qiu, Y. Q.  
*Theoretical Study on Redox-adjustable Second-order Nonlinear Optical Responses of 12-Vertex 1-R-CB11-Me-11 (-) Carborane Complexes*  
Chemical Journal of Chinese Universities-Chinese, (34): 2791-2797 2013.
- Wang, J. C.; Ding, Y. Q.; Wang, S. J.; Yang, P. F.  
*Diamine-catalyzed urethane reaction of 1,3-propanediol with phenyl isocyanate*  
Journal of Coatings Technology and Research, (10): 859-864 2013.
- Wang, J. M.; Li, Z. M.; Wang, Q. R.; Tao, F. G.  
*A DFT study on the mechanisms for the cycloaddition reactions between 1-aza-2-azoniaallene cations and acetylenes*  
Journal of Molecular Modeling, (19): 83-95 2013.
- Wang, J. Y.; Cai, D. L.; Zhang, M.; Wang, M.  
*The addition mechanism of TMSCN into N-acetylpyridinum to give 2-cyanoacetylpyridinum: The roles of TpW(NO)(PMe<sub>3</sub>) and DABCO*  
Journal of Organometallic Chemistry, (724): 117-128 2013.
- Wang, L.; Ni, L.; Yao, J.  
*Syntheses, structures, fluorescent properties and natural bond orbital analyses of metal-organic complexes based on 5,6-substituted 1,10-phenanthroline derivatives*  
Polyhedron, (59): 115-123 2013.
- Wang, L. F.; Kefalidis, C. E.; Sinbandhit, S.; Dorcet, V.; Carpentier, J. F.; Maron, L.; Sarazin, Y.  
*Heteroleptic Tin(II) Initiators for the Ring-Opening (Co)Polymerization of Lactide and Trimethylene Carbonate: Mechanistic Insights from Experiments and Computations*  
Chemistry-a European Journal, (19): 13463-13478 2013.
- Wang, M.; Zhao, J.; Bu, Y. X.  
*Theoretical exploration of structures and electronic properties of double-electron oxidized guanine-cytosine base pairs with intriguing radical-radical interactions*  
Physical Chemistry Chemical Physics, (15): 18453-18463 2013.
- Wang, P. C.; Zhu, Z. S.; Xu, J.; Zhao, X. J.; Lu, M.  
*Theoretical study of the thermodynamic and burning properties of oxygen-rich hydrazine derivatives-green and powerful oxidants for energetic materials*  
Journal of Molecular Modeling, (19): 2583-2591 2013.
- Wang, Q.; Jia, J. F.; Guo, C. H.; Wu, H. S.  
*Mechanistic investigation of Cu(I)-mediated three-component domino reaction of asymmetrical alkynes with carbon dioxide: Theoretical rationale for the regioselectivity*  
Journal of Organometallic Chemistry, (748): 84-88 2013.
- Wang, S. J.; Li, Y.; Wang, Y. F.; Wu, D.; Li, Z. R.  
*Structures and nonlinear optical properties of the endohedral metallofullerene-superhalogen compounds Li@C-60-BX<sub>4</sub> (X = F, Cl, Br)*  
Physical Chemistry Chemical Physics, (15): 12903-12910 2013.

- Wang, X. F.; Andrews, L.; Thanthiriwatte, K. S.; Dixon, D. A.  
*Infrared Spectra of H<sub>2</sub>ThS and H<sub>2</sub>US in Noble Gas Matrixes: Enhanced H-An-S Covalent Bonding*  
Inorganic Chemistry, (52): 10275-10285 2013.
- Wang, Y.; Shi, W. J.; Ren, F. D.; Cao, D. L.; Chen, F.  
*A B3LYP AND MP2(FULL) THEORETICAL INVESTIGATION INTO THE C-NO<sub>2</sub> BOND STRENGTH UPON THE FORMATION OF HF OR Na<sup>+</sup> COMPLEX INVOLVING THE NITRO GROUP OF NITRO-1,2,4-TRIAZOLE*  
Journal of Theoretical & Computational Chemistry, (12) 2013.
- Wang, Y. Q.; Han, Q. Z.; Wen, H.  
*Theoretical discussion on the mechanism of binding CO<sub>2</sub> by DBU and alcohol*  
Molecular Simulation, (39): 822-827 2013.
- Wang, Z. J.; Ye, H. D.; Li, Y. G.; Li, Y. Z.; Yan, H.  
*Unprecedented Boron-Functionalized Carborane Derivatives by Facile and Selective Cobalt-Induced B-H Activation*  
Journal of the American Chemical Society, (135): 11289-11298 2013.
- Wei, F. D.; Liu, W.; Lv, G.; Wang, H.; Wang, X. M.  
*Density Functional Theory Study on the Interactions Between Ni-n (n=1, ..., 6) and Methylamine or Acetic Acid*  
Journal of Nanoscience and Nanotechnology, (13): 4223-4227 2013.
- Wei, W.; Bai, F. Q.; Xia, B. H.; Chen, H. B.; Zhang, H. X.  
*Theoretical analysis on magnetic properties of conjugated organic molecules containing borepin*  
Chemical Research in Chinese Universities, (29): 962-968 2013.
- Wei, X. F.; Han, Z.; Zhang, D. J.  
*Theoretical study on the mechanism of the side reaction of 1-butyl-3-methylimidazolium cation with D-glucose*  
Carbohydrate Research, (374): 40-44 2013.
- Wei, X. F.; Zhang, D. J.  
*Theoretical study on the mechanism of the reaction of alkylmethylimidazolium cation with benzaldehyde involved in the base-catalyzed Baylis-Hillman reaction*  
Computational and Theoretical Chemistry, (1014): 24-28 2013.
- Weingartner, W.; Maas, G.  
*Molecular and Crystal Structure of Chlorido 2-(N,N,N',N'-tetramethylamidinio)ethynido silver*  
Zeitschrift Fur Naturforschung Section B-a Journal of Chemical Sciences, (68): 687-692 2013.
- Weinhold, F.; West, R.  
*Hyperconjugative Interactions in Permethylated Siloxanes and Ethers: The Nature of the SiO Bond*  
Journal of the American Chemical Society, (135): 5762-5767 2013.
- Wen, M. W.; Huang, F.; Lu, G.; Wang, Z. X.  
*Density Functional Theory Mechanistic Study of the Reduction of CO<sub>2</sub> to CH<sub>4</sub> Catalyzed by an Ammonium Hydridoborate Ion Pair: CO<sub>2</sub> Activation via Formation of a Formic Acid Entity*  
Inorganic Chemistry, (52): 12098-12107 2013.
- Werkema, E. L.; Castro, L.; Maron, L.; Eisenstein, O.; Andersen, R. A.  
*Cleaving bonds in CH<sub>3</sub>OSO<sub>2</sub>CF<sub>3</sub> with 1,2,4-(Me<sub>3</sub>C)(3)C<sub>5</sub>H<sub>2</sub> (2)CeH; an experimental and computational study*

