NBO 2015 – 1592 references
Compiled/Updated by Ariel Andrea on 4/01/2016

Abbat, S.; Dhaked, D.; Arfeen, M.; Bharatam, P. V.
Mechanism of the Paal-Knorr reaction: the importance of water mediated hemialcohol pathway
Rsc Advances, (5): 88353-88366 2015.

Abdel-Ghani, N. T.; Mansour, A. M.; El-Ghar, M. F. A.; El-Borady, O. M.; Shorafa, H.
Co(II), Ni(II) and Cu(II) complexes of azo-aminopyrazole ligand: Spectroscopic, crystal structure and quantum chemical calculations
Inorganica Chimica Acta, (435): 187-193 2015.

Abdulsattar, M. A.
Molecular approach to hexagonal and cubic diamond nanocrystals
Carbon Letters, (16): 192-197 2015.

Abdulsattar, M. A.; Almaroof, S. M.
Electronic and spectroscopic properties of GeC superlattice nanocrystals: A first-principle study using diamondoid structures
Superlattices and Microstructures, (79): 63-71 2015.

Abedini, M.; Izadyar, M.; Nakhaipour, A.
Different Aspects of Single Wall Carbon Nanotube Functionalization by Aniline Adsorption; Quantum Mechanics/Molecular Mechanics Study
Journal of Nano Research, (32): 1-U21 2015.

Adrover, M.; Howes, B. D.; Iannuzzi, C.; Smulevich, G.; Pastore, A.
Anatomy of an iron-sulfur cluster scaffold protein: Understanding the determinants of 2Fe-2S cluster stability on IscU
Biochimica Et Biophysica Acta-Molecular Cell Research, (1853): 1448-1456 2015.

Afaneh, A. T.; Schreckenbach, G.
Fluorescence Enhancement/Quenching Based on Metal Orbital Control: Computational Studies of a 6-Thienyllumazine-Based Mercury Sensor
Journal of Physical Chemistry A, (119): 8106-8116 2015.

Aggarwal, K.; Khurana, J. M.
X-ray diffraction, spectroscopic characterization and quantum chemical calculations by DFT and HF of novel 2-hydroxy-12-(4-hydroxypheny1)-9, 9-dimethyl-9,10-dihydro-8H-benzo a xanthen-11(12H)-one
Journal of Molecular Structure, (1079): 21-34 2015.

Ahmadi, A. A.; Fattahi, A.
Influence of a beta-OH substituent on S(N)2 reactions of fluoroethane: Intramolecular hydrogen bonding catalysis or inhibition? A theoretical study
Computational and Theoretical Chemistry, (1067): 71-83 2015.

Ahmadinejad, N.; Tahan, A.
The comparison of NMR tensors and NQR frequencies of hallucinogenic Harmine compound in the gas phase
Russian Journal of Physical Chemistry B, (9): 19-21 2015.

Akbari, A.; Golzadeh, B.; Arshadi, S.; Kassaee, M. Z.
A quest for stable 2,5-bis(halobora)cyclopentenylidene and its Si, Ge, Sn and Pb analogs at theoretical levels
Rsc Advances, (5): 43319-43327 2015.

Akher, F. B.; Ebrahimi, A.
pi-Stacking effects on the hydrogen bonding capacity of methyl 2-naphthoate
Journal of Molecular Graphics and Modelling, (61): 115-122 2015.

Akhtari, K.; Hassanzadeh, K.; Fakhraei, B.; Fakhraei, N.; Hassanzadeh, H.; Akhtari, G.; Zarei, S. A.; Hassanzadeh, K.
Mechanisms of the hydroxyl and superoxide anion radical scavenging activity and protective effect on lipid peroxidation of thymoquinone: a DFT study
Monatshefte fur Chemie, (146): 601-611 2015.

Akilandeswari, L.; Prathipa, C.
Competitive and Cooperative Torquoselectivity in the thermal ring opening of cyclobutene: A density functional insight
Journal of Chemical Sciences, (127): 1505-1511 2015.

Aksakal, F.; Shvets, N.; Dimoglo, A.
The study of dual COX-2/5-LOX inhibitors by using electronic-topological approach based on data on the ligand-receptor interactions
Journal of Molecular Graphics and Modelling, (60): 79-88 2015.

Alabugin, I. V.; Bresch, S.; Gomes, G. D.
Orbital hybridization: a key electronic factor in control of structure and reactivity
Journal of Physical Organic Chemistry, (28): 147-162 2015.

Alagona, G.; Ghio, C.
Rhodium-Catalyzed Hydroformylation of Ketal-Masked beta-Isophorone: Computational Explanation for the Unexpected Reaction Evolution of the Tertiary Rh-Alkyl via an Exocyclic beta-Elimination Derivative
Journal of Physical Chemistry A, (119): 5117-5133 2015.

Alam, M. J.; Ahmad, S.
FTIR, FT-Raman, UV-Visible spectra and quantum chemical calculations of allantoin molecule and its hydrogen bonded dimers
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (136): 961-978 2015.

Alaniz, V.; Rocha-Rinza, T.; Cuevas, G.
Assessment of Hydrophobic Interactions and Their Contributions Through the Analysis of the Methane Dimer
Journal of Computational Chemistry, (36): 361-375 2015.

Alauddin, M.; Gloaguen, E.; Brenner, V.; Tardivel, B.; Mons, M.; Zehnacker-Rentien, A.; Declerck, V.; Aitken, D. J.
Intrinsic Folding Proclivities in Cyclic -Peptide Building Blocks: Configuration and Heteroatom Effects Analyzed by Conformer-Selective Spectroscopy and Quantum Chemistry
Chemistry-a European Journal, (21): 16479-16493 2015.

Albury, R. M.; Pruitt, C. J. M.; Hester, T. H.; Goebbert, D. J.
Fragmentation of Cr(NO3)(4)(-): Metal Oxidation upon O circle- Abstraction
Journal of Physical Chemistry A, (119): 11471-11478 2015.

Alcaide, B.; Almendros, P.; Carrascosa, R.; Casarrubios, L.; Soriano, E.
A Versatile Synthesis of beta-Lactam-Fused Oxacycles through the Palladium-Catalyzed Chemo-, Regio-, and Diastereoselective Cyclization of Allenic Diols
Chemistry-a European Journal, (21): 2200-2213 2015.

Aleksic, J.; Stojanovic, M.; Baranac-Stojanovic, M.
Origin of Fluorine/Sulfur Gauche Effect of beta-Fluorinated Thiol, Sulfoxide, Sulfone, and Thionium Ion
Journal of Organic Chemistry, (18): 10197-10207 2015.

Alen, S.; Sajan, D.; Joseph, L.; Chaitanya, K.; Shettigar, V.; Jothy, V. B.
Synthesis, growth, vibrational spectral investigations and structure-property relationship of an organic NLO crystal: 3,4-Dimethoxy chalcone
Chemical Physics Letters, (636): 208-215 2015.

Alen, S.; Sajan, D.; Sabu, K. J.; Sundius, T.; Chaitanya, K.; Blockhuys, F.; Jothy, V. B.
Vibrational spectral analysis, electronic absorption and non-linear optical behavior of (E)-1-(2,4,6-trimethoxyphenyl)pent-1-en-3-one

Vibrational Spectroscopy, (79): 1-10 2015.

Alen, S.; Sajan, D.; Umadevi, T.; Nemec, I.; Baburaj, M. S.; Jothy, V. B.; Joy, B. H. S.
Twisted intramolecular charge transfer and its contribution to the NLO activity of Diglycine Picrate: A vibrational spectroscopic study
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (135): 720-731 2015.

Alfonso, M.; Ferao, A. E.; Tarraga, A.; Molina, P.
Electrochemical and Fluorescent Ferrocene-Imidazole-Based Dyads as Ion-Pair Receptors for Divalent Metal Cations and Oxoanions
Inorganic Chemistry, (54): 7461-7473 2015.

Ali, M. M.; George, G.; Ramalingam, S.; Periandy, S.; Gokulakrishnan, V.
Vibrational FT-IR, FT-Raman analysis, NMR and mass - Spectroscopic investigation on 3,6-Dimethylphenanthrene using computational calculation
Journal of Molecular Structure, (1099): 463-481 2015.

Alisir, S. H.; Demir, S.; Sariboga, B.; Buyukgungor, O.
A disparate 3-D silver(I) coordination polymer of pyridine-3,5-dicarboxylate and pyrimidine with strong intermetallic interactions: X-ray crystallography, photoluminescence and antimicrobial activity
Journal of Coordination Chemistry, (68): 155-168 2015.

Alkorta, I.; Elguero, J.; Del Bene, J. E.
Exploring the PX3:NCH and PX3:NH3 potential surfaces, with X = F, Cl, and Br
Chemical Physics Letters, (641): 84-89 2015.

Alkorta, I.; Elguero, J.; Grabowski, S. J.
Pnicogen and hydrogen bonds: complexes between PH3X+ and PH2X systems
Physical Chemistry Chemical Physics, (17): 3261-3272 2015.

Alkorta, I.; Elguero, J.; Mo, O.; Yanez, M.; Del Bene, J. E.
Using beryllium bonds to change halogen bonds from traditional to chlorine-shared to ion-pair bonds
Physical Chemistry Chemical Physics, (17): 2259-2267 2015.

Allehyani, B. H.; Elroby, S. A.; Aziz, S. G.; Hilal, R. H.
Electronic structure of alloxan and its dimers: QM/QD simulations and quantum chemical topology analysis
Journal of Biomolecular Structure and Dynamics, (33): 2121-2132 2015.

Allehyani, B. H.; Elroby, S. A.; Aziz, S. G.; Hilal, R. H.
Protonation and deprotonation enthalpies of alloxan and implications for the structure and energy of its complexes with water: a computational study
Journal of Biomolecular Structure and Dynamics, (33): 897-910 2015.

Al-Mogren, M. M.; El-Gogary, T. M.
Structure, stability, energy barrier and ionization energies of chemically modified DNA-bases: Quantum chemical calculations on 37 favored and rare tautomeric forms of tetraphosphoadenine
Computational and Theoretical Chemistry, (1052): 35-41 2015.

Almutairi, M. S.; Alanazi, A. M.; Al-Abdullah, E. S.; El-Emam, A. A.; Pathak, S. K.; Srivastava, R.; Prasad, O.; Sinha, L.
FT-IR and FT-Raman spectroscopic signatures, vibrational assignments, NBO, NLO analysis and molecular docking study of 2-{ 5-(adamantan-1-yl)-4-methyl-4H-1,2,4-triazol-3-yl sulfanyl}-N,N-dime thylethanamine
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (140): 1-14 2015.

Al-Omary, F. A. M.; Raj, A.; Raju, K.; Panicker, C. Y.; Haress, N. G.; El-Emam, A. A.; El-Ashmawy, M. B.; Al-Saadi, A. A.; Van Alsenoy, C.; War, J. A.
Spectroscopic investigation (FT-IR, FT-Raman), HOMO-LUMO, NBO analysis and molecular docking study of 2- (4-chlorobenzyl)sulfanyl -4-(2-methylpropyl)-6- 3-trifluoromethyl)-an ilino pyrimidine-5-carbonitrile, a potential chemotherapeutic agent

Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (136): 520-533 2015.

Alturk, S.; Tamer, O.; Avci, D.; Atalay, Y.
Synthesis, spectroscopic characterization, second and third-order nonlinear optical properties, and DFT calculations of a novel Mn(II) complex
Journal of Organometallic Chemistry, (797): 110-119 2015.

Alves, L. G.; Madeira, F.; Munha, R. F.; Barroso, S.; Veiros, L. F.; Martins, A. M.
Reactions of heteroallenes with cyclam-based Zr(IV) complexes
Dalton Transactions, (44): 1441-1455 2015.

Alzoman, N. Z.; Mary, Y. S.; Panicker, C. Y.; Al-Swaidan, I. A.; El-Emam, A. A.; Al-Deeb, O. A.; Al-Saadi, A. A.; Van Alsenoy, C.; War, J. A.
Spectroscopic investigation (FT-IR and FT-Raman), vibrational assignments, HOMO-LUMO, NBO, MEP analysis and molecular docking study of 2- (4-chlorobenzyl)sulfanyl -4-(2-methylpropyl)-6-(phenylsulfanyl)-pyrim idine-5-carbonitrile, a potential chemotherapeutic agent
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (139): 413-424 2015.

Amaral, L.; Szterner, P.; Morais, V. M. F.; da Silva, M.
Thermochemical study of the isomeric compounds: 3-acetylbenzonitrile and benzoylacetonitrile
Journal of Chemical Thermodynamics, (91): 452-458 2015.

Aminova, R. M.; Galiullina, L. F.; Klochkov, V. V.; Aganov, A. V.
A quantum chemical study of an interaction between collagen fragments and calcium ions using calculations of model complexes
Russian Chemical Bulletin, (64): 210-215 2015.

Anandhan, K.; Boobalan, M. S.; Venkatesan, P.; Ilangovan, A.; Kaushik, M. P.; Arunagiri, C.
Crystallography and computational electronic structure investigations on 14-(3, 4, 5-trimethoxyphenyl)-14H-dibenzo a,j xanthene
Journal of Molecular Structure, (1097): 185-198 2015.

Anbarasan, R.; Dhandapani, A.; Manivarman, S.; Subashchandrabose, S.; Saleem, H.
Synthesis and spectroscopical study of rhodanine derivative using DFT approaches
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (146): 261-272 2015.

Andersen, K. A.; Aronoff, M. R.; McGrath, N. A.; Raines, R. T.
Diazo Groups Endure Metabolism and Enable Chemoselectivity in Cellulo
Journal of the American Chemical Society, (137): 2412-2415 2015.

Andrada, D. M.; Holzmann, N.; Hamadi, T.; Frenking, G.
Direct estimate of the internal Pi-donation to the carbene centre within N-heterocyclic carbenes and related molecules
Beilstein Journal of Organic Chemistry, (11): 2727-2736 2015.

Andrejeva, A.; Breckenridge, W. H.; Wright, T. G.
A Surprisingly Simple Electrostatic Model Explains Bent Versus Linear Structures in M+-RG(2) Species (M = Group 1 Metal, Li-Fr; RG = Rare Gas, He-Rn)
Journal of Physical Chemistry A, (119): 10959-10970 2015.

Andrejeva, A.; Gardner, A. M.; Graneek, J. B.; Breckenridge, W. H.; Wright, T. G.
Theoretical Study of M+-RG(2): (M+ = Ca, Sr, Ba, and Ra; RG = He-Rn)
Journal of Physical Chemistry A, (119): 5995-6005 2015.

Andres, J.; Gracia, L.; Gonzalez-Navarrete, P.; Safont, V. S.
Chemical structure and reactivity by means of quantum chemical topology analysis
Computational and Theoretical Chemistry, (1053): 17-30 2015.

Andrzejak, M.; Szczepanik, D. W.; Orzel, L.

The lowest triplet states of bridged cis-2,2 '-bithiophenes - theory vs. experiment
Physical Chemistry Chemical Physics, (17): 5328-5337 2015.

Anitha, E. G.; Vedhagiri, S. J.; Parimala, K.
Spectroscopic (FT-IR, FT-Raman and UV-Visible) investigations, NMR chemical shielding anisotropy (CSA) parameters of 2,6-Diainino-4-chloropyrimidine for dye sensitized solar cells using density functional theory
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (136): 1557-1568 2015.

Anitha, K.; Balachandran, V.
Assessment of long-range corrected and conventional DFT functional for the prediction of second - Order NLO properties and other molecular properties of N-(2-cyanoethyl)-N-butylaniline - A vibrational spectroscopy study
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (146): 66-79 2015.

Anitha, R.; Gunasekaran, M.; Kumar, S. S.; Athimoolam, S.; Sridhar, B.
Single crystal XRD, vibrational and quantum chemical calculation of pharmaceutical drug paracetamol: A new synthesis form
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (150): 488-498 2015.

Anjos, I. C.; Rocha, G. B.
A topological assessment of the electronic structure of mesoionic compounds
Journal of Computational Chemistry, (36): 1907-1918 2015.

Anju, R. S.; Saha, K.; Mondal, B.; Roisnel, T.; Halet, J. F.; Ghosh, S.
In search for new bonding modes of the methylenedithiolato ligand: novel tri- and tetra-metallic clusters
Dalton Transactions, (44): 11306-11313 2015.

Antinolo, A.; Garcia-Yuste, S.; Otero, A.; Espinosa, A.
Unusual Mechanism for the Reaction of a Niobocene Hydride Complex with Activated Alkynes. Experimental and DFT Studies
Organometallics, (34): 2695-2698 2015.

Ao, M. Z.; Tao, Z. Q.; Liu, H. X.; Wu, D. Y.; Wang, X.
A theoretical investigation of the competition between hydrogen bonding and lone pair center dot center dot center dot pi interaction in complexes of TNT with NH3
Computational and Theoretical Chemistry, (1064): 25-34 2015.

Aoki, Y.; Ohmori, K.; Suzuki, K.
Dioxanone-Fused Dienes Enable Highly Endo-Selective Intramolecular Diels-Alder Reactions
Organic Letters, (17): 2756-2759 2015.

Appell, M.; Bosma, W. B.
Assessment of the electronic structure and properties of trichothecene toxins using density functional theory
Journal of Hazardous materials, (288): 113-123 2015.

Arabieh, M.; Khodabandeh, M. H.; Karimi-Jafari, M. H.; Platas-Iglesias, C.; Zare, K.
Complexation of Sm3+ and pamidronate: A DFT study
Journal of Rare Earths, (33): 310-319 2015.

Araghi, S. H.; Entezari, M. H.; Googheri, M. S. S.
Configurational study of amino-functionalized silica surfaces: A density functional theory modeling
Journal of Molecular Graphics and Modelling, (59): 21-30 2015.

Arakawa, M.; Kohara, K.; Terasaki, A.
Reaction of Aluminum Cluster Cations with a Mixture of O-2 and H2O Gases: Formation of Hydrated-Alumina Clusters
Journal of Physical Chemistry C, (119): 10981-10986 2015.

Arce, E. R.; Mosquillo, M. F.; Perez-Diaz, L.; Echeverria, G. A.; Piro, O. E.; Merlino, A.; Coitino, E. L.; Ribeiro, C. M.; Leite, C. Q. F.; Pavan, F. R.; Otero, L.; Gambino, D.

Aromatic amine N-oxide organometallic compounds: searching for prospective agents against infectious diseases
Dalton Transactions, (44): 14453-14464 2015.

Arenzano, J. A.; Virues, J. O.; Colorado-Peralta, R.; Ramirez-Montes, P. I.; Santillan, R.; Sanchez, M.; Rivera, J. M.
Heterometallic coordination framework by sodium carboxylate subunits and cobalt (III) centers obtained from a highly hydrogen bonding stabilized cobalt (II) monomeric complex
Inorganic Chemistry Communications, (51): 55-60 2015.

Arivazhagan, G.; Elangovan, A.; Shanmugam, R.; Vijayalakshmi, R.; Kannan, P. P.
Spectroscopic studies, NBO analysis and dielectric studies on the behaviour of acetone molecules in non-polar solvent environment
Chemical Physics Letters, (627): 101-106 2015.

Arivazhagan, M.; Manivel, S.; Jeyavijayan, S.; Meenakshi, R.
Vibrational spectroscopic (FTIR and FT-Raman), first-order hyperpolarizablity, HOMO, LUMO, NBO, Mulliken charge analyses of 2-ethylimidazole based on Hartree-Fock and DFT calculations
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (134): 493-501 2015.

Arjunan, V.; Anitha, R.; Devi, L.; Mohan, S.; Yang, H. F.
Comprehensive quantum chemical and spectroscopic (FTIR, FT-Raman, H-1, C-13 NMR) investigations of (1,2-epoxyethyl)benzene and (1,2-epoxy-2-phenyl)propane
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (135): 120-136 2015.

Arjunan, V.; Anitha, R.; Marchewka, M. K.; Mohan, S.; Yang, H. F.
Conformational, structural, vibrational, electronic and quantum chemical investigations of cis-2-methoxycinnamic acid
Journal of Molecular Structure, (1080): 122-136 2015.

Arjunan, V.; Marchewka, M. K.; Raj, A.; Yang, H. F.; Mohan, S.
Structural and vibrational spectral investigations of melaminium glutarate monohydrate by FTIR, FT-Raman and DFT methods
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (135): 540-550 2015.

Arjunan, V.; Santhanam, R.; Marchewka, M. K.; Mohan, S.; Yang, H. F.
Structure activity studies of an analgesic drug tapentadol hydrochloride by spectroscopic and quantum chemical methods
Journal of Molecular Structure, (1100): 188-202 2015.

Arjunan, V.; Thirunarayanan, S.; Devi, G. D.; Mohan, S.
Substituent influence on the structural, vibrational and electronic properties of 2,5-dihydrothiophene-1,1-dioxide by experimental and DFT methods
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (150): 641-651 2015.

Arkan, F.; Izadyar, M.; Nakhaeipour, A.
A quantum chemistry study on the performance of porphyrin-based solar cell sensitisers; Zinc and anchor group position effects
Molecular Physics, (113): 3815-3825 2015.

Arshad, M. N.; Asiri, A. M.; Alamry, K. A.; Mahmood, T.; Gilani, M. A.; Ayub, K.; Birinji, A. S.
Synthesis, crystal structure, spectroscopic and density functional theory (DFT) study of N- 3-anthracen-9-yl-1-(4-bromo-phenyl)-allylidene -N-benzenesulfonohydra zine
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (142): 364-374 2015.

Arulmani, R.; Balachander, R.; Vijaya, P.; Sankaran, K. R.
Spectral and conformational studies on 3-pyridinealdazine by DFT approach
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (138): 660-666 2015.

Arulmozhiraja, S.; Nakatani, N.; Nakayama, A.; Hasegawa, J. Y.

Energy dissipative photoprotective mechanism of carotenoid spheroidene from the photoreaction center of purple bacteria Rhodobacter sphaeroides
Physical Chemistry Chemical Physics, (17): 23468-23480 2015.

Attoui-Yahia, O.; Khatmi, D.; Kraim, K.; Ferkous, F.
Hydrogen bonding investigation in Pyridoxine/beta-cyclodextrin complex based on QTAIM and NBO approaches
Journal of the Taiwan Institute of Chemical Engineers, (47): 91-98 2015.

Avi, M. D. R.; Garcia, A. A. M.; Urena, F. P.
Electronic structure of kaempferol-Cu2+ coordination compounds: a DFT, QTAIM and NBO study in the gas phase
Theoretical Chemistry Accounts, (134) 2015.

Azam, M.; Al-Resayes, S. I.; Velmurugan, G.; Venuvanalingam, P.; Wagler, J.; Kroke, E.
Novel uranyl(VI) complexes incorporating propylene-bridged salen-type N2O2-ligands: a structural and computational approach
Dalton Transactions, (44): 568-577 2015.

Azami, S. M.
Electron Density Analysis of Hyperconjugation
Chemphyschem, (16): 3842-3845 2015.

Aziz, S. G.; Alyoubi, A. O.; Elroby, S. A.; Osman, O. I.; Hilal, R. H.
Towards Understanding the Decomposition/Isomerism Channels of Stratospheric Bromine Species: Ab Initio and Quantum Topology Study
International Journal of Molecular Sciences, (16): 6783-6800 2015.

Aziz, S. G.; Osman, O. I.; Elroby, S. A.; Hilal, R. H.
Gas-Phase Thermal Tautomerization of Imidazole-Acetic Acid: Theoretical and Computational Investigations
International Journal of Molecular Sciences, (16): 26347-26362 2015.

Azofra, L. M.
Towards an understanding of the CO2-philicity in glycine: Deepening into the CO2:Aminoacid interactions
Chemical Physics, (453): 1-6 2015.

Azofra, L. M.; Alkorta, I.; Scheiner, S.
Chalcogen Bonds in Complexes of SOXY (X, Y = F, Cl) with Nitrogen Bases
Journal of Physical Chemistry A, (119): 535-541 2015.

Azofra, L. M.; Scheiner, S.
Tetrel, chalcogen, and CH center dot center dot O hydrogen bonds in complexes pairing carbonyl-containing molecules with 1, 2, and 3 molecules of CO2
Journal of Chemical Physics, (142) 2015.

Badieyan, S.; Bach, R. D.; Sobrado, P.
Mechanism of N-Hydroxylation Catalyzed by Flavin-Dependent Monooxygenases
Journal of Organic Chemistry, (80): 2139-2147 2015.

Badoglu, S.; Temel, E.; Yurdakul, A.; Buyukgungor, O.
XRD, FT-IR, and DFT study on a novel ethyl derivative of 3-hydroxy-2-quinoxalinecarboxylic acid
Optics and Spectroscopy, (119): 987-996 2015.

Bagheri, S.; Masoodi, H. R.
Theoretical study of the influence of cation-pi and anion-pi interactions on some NMR data of borazine complexes
Chemical Physics Letters, (629): 46-52 2015.

Bagheri, S.; Masoodi, H. R.; Abadi, M. N.
Estimation of individual NH center dot center dot center dot X (X = N, O) hydrogen bonding energies in some complexes involving multiple hydrogen bonds using NBO calculations

Theoretical Chemistry Accounts, (134) 2015.

Bahgat, K.; Fraihat, S.
Normal coordinate analysis, molecular structure, vibrational, electronic spectra and NMR investigation of 4-Amino-3-phenyl-1H-1,2,4-triazole-5(4H)-thione by ab initio HF and DFT method
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (135): 1145-1155 2015.

Baillie, R. A.; Holmes, A. S.; Lefevre, G. P.; Patrick, B. O.; Shree, M. V.; Wakeham, R. J.; Legzdins, P.; Rosenfeld, D. C.
*Synthesis, Characterization, and Some Properties of Cp*W(NO)(H)(eta(3)-allyl) Complexes*
Inorganic Chemistry, (54): 5915-5929 2015.

Baillie, R. A.; Lefevre, G. P.; Wakeham, R. J.; Holmes, A. S.; Legzdins, P.
*Unsymmetrical Saturated Ketones Resulting from Activations of Hydrocarbon C(sp(3))-H and C(sp(2))-H Bonds Effected by Cp*W(NO)(H)(eta(3)-allyl) Complexes*
Organometallics, (34): 4085-4092 2015.

Balachandran, V.; Karpagam, V.; Revathi, B.; Kavimani, M.; Ilango, G.
Conformational stability, spectroscopic and computational studies, HOMO-LUMO, NBO, ESP analysis, thermodynamic parameters of natural bioactive compound with anticancer potential of 2-(hydroxymethyl)anthraquinone
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (150): 631-640 2015.

Balachandran, V.; Karpagam, V.; Santhi, G.; Revathi, B.; Ilango, G.; Kavimani, M.
Conformational stability, vibrational (FT-IR and FT-Raman) spectra and computational analysis of m-trifluoromethyl benzoic acid
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (137): 165-175 2015.

Balachandrana, V.; Santhi, G.; Karpagam, V.; Revathi, B.; Karabacak, M.
Spectroscopic investigation, natural bond orbital analysis, HOMO-LUMO and thermodynamic functions of 2-tert-butyl-5-methyl anisole using DFT (B3LYP) calculations
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (136): 451-463 2015.

Balakrishnan, C.; Subha, L.; Neelakantan, M. A.; Mariappan, S. S.
Synthesis, spectroscopy, X-ray crystallography, DFT calculations, DNA binding and molecular docking of a propargyl arms containing Schiff base
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (150): 671-681 2015.

Banerjee, P.; Mukhopadhyay, D. P.; Chakraborty, T.
On the origin of donor O-H bond weakening in phenol-water complexes
Journal of Chemical Physics, (143) 2015.

Banerjee, S.
Understanding the ring-opening, chelation and non-chelation reactions between nedaplatin and thiosulfate: a DFT study based on NBO, ETS-NOCV and QTAIM
Theoretical Chemistry Accounts, (135) 2015.

Bansar, R. K.; Gupta, R.; Kour, M.
Diels-Alder Reactions with the > C=P- Functionality of Annelated Azaphospholes
Synlett, (26): 294-303 2015.

Banu, T.; Ghosh, D.; Debnath, T.; Sen, K.; Das, A. K.
Molecular hydrogen binding affinities of metal cation decorated substituted benzene systems: insight from computational exploration
Rsc Advances, (5): 57647-57656 2015.