- New Journal of Chemistry, (37): 132-142 2013.
- Werle, C.; Bailly, C.; Karmazin-Brelot, L.; Le Goff, X. F.; Ricard, L.; Djukic, J. P.  
*Hemichelation, a Way To Stabilize Electron-Unsaturated Complexes: The Case of T-Shaped Pd and Pt Metallacycles*  
Journal of the American Chemical Society, (135): 17839-17852 2013.
- West, A. C.; Schmidt, M. W.; Gordon, M. S.; Ruedenberg, K.  
*A comprehensive analysis of molecule-intrinsic quasi-atomic, bonding, and correlating orbitals. I. Hartree-Fock wave functions*  
Journal of Chemical Physics, (139) 2013.
- Wiberg, K. B.; Ellison, G. B.; McBride, J. M.; Petersson, G. A.  
*Substituent Effects on O-H Bond Dissociation Enthalpies: A Computational Study*  
Journal of Physical Chemistry A, (117): 213-218 2013.
- Wiegand, T.; Eckert, H.; Grimme, S.  
*Solid-State NMR as a Spectroscopic Tool for Characterizing Phosphane-Borane Frustrated Lewis Pairs*  
Frustrated Lewis Pairs I: Uncovering and Understanding, (332): 291-345 2013.
- Wierzbinski, E.; Yin, X.; Werling, K.; Waldeck, D. H.  
*The Effect of Oxygen Heteroatoms on the Single Molecule Conductance of Saturated Chains*  
Journal of Physical Chemistry B, (117): 4431-4441 2013.
- Wilson, C. R.; Fagenson, A. M.; Ruangpradit, W.; Muller, M. T.; Munro, O. Q.  
*Gold(III) Complexes of Pyridyl- and Isoquinolylamido Ligands: Structural, Spectroscopic, and Biological Studies of a New Class of Dual Topoisomerase I and II Inhibitors*  
Inorganic Chemistry, (52): 7889-7906 2013.
- Winkelhaus, D.; Vishnevskiy, Y. V.; Berger, R. J. F.; Stammer, H. G.; Neumann, B.; Mitzel, N. W.  
*B=N Bonds and BCN Rings - Reactivity and Charge Density Studies*  
Zeitschrift für Anorganische und Allgemeine Chemie, (639): 2086-2095 2013.
- Witt, A.; Hellweg, A.  
*On the formation of the formate anion: Insights from population analyses*  
Computational and Theoretical Chemistry, (1012): 8-13 2013.
- Witts, R. N.; Hopson, E. C.; Koballa, D. E.; Van Boening, T. A.; Hopkins, N. H.; Patterson, E. V.; Nagan, M. C.  
*Backbone-Base Interactions Critical to Quantum Stabilization of Transfer RNA Anticodon Structure*  
Journal of Physical Chemistry B, (117): 7489-7497 2013.
- Wojciechowski, P.  
*Theoretical anharmonic Raman and infrared spectra with vibrational assignments and NBO analysis for 2,3,4,5,6-pentafluoroaniline*  
Journal of Fluorine Chemistry, (154): 7-15 2013.
- Wong, M. W.; Xie, H. F.; Kwa, S. T.  
*Anion recognition by azophenol thiourea-based chromogenic sensors: a combined DFT and molecular dynamics investigation*  
Journal of Molecular Modeling, (19): 205-213 2013.
- Wright, A. M.; Howard, A. A.; Howard, C.; Tschumper, G. S.; Hammer, N. I.  
*Charge Transfer and Blue Shifting of Vibrational Frequencies in a Hydrogen Bond Acceptor*