Barakat, A.; Al-Majid, A. M.; Islam, M. S.; Ali, M.; Soliman, S. M.; Siddiqui, M. R. H.; Ghabbour, H. A.; Fun, H. K.
Molecular structure investigation and tautomerism aspects of (E)-3-benzylideneindolin-2-one
Journal of Chemical Sciences, (127): 1547-1556 2015.

Barakat, A.; Al-Majid, A. M.; Soliman, S. M.; Mabkhot, Y. N.; Ali, M.; Ghabbour, H. A.; Fun, H. K.; Wadood, A.
Structural and spectral investigations of the recently synthesized chalcone (E)-3-mesityl-1-(naphthalen-2-yl) prop-2-en-1-one, a potential chemotherapeutic agent
Chemistry Central Journal, (9) 2015.

Barakat, A.; Al-Najjar, H. J.; Al-Majid, A. M.; Soliman, S. M.; Mabkhot, Y. N.; Shaik, M. R.; Ghabbour, H. A.; Fun, H. K.
Synthesis, NMR, FT-IR, X-ray structural characterization, DFT analysis and isomerism aspects of 5-(2,6-dichlorobenzylidene)pyrimidine-2,4,6(1H,3H,5H)-trione
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (147): 107-116 2015.

Baranac-Stojanovic, M.; Aleksic, J.; Stojanovic, M.
Energy decomposition analysis of gauche preference in 2-haloethanol, 2-haloethylamine (halogen = F, Cl), their protonated forms and anti preference in 1-chloro-2-fluoroethane
Rsc Advances, (5): 22980-22995 2015.

Barik, S. K.; Dorcet, V.; Roisnel, T.; Halet, J. F.; Ghosh, S.
Synthesis and chemistry of the open-cage cobaltaheteroborane cluster {(eta(5)-C5Me5)Co}(2)B2H2Se2 : a combined experimental and theoretical study
Dalton Transactions, (44): 14403-14410 2015.

Barik, S. K.; Rao, C. E.; Yuvaraj, K.; Jagan, R.; Kahlal, S.; Halet, J. F.; Ghosh, S.
Electron-Precise 1,3-Bishomocubanes - A Combined Experimental and Theoretical Study
European Journal of Inorganic Chemistry: 5556-5562 2015.

Barone, V.; Bellina, F.; Biczysko, M.; Bloino, J.; Fornaro, T.; Latouche, C.; Lessi, M.; Marianetti, G.; Minei, P.; Panattoni, A.; Pucci, A.
Toward the design of alkynylimidazole fluorophores: computational and experimental characterization of spectroscopic features in solution and in poly(methyl methacrylate)
Physical Chemistry Chemical Physics, (17): 26710-26723 2015.

Bartocci, A.; Belpassi, L.; Cappelletti, D.; Falcinelli, S.; Grandinetti, F.; Tarantelli, F.; Pirani, F.
Catching the role of anisotropic electronic distribution and charge transfer in halogen bonded complexes of noble gases
Journal of Chemical Physics, (142) 2015.

Baskar, A. J. A.; Kumar, R.; Solomon, R. V.; Sundararajan, M.; Kannappan, V.; Singh, D. R.; Jaccob, M.
Ultrasonic, spectrophotometric and theoretical studies of sigma and PI interactions of iodine with substituted benzene
Rsc Advances, (5): 44873-44885 2015.

Batista, M. L. S.; Perez-Sanchez, G.; Gomes, J. R. B.; Coutinho, J. A. P.; Maginn, E. J.
Evaluation of the GROMOS 56A(CARBO) Force Field for the Calculation of Structural, Volumetric, and Dynamic Properties of Aqueous Glucose Systems
Journal of Physical Chemistry B, (119): 15310-15319 2015.

Bauza, A.; Frontera, A.
Aerogen Bonding Interaction: A New Supramolecular Force?
Angewandte Chemie-International Edition, (54): 7340-7343 2015.

Bauza, A.; Frontera, A.
pi-Hole aerogen bonding interactions
Physical Chemistry Chemical Physics, (17): 24748-24753 2015.

Bauza, A.; Frontera, A.
Theoretical Study on the Dual Behavior of XeO3 and XeF4 toward Aromatic Rings: Lone Pair-pi versus Aerogen-pi Interactions
Chemphyschem, (16): 3625-3630 2015.

Bauza, A.; Frontera, A.

Unveiling NO2 pi center dot center dot center dot C=C pi-hole interactions: A combined computational and crystallographic study
Chemical Physics Letters, (633): 282-286 2015.

Bazzi, S.; Novotny, J.; Yurenko, Y. P.; Marek, R.
Designing a New Class of Bases for Nucleic Acid Quadruplexes and Quadruplex-Active Ligands
Chemistry-a European Journal, (21): 9414-9425 2015.

Behjatmanesh-Ardakani, R.
NBO-NEDA, NPA, and QTAIM studies on the interactions between aza-, diaza-, and triaza-12-crown-4 (A(n)-12-crown-4, n=1, 2, 3) and Li+, Na+, and K+ ions
Computational and Theoretical Chemistry, (1051): 62-71 2015.

Bellow, J. A.; Yousif, M.; Fang, D.; Kratz, E. G.; Cisneros, G. A.; Groysman, S.
Synthesis and Reactions of 3d Metal Complexes with the Bulky Alkoxide Ligand (OCBu2Ph)-Bu-t
Inorganic Chemistry, (54): 5624-5633 2015.

Belskaya, N. P.; Lesogorova, S. G.; Subbotina, J. O.; Koksharov, A. V.; Slepukhin, P. A.; Dehaen, W.; Bakulev, V. A.
1,3-Dipolar cycloaddition of 3-alkylsulfanyl-2-arylazo-3-(tert-cycloalkylamino)acrylonitriles with N-methyl- and N-phenylmaleimides
Tetrahedron, (71): 1438-1447 2015.

Belyakov, A. V.; Gureev, M. A.; Garabadzhiu, A. V.; Losev, V. A.; Rykov, A. N.
Determination of the molecular structure of gaseous proline by electron diffraction, supported by microwave and quantum chemical data
Structural Chemistry, (26): 1489-1500 2015.

Belyakov, A. V.; Sigolaev, Y.; Shlykov, S. A.; Wallevik, S. O.; Jonsdottir, N. R.; Bjornsson, R.; Jonsdottir, S.; Kvaran, A.; Kern, T.; Hassler, K.; Arnason, I.
Conformational properties of 1-tert-butyl-1-silacyclohexane, C5H10SiH(t-Bu): gas-phase electron diffraction, temperature-dependent Raman spectroscopy, and quantum chemical calculations
Structural Chemistry, (26): 445-453 2015.

Benchouk, W.; Mekelleche, S. M.
Regio- and diastereoselectivity of the 1,3-dipolar cycloaddition of alpha-aryl nitrone with methacrolein. A theoretical investigation
Rsc Advances, (5): 22126-22134 2015.

Benhamada, N.; Bouchene, R.; Bouacida, S.; Zouchoune, B.
Molecular structure, bonding analysis and redox properties of transition metal-Hapca bis(3-aminopyrazine-2-carboxylic acid) complexes: A theoretical study
Polyhedron, (91): 59-67 2015.

Berardozzi, R.; Di Bari, L.
Optical Activity in the Near-IR Region: The=980 nm Multiplet of Chiral Yb3+ Complexes
Chemphyschem, (16): 2868-2875 2015.

Berger, G.; Fusaro, L.; Luhmer, M.; Czapla-Masztafiak, J.; Lipiec, E.; Szlachetko, J.; Kayser, Y.; Fernandes, D. L. A.; Sa, J.; Dufrasne, F.; Bombard, S.
Insights into the structure-activity relationships of chiral 1,2-diaminophenylalkane platinum(II) anticancer derivatives
Journal of Biological Inorganic Chemistry, (20): 841-853 2015.

Beryozkina, T. V.; Efimov, I. V.; Fabian, W. M. F.; Beliaev, N. A.; Slepukhin, P. A.; Isenov, M. L.; Dehaen, W.; Lubec, G.; Eltsov, O. S.; Fan, Z.; Thomas, J.; Bakulev, V. A.
Reactivity of 1,2,3-triazoles towards sulfonyl chlorides. A novel approach to 1-and 2-sulfonyl-4-azolyl-1,2,3-triazoles
Tetrahedron, (71): 6189-6195 2015.

Bezpalko, M. W.; Foxman, B. M.; Thomas, C. M.

Use of a Bidentate Ligand Featuring an N-Heterocyclic Phosphenium Cation (NHP+) to Systematically Explore the Bonding of NHP+ Ligands with Nickel
Inorganic Chemistry, (54): 8717-8726 2015.

Bhardwaj, S.; Rai, S.; Sau, T. K.; Singh, H.
Theoretical studies of Raman scattering properties of methylphosphine and methylamine adsorbed on gold clusters
Vibrational Spectroscopy, (76): 38-47 2015.

Bhargava, M.; Maheshwari, P.; Kour, M.; Bansal, R. K.
Fluxional behaviour of tricyclo 2.2.1.0(2,6) heptaphosphide trisanion: a DFT investigation
Zeitschrift Fur Naturforschung Section B-a Journal of Chemical Sciences, (70): 871-878 2015.

Bhattacherjee, A.; Matsuda, Y.; Fujii, A.; Wategaonkar, S.
Acid-Base Formalism in Dispersion-Stabilized S-H center dot center dot center dot Y (Y=O,S) Hydrogen-Bonding Interactions
Journal of Physical Chemistry A, (119): 1117-1126 2015.

Bhavani, K.; Renuga, S.; Muthu, S.; Narayanan, K. S.
Quantum mechanical study and spectroscopic (FT-IR, FT-Raman, C-13, H-1) study, first order hyperpolarizability, NBO analysis, HOMO and LUMO analysis of 2-acetoxybenzoic acid by density functional methods
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (136): 1260-1268 2015.

Bhowmick, D.; Mugesh, G.
Introduction of a catalytic triad increases the glutathione peroxidase-like activity of diaryl diselenides
Organic & Biomolecular Chemistry, (13): 9072-9082 2015.

Bickelhaupt, F. M.; Sola, M.; Fernandez, I.
Understanding the Reactivity of Endohedral Metallofullerenes: C-78 versus Sc3N@C-78
Chemistry-a European Journal, (21): 5760-5768 2015.

Billes, F.; Eleckova, L.; Mikosch, H.; Andruch, V.
Vibrational spectroscopic study of dehydroacetic acid and its cinnamoyl pyrone derivatives
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (146): 97-112 2015.

Binder, J. F.; Swidan, A.; Tang, M.; Nguyen, J. H.; Macdonald, C. L. B.
Remarkably stable chelating bis-N-heterocyclic carbene adducts of phosphorus(I) cations
Chemical Communications, (51): 7741-7744 2015.

Biswal, H. S.; Bhattacharyya, S.; Bhattacherjee, A.; Wategaonkar, S.
Nature and strength of sulfur-centred hydrogen bonds: laser spectroscopic investigations in the gas phase and quantum-chemical calculations
International Reviews in Physical Chemistry, (34): 99-160 2015.

Biswas, B.; Singh, P. C.
Effect of hydration on the organo-noble gas molecule HKrCCH: role of krypton in the stabilization of hydrated HKrCCH complexes
Physical Chemistry Chemical Physics, (17): 30632-30641 2015.

Bogdan, E.; Compain, G.; Mtashobya, L.; Le Questel, J. Y.; Besseau, F.; Galland, N.; Linclau, B.; Graton, J.
Influence of Fluorination on the Conformational Properties and Hydrogen-Bond Acidity of Benzyl Alcohol Derivatives
Chemistry-a European Journal, (21): 11462-11474 2015.

Boixel, J.; Guerchais, V.; Le Bozec, H.; Chantzis, A.; Jacquemin, D.; Colombo, A.; Dragonetti, C.; Marinotto, D.; Robertode, D.
Sequential double second-order nonlinear optical switch by an acido-triggered photochromic cyclometallated platinum(II) complex
Chemical Communications, (51): 7805-7808 2015.

Bolano, T.; Esteruelas, M. A.; Fernandez, I.; Onate, E.; Palacios, A.; Tsai, J. Y.; Xia, C. J.

Osmium(II)-Bis(dihydrogen) Complexes Containing C-aryl,C-NHC- Chelate Ligands: Preparation, Bonding Situation, and Acidity
Organometallics, (34): 778-789 2015.

Boobalan, M. S.; Amaladasan, M.; Ramalingam, S.; Tamilvendan, D.; Prabhu, G. V.; Bououdina, M.
First principles and DFT supported investigations on vibrational spectra and electronic structure of 2-((phenylamino)methyl)isoindoline-1, 3-dione - An antioxidant active Mannich
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (137): 962-978 2015.

Boobalan, M. S.; Tamilvendan, D.; Amaladasan, M.; Ramalingam, S.; Prabhu, G. V.; Bououdina, M.
Vibrational spectra and electronic structure of 3-((1H-pyrrol-1-yl) methyl) naphthalen-2-ol - A computational insight on antioxidant active Mannich base
Journal of Molecular Structure, (1081): 159-174 2015.

Boopathi, S.; Kolandaivel, P.
Study on the inter- and intra-peptide salt-bridge mechanism of A beta(23-28) oligomer interaction with small molecules: QM/MM method
Molecular Biosystems, (11): 2031-2041 2015.

Borgohain, R.; Guha, A. K.; Pratihar, S.; Handique, J. G.
Antioxidant activity of some phenolic aldehydes and their diimine derivatives: A DFT study
Computational and Theoretical Chemistry, (1060): 17-23 2015.

Borocci, S.; Cecchi, P.; Giordani, M.; Grandinetti, F.
Complexes of the noble gases with H3O+: a theoretical investigation of Ng(H3O+) (Ng = He-Xe)
European Journal of Mass Spectrometry, (21): 171-181 2015.

Borocci, S.; Giordani, M.; Grandinetti, F.
Complexes of XeHXe+ with Simple Ligands: A Theoretical Investigation on (XeHXe+) (L = N-2, CO, H2O, NH3)
Journal of Physical Chemistry A, (119): 2383-2392 2015.

Borpuzari, M. P.; Guha, A. K.; Kar, R.
Structural, electronic and reactivity studies on group 15 analogues of N-heterocyclic carbene
Structural Chemistry, (26): 859-871 2015.

Borthakur, B.; Phukan, A. K.
Moving toward Ylide-Stabilized Carbenes
Chemistry-a European Journal, (21): 11603-11609 2015.

Boshra, A.; Oliaey, A. R.; Rezaie, F.; Bazvand, Y.; Hamid, S. B. A.
Novel cations of xenon trifluoroborazine complexes: Structures, reactivities, and natural bonding orbital analysis
Journal of Fluorine Chemistry, (178): 99-106 2015.

Bouchet, A.; Klyne, J.; Piani, G.; Dopfer, O.; Zehnacker, A.
Diastereo-specific conformational properties of neutral, protonated and radical cation forms of (1R,2S)-cis- and (1R,2R)-trans-amino-indanol by gas phase spectroscopy
Physical Chemistry Chemical Physics, (17): 25809-25821 2015.

Bourque, J. L.; Boyle, P. D.; Baines, K. M.
Synthesis and Characterization of Cationic Low-Valent Gallium Complexes of Cryptand 2.2.2
Chemistry-a European Journal, (21): 9790-9796 2015.

Bousquet, B.; Cherif, M.; Huang, K. Q.; Rabilloud, F.
Absorption Spectra of Aryl Thiol-Coated Silver Nanoclusters: A Time-Dependent Density-Functional Study
Journal of Physical Chemistry C, (119): 4268-4277 2015.

Bouten, P. J. M.; Hertsen, D.; Vergaelen, M.; Monnery, B. D.; Boerman, M. A.; Goossens, H.; Catak, S.; van Hest, J. C. M.; Van Speybroeck, V.; Hoogenboom, R.

Accelerated living cationic ring-opening polymerization of a methyl ester functionalized 2-oxazoline monomer
Polymer Chemistry, (6): 514-518 2015.

Braga, C. B.; Ducati, L. C.; Rittner, R.
Experimental and theoretical evaluation on the conformational behavior of L-aspartic acid dimethyl ester and its N-acetylated derivative
Rsc Advances, (5): 18013-18024 2015.

Brahmachari, G.; Kumar, A.; Srivastava, A. K.; Gangwar, S.; Misra, N.; Gupta, V. K.; Rajnikant
Synthesis, spectroscopic characterization, X-ray analysis and theoretical studies on the spectral features (FT-IR, H-1-NMR), chemical reactivity, NBO analyses of 2-(4-fluorophenyl)-2-(4-fluorophenylamino)acetonitrile and its docking into IDO enzyme
Rsc Advances, (5): 80967-80977 2015.

Branzanic, A. M. V.; Lupan, A.; King, R. B.
Dimetallaborane analogues of pentaborane
Dalton Transactions, (44): 7355-7363 2015.

Branzanic, A. M. V.; Lupan, A.; King, R. B.
The Wade Mingos rules in seven-vertex dimetallaborane chemistry: Hydrogen-rich Cp2M2B5H9 systems of the second and third row transition metals
Journal of Organometallic Chemistry, (792): 74-80 2015.

Braunschweig, H.; Celik, M. A.; Dewhurst, R. D.; Heid, M.; Hupp, F.; Sen, S. S.
Stepwise isolation of low-valent, low-coordinate Sn and Pb mono- and dications in the coordination sphere of platinum
Chemical Science, (6): 425-435 2015.

Brea, O.; Mo, O.; Yanez, M.
Ga+ Basicity and Affinity Scales Based on High-Level AbInitio Calculations
Chemphyschem, (16): 3206-3213 2015.

Brea, O.; Mo, O.; Yanez, M.; Alkorta, I.; Elguero, J.
Creating sigma-Holes through the Formation of Beryllium Bonds
Chemistry-a European Journal, (21): 12676-12682 2015.

Brovarets, O. O.; Yurenko, Y. P.; Hovorun, D. M.
The significant role of the intermolecular CHMIDLINE HORIZONTAL ELLIPSISO/N hydrogen bonds in governing the biologically important pairs of the DNA and RNA modified bases: a comprehensive theoretical investigation
Journal of Biomolecular Structure and Dynamics, (33): 1624-1652 2015.

Bruna, S.; Martinez-Montero, I.; Gonzalez-Vadillo, A. M.; Martin-Fernandez, C.; Montero-Campillo, M. M.; Mo, O.; Cuadrado, I.
Ferrocene and Silicon-Containing Oxathiacrown Macrocycles and Linear Oligo-Oxathioethers Obtained via Thiol-Ene Chemistry of a Redox-Active Bifunctional Vinyldisiloxane
Macromolecules, (48): 6955-6969 2015.

Buchalski, P.; Pacholski, R.; Shkurenko, A.; Suwinska, K.
Novel, axially chiral analogues of nickelocene with nickeladibenzofluorenyl ligand
Journal of Organometallic Chemistry, (785): 26-31 2015.

Bueno, M. A.; Oliveira, B. G.
THE INFLUENCE OF H-BONDS ON CHEMICAL REACTIONS: PRILESCHAJEW REACTION
Quimica Nova, (38): 1-7 2015.

Bultinck, P.; Jayatilaka, D.; Cardenas, C.
A problematic issue for atoms in molecules: Impact of (quasi-)degenerate states on Quantum Theory Atoms in Molecules and Hirshfeld-I properties
Computational and Theoretical Chemistry, (1053): 106-111 2015.

Buszek, R. J.; Boatz, J. A.
On the Comparison of Small Nitrogen and Phosphorus Oxide Cages
Propellants Explosives Pyrotechnics, (40): 803-807 2015.

Cagide, F.; Borges, F.; Gomes, L. R.; Low, J. N.
Synthesis and characterisation of new 4-oxo-N-(substituted-thiazol-2-yl)-4H-chromene-2-carboxamides as potential adenosine receptor ligands
Journal of Molecular Structure, (1089): 206-215 2015.

Calderon, L. A.; Garza, J.; Espinal, J. F.
Theoretical Study of Sodium Effect on the Gasification of Carbonaceous Materials with Carbon Dioxide
Journal of Physical Chemistry A, (119): 12756-12766 2015.

Calichman, M.; Allen, C. W.
ORGANOPHOPHAZENES 28: THE NATURE OF THE EXOCYCLIC PHOSPHORUS-CARBON BOND IN ORGANOPHOSPHAZENES
Phosphorus Sulfur and Silicon and the Related Elements, (190): 2110-2115 2015.

Campanelli, A. R.; Domenicano, A.
Transmission of electronic substituent effects along polyenic chains: a quantum chemical study based on structural variation and pi-charge distribution
Structural Chemistry, (26): 1259-1271 2015.

Campanelli, A. R.; Domenicano, A.; Hnyk, D.
Transmission of Electronic Substituent Effects across the 1,12-Dicarba-doso-dodecaborane Cage: A Computational Study Based on Structural Variation, Atomic Charges, and C-13 NMR Chemical Shifts
Journal of Physical Chemistry A, (119): 205-214 2015.

Cao, G. J.; Schwarz, W. H. E.; Li, J.
An 18-Electron System Containing a Superheavy Element: Theoretical Studies of Sg@Au-12
Inorganic Chemistry, (54): 3695-3701 2015.

Cao, J. S.; Ren, Q.; Chen, F. W.; Lu, T.
Comparative study on the methods for predicting the reactive site of nucleophilic reaction
Science China-Chemistry, (58): 1845-1852 2015.

Cao, W.; Tian, D. X.; Han, D. X.
DFT studies on the palladium-catalyzed dearomatization reaction between naphthalene allyl chloride and allyltributylstannane
Journal of Molecular Modeling, (21) 2015.

Caramori, G. F.; Ortolan, A. O.; Parreira, R. L. T.; da Silva, E. H.
Ruthenium nitrosyl complexes containing pyridine-functionalized carbenes - A theoretical insight
Journal of Organometallic Chemistry, (799-800): 54-60 2015.

Caramori, G. F.; Piccoli, R. M.; Segala, M.; Munoz-Castro, A.; Guajardo-Maturana, R.; Andrada, D. M.; Frenking, G.
Cyclic trinuclear copper(I), silver(I), and gold(I) complexes: a theoretical insight
Dalton Transactions, (44): 377-385 2015.

Cardoso, B. D.; Royo, B.; Calhorda, M. J.
Preference for sulfoxide S- or O-bonding to 3d transition metals - DFT insights
Journal of Organometallic Chemistry, (792): 167-176 2015.

Carrizo, E. D. S.; Bickelhaupt, F. M.; Fernandez, I.
Factors Controlling beta-Elimination Reactions in Group 10 Metal Complexes
Chemistry-a European Journal, (21): 14362-14369 2015.

Carrizo, E. D. S.; Fernandez, I.; Martin, S. E.

Computational Study on the C-Heteroatom Bond Formation via Stille Cross-Coupling Reaction: Differences between Organoheterostannanes Me3SnAsPh2 vs Me3SnPPh2
Organometallics, (34): 159-166 2015.

Carvalho, A. T. P.; O'Donoghue, A. C.; Hodgson, D. R. W.; Kamerlin, S. C. L.
Understanding thio-effects in simple phosphoryl systems: role of solvent effects and nucleophile charge
Organic & Biomolecular Chemistry, (13): 5391-5398 2015.

Castillo, M. V.; Pergomet, J. L.; Carnavale, G. A.; Davies, L.; Zinczuk, J.; Brandan, S. A.
A complete vibrational study on a potential environmental toxicant agent, the 3,3 ',4,4 '-tetrachloroazobenzene combining the FTIR, FTRaman, UV-Visible and NMR spectroscopies with DFT calculations
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (134): 577-586 2015.

Castro, L.; Kirillov, E.; Miserque, O.; Welle, A.; Haspeslagh, L.; Carpentier, J. F.; Maron, L.
Are Solvent and Dispersion Effects Crucial in Olefin Polymerization DFT Calculations? Some Insights from Propylene Coordination and Insertion Reactions with Group 3 and 4 Metallocenes
Acs Catalysis, (5): 416-425 2015.

Cazacu, M.; Shova, S.; Soroceanu, A.; Machata, P.; Bucinsky, L.; Breza, M.; Rapta, P.; Telser, J.; Krzystek, J.; Arion, V. B.
Charge and Spin States in Schiff Base Metal Complexes with a Disiloxane Unit Exhibiting a Strong Noninnocent Ligand Character: Synthesis, Structure, Spectroelectrochemistry, and Theoretical Calculations
Inorganic Chemistry, (54): 5691-5706 2015.

Cebollada, A.; Viguri, M. E.; Perez, J.; Diaz, J.; Lopez, R.; Riera, L.
Influence of the N-N Coligand: C-C Coupling Instead of Formation of Imidazol-2-yl Complexes at {Mo(eta(3)-allyl)(CO)(2)} Fragments. Theoretical and Experimental Studies
Inorganic Chemistry, (54): 2580-2590 2015.

Cerqueira, C. R.; Olivato, P. R.; Rodrigues, D. N. S.; Zukerman-Schpector, J.; Tiekink, E. R. T.; Dal Colle, M.
Conformational study of some 4 '-substituted 2-(phenylselanyl)-2-(ethylsulfonyl)-acetophenones
Journal of Molecular Structure, (1084): 190-199 2015.

Ceylan, U.; Durgun, M.; Turkmen, H.; Yalcin, S. P.; Kilic, A.; Ozdemir, N.
Theoretical and experimental investigation of 4- (2-hydroxy-3-methylbenzylidene)amino benzenesulfonamide: Structural and spectroscopic properties, NBO, NLO and NPA analysis
Journal of Molecular Structure, (1089): 222-232 2015.

Chain, F. E.; Leyton, P.; Paipa, C.; Fortuna, M.; Brandan, S. A.
FT-IR, FT-Raman, UV-Visible, and NMR spectroscopy and vibrational properties of the labdane-type diterpene 13-epi-sclareol
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (138): 303-313 2015.

Chain, F. E.; Romano, E.; Leyton, P.; Paipa, C.; Catalan, C. A. N.; Fortuna, M.; Brandan, S. A.
Vibrational and structural study of onopordopicrin based on the FTIR spectrum and DFT calculations
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (150): 381-389 2015.

Chalmers, B. A.; Buhl, M.; Arachchige, K. S. A.; Slawin, A. M. Z.; Kilian, P.
Structural, Spectroscopic and Computational Examination of the Dative Interaction in Constrained Phosphine-Stibines and Phosphine-Stiboranes
Chemistry-a European Journal, (21): 7520-7531 2015.

Chamorro, E.; Duque-Norena, M.
Understanding the Highly Varying pK(a) of Arylamines. A Perspective from the Average Local Ionization Condensed-to-Atom Framework
Journal of Physical Chemistry A, (119): 8156-8162 2015.

Chand, S.; Al-Omary, F. A. M.; El-Emam, A. A.; Shukla, V. K.; Prasad, O.; Sinha, L.
Study on molecular structure, spectroscopic behavior, NBO, and NLO analysis of 3-methylbezothiazole-2-thione

Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (146): 129-141 2015.

Chandrasekaran, K.; Kumar, R. T.
Structural, spectral, thermodynamical, NLO, HOMO, LUMO and NBO analysis of fluconazole
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (150): 974-991 2015.

Chen, C.; Liu, Y. L.; Zhang, J.; Zhang, M. Z.; Zheng, J.; Teng, Y.; Liang, G. Z.
A quantitative sequence-aggregation relationship predictor applied as identification of self-assembled hexapeptides
Chemometrics and Intelligent Laboratory Systems, (145): 7-16 2015.

Chen, D. M.; Gau, M. R.; Dobereiner, G. E.
Palladium and Platinum Acyl Complexes and Their Lewis Acid Adducts. Experimental and Computational Study of Thermodynamics and Bonding
Organometallics, (34): 4069-4075 2015.

Chen, F.; Wang, C. Z.; Li, Z. J.; Lan, J. H.; Ji, Y. Q.; Chai, Z. F.
New Three-Fold Interpenetrated Uranyl Organic Framework Constructed by Terephthalic Acid and Imidazole Derivative
Inorganic Chemistry, (54): 3829-3834 2015.

Chen, H.; Lin, W. Y.; Cui, H. J.; Jiang, W. Q.
Development of Unique Xanthene-Cyanine Fused Near-Infrared Fluorescent Fluorophores with Superior Chemical Stability for Biological Fluorescence Imaging
Chemistry-a European Journal, (21): 733-745 2015.