- Journal of Physical Chemistry A, (117): 5435-5446 2013.
- Wright, J. H.; Kefaidis, C. E.; Tham, F. S.; Maron, L.; Lavallo, V.  
*Click-Like Reactions with the Inert HCB11Cl11- Anion Lead to Carborane-Fused Heterocycles with Unusual Aromatic Character*  
Inorganic Chemistry, (52): 6223-6229 2013.
- Wu, H. Q.; Zhong, R. L.; Kan, Y. H.; Sun, S. L.; Zhang, M.; Xu, H. L.; Su, Z. M.  
*After the electronic field: Structure, bonding, and the first hyperpolarizability of HARF*  
Journal of Computational Chemistry, (34): 952-957 2013.
- Wu, J. I. C.; Schleyer, P. V.  
*Hyperconjugation in hydrocarbons: Not just a "mild sort of conjugation"*  
Pure and Applied Chemistry, (85): 921-940 2013.
- Wu, J. X.; Wang, M.; Wang, L. S.; Wang, J. Y.; Jiang, L. B.  
*How the Bicyclo 4.1.0 Substrate Isomerizes into 4,5-Dihydrobenzo b furan: The Contribution from W(CO)(5) and NEt3*  
Journal of Organic Chemistry, (78): 10812-10820 2013.
- Wu, X. M.; Yang, G.; Zhou, L. J.; Han, X. W.  
*How significant the charge density of olefins to their epoxidation reactions over M4+-substituted zeolitic catalysts: A DFT investigation*  
Computational and Theoretical Chemistry, (1017): 109-116 2013.
- Xavier, R. J.; Dinesh, P.  
*Conformational stability, vibrational spectra, HOMO-LUMO and NBO analysis of 1,3,4-thiadiazolidine-2,5-dithione with experimental (FT-IR and FT-Raman) techniques and scaled quantum mechanical calculations*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (113): 171-181 2013.
- Xavier, R. J.; Raj, S. A.  
*Ab initio, density functional computations, FT-IR, FT-Raman and molecular geometry of 4-morpholine carbonitrile*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (101): 148-155 2013.
- Xi, H. W.; Bedoura, S.; Lim, K. H.  
*Hydrogen bond and internal rotations barrier: DFT study on heavier group-14 analogues of formamide*  
Journal of Physical Organic Chemistry, (26): 420-431 2013.
- Xia, Y.; Qu, S. L.; Xiao, Q.; Wang, Z. X.; Qu, P. Y.; Chen, L.; Liu, Z.; Tian, L. M.; Huang, Z. X.; Zhang, Y.; Wang, J. B.  
*Palladium-Catalyzed Carbene Migratory Insertion Using Conjugated Ene-Yne-Ketones as Carbene Precursors*  
Journal of the American Chemical Society, (135): 13502-13511 2013.
- Xiang, J. Y.; Ponder, J. W.  
*A valence bond model for aqueous Cu(II) and Zn(II) ions in the AMOEBA polarizable force field*  
Journal of Computational Chemistry, (34): 739-749 2013.
- Xiao, Y.; Chen, X. Y.; Qiu, Y. X.; Wang, S. G.  
*Spin-flip reactions of Zr + C2H6 researched by relativistic density functional theory*  
Journal of Molecular Modeling, (19): 4003-4012 2013.
- Xie, J.; Feng, W. L.; Lu, P. F.; Meng, Y.

- Theoretical study on halide anion recognitions by pyrrole- and benzene-strapped calix 4 pyrroles*  
Computational and Theoretical Chemistry, (1007): 1-8 2013.
- Xie, X. H.; Shen, W.; He, R. X.; Li, M.  
*A Density Functional Study of Furofuran Polymers as Potential Materials for Polymer Solar Cells*  
Bulletin of the Korean Chemical Society, (34): 2995-3004 2013.
- Xie, X. H.; Shen, W.; He, R. X.; Li, M.  
*Theoretical design study on photophysical property on oligomers based on spirobifluorene and carbazole-triphenylamine for PLED applications*  
Journal of Molecular Modeling, (19): 139-149 2013.
- Xu, F.; Matsumoto, K.; Hagiwara, R.  
*The first crystallographic example of a face-sharing fluoroaluminate anion Al<sub>2</sub>F<sub>9</sub>*  
Dalton Transactions, (42): 1965-1968 2013.
- Xu, H. Y.; Wang, W.; Zhu, J. Q.; Xu, X. L.; Zhang, D. Y.  
*Interaction between Metalloporphyrins and Diazine Tautomers*  
Bulletin of the Korean Chemical Society, (34): 3727-3732 2013.
- Xu, H. Y.; Wang, W.; Zou, J. W.  
*Theoretical Study of Pnictogen Bonding Interactions between PH<sub>2</sub>X and Five-membered Heterocycles*  
Acta Chimica Sinica, (71): 1175-1182 2013.
- Xu, Q. Q.; Yang, H. Q.; Gao, C.; Hu, C. W.  
*Theoretical study on the reaction mechanism of NO and CO catalyzed by Rh atom*  
Structural Chemistry, (24): 13-23 2013.
- Yamada, K.; Koga, N.  
*Variationally determined electronic states for the theoretical analysis of intramolecular interaction. II. Qualitative nature of the P?O bond in phosphine oxides*  
Journal of Computational Chemistry, (34): 149-161 2013.
- Yan, L. L.; Liu, Y. R.; Huang, T.; Jiang, S.; Wen, H.; Gai, Y. B.; Zhang, W. J.; Huang, W.  
*Structure, stability, and electronic property of carbon-doped gold clusters AunC- (n=1-10): A density functional theory study*  
Journal of Chemical Physics, (139) 2013.
- Yanez, M.; Mo, O.; Alkorta, I.; Elguero, J.  
*Can Conventional Bases and Unsaturated Hydrocarbons Be Converted into Gas-Phase Superacids That Are Stronger than Most of the Known Oxyacids? The Role of Beryllium Bonds*  
Chemistry-a European Journal, (19): 11637-11643 2013.
- Yanez, M.; Mo, O.; Alkorta, I.; Elguero, J.  
*Spontaneous ion-pair formation in the gas phase induced by Beryllium bonds*  
Chemical Physics Letters, (590): 22-26 2013.
- Yang, H.; Wong, M. W.  
*Oxyanion Hole Stabilization by C-H center dot center dot center dot O Interaction in a Transition State-A Three-Point Interaction Model for Cinchona Alkaloid-Catalyzed Asymmetric Methanolysis of meso-Cyclic Anhydrides*  
Journal of the American Chemical Society, (135): 5808-5818 2013.

- Yang, J.; Miao, J. K.; Li, X. J.; Xu, W. G.  
*Cycloaddition of ozone to allyl alcohol, acrylic acid and allyl aldehyde: A comparative DFT study*  
Chemical Physics, (415): 161-167 2013.
- Yang, N.; Dong, L.; Su, Z. S.; Hu, C. W.  
*Theoretical study on the mechanism of Pd(OAc)<sub>2</sub> catalyzed dehydrogenative cross-coupling of two heteroarenes*  
Rsc Advances, (3): 20772-20781 2013.
- Yang, Q. W.; Xing, H. B.; Su, B. G.; Bao, Z. B.; Wang, J.; Yang, Y. W.; Ren, Q. L.  
*The Essential Role of Hydrogen-Bonding Interaction in the Extractive Separation of Phenolic Compounds by Ionic Liquid*  
AIChE Journal, (59): 1657-1667 2013.
- Yang, X.; Li, Q. Z.; Cheng, J. B.; Li, W. Z.  
*A new interaction mechanism of LiNH<sub>2</sub> with MgH<sub>2</sub>: magnesium bond*  
Journal of Molecular Modeling, (19): 247-253 2013.
- Yang, Y.; Yu, L.  
*Theoretical investigations of ferrocene/ferrocenium solvation in imidazolium-based room-temperature ionic liquids*  
Physical Chemistry Chemical Physics, (15): 2669-2683 2013.
- Yang, Y. F.; Foo, C.; Xi, H. W.; Li, Y. X.; Lim, K. H.; So, C. W.  
*A Base-Stabilized 2-Silaallene*  
Organometallics, (32): 2267-2270 2013.
- Yang, Z.; Hao, L. K.; Yin, B.; She, M.; Obst, M.; Kappler, A.; Li, J. L.  
*Six-Membered Spirocyclic Triggered Probe for Visualizing Hg<sup>2+</sup> in Living Cells and Bacteria-EPS-Mineral Aggregates*  
Organic Letters, (15): 4334-4337 2013.
- Yang, Z.; Zhang, B. L.; Liu, X. G.; Yang, Y. Z.; Li, X. Y.; Xiong, S. J.; Xu, B. S.  
*The structural and optical properties of the CpTMC60 (TM = Sc-Fe) sandwich cluster*  
Journal of Physics B-Atomic Molecular and Optical Physics, (46) 2013.
- Yao, S. L.; Hrobarik, P.; Meier, F.; Rudolph, R.; Bill, E.; Irran, E.; Kaupp, M.; Driess, M.  
*A Heterobimetallic Approach To Stabilize the Elusive Disulfur Radical Trianion ("Subsulfide")  $S_3^{3-}$*   
Chemistry-a European Journal, (19): 1246-1253 2013.
- Ye, S. Y.; Peng, L.; Song, K. S.; Gu, F. L.  
*Halogen Doping Effect on Electronic Structure of Poly(methylphenyl)silane: a Theoretical Study*  
Acta Chimica Sinica, (71): 271-278 2013.
- Yi, P. G.; Hou, B.; Wang, Z. X.; Liu, Z. J.; Yu, X. Y.; Xu, B. Y.  
*Study on the Aromaticity of Heterobenzenes C<sub>5</sub>H<sub>5</sub>X (X=N, P, As, Sb, Bi) by Nucleus Independent Chemical Shifts (NICS) and Isomerization Stabilization Energies (ISE)*  
Acta Chimica Sinica, (71): 126-132 2013.
- Yildizab, C. B.; Azizoglu, A.  
*Computational investigations on the electronic and structural properties of germacyclopropylidenoids*  
Computational and Theoretical Chemistry, (1023): 24-28 2013.

- Yogeswari, B.; Kanakaraju, R.; Boopathi, S.; Kolandaivel, P.  
*Molecular dynamics and quantum chemical studies of solvent effects on cyclo glycylglycine and glycylalanine dipeptides*  
Molecular Simulation, (39): 670-687 2013.
- Yoon, J. H.; Lim, J. S.; Woo, K. C.; Kim, M. S.; Kim, S. K.  
*Chemical Substitution Effect on Energetic and Structural Differences between Ground and First Electronically Excited States of Thiophenoxyl Radicals*  
Bulletin of the Korean Chemical Society, (34): 415-420 2013.
- Young, N. A.  
*Main group coordination chemistry at low temperatures: A review of matrix isolated Group 12 to Group 18 complexes*  
Coordination Chemistry Reviews, (257): 956-1010 2013.
- Yu, S. P.; Zeng, Q.; Lou, Z. Y.; Yang, M. L.; Wu, D. Y.  
*First-principles study of O-2 activation on ligand-protected Au-32 clusters*  
Physical Chemistry Chemical Physics, (15): 9742-9751 2013.
- Yu, X. L.; Yu, R. Q.  
*Setschenow Constant Prediction Based on the IEF-PCM Calculations*  
Industrial & Engineering Chemistry Research, (52): 11182-11188 2013.
- Yu, Y.; Li, C.; Yin, B.; Li, J. L.; Huang, Y. H.; Wen, Z. Y.; Jiang, Z. Y.  
*Are trinuclear superhalogens promising candidates for building blocks of novel magnetic materials? A theoretical prospect from combined broken-symmetry density functional theory and ab initio study*  
Journal of Chemical Physics, (139) 2013.
- Yuan, L. W.; Hu, Q. Z.; Yang, Q. W.; Zhang, W. Q.  
*A detailed study on thiocarbonyl ene reactions*  
Computational and Theoretical Chemistry, (1019): 71-77 2013.
- Yuan, Y.; Cheng, L. J.  
*Ferrocene analogues of sandwich B-12 center dot Cr center dot B-12: A theoretical study*  
Journal of Chemical Physics, (138) 2013.
- Yurdakul, S.; Tanribuyurdu, S.  
*Theoretical and experimental study of solvent effects on the structure, vibrational spectra, and tautomerism of 3-amino-1,2,4-triazine*  
Journal of Molecular Structure, (1052): 57-66 2013.
- Yurkerwich, K.; Rong, Y.; Parkin, G.  
*Gallium hydride and monovalent indium compounds that feature tris(pyrazolyl)hydroborate ligands*  
Acta Crystallographica Section C-Crystal Structure Communications, (69): 963-967 2013.
- Zabaradsti, A.; Kakanejadifard, A.; Ghasemian, M.; Esmailifar, M.  
*Theoretical study of molecular interactions of sulfur ylide with HSX (X = F, Cl, and Br) molecules*  
Structural Chemistry, (24): 1607-1614 2013.
- Zabaradsti, A.; Kakanejadifard, A.; Ghasemian, M.; Jamshidi, Z.  
*Theoretical study of molecular interactions of sulfur ylide with HF, HCN, and HN3*  
Structural Chemistry, (24): 271-277 2013.