Chen, J. L.; Liu, Z. G.; Feng, H.; Xie, Y. M.; King, R. B.
Binuclear 1,2-diaza-3,5-diborolyl iron carbonyls: Effect of replacing ring CC units with isoelectronic BN units
Inorganica Chimica Acta, (425): 169-175 2015.

Chen, M. Y.; Serna, P.; Lu, J.; Gates, B. C.; Dixon, D. A.
Molecular models of site-isolated cobalt, rhodium, and iridium catalysts supported on zeolites: Ligand bond dissociation energies
Computational and Theoretical Chemistry, (1074): 58-72 2015.

Chen, P. Y.; Zhang, L.; Zhu, S. G.; Cheng, G. B.
Intermolecular interactions, thermodynamic properties, crystal structure, and detonation performance of CL-20/TEX cocrystal explosive
Canadian Journal of Chemistry, (93): 632-638 2015.

Chen, R.; Luo, X. L.; Liang, G. M.
Theoretical studies on the aminolysis mechanism of propylene carbonate with ammonia
Theoretical Chemistry Accounts, (134) 2015.

Chen, R.; Zhou, W. H.; Wu, Z. W.; Xu, X.; Xu, Z. G.
Theoretical Study on the Structures and Magnetic Properties of Metal String Complexes Ni-3(L)(4)(NCS)(2) (L = dpa(-), mpta(-), mdpa(-), mppa(-))
Acta Physico-Chimica Sinica, (31): 1683-1689 2015.

Chen, S.; Yang, H. Q.; Hu, C. W.
Theoretical study on the reaction mechanisms of the aldol-condensation of 5-hydroxymethylfurfural with acetone catalyzed by MgO and MgO+
Catalysis Today, (245): 100-107 2015.

Chen, Y. S.; Wang, F.
Theoretical study of interactions between electron-deficient arenes and coinage metal anions
Journal of Molecular Modeling, (21) 2015.

Chermahini, Z. J.; Chermahini, A. N.; Dabbagh, H. A.; Teimouri, A.
Complexation of all-cis cyclo(L-Pro)(3) and alkali metal cations: a DFT study

Journal of Inclusion Phenomena and Macrocyclic Chemistry, (81): 465-473 2015.

Chermahini, Z. J.; Chermahini, A. N.; Dabbagh, H. A.; Teimouri, A.
Metal ion binding of s-block cations and nanotubular cyclic (proline)(4): A theoretical study
Structural Chemistry, (26): 675-684 2015.

Chernikova, I. B.; Khursan, S. L.; Yunusov, M. S.; Yumagulov, R. A.
Chlorination of 5-nitro-6-methyluracil and its N(1),N(3)-dimethyl analogue with molecular chlorine
Mendeleev Communications, (25): 221-223 2015.

Chernyshev, V. M.; Vlasova, A. G.; Astakhov, A. V.; Shishkina, S. V.; Shishkin, O. V.
Reactivity of C-Amino-1,2,4-triazoles toward Electrophiles: A Combined Computational and Experimental Study of Alkylation by Halogen Alkanes
Journal of Organic Chemistry, (80): 375-385 2015.

Chethana, B. K.; Lee, D.; Mushrif, S. H.
First principles investigation into the metal catalysed 1,2 carbon shift reaction for the epimerization of sugars
Journal of Molecular Catalysis a-Chemical, (410): 66-73 2015.

Chiniforoshan, H.; Khalesi, S. B.; Tabrizi, L.; Hajipour, A. R.; Chermahini, A. N.; Karimzadeh, M.
Silver nanoparticles with 4,4 '-dicyanamidobiphenyl ligand: Synthesis, photoluminescent and electroluminescent properties and DFT calculations
Journal of Molecular Structure, (1082): 56-61 2015.

Chiniforoshan, H.; Radani, Z. S.; Tabrizi, L.; Tavakol, H.; Sabzalian, M. R.; Mohammadnezhad, G.; Gorls, H.; Plass, W.
Pyrazinamide drug interacting with Co(III) and Zn(II) metal ions based on 2,2 '-bipyridine and 1,10-phenanthroline ligands: Synthesis, studies and crystal structure, DFT calculations and antibacterial assays
Journal of Molecular Structure, (1081): 237-243 2015.

Chipanina, N. N.; Lazareva, N. F.; Oznobikhina, L. P.; Lazarev, I. M.; Shainyan, B. A.
The hydrolysis of (O-Si)-chelate N-(acetamido)methyl dimethylchlorosilanes. DFT and MP2 study, QTAIM and NBO analysis
Computational and Theoretical Chemistry, (1070): 162-173 2015.

Chitradevi, A.; Kumar, S. S.; Athimoolam, S.; Bahadur, S. A.; Sridhar, B.
Single crystal XRD, vibrational spectra, quantum chemical and thermal studies on a new semi-organic crystal: 4-Aminium antipyrine chloride
Journal of Molecular Structure, (1099): 58-67 2015.

Cho, B. K.; Wong, M. W.
Unconventional Bifunctional Lewis-Bronsted Acid Activation Mode in Bicyclic Guanidine-Catalyzed Conjugate Addition Reactions
Molecules, (20): 15108-15121 2015.

Cho, H. G.; Andrews, L.
Infrared spectra of M-eta(2)-C2H2 and HM-CCH produced in reactions of laser-ablated Fe and Os atoms with acetylene
Journal of Molecular Spectroscopy, (310): 84-91 2015.

Cho, H. G.; Andrews, L.
Infrared Spectra of Planar and Agostic-Like Bridged Scandium Methylidene Complexes Prepared in Reactions of Laser-Ablated Sc Atoms with Di-, Tri-, and Tetrahalomethanes
Organometallics, (34): 3390-3399 2015.

Cho, H. G.; Andrews, L.
IR Spectra and DFT Calculations of M-(2)-(NC)-CH3, CH3-MNC, and CH2=M(H)NC Prepared by Reactions of Laser-Ablated Hf and Ti Atoms with Acetonitrile
European Journal of Inorganic Chemistry: 4379-4387 2015.

Cho, H. G.; Andrews, L.
Matrix Infrared Spectra and Density Functional Calculations of CH2Cl-Cl and CH2Br-Br Produced by Laser-ablated Metal Plume Irradiation
Bulletin of the Korean Chemical Society, (36): 1580-1585 2015.

Choudhary, A.; Kamer, K. J.; Shoulders, M. D.; Raines, R. T.
4-Ketoproline: An Electrophilic Proline Analog for Bioconjugation
Biopolymers, (104): 110-115 2015.

Chowdhury, M. A. H.; Rajbangshi, S.; Karim, M.; Ghosh, S.; Kabir, S. E.; Siddiquee, T. A.; Nesterov, V. N.; Richmond, M. G.
Reactivity of CpMo(CO)(2) (2) towards heterocyclic thiols: Synthesis, structure, and bonding in the sulfido-ligated cluster Cp3Mo3(mu-CO)(2)(mu-kappa(2)-C7H4NS)(mu-S)(mu(3)-S)
Inorganica Chimica Acta, (434): 97-103 2015.

Chu, K. T.; Liu, Y. C.; Huang, Y. L.; Lee, G. H.; Tseng, M. C.; Chiang, M. H.
Redox Communication within Multinuclear Iron-Sulfur Complexes Related to Electronic Interplay in the Active Site of FeFe Hydrogenase
Chemistry-a European Journal, (21): 6852-6861 2015.

Cinar, M.; Karabacak, M.; Chand, S.; Shukla, V. K.; Sinha, L.; Prasad, O.; Singh, M. P.; Asiri, A. M.
Conformational and spectroscopic behaviors of 2,4-xylyl isothiocyanate
Journal of Molecular Structure, (1087): 113-120 2015.

Clark, A. E.; Samuels, A.; Wisuri, K.; Landstrom, S.; Saul, T.
Sensitivity of Solvation Environment to Oxidation State and Position in the Early Actinide Period
Inorganic Chemistry, (54): 6216-6225 2015.

Clark, T.; Politzer, P.; Murray, J. S.
Correct electrostatic treatment of noncovalent interactions: the importance of polarization
Wiley Interdisciplinary Reviews-Computational Molecular Science, (5): 169-177 2015.

Clauss, A. D.; Ayoub, M.; Moore, J. W.; Landis, C. R.; Weinhold, F.
Rabbit ears concepts of water lone pairs: a reply to comments of Hiberty, Danovich, and Shaik
Chemistry Education Research and Practice, (16): 694-696 2015.

Clough, M. T.; Crick, C. R.; Grasvik, J.; Hunt, P. A.; Niedermeyer, H.; Welton, T.; Whitaker, O. P.
A physicochemical investigation of ionic liquid mixtures
Chemical Science, (6): 1101-1114 2015.

Collins, M. A.; Bettens, R. P. A.
Energy-Based Molecular Fragmentation Methods
Chemical Reviews, (115): 5607-5642 2015.

Cooper, M.; Wagner, A.; Wondrousch, D.; Sonntag, F.; Sonnabend, A.; Brehm, M.; Schuurmann, G.; Adrian, L.
Anaerobic Microbial Transformation of Halogenated Aromatics and Fate Prediction Using Electron Density Modeling
Environmental Science & Technology, (49): 6018-6028 2015.

Cooper, R. J.; Heiles, S.; Williams, E. R.
Effects of electronic structure on the hydration of PbNO3+ and SrNO3+ ion pairs
Physical Chemistry Chemical Physics, (17): 15963-15975 2015.

Corbey, J. F.; Woen, D. H.; Palumbo, C. T.; Fieser, M. E.; Ziller, J. W.; Furche, F.; Evans, W. J.
Ligand Effects in the Synthesis of Ln(2+) Complexes by Reduction of Tris(cyclopentadienyl) Precursors Including C-H Bond Activation of an Indenyl Anion
Organometallics, (34): 3909-3921 2015.

Cormanich, R. A.; Buhl, M.; Rittner, R.
Understanding the conformational behaviour of Ac-Ala-NHMe in different media. A joint NMR and DFT study

Organic & Biomolecular Chemistry, (13): 9206-9213 2015.

Cormanich, R. A.; Rittner, R.; Buhl, M.
Conformational preferences of Ac-Gly-NHMe in solution
Rsc Advances, (5): 13052-13060 2015.

Crandell, D. W.; Ghosh, S.; Berlinguette, C. P.; Baik, M. H.
How a Co-IV - O (2+) Fragment Oxidizes Water: Involvement of a Biradicaloid Co-II-(center dot O center dot) (2+) Species in Forming the O-O Bond
Chemsuschem, (8): 844-852 2015.

Crawford, L.; Cole-Hamilton, D. J.; Buhl, M.
Uncovering the Mechanism of Homogeneous Methyl Methacrylate Formation with P,N Chelating Ligands and Palladium: Favored Reaction Channels and Selectivities
Organometallics, (34): 438-449 2015.

Cruz, C. D.; Christensen, P. R.; Chronister, E. L.; Casanova, D.; Wolf, M. O.; Bardeen, C. J.
Sulfur-Bridged Terthiophene Dimers: How Sulfur Oxidation State Controls Interchromophore Electronic Coupling
Journal of the American Chemical Society, (137): 12552-12564 2015.

Cuerva, C.; Ovejero, P.; Torres, M. R.; Cano, M.; Campo, J. A.
Dicatenar pyridylpyrazoles: An opportunity to induce mesomorphism. Synthesis, X-ray characterisation and DFT calculations
Polyhedron, (100): 100-107 2015.

Cui, Y. L.; Zhao, H.; Zhao, J. F.; Li, P. Y.; Song, P.; Xia, L. X.
The excited-state multiple proton transfer mechanism of the 7-hydroxyquinoline-(CH3OH)(3) cluster
New Journal of Chemistry, (39): 9910-9917 2015.

Cui, Z. H.; Ding, Y. H.; Cabellos, J. L.; Osorio, E.; Islas, R.; Restrepo, A.; Merino, G.
Planar tetracoordinate carbons with a double bond in CAl3E clusters
Physical Chemistry Chemical Physics, (17): 8769-8775 2015.

Curado, N.; Carrasco, M.; Alvarez, E.; Maya, C.; Peloso, R.; Rodriguez, A.; Lopez-Serrano, J.; Carmona, E.
Lithium Di- and Trimethyl Dimolybdenum(II) Complexes with Mo-Mo Quadruple Bonds and Bridging Methyl Groups
Journal of the American Chemical Society, (137): 12378-12387 2015.

Dai, Y. F.; Qu, Y. X.; Wang, S.; Wang, J. D.
Structures and hydrogen bonding investigation of 1,3-dimethylimidazolium methylsulfate and 1,3-dimethylimidazolium dimethylphosphate with theoretical methods
Computational and Theoretical Chemistry, (1055): 33-41 2015.

Dai, Z. H.; Qiang, L.; Tang, L. M.; Guo, B. H.
A novel supramolecular polymer fabricated via stronger hydrogen-bonding interactions between substituted amide groups: design, synthesis, properties and mechanism
Rsc Advances, (5): 84104-84112 2015.

Dargent, D.; Zins, E. L.; MadebSne, B.; Alikhani, M. E.
Topological insights into the 1/1 diacetyl/water complex gained using a new methodological approach
Journal of Molecular Modeling, (21) 2015.

Das, K. G. V.; Panicker, C. Y.; Narayana, B.; Nayak, P. S.; Sarojini, B. K.; Al-Saadi, A. A.
FT-IR, molecular structure, first order hyperpolarizability, NBO analysis, HOMO and LUMO and MEP analysis of 1-(10H-phenothiazin-2-yl)ethanone by HF and density functional methods
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (135): 162-171 2015.

Das, M.; Ghosh, B. N.; Bauza, A.; Rissanen, K.; Frontera, A.; Chattopadhyay, S.

Observation of novel oxygen center dot center dot center dot oxygen interaction in supramolecular assembly of cobalt(III) Schiff base complexes: a combined experimental and computational study
Rsc Advances, (5): 73028-73039 2015.

Das, S.; Singh, H. B.; Butcher, R. J.
Isolation of organomercury(II) azides stabilized by intramolecular coordination
Journal of Organometallic Chemistry, (799-800): 184-194 2015.