- Zabardasti, A.; Kakanejadifard, A.; Goudarziafshar, H.; Salehnassaj, M.; Zohrehband, Z.; Jaberansari, F.; Solimannejad, M.  
*Theoretical study of hydrogen and halogen bond interactions of methylphosphines with hypohalous acids*  
Computational and Theoretical Chemistry, (1014): 1-7 2013.
- Zabula, A. V.; Rogachev, A. Y.; Guzei, I. A.; West, R.  
*Silicon in a Negatively Charged Shell: Anions of Spirosilabifluorene*  
Organometallics, (32): 3760-3768 2013.
- Zaccaron, S.; Ganzerla, R.; Bortoluzzi, M.  
*Iron complexes with gallic acid: a computational study on coordination compounds of interest for the preservation of cultural heritage*  
Journal of Coordination Chemistry, (66): 1709-1719 2013.
- Zahedi-Tabrizi, M.; Badalkhani-Khamseh, F.  
*Effect of methyl groups substitution on the strength of intramolecular hydrogen bonding of naphthazarin: DFT and NBO studies*  
Journal of the Iranian Chemical Society, (10): 685-694 2013.
- Zakarianejad, M.; Ghasempour, H.; Habibi-Khorassani, S. M.; Maghsoodlou, M. T.; Makiabadi, B.; Nassiri, M.; Ghahghayi, Z.; Abedi, A.  
*Theoretical study, synthesis, kinetics and mechanistic investigation of a stable phosphorus ylide in the presence of methyl carbamate as a NH-acid*  
Arkivoc: 171-190 2013.
- Zamora, A.; Rodriguez, V.; Cutillas, N.; Yellol, G. S.; Espinosa, A.; Samper, K. G.; Capdevila, M.; Palacios, O.; Ruiz, J.  
*New steroidal 7-azaindole platinum (II) antitumor complexes*  
Journal of Inorganic Biochemistry, (128): 48-56 2013.
- Zanjanchi, F.; Hadipour, N. L.; Sabzyan, H.; Beheshtian, J.  
*Theoretical investigation of azo dyes adsorbed on cellulose fibers: 1. Electronic and bonding structures*  
Journal of the Iranian Chemical Society, (10): 985-999 2013.
- Zanti, G.; Peeters, D.  
*Electronic structure analysis of small gold clusters Au-m (m <= 16) by density functional theory*  
Theoretical Chemistry Accounts, (132) 2013.
- Zardoost, M. R.  
*Kinetics and mechanism of intramolecular aldol condensation of 2,5-hexadione, a DFT and MP2 study*  
Russian Journal of Physical Chemistry B, (7): 540-547 2013.
- Zardoost, M. R.; Siadati, S. A.  
*A DFT study on the effect of functional groups on the formation kinetics of 1,2,3-triazolo-1,4-benzoxazine via intramolecular 1,3-dipolar cycloaddition*  
Progress in Reaction Kinetics and Mechanism, (38): 191-196 2013.
- Zardoost, M. R.; Siadati, S. A.  
*A Theoretical Study of Substitution Effect on an Electrocyclization Reaction*  
Combinatorial Chemistry & High Throughput Screening, (16): 408-412 2013.
- Zardoost, M. R.; Siadati, S. A.; Oghani, B. G.  
*A DFT study on the 1,3-dipolar cycloaddition of benzonitrile oxide and N-ethylmaleimide*

- Progress in Reaction Kinetics and Mechanism, (38): 316-322 2013.
- Zborowski, K. K.; Mohammadpour, M.; Sadeghi, A.; Proniewicz, L. M.  
*Theoretical study on the molecular tautomerism of the 3-hydroxy-pyridin-4-one system*  
Molecular Physics, (111): 958-967 2013.
- Zeegers-Huyskens, T.; Lily, M.; Sutradhar, D.; Chandra, A. K.  
*Theoretical Study of the O center dot center dot center dot Cl Interaction in Fluorinated Dimethyl Ethers Complexed with a Cl Atom: Is It through a Two-Center-Three-Electron Bond?*  
Journal of Physical Chemistry A, (117): 8010-8016 2013.
- Zeinalinezhad, A.; Sahnoun, R.; Aziz, M.  
*Ab initio molecular orbitals studies and NBO analysis of conformational preference in 2-hydroxypiperidine*  
Computational and Theoretical Chemistry, (1024): 52-60 2013.
- Zen, A.; Luo, Y.; Sorella, S.; Guidoni, L.  
*Molecular Properties by Quantum Monte Carlo: An Investigation on the Role of the Wave Function Ansatz and the Basis Set in the Water Molecule*  
Journal of Chemical Theory and Computation, (9): 4332-4350 2013.
- Zendaoui, S. M.; Zouchoune, B.  
*Molecular properties and electronic structure of phenazine ligand in binuclear molybdenum and manganese metal complexes: A density functional theory study*  
Polyhedron, (51): 123-131 2013.
- Zeng, H. L.; Pei, X. L.; Chen, G. F.; Cao, L. J.; Chen, L.; Fang, X. Z.  
*Comparative studies on melt processable polyimides derived from 2,3,3',4'-oxydiphthalic anhydride and 2,3,3',4'-thioetherdiphthalic anhydride*  
High Performance Polymers, (25): 454-463 2013.
- Zeng, J.; Duan, L. L.; Zhang, J. Z. H.; Mei, Y.  
*A numerically stable restrained electrostatic potential charge fitting method*  
Journal of Computational Chemistry, (34): 847-853 2013.
- Zeng, Q.; Shi, J.; Jiang, G.; Yang, M. L.; Wang, F.; Chen, J.  
*Structures and optical absorptions of PbSe clusters from ab initio calculations*  
Journal of Chemical Physics, (139) 2013.
- Zeng, Y.; Feng, H.; Xie, Y. M.; King, R. B.; Schaefer, H. F.  
*Metallametalloenes: Sandwich Compounds of the First-Row Transition Metals (M, M = Fe, Co, Ni) Containing a Metallacyclopentadiene Ring*  
European Journal of Inorganic Chemistry: 2070-2077 2013.
- Zeng, Y. L.; Wu, W. J.; Li, X. Y.; Zheng, S. J.; Meng, L. P.  
*Influence of the Li Interaction on the H/X Interactions in HOLLiC6H6HOX/XOH (X=F, Cl, Br, I) Complexes*  
Chemphyschem, (14): 1591-1600 2013.
- Zeonjuk, L. L.; Vankova, N.; Knapp, C.; Gabel, D.; Heine, T.  
*On the gas-phase dimerization of negatively charged closo-dodecaborates: a theoretical study*  
Physical Chemistry Chemical Physics, (15): 10358-10366 2013.
- Zeonjuk, L. L.; Vankova, N.; Mavrandonakis, A.; Heine, T.; Roschenthaler, G. V.; Eicher, J.  
*On the Mechanism of Hydrogen Activation by Frustrated Lewis Pairs*