Davis, J. G.; Zukowski, S. R.; Rankin, B. M.; Ben-Amotz, D.
Influence of a Neighboring Charged Group on Hydrophobic Hydration Shell Structure
Journal of Physical Chemistry B, (119): 9417-9422 2015.

de Aguiar, I.; Tavares, A.; Roveda, A. C.; da Silva, A. C. H.; Marino, L. B.; Lopes, E. O.; Pavan, F. R.; Lopes, L. G. F.; Franco, D. W.
Antitubercular activity of Ru (II) isoniazid complexes
European Journal of Pharmaceutical Sciences, (70): 45-54 2015.

de la Luz, A. P.; Mendez-Maldonado, G. A.; Nunez-Rojas, E.; Bresme, F.; Alejandre, J.
A New Force Field of Formamide and the Effect of the Dielectric Constant on Miscibility
Journal of Chemical Theory and Computation, (11): 2792-2800 2015.

de Melo, U. Z.; Silva, R. G. M.; Yamazaki, D. A. S.; Pontes, R. M.; Gauze, G. F.; Rosa, F. A.; Rittner, R.; Basso, E. A.
NMR Spectroscopy and Theoretical Calculations in the Conformational Analysis of 1-Methylpyrrolidin-2-one 3-Halo-derivatives
Journal of Physical Chemistry A, (119): 2111-2121 2015.

Deb, A. K. S.; Ali, S. M.; Shenoy, K. T.
Unanticipated favoured adsorption affinity of Th(IV) ions towards bidentate carboxylate functionalized carbon nanotubes (CNT-COOH) over tridentate diglycolamic acid functionalized CNT: density functional theoretical investigation
Rsc Advances, (5): 80076-80088 2015.

Deb, A. K. S.; Ali, S. M.; Shenoy, K. T.; Ghosh, S. K.
Adsorption of Eu3+ and Am3+ ion towards hard donor-based diglycolamic acid-functionalised carbon nanotubes: density functional theory guided experimental verification
Molecular Simulation, (41): 490-503 2015.

DeBackere, J. R.; Mercier, H. P. A.; Schrobilgen, G. J.
Pentafluoro-oxotellurate(VI) Anions of Mercury(II); Syntheses and Structures of Hg(OTeF5)(4) (2-), Hg(OTeF5)(5) (3-), Hg-2(OTeF5)(6) (2-), Hg(OTeF5)(4) (2-)center dot Hg(OTeF5)(2), and Hg-2(OTeF5)(7) (3-).Hg(OTeF5)(2)
Inorganic Chemistry, (54): 1606-1626 2015.

Deepha, V.; Praveena, R.; Sadasivam, K.
DFT studies on antioxidant mechanisms, electronic properties, spectroscopic (FT-IR and UV) and NBO analysis of C-glycosyl flavone, an isoorientin
Journal of Molecular Structure, (1082): 131-142 2015.

Deimler, R. E.; Sander, M.; Jackson, G. P.
Radical-induced fragmentation of phospholipid cations using metastable atom-activated dissociation mass spectrometry (MAD-MS)
International Journal of Mass Spectrometry, (390): 178-186 2015.

Del Bene, J. E.; Alkorta, I.; Elguero, J.
Can HN=NH, FN=NH, or HN=CHOH bridge the sigma-hole and the lone pair at P in binary complexes with H2XP, for X = F, Cl, NC, OH, CN, CCH, CH3, and H?
Physical Chemistry Chemical Physics, (17): 30729-30735 2015.

Del Bene, J. E.; Alkorta, I.; Elguero, J.
Exploring the (H2C=PH2)(+):N-Base Potential Surfaces: Complexes Stabilized by Pnicogen, Hydrogen, and Tetrel Bonds

Journal of Physical Chemistry A, (119): 11701-11710 2015.

Del Bene, J. E.; Alkorta, I.; Elguero, J.
P center dot center dot center dot N Pnicogen Bonds in Cationic Complexes of F4P+ and F3HP+ with Nitrogen Bases
Journal of Physical Chemistry A, (119): 3125-3133 2015.

Del Bene, J. E.; Alkorta, I.; Elguero, J.
Properties of Cationic Pnicogen-Bonded Complexes F4-nHnP+:N-Base with F-P center dot center dot center dot N Linear and n=0-3
Journal of Physical Chemistry A, (119): 5853-5864 2015.

Del Bene, J. E.; Alkorta, I.; Elguero, J.
Substituent Effects on the Properties of Pnicogen-Bonded Complexes H2XP:PYH2, for X, Y = F, Cl, OH, NC, CCH, CH3, CN, and H
Journal of Physical Chemistry A, (119): 224-233 2015.

Del Giacco, T.; Lanzalunga, O.; Lapi, A.; Mazzonna, M.; Mencarelli, P.
Photosensitized Oxidation of Aryl Benzyl Sulfoxides. Evidence for Nucleophilic Assistance to the C-S Bond Cleavage of Aryl Benzyl Sulfoxide Radical Cations
Journal of Organic Chemistry, (80): 2310-2318 2015.

del Rosal, I.; Brignou, P.; Guillaume, S. M.; Carpentier, J. F.; Maron, L.
DFT investigations on the ring-opening polymerization of substituted cyclic carbonates catalyzed by zinc-{beta-diketiminate} complexes
Polymer Chemistry, (6): 3336-3352 2015.

Del Rosal, I.; Gerber, I. C.; Poteau, R.; Maron, L.
Grafting of lanthanide complexes on silica surfaces dehydroxylated at 200 degrees C: a theoretical investigation
New Journal of Chemistry, (39): 7703-7715 2015.

Delgado-Camon, A.; Jarne, C.; Cebolla, V. L.; Larranaga, O.; de Cozar, A.; Cossio, F. P.; Vara, Y.; Dominguez, A.; Membrado, L.; Galban, J.; Garriga, R.
Resonance driven regioselective demethylation of berberine. Microwave assisted synthesis of berberrubine and its assessment as fluorescent chemosensor for alkanes
Tetrahedron, (71): 6148-6154 2015.

Della Rosa, C. D.; Mancini, P. M. E.; Kneeteman, M. N.; Baena, A. F. L.; Suligoy, M. A.; Domingo, L. R.
Polar Diels-Alder reactions using electrophilic nitrobenzothiophenes. A combined experimental and DFT study
Journal of Molecular Structure, (1079): 47-53 2015.

Demircioglu, Z.; Kastas, C. A.; Buyukgungor, O.
The spectroscopic (FT-IR, UV-vis), Fukui function, NLO, NBO, NPA and tautomerism effect analysis of (E)-2- (2-hydroxy-6-methoxybenzylidene)amino benzonitrile
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (139): 539-548 2015.

Demircioglu, Z.; Kastas, C. A.; Buyukgungor, O.
Theoretical analysis (NBO, NPA, Mulliken Population Method) and molecular orbital studies (hardness, chemical potential, electrophilicity and Fukui function analysis) of (E)-2-((4-hydroxy-2-methylphenylimino)methyl)-3-methoxyphenol
Journal of Molecular Structure, (1091): 183-195 2015.

Deng, J.; Wang, Y.; Yang, B.; Ma, Y. G.
Terahertz radiation from pentacene organic diode at room temperature
Chinese Optics Letters, (13) 2015.

Deng, J. S.; Lei, Y. H.; Wen, S. M.; Chen, Z. X.
Modeling interactions between ethyl xanthate and Cu/Fe ions using DFT/B3LYP approach
International Journal of Mineral Processing, (140): 43-49 2015.

Deng, X. J.; Kong, X. Y.; Xu, H. G.; Xu, X. L.; Feng, G.; Zheng, W. J.
Photoelectron Spectroscopy and Density Functional Calculations of VGen- (n=3-12) Clusters
Journal of Physical Chemistry C, (119): 11048-11055 2015.

Derikvand, Z.; Zabardasti, A.; Amini, N.
Theoretical investigation of H center dot center dot center dot F and H center dot center dot center dot H intermolecular interactions of nido-CB4H8 with HF molecule
Structural Chemistry, (26): 207-211 2015.

Derikvand, Z.; Zabardasti, A.; Azadbakht, A.
Theoretical study of intermolecular interactions in CB4H8-HOX (X = F, Cl, Br, I) complexes
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (150): 778-785 2015.

Devi, T. S. R.; Kumar, J. S.; Ramkumaar, G. R.
DFT analysis on the molecular structure, vibrational and electronic spectra of 2-(cyclohexylamino)ethanesulfonic acid
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (137): 761-777 2015.

Devi, T. S. R.; Kumar, J. S.; Ramkumaar, G. R.
Quantum chemical studies on structural, vibrational, NBO and hyperpolarizability of N-(1,1-Dimethyl-2-hydroxyethyl)-3-amino-2-hydroxypropanesulfonic acid
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (136): 1500-1514 2015.

Dey, G.; Elliot, S. D.
Quantum Chemical Study of the Effect of Precursor Stereochemistry on Dissociative Chemisorption and Surface Redox Reactions During the Atomic Layer Deposition of the Transition Metal Copper
Journal of Physical Chemistry C, (119): 5914-5927 2015.

Dhas, D. A.; Joe, I. H.; Roy, S. D. D.; Balachandran, S.
Spectroscopic analysis and charge transfer interaction studies of 4-benzyloxy-2-nitroaniline insecticide: A density functional theoretical approach
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (135): 583-596 2015.

Dheivamalar, S.; Sugi, L.
Density functional theory (DFT) investigations on doped fullerene with heteroatom substitution
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (151): 687-695 2015.

Di Palma, T. M.; Bende, A.
Encasing of Na+ ion in dimer-formed acetic acid clusters
Journal of Mass Spectrometry, (50): 1136-1143 2015.

Diller, K.; Ma, Y.; Luo, Y.; Allegretti, F.; Liu, J. Z.; Tang, B. Z.; Lin, N. A.; Barth, J. V.; Klappenberger, F.
Polyphenylsilole multilayers - an insight from X-ray electron spectroscopy and density functional theory
Physical Chemistry Chemical Physics, (17): 31117-31124 2015.

Ding, K. W.; Li, X. W.; Xu, H. G.; Li, T. Q.; Ge, Z. X.; Wang, Q.; Zheng, W. J.
Experimental observation of TiN12+ cluster and theoretical investigation of its stable and metastable isomers
Chemical Science, (6): 4723-4729 2015.

Ding, L. L.; Zheng, W. R.; Wang, Y. X.
Homolytic C-O Cleavage in Phosphates and Sulfonates
Journal of Physical Chemistry A, (119): 3488-3499 2015.

Ding, L. L.; Zheng, W. R.; Wang, Y. X.
Theoretical study on homolytic C(sp(2))-O cleavage in ethers and phenols
New Journal of Chemistry, (39): 6935-6943 2015.

Ding, Y. Q.; Cui, Y. Z.; Li, T. D.

New Views on the Reaction of Primary Amine and Aldehyde from DFT Study
Journal of Physical Chemistry A, (119): 4252-4260 2015.

Diwaker; Kumar, C. S. C.; Kumar, A.; Chandraju, S.
Spectroscopic (FT-IR, H-1, C-13 NMR and UV-vis) characterization and DFT studies of novel 8-((4-(methylthio)-2,5-diphenylfuran-yl)methoxy)quinoline
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (150): 602-613 2015.

Djemil, R.; Attoui-Yahia, O.; Khatmi, D.
DFT-ONIOM study of the dopamine-beta-CD complex: NBO and AIM analysis
Canadian Journal of Chemistry, (93): 1115-1121 2015.

Djordjevic, I.; Grubisic, S.; Milcic, M.; Niketic, S.
Derivation of a new set of force field parameters for ammine complexes of chromium(III) containing halogenido ligands: modeling of the trans-influence of halogenido ligands
Journal of the Serbian Chemical Society, (80): 329-342 2015.

Dobrydnev, A. V.; Volovenko, Y. M.; Turov, A. V.; Medviediev, V. V.; Shishkin, O. V.; Volovnenko, T. A.
Synthesis of spiro 2-(5-amino-2,3-dihydro-3-oxopyrrol-4-yl)-1,3-dialkylbenzimidazolium chlorides
Monatshefte fur Chemie, (146): 931-939 2015.

Dolati, F.; Tayyari, S. F.; Vakili, M.
Tautomerism, conformational analysis, and spectroscopy studies of 3-bromo-pentane-2,4-dione
Journal of Molecular Structure, (1094): 264-273 2015.

Dolyniuk, J. A.; He, H.; Ivanov, A. S.; Boldyrev, A. I.; Bobev, S.; Kovnir, K.
Ba and Sr Binary Phosphides: Synthesis, Crystal Structures, and Bonding Analysis
Inorganic Chemistry, (54): 8608-8616 2015.

Domancich, N. F.; Ferullo, R. M.; Castellani, N. J.
Interaction of aluminum dimer with defective graphene
Computational and Theoretical Chemistry, (1059): 27-34 2015.

Domingo, L. R.; Aurell, M. J.; Perez, P.
A mechanistic study of the participation of azomethine ylides and carbonyl ylides in 3+2 cycloaddition reactions
Tetrahedron, (71): 1050-1057 2015.

Domingo, L. R.; Rios-Gutierrez, M.; Perez, P.
A DFT study of the ionic 2+2 cycloaddition reactions of keteniminium cations with terminal acetylenes
Tetrahedron, (71): 2421-2427 2015.

Domingo, L. R.; Rios-Gutierrez, M.; Saez, J. A.
Unravelling the mechanism of the ketene-imine Staudinger reaction. An ELF quantum topological analysis
Rsc Advances, (5): 37119-37129 2015.

Domingo, L. R.; Saez, J. A.; Emamian, S. R.
Understanding the domino reaction between 3-chloroindoles and methyl coumalate yielding carbazoles. A DFT study
Organic & Biomolecular Chemistry, (13): 2034-2043 2015.

Donald, K. J.; Stewart, J.; Guarino, M.
Structure, bonding, relativistic effects, and dispersion in the group 12 dihalide (MX2)(3) clusters, with lessons from the extended solids
Structural Chemistry, (26): 1179-1195 2015.

Dong, C. H.; Yang, X. Z.; Yao, J. N.; Chen, H.
Mechanistic Study and Ligand Design for the Formation of Zinc Formate Complexes from Zinc Hydride Complexes and Carbon Dioxide
Organometallics, (34): 121-126 2015.

Dong, X.; Tian, Z. Y.; Yang, X.; Xue, Y.
Theoretical study on the mechanism of self-cleavage reaction of the glmS ribozyme
Theoretical Chemistry Accounts, (134) 2015.

Doss, M. A.; Savithiri, S.; Rajarajan, G.; Thanikachalam, V.; Anbuselvan, C.
Synthesis, electronic structure investigation of 3-penty1-2,6-di(furan-2yl)piperidin-4-one by FT-IR, FT-Raman and UV-Visible spectral studies and ab initio/DFT calculations
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (151): 773-784 2015.

Dostal, L.; Jambor, R.; Ruzicka, A.; Jirasko, R.; Lycka, A.; Beckmann, J.; Ketkov, S.
From Stiba- and Bismaheteroboroxines to N,C,N-Chelated Diorganoantimony(III) and Bismuth(III) Cations-An Unexpected Case of Aryl Group Migration
Inorganic Chemistry, (54): 6010-6019 2015.

Douvali, A.; Papaefstathiou, G. S.; Gullo, M. P.; Barbieri, A.; Tsipis, A. C.; Malliakas, C. D.; Kanatzidis, M. G.; Papadas, I.; Armatas, G. S.; Hatzidimitriou, A. G.; Lazarides, T.; Manos, M. J.
Alkaline Earth Metal Ion/Dihydroxy-Terephthalate MOFs: Structural Diversity and Unusual Luminescent Properties
Inorganic Chemistry, (54): 5813-5826 2015.

Duarte, D. J. R.; Peruchena, N. M.; Alkorta, I.
Double Hole-Lump Interaction between Halogen Atoms
Journal of Physical Chemistry A, (119): 3746-3752 2015.

Dudev, T.; Lim, C.
Ion Selectivity in the Selectivity Filters of Acid-Sensing Ion Channels
Scientific Reports, (5) 2015.

Dudev, T.; Musset, B.; Morgan, D.; Cherny, V. V.; Smith, S. M. E.; Mazmanian, K.; DeCoursey, T. E.; Lim, C.
Selectivity Mechanism of the Voltage-gated Proton Channel, H(V)1
Scientific Reports, (5) 2015.

Dunnington, B. D.; Schmidt, J. R.
Molecular bonding-based descriptors for surface adsorption and reactivity
Journal of Catalysis, (324): 50-58 2015.

Dunnington, B. D.; Schmidt, J. R.
A projection-free method for representing plane-wave DFT results in an atom-centered basis
Journal of Chemical Physics, (143) 2015.

Dutta, B.; De, R. N.; Chowdhury, J.
Prototropic tautomerism of 4-Methyl 1,2,4-Triazole-3-Thione molecule in solvent water medium: DFT and Car-Parrinello molecular dynamics study
Chemical Physics, (463): 30-37 2015.

Ehsani, A.; Babaei, F.; Mostaanzadeh, H.
Electrochemical and Optical Investigation of Conductive Polymer and MWCNT Nanocomposite Film
Journal of the Brazilian Chemical Society, (26): 331-337 2015.

Eid, S.; Hassan, W. M. I.
Chemical and Theoretical Studies for Corrosion Inhibition of Magnesium in Hydrochloric Acid by Tween 80 Surfactant
International Journal of Electrochemical Science, (10): 8017-8027 2015.

El-Amri, A.; Elroby, S. A.; Kuhn, O.; Hilal, R. H.
Toward understanding tautomeric switching in 4-hydroxynaphthaldehyde and its dimers: A DFT and quantum topology study
Journal of Theoretical & Computational Chemistry, (14) 2015.

Elanthiraiyan, M.; Jayasudha, B.; Arivazhagan, M.
Molecular structure, vibrational spectroscopy, NBO and HOMO, LUMO studies of o-methoxybenzonitrile
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (134): 543-552 2015.

Elroby, S. A.; Aboud, S.; Aziz, S. G.; Hilal, R.
Substituent effects on the absorption and vibrational spectra of some 2-hydroxy Schiff bases: DFT/TDDFT, natural bond orbital and experimental study
Journal of Structural Chemistry, (56): 414-427 2015.

El-Sayed, A. A.; Molina, A. T.; Alvarez-Ros, M. C.; Palafox, M. A.
Conformational analysis of the anti-HIV Nikavir prodrug: comparisons with AZT and Thymidine, and establishment of structure-activity relationships/tendencies in other 6 '-derivatives
Journal of Biomolecular Structure and Dynamics, (33): 723-748 2015.

El-Sheshtawy, H. S.; Ibrahim, M. M.; El-Mehasseb, I.; El-Kemary, M.
Orthogonal hydrogen/halogen bonding in 1-(2-methoxyphenyl)-1H-imidazole-2(3H)-thione-I-2 adduct: An experimental and theoretical study
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (143): 120-127 2015.

Ema, T.; Fukuhara, K.; Sakai, T.; Ohbo, M.; Bai, F. Q.; Hasegawa, J. Y.
Quaternary ammonium hydroxide as a metal-free and halogen-free catalyst for the synthesis of cyclic carbonates from epoxides and carbon dioxide
Catalysis Science & Technology, (5): 2314-2321 2015.

Emamian, S.
Generation of a substituted 1,2,4-thiadiazole ring via the 3+2 cycloaddition reaction of benzonitrile sulfide toward trichloroacetonitrile. A DFT study of the regioselectivity and of the molecular mechanism
Comptes Rendus Chimie, (18): 1277-1283 2015.

Emamian, S.
Polar Diels-Alder reaction of isoprene toward 2-bromocyclobutenone followed by a subsequent sodium hydroxide-assisted ring contraction reaction. A regio- and stereoselectivity and molecular mechanism study using DFT
New Journal of Chemistry, (39): 9525-9534 2015.

Emamian, S.
Understanding the molecular mechanism and regioselectivity in the synthesis of celecoxib via a domino reaction: A DFT study
Journal of Molecular Graphics and Modelling, (60): 155-161 2015.

Emamian, S.
Understanding the molecular mechanism in a regiospecific 3+2 cycloaddition reaction including C-O and C-S interactions: an ELF topological analysis
Rsc Advances, (5): 72959-72970 2015.

Emamian, S.
Understanding the regioselectivity and molecular mechanism in the synthesis of isoxazoles containing pentafluorosulfanyl substitution via a 3+2 cycloaddition reaction: A DFT study
Journal of Fluorine Chemistry, (178): 165-172 2015.

Emamian, S.; Hosseini, S. J.; Ravani, K. S.
Ionic Diels-Alder reaction of 3-bromofuran toward the highly electron deficient cyclobuteniminium cation: a regio- and stereoselectivity, and molecular mechanism study using DFT
Rsc Advances, (5): 98538-98548 2015.

Emamian, S.; Lu, T.; Moeinpour, F.
Can the high reactivity of azomethine betaines in 3+2 cycloaddition reactions be explained using singlet-diradical character descriptors? What molecular mechanism is actually involved in these cycloadditions?
Rsc Advances, (5): 62248-62259 2015.

Erdogdu, Y.; Saglam, S.; Dereli, O.
Theoretical (DFT) and experimental (FT-IR, FT-Raman, FT-NMR) investigations on 7-Acetoxy-4-(bromomethyl)coumarin
Optics and Spectroscopy, (119): 411-423 2015.

Escudero-Adan, E. C.; Bauza, A.; Frontera, A.; Ballester, P.
Nature of Noncovalent Carbon-Bonding Interactions Derived from Experimental Charge-Density Analysis
Chemphyschem, (16): 2530-2533 2015.

Esmkhani, R.; Monajjemi, M.
Electronic Structural Investigation of Boron Nitride Nano Cage (B30N20) in Point of Exchange and Correlation Energy
Journal of Computational and Theoretical Nanoscience, (12): 652-659 2015.

Espada, M. F.; Campos, J.; Lopez-Serrano, J.; Poveda, M. L.; Carmona, E.
Methyl-, Ethenyl-, and Ethynyl-Bridged Cationic Digold Complexes Stabilized by Coordination to a Bulky Terphenylphosphine Ligand
Angewandte Chemie-International Edition, (54): 15379-15384 2015.

Espelt, L. R.; McPherson, I. S.; Wiensch, E. M.; Yoon, T. P.
Enantioselective Conjugate Additions of alpha-Amino Radicals via Cooperative Photoredox and Lewis Acid Catalysis
Journal of the American Chemical Society, (137): 2452-2455 2015.

Esrafili, M. D.; Ghanbari, M.; Nurazar, R.; Nematollahi, P.
Theoretical study of formamide decomposition pathways over (6,0) silicon-carbide nanotube
Journal of Molecular Modeling, (21) 2015.

Esrafili, M. D.; Mohammadian-Sabet, F.
Bifurcated chalcogen bonds: A theoretical study on the structure, strength and bonding properties
Chemical Physics Letters, (634): 210-215 2015.

Esrafili, M. D.; Mohammadian-Sabet, F.
Exploring sigma-hole bonding in XH3Si center dot center dot center dot HMY (X=H, F, CN; M=Be, Mg; Y=H, F, CH3) complexes: a "tetrel-hydride" interaction
Journal of Molecular Modeling, (21) 2015.

Esrafili, M. D.; Mohammadian-Sabet, F.
Prediction and characterisation of a chalcogen center dot center dot center dot pi interaction with acetylene as a potential electron donor in XHS center dot center dot center dot HCCH and XHSe center dot center dot center dot HCCH (X = F, Cl, Br, CN, OH, OCH3, NH2, CH3) sigma-hole complexes
Molecular Physics, (113): 3559-3566 2015.

Esrafili, M. D.; Mohammadian-Sabet, F.; Solimannejad, M.
Mutual influence between anion-pi and pnicogen bond interactions: The enhancement of P center dot center dot center dot N and P center dot center dot center dot O interactions by an anion-pi bond
Journal of Molecular Graphics and Modelling, (57): 99-105 2015.

Esrafili, M. D.; Mohammadirad, N.
Effect of cation-pi interaction on lithium and halogen bonds: a comparative study
Molecular Physics, (113): 711-718 2015.

Esrafili, M. D.; Mohammad-Valipour, R.; Mousavi-Khoshdel, S. M.; Nematollahi, P.
A Comparative Study of CO Oxidation on Nitrogen- and Phosphorus-Doped Graphene
Chemphyschem, (16): 3719-3727 2015.

Esrafili, M. D.; Nurazar, R.
Hydrogen generation from methylamine using silicon carbide nanotubes as a dehydrogenation catalyst: A density functional theory study
Journal of Molecular Graphics and Modelling, (55): 41-47 2015.

Esrafili, M. D.; Nurazar, R.
Metal-Free Decomposition of Formic Acid on Pristine and Carbon-Doped Boron Nitride Fullerene: A DFT Study
Journal of Cluster Science, (26): 595-608 2015.

Esrafili, M. D.; Nurazar, R.; Masumi, V.
Adsorption and decomposition of formamide over zigzag (n,0) silicon-carbide nanotubes (n=5-7): Investigation of curvature effects
Surface Science, (637): 69-76 2015.

Esrafili, M. D.; Nurazar, R.; Mohammadian-Sabet, F.
Cooperative effects between tetrel bond and other s- hole bond interactions: a comparative investigation
Molecular Physics, (113): 3703-3711 2015.

Esrafili, M. D.; Saeidi, N.
Si-embedded boron-nitride nanotubes as an efficient and metal-free catalyst for NO oxidation
Superlattices and Microstructures, (81): 7-15 2015.

Esrafili, M. D.; Saeidi, N.; Baneshi, M. M.
Chalcogen-Chalcogen Interactions in Furan-YHX and Thiophene-YHX Complexes (X = F, Cl, Br; Y = S, Se): An Ab Initio Study
Bulletin of the Chemical Society of Japan, (88): 1683-1692 2015.

Esrafili, M. D.; Saeidi, N.; Nematollahi, P.
Can Si-embedded boron nitride nanotubes act as a favorable metal-free catalyst for CO oxidation by N2O?
Rsc Advances, (5): 100290-100298 2015.

Esrafili, M. D.; Teymurian, V. M.; Nurazar, R.
Catalytic dehydrogenation of hydrazine on silicon-carbide nanotubes: A DFT study on the kinetic issue
Surface Science, (632): 118-125 2015.

Esselman, B. J.; Hill, N. J.
Proper Resonance Depiction of Acylium Cation: A High-Level and Student Computational Investigation
Journal of Chemical Education, (92): 660-663 2015.

Esser, M.; Deringer, V. L.; Wuttig, M.; Dronskowski, R.
Orbital mixing in solids as a descriptor for materials mapping
Solid State Communications, (203): 31-34 2015.

Eussner, J. P.; Kusche, R. O.; Dehnen, S.
Synthesis and Thorough Investigation of Discrete Organotin Telluride Clusters
Chemistry-a European Journal, (21): 12376-12388 2015.

Fabig, S.; Haberhauer, G.; Gleiter, R.
Dimerization of Two Alkyne Units: Model Studies, Intermediate Trapping Experiments, and Kinetic Studies
Journal of the American Chemical Society, (137): 1833-1843 2015.

Faghih, Z.; Fereidoonnezhad, M.; Tabaei, S. M. H.; Rezaei, Z.; Zolghadr, A. R.
The binding of small carbazole derivative (P7C3) to protofibrils of the Alzheimer's disease and beta-secretase: Molecular dynamics simulation studies
Chemical Physics, (459): 31-39 2015.

Fan, S. H.; Lv, K.; Sun, H.; Zhou, G.; Wang, Z. S.
The position effect of electron-deficient quinoxaline moiety in porphyrin based sensitizers
Journal of Power Sources, (279): 36-47 2015.

Fang, H. L.; Xu, L.; Li, J.; Wang, B.; Zhang, Y. F.; Huang, X.
Catalytic oxidation of CO by N2O on neutral Y2MO5 (M = Y, Al) clusters: a density functional theory study

Rsc Advances, (5): 76651-76659 2015.

Fang, W. W.; Liu, C.; Chen, J. B.; Lu, Z. W.; Li, Z. M.; Bao, X. L.; Tu, T.
The electronic effects of ligands on metal-coordination geometry: a key role in the visual discrimination of dimethylaminopyridine and its application towards chemo-switch
Chemical Communications, (51): 4267-4270 2015.