- Chemistry-a European Journal, (19): 17413-17424 2013.
- Zhan, W. S.; Li, R.; Pan, S.; Guo, Y. N.; Zhang, Y.  
*Extension of Conjugate pi Bridge in Dye Molecules for Dye-Sensitized Solar Cells*  
Acta Physico-Chimica Sinica, (29): 255-262 2013.
- Zhang, C. G.; Zhang, L. Y.; Li, H. Y.; Yu, S. Y.; Wang, Z. X.  
*Differences between insertions of ethylene into metallocene and non-metallocene ethylene polymerization catalysts*  
Journal of Physical Organic Chemistry, (26): 70-76 2013.
- Zhang, D. X.; Li, J.; Dong, X.; Zhou, X.; Yang, Z.; Roesky, H. W.  
*N-Heterocyclic Carbene-facilitated Condensation of 3-Methylphenylboronic Acid to the Boroxine*  
Zeitschrift Fur Naturforschung Section B-a Journal of Chemical Sciences, (68): 453-457 2013.
- Zhang, F. Y.; Zhao, L. M.; Sui, H. G.; Lu, X. Q.; Yang, G. W.; Guo, Y. H.; Guo, W. Y.; Fu, Q. T.  
*Reactivity of ethanol with ground state Ni+(D-2) in the gas phase: A density functional study*  
Computational and Theoretical Chemistry, (1023): 29-37 2013.
- Zhang, G. Q.; Li, X. W.; Li, Y.; Chen, D. Z.  
*Electron density characteristics and charge transfer effect of hydrogen bond O-H center dot center dot center dot Pt(II): atoms in molecules study and natural bond orbital analysis*  
Molecular Physics, (111): 3276-3282 2013.
- Zhang, G. Q.; Zhao, X. J.; Chen, D. Z.  
*Dual Bonding between H2O/H2S and AgCl/CuCl: Cu/Ag Bond, Sister Bond to Au Bond*  
Journal of Physical Chemistry A, (117): 10944-10950 2013.
- Zhang, L.; Ren, F. D.; Cao, D. L.; Wang, J. L.; Gao, J. F.  
*A comparative theoretical investigation into the strength of the trigger-bond in the Na+, Mg2+ and HF complexes involving the nitro group of R-NO2 (R = -CH3, -NH2 and -OCH3) or the C = C bond of (E)-O2N-CH = CH-NO2*  
Journal of Molecular Modeling, (19): 2499-2507 2013.
- Zhang, L. B.; Ren, T. Q.; Yang, X. Q.; Zhou, L. Z.; Li, X. M.  
*Intermolecular interactions of a size-expanded guanine analogue with gold nanoclusters*  
International Journal of Quantum Chemistry, (113): 2234-2242 2013.
- Zhang, L. B.; Ren, T. Q.; Zhou, L. Z.; Tian, J. X.; Li, X. M.  
*DFT investigation of the intermolecular interactions of a thieno-separated tricyclic guanine analog with gold nanoclusters*  
Computational and Theoretical Chemistry, (1019): 1-10 2013.
- Zhang, M.; Sheng, L.  
*Ab initio study of the organic xenon insertion compound into ethylene and ethane*  
Journal of Chemical Physics, (138) 2013.
- Zhang, M.; Zhao, J.; Liu, J. X.; Zhou, L. W.; Bu, Y. X.  
*Coexistence of solvated electron and benzene-centered valence anion in the negatively charged benzene-water clusters*  
Journal of Chemical Physics, (138) 2013.
- Zhang, Q.; Wu, C. H.; Zhou, L. X.; Li, J.

- Theoretical Studies on Intramolecular C-H Amination of Biaryl Azides Catalyzed by Four Different Late Transition Metals*  
Organometallics, (32): 415-426 2013.
- Zhang, R. H.; Li, X.; Liang, Z. J.; Zhu, K. K.; Lu, J. Y.; Kong, X. Q.; Ouyang, S. S.; Li, L.; Zheng, Y. G.; Luo, C.  
*Theoretical Insights into Catalytic Mechanism of Protein Arginine Methyltransferase 1*  
Plos One, (8) 2013.
- Zhang, S. L.; Fan, H. J.  
*Theoretical Study on Copper-Catalyzed S-Arylation of Thiophenols with Aryl Halides: Evidence Supporting the LCu(I)-SPh Active Catalyst and Halogen Atom Transfer Mechanism*  
Organometallics, (32): 4944-4951 2013.
- Zhang, W. J.; Wei, D. H.; Tang, M. S.  
*DFT Investigation on Mechanisms and Stereoselectivities of 2+2+2 Multimolecular Cycloaddition of Ketenes and Carbon Disulfide Catalyzed by N-Heterocyclic Carbenes*  
Journal of Organic Chemistry, (78): 11849-11859 2013.
- Zhang, X. R.; Wang, Y. Y.; Li, W. J.; Yuan, A. H.  
*Density functional theory study of the adsorption of CO on W-n (n=1-6) clusters*  
Acta Physica Sinica, (62) 2013.
- Zhang, Y.; Shen, W.; He, R. X.; Liu, X. R.; Li, M.  
*Molecular design of copolymers based on polyfluorene derivatives for Bulk-heterojunction-type solar cells*  
Journal of Materials Science, (48): 1205-1213 2013.
- Zhang, Z. T.; Turner, C. H.  
*Structural and Electronic Properties of Carbon Nanotubes and Graphenes Functionalized with Cyclopentadienyl-Transition Metal Complexes: A DFT Study*  
Journal of Physical Chemistry C, (117): 8758-8766 2013.
- Zhao, D. B.; Rong, C. Y.; Jenkins, S.; Kirk, S. R.; Yin, D. L.; Liu, S. B.  
*Origin of the cis-Effect: a Density Functional Theory Study of Doubly Substituted Ethylenes*  
Acta Physico-Chimica Sinica, (29): 43-54 2013.
- Zhao, G. Z.; Lu, M.  
*Theoretical Studies on 4-amino-3,5-dinitropyrazole and Its Analogues*  
Journal of Energetic Materials, (31): 60-71 2013.
- Zhao, J. F.; Sun, C. Z.; Sun, N.; Meng, L.; Chen, D. Z.  
*Theoretical Study on the Mechanism of the Reaction for Alkene Hydroaminations Catalyzed by Chiral Aldehyde*  
International Journal of Quantum Chemistry, (113): 2457-2463 2013.
- Zhao, J. W.; Nie, L.; Zhang, L. Y.; Jin, Y.; Peng, Y.; Du, S. H.; Jiang, N.  
*Molecularly imprinted layer-coated silica nanoparticle sensors with guest-induced fluorescence enhancement: theoretical prediction and experimental observation*  
Analytical Methods, (5): 3009-3015 2013.
- Zhao, L. H.; Weng, J. Y.; Zhao, W.; Ruan, W. J.; Xin, F.; Zhang, Y. H.  
*Density functional theory study on the influence of pyrrolidine substituent of C-60 bisadduct on its supramolecular interaction with porphine*  
Chemical Physics, (423): 43-48 2013.

- Zhao, L. M.; Tan, M.; Chen, J.; Ding, Q. Y.; Lu, X. Q.; Chi, Y. H.; Yang, G. W.; Guo, W. Y.; Fu, Q. T.  
*The Competitive O-H versus C-H Bond Activation of Ethanol and Methanol by VO<sub>2</sub><sup>+</sup> in Gas Phase: A DFT Study*  
Journal of Physical Chemistry A, (117): 5161-5170 2013.
- Zhao, N.; Hastings, G.  
*On the Nature of the Hydrogen Bonds to Neutral Ubiquinone in the Q(A) Binding Site in Purple Bacterial Photosynthetic Reaction Centers*  
Journal of Physical Chemistry B, (117): 8705-8713 2013.
- Zhao, N. N.; Zhao, Y. L.; Hu, Y.; Ma, H. X.; Zhao, F. Q.; Song, J. R.  
*Intermolecular Interactions and Thermodynamic Properties of 3,6-Diamino-1,2,4,5-tetrazine-1,4-dioxide Dimers: A Density Functional Theoretical Study*  
South African Journal of Chemistry-Suid-Afrikaanse Tydskrif Vir Chemie, (66): 167-172 2013.
- Zhao, Q.; Feng, D. C.  
*Influence of transition metals on halogen-bonded complexes of MCCBr center dot center dot center dot NCH and HCCBra center dot center dot center dot NCM' (M, M' = Cu, Ag, and Au)*  
Journal of Molecular Modeling, (19): 1267-1271 2013.
- Zhao, S.; Ren, Y. L.; Lu, W. W.; Wang, J. J.; Yin, W. P.  
*Density functional study of Ag<sub>n</sub>Au<sub>m</sub> and Ag<sub>n</sub>Au<sub>m</sub><sup>+</sup> (n+m ≤ 5) clusters interaction with a single S atom*  
Computational and Theoretical Chemistry, (1017): 188-193 2013.
- Zhao, S. S.; Shi, W. J.; Wang, J. L.  
*Theoretical investigation on the structure and thermodynamic properties of the 2,4-dinitroimidazole complex with methanol*  
Journal of Molecular Modeling, (19): 163-171 2013.
- Zhao, X. R.; Pang, X.; Yan, X. Q.; Jin, W. J.  
*Halogen Bonding or Hydrogen Bonding between 2,2,6,6-Tetramethylpiperidine-noxyl Radical and Trihalomethanes CHX<sub>3</sub> (X=Cl, Br, I)*  
Chinese Journal of Chemical Physics, (26): 172-180 2013.
- Zhao, Y.; Yang, L. J.; Chen, S.; Wang, X. Z.; Ma, Y. W.; Wu, Q.; Jiang, Y. F.; Qian, W. J.; Hu, Z.  
*Can Boron and Nitrogen Co-doping Improve Oxygen Reduction Reaction Activity of Carbon Nanotubes?*  
Journal of the American Chemical Society, (135): 1201-1204 2013.
- Zhao, Y. X.; Zhou, F.; Zhou, H. C.; Su, H. B.  
*The structural and bonding evolution in cysteine-gold cluster complexes*  
Physical Chemistry Chemical Physics, (15): 1690-1698 2013.
- Zheng, B. S.; Hou, B.; Wang, Z. X.; Yi, P. G.; Wu, J. Y.; Ding, X. L.  
*Theoretical characters and nature of the intermolecular lithium bonded interactions B center dot center dot center dot LiCN/LiNC (B = pyridine, furan and thiophene)*  
Computational and Theoretical Chemistry, (1017): 153-158 2013.
- Zheng, W. R.; Chen, Z. C.; Xu, W. X.  
*DFT Study on Homolytic Dissociation Enthalpies of C-I Bonds*  
Chinese Journal of Chemical Physics, (26): 541-548 2013.
- Zheng, X. Y.; Shuai, Z. G.; Wang, D.