Fang, Y.; Li, A. Y.; Ma, F. Y.
A comparative study of the chalcogen bond, halogen bond and hydrogen bond S center dot center dot center dot O/Cl/H formed between SHX and HOCl
Journal of Molecular Modeling, (21) 2015.

Farag, M. H.; Ruiz-Lopez, M. F.; Bastida, A.; Monard, G.; Ingrosso, F.
Hydration Effect on Amide I Infrared Bands in Water: An Interpretation Based on an Interaction Energy Decomposition Scheme
Journal of Physical Chemistry B, (119): 9056-9067 2015.

Farmanzadeh, D.; Najafi, M.
Benzimidazole derivatives as anticancer drugs: A theoretical investigation
Journal of Theoretical & Computational Chemistry, (14) 2015.

Farmanzadeh, D.; Najafi, M.
Theoretical study of anticancer properties of indolyl-oxazole drugs and their interactions with DNA base pairs in gas phase and solvent
Structural Chemistry, (26): 831-844 2015.

Fasfous, II; Dawoud, J. N.; Sallabi, A. K.; Hassouneh, T. S.
A density functional theory study of the Cu+ center dot (CO)(n) (n=1-3) complexes
Journal of Coordination Chemistry, (68): 1528-1543 2015.

Fatma, S.; Bishnoi, A.; Verma, A. K.
Synthesis, spectral analysis (FT-IR, H-1 NMR, C-13 NMR and UV-visible) and quantum chemical studies on molecular geometry, NBO, NLO, chemical reactivity and thermodynamic properties of novel 2-amino-4-(4-(dimethylamino)phenyl)-5-oxo-6-phenyl-5,6-dihydro-4H-pyrano 3,2-c quinoline-3-carbonitrile
Journal of Molecular Structure, (1095): 112-124 2015.

Fatynowicz, H.; Daszkiewicz, M.; Wysokinski, R.; Adach, A.; Cieslak-Golonka, M.
Ni(II) complex with sarcosine derived from in situ generated ligand: structural, spectroscopic, and DFT studies
Structural Chemistry, (26): 1555-1563 2015.

Feixas, F.; Matito, E.; Poater, J.; Sola, M.
Quantifying aromaticity with electron delocalisation measures
Chemical Society Reviews, (44): 6434-6451 2015.

Feixas, F.; Rodriguez-Mayorga, M.; Matito, E.; Sola, M.
Three-center bonding analyzed from correlated and uncorrelated third-order reduced density matrices
Computational and Theoretical Chemistry, (1053): 173-179 2015.

Feldmann, K. O.; Wiegand, T.; Ren, J. J.; Eckert, H.; Breternitz, J.; Groh, M. F.; Muller, U.; Ruck, M.; Maryasin, B.; Ochsenfeld, C.; Schon, O.; Karaghiosoff, K.; Weigand, J. J.
P3Se4 (+): A Binary Phosphorus-Selenium Cation
Chemistry-a European Journal, (21): 9697-9712 2015.

Fernandez, E.; Boronat, M.; Corma, A.
Trends in the Reactivity of Molecular O-2 with Copper Clusters: Influence of Size and Shape
Journal of Physical Chemistry C, (119): 19832-19846 2015.

Filippi, A.; Fraschetti, C.; Grandinetti, F.; Speranza, M.; Ponzi, A.; Decleva, P.; Stranges, S.

Electronic structure and conformational flexibility of D-cycloserine
Physical Chemistry Chemical Physics, (17): 25845-25853 2015.

Filippov, O. A.; Golub, I. E.; Osipova, E. S.; Kirkina, V. A.; Gutsul, E. I.; Belkova, N. V.
Activation of M-H bond upon the complexation of transition metal hydrides with acids and bases
Russian Chemical Bulletin, (63): 2428-2433 2015.

Fogler, E.; Efremenko, I.; Gargir, M.; Leitus, G.; Diskin-Posner, Y.; Ben-David, Y.; Martin, J. M. L.; Milstein, D.
New Ruthenium Nitrosyl Pincer Complexes Bearing an O-2 Ligand. Mono-Oxygen Transfer
Inorganic Chemistry, (54): 2253-2263 2015.

Ford, T. A.
The molecular complexes of boron trifluoride with nitrosyl fluoride and nitrosyl chloride. Ion-pair formation
Journal of Molecular Structure, (1090): 7-13 2015.

Foroutan-Nejad, C.; Badri, Z.; Marek, R.
Multi-center covalency: revisiting the nature of anion-pi interactions
Physical Chemistry Chemical Physics, (17): 30670-30679 2015.

Foroutan-Nejad, C.; Vicha, J.; Marek, R.; Patzschke, M.; Straka, M.
Unwilling U-U bonding in U-2@C-80: cage-driven metal-metal bonds in di-uranium fullerenes
Physical Chemistry Chemical Physics, (17): 24182-24192 2015.

Fortino, M.; Marino, T.; Russo, N.; Sicilia, E.
Mechanism of Thyroxine Deiodination by Naphthyl-Based Iodothyronine Deiodinase Mimics and the Halogen Bonding Role: A DFT Investigation
Chemistry-a European Journal, (21): 8554-8560 2015.

Fox, S. J.; Gourdain, S.; Coulthurst, A.; Fox, C.; Kuprov, I.; Essex, J. W.; Skylaris, C. K.; Linclau, B.
A Computational Study of Vicinal Fluorination in 2,3-Difluorobutane: Implications for Conformational Control in Alkane Chains
Chemistry-a European Journal, (21): 1682-1691 2015.

Franco, J. M. V.; Sasamori, T.; Schnakenburg, G.; Ferao, A. E.; Streubel, R.
Going for strain: synthesis of the first 3-iminoazaphosphiridine complexes and their conversion into oxaphosphirane complex valence isomers
Chemical Communications, (51): 3878-3881 2015.

Franco, J. M. V.; Schnakenburg, G.; Ferao, A. E.; Streubel, R.
Unprecedented Ring-Ring Interconversion of N,P,C-Cage Ligands
Chemistry-a European Journal, (21): 3727-3735 2015.

Freeman, F.
Mechanisms of Reactions of Sulfur Hydride Hydroxide: Tautomerism, Condensations, and C-Sulfenylation and O-Sulfenylation of 2,4-Pentanedione
Journal of Physical Chemistry A, (119): 3500-3517 2015.

Frenking, G.; Caramori, G. F.
No Need for a Re-examination of the Electrostatic Notation of the Hydrogen Bonding: A Comment
Angewandte Chemie-International Edition, (54): 2596-2599 2015.

Fry, A. J.
Computational Studies of Ion Pairing. 10. Ion Pairing between Tetrabutylammonium ion and Inorganic Ions: A General Motif Confirmed
Journal of Organic Chemistry, (80): 3758-3765 2015.

Fu, G.; Yuan, R. M.; Wang, P.; Wan, H. L.
DFT studies on the activation of C-H bonds on V/P mixed oxides

Chinese Journal of Catalysis, (36): 1528-1534 2015.

Fu, H. Q.; Su, B. F.; Yang, H. Q.; Hu, C. W.
Theoretical insight into the C-H and C-C scission mechanism of ethane on a tetrahedral Pt-4 subnanocluster
Rsc Advances, (5): 40978-40988 2015.

Fu, H. Y.; Cao, M. J.; She, Y. B.; Sun, Z. C.; Yu, Y. M.
Electronic effects of the substituent on the dioxygen-activating abilities of substituted iron tetraphenylporphyrins: a theoretical study
Journal of Molecular Modeling, (21) 2015.

Fuente, S. A.; Ferretti, C. A.; Domancich, N. F.; Diez, V. K.; Apesteguia, C. R.; Di Cosimo, J. I.; Ferullo, R. M.; Castellani, N. J.
Adsorption of 2-propanol on MgO surface: A combined experimental and theoretical study
Applied Surface Science, (327): 268-276 2015.

Fuertes, P.; Garcia-Valverde, M.; Pascual, R.; Rodriguez, T.; Rojo, J.; Garcia-Calvo, J.; Calvo, P.; Cuevas, J. V.; Garcia-Herbosa, G.; Torroba, T.
Structural Conformers of (1,3-Dithiol-2-ylidene)ethanethioamides: The Balance between Thioamide Rotation and Preservation of Classical Sulfur-Sulfur Hypervalent Bonds
Journal of Organic Chemistry, (80): 30-39 2015.

Fukuzawa, K.; Kurisaki, I.; Watanabe, C.; Okiyama, Y.; Mochizuki, Y.; Tanaka, S.; Komeiji, Y.
Explicit solvation modulates intra- and inter-molecular interactions within DNA: Electronic aspects revealed by the ab initio fragment molecular orbital (FMO) method
Computational and Theoretical Chemistry, (1054): 29-37 2015.

Furer, V. L.; Vandyukov, A. E.; Majoral, J. P.; Caminade, A. M.; Gottis, S.; Laurent, R.; Kovalenko, V. I.
Comparative DFT study of structure, reactivity and IR spectra of phosphorus-containing dendrons with P=N-P=S linkages, vinyl and azide functional groups
Journal of Molecular Structure, (1091): 6-15 2015.

Furer, V. L.; Vandyukov, A. E.; Majoral, J. P.; Caminade, A. M.; Gottis, S.; Laurent, R.; Kovalenko, V. I.
DFT study of structure, IR and Raman spectra of dendrimer with P=N-P=S linkages and its complexation with gold
Journal of Molecular Structure, (1084): 103-113 2015.

Furer, V. L.; Vandyukov, A. E.; Padie, C.; Majoral, J. P.; Caminade, A. M.; Kovalenko, V. I.
Raman spectroscopy studies of phosphorus dendrimers with phenoxy and deuterophenoxy terminal groups
Vibrational Spectroscopy, (80): 17-23 2015.

Fustier, M.; Le Goff, X. F.; Lutz, M.; Slootweg, J. C.; Mezailles, N.
Scandium Carbene Complexes: Synthesis of Mixed Alkyl, Amido, and Phosphido Derivatives
Organometallics, (34): 63-72 2015.

Gajalakshmi, D.; Solomon, R. V.; Tamilmani, V.; Boobalan, M.; Venuvanalingam, P.
A DFT/TDDFT mission to probe push-pull vinyl coupled thiophene oligomers for optoelectronic applications
Rsc Advances, (5): 50353-50364 2015.

Gal, J. F.; Yanez, M.; Mo, O.
Aluminum monocation basicity and affinity scales
European Journal of Mass Spectrometry, (21): 517-532 2015.

Gamez, F.; Hortal, A. R.; Hurtado, P.; Aviles-Moreno, J. R.; Hamad, S.; Martinez-Haya, B.
Binding Selectivity of Macrocycle Ionophores in Ionic Liquids versus Aqueous Solution and Solvent-free Conditions
Chemphyschem, (16): 3672-3680 2015.

Gangadharan, R. P.; Krishnan, S. S.
First Order Hyperpolarizabilities, NPA and Fukui Functions of Cyclohexanone by Density Functional Theory Method
Acta Physica Polonica A, (127): 748-752 2015.

Gangadharan, R. P.; Krishnan, S. S.
Natural Bond Orbital (NBO) Population Analysis, First Order Hyperpolarizabilities and Thermodynamic Properties of Cyclohexanone
Spectroscopy and Spectral Analysis, (35): 1506-1511 2015.

Gangarapu, S.; Marcelis, A. T. M.; Alhamed, Y. A.; Zuilhof, H.
The Transition States for CO2 Capture by Substituted Ethanolamines
Chemphyschem, (16): 3000-3006 2015.

Gao, F. W.; Gao, Y.; Wang, L. J.; Xu, H. L.; Sun, S. L.; Su, Z. M.
"Dancing inside the ball": the structures and nonlinear optical properties of three Sc2S@C-3v(8)-C-82 isomers
Journal of Molecular Modeling, (21) 2015.

Gao, F. W.; Zhong, R. L.; Sun, S. L.; Xu, H. L.; Zhao, L.; Su, Z. M.
Charge transfer and first hyperpolarizability: cage-like radicals C59X and lithium encapsulated Li@ C59X (X= B, N)
Journal of Molecular Modeling, (21) 2015.

Gao, H. F.; Zhang, S. H.; Ren, F. D.; Liu, F.; Gou, R. J.; Ding, X.
Theoretical insight into the co-crystal explosive of 2,4,6,8,10,12-hexanitrohexaazaisowurtzitane (CL-20)/1,1-diamino-2,2-dinitroethylene (FOX-7)
Computational Materials Science, (107): 33-41 2015.

Gao, K. Q.; Sheng, L.
Theoretical investigation of HNgNH(3)(+) ions (Ng = He, Ne, Ar, Kr, and Xe)
Journal of Chemical Physics, (142) 2015.

Gao, L. G.; Song, X. L.; Cao, W.; Lu, L. L.
Luteolin and Luteolin-Cr(III) Complexes: Antioxidation and Reaction Mechanism with Hydrogen Peroxide Radical
Chinese Journal of Inorganic Chemistry, (31): 2229-2235 2015.

Gao, M.; Gao, G. Q.; Li, Q. Z.; Yang, X.; Li, W. Z.; Cheng, J. B.
Theoretical study of synergistic effects between anion-pi and metal-Lp interactions
Rsc Advances, (5): 76912-76918 2015.

Gao, M.; Li, Q. Z.; Cheng, J. B.; Li, W. Z.; Li, H. B.
Complicated synergistic effects between metal-pi interaction and halogen bonding involving MCCX
Rsc Advances, (5): 105160-105168 2015.

Gao, M.; Li, Q. Z.; Li, H. B.; Li, W. Z.; Cheng, J. B.
How do organic gold compounds and organic halogen molecules interact? Comparison with hydrogen bonds
Rsc Advances, (5): 12488-12497 2015.

Gao, M.; Li, Q. Z.; Li, W. Z.; Cheng, J. B.
Interplay between Cation-pi and Coinage-Metal-Oxygen Interactions: An Ab Initio Study and Cambridge Structural Database Survey
Chemphyschem, (16): 1008-1016 2015.

Gao, W.; Tian, Y.; Xuan, X. P.
How the cation-cation pi-pi stacking occurs: A theoretical investigation into ionic clusters of imidazolium
Journal of Molecular Graphics and Modelling, (60): 118-123 2015.

Gao, X. Z.; Gong, S. D.; Li, N.; King, R. B.
Sulfur difluoride and sulfur monofluoride as ligands in iron carbonyl chemistry
New Journal