- Anion-Binding Properties of pi-Electron Deficient Cavities in Bis(tetraoxacalix 2 arene 2 triazine): A Theoretical Study*  
Journal of Physical Chemistry A, (117): 3844-3851 2013.
- Zheng, Y. S.; Zhuo, Z. H.; He, Y.; Mo, Q.  
*Structure and Spectral Studies of N-Ethyl Pyridinium Bromide Ionic Liquids: DFT and ab initio Study*  
Asian Journal of Chemistry, (25): 3233-3236 2013.
- Zhou, D. H.; Li, M. M.; Cui, L. L.  
*Photophysical Properties and Photoinduced Electron Transfer Mechanism in a Near-IR Fluorescent Probe for Monitoring Peroxynitrite*  
Acta Physico-Chimica Sinica, (29): 1453-1460 2013.
- Zhou, G. F.; Ren, J.; Zhang, S. W.  
*Initial growth mechanisms of ZrO<sub>2</sub> and TiO<sub>2</sub> thin films using cycloheptatrienyl-cyclopentadienyl heteroleptic precursors: A comparative study by density functional theory*  
Applied Surface Science, (283): 968-974 2013.
- Zhou, K.  
*Theoretical studies on the pentaatomic planar tetracoordinate carbon molecules CGa<sub>3</sub>Si and CGa<sub>3</sub>Si*  
Computational and Theoretical Chemistry, (1009): 30-34 2013.
- Zhou, W. X.; Yin, B.; Li, J.; Sun, W. J.; Zhang, F. X.  
*A C-S cross-coupling observed in situ reaction of 2-mercaptobenzothiazole with CuI*  
Inorganica Chimica Acta, (408): 209-213 2013.
- Zhou, Z. J.; Li, X. P.; Huang, X. R.; Wu, Z. J.; Li, Z. R.  
*Theoretical Study on Second-order Nonlinear Optical Response of Lithiation Boron Nitride Nanotube*  
Chemical Journal of Chinese Universities-Chinese, (34): 2152-2157 2013.
- Zhu, H. J.; Cao, H.; Li, T. H.  
*A theoretical study on the decomposition mechanisms of deprotonated glycolic acid*  
Computational and Theoretical Chemistry, (1008): 32-38 2013.
- Zhu, Y. Y.; Day, C. S.; Zhang, L.; Hauser, K. J.; Jones, A. C.  
*A Unique Au-Ag-Au Triangular Motif in a Trimetallic Halonium Dication: Silver Incorporation in a Gold(I) Catalyst*  
Chemistry-a European Journal, (19): 12264-12271 2013.
- Zielinski, F.; Tognetti, V.; Joubert, L.  
*A theoretical study on the gas-phase protonation of pyridine and phosphinine derivatives*  
Journal of Molecular Modeling, (19): 4049-4058 2013.
- Zierkiewicz, W.  
*Reaction of volatile anaesthetic desflurane with chlorine atom. Theoretical investigation*  
Chemical Physics Letters, (555): 72-78 2013.
- Zimmerman, H. E.; Weinhold, F.  
*Natural Bond-Bond Polarizability: A Huckel-Like Electronic Delocalization Index*  
Journal of Organic Chemistry, (78): 1844-1850 2013.
- Zimmerman, P. M.  
*Automated discovery of chemically reasonable elementary reaction steps*

Journal of Computational Chemistry, (34): 1385-1392 2013.

Zimnicka, M.; Chung, T. W.; Moss, C. L.; Turecek, F.

*Perturbing Peptide Cation-Radical Electronic States by Thioamide Groups: Formation, Dissociations, and Energetics of Thiopeptide Cation-Radicals*

Journal of Physical Chemistry A, (117): 1265-1275 2013.

Zorlu, Y.; Can, H.

*A novel 1D silver(I) coordination polymer constructed from indol-3-butyric acid: Synthesis, crystal structure and natural bond orbital analysis by DFT*

Journal of Molecular Structure, (1037): 109-115 2013.

Zorlu, Y.; Can, H.; Aksakal, F.

*A novel 2D chiral silver(I) coordination polymer assembled from 5-sulfosalicylic acid and (2S,4R)-4-hydroxyproline: Synthesis, crystal structure, HOMO-LUMO and NBO analysis*

Journal of Molecular Structure, (1049): 368-376 2013.

Zou, H. Y.; Ma, N. N.; Sun, S. L.; Li, X.; Qiu, Y. Q.

*Structures and redox-switchable second-order nonlinear optics properties of N-legged piano stool shaped 12-vertex rhenacarborane half-sandwich complexes*

Journal of Organometallic Chemistry, (728): 6-15 2013.

Zou, W. L.; Filatov, M.; Atwood, D.; Cremer, D.

*Removal of Mercury from the Environment: A Quantum-Chemical Study with the Normalized Elimination of the Small Component Method*

Inorganic Chemistry, (52): 2497-2504 2013.

Zou, W. L.; Nori-Shargh, D.; Boggs, J. E.

*On the Covalent Character of Rare Gas Bonding Interactions: A New Kind of Weak Interaction*

Journal of Physical Chemistry A, (117): 207-212 2013.

Zubieta, C.; Castellani, N. J.; Ferullo, R. M.

*High reactivity of nitric oxide with peroxy groups on BaO particles. DFT calculations*

Computational and Theoretical Chemistry, (1009): 1-7 2013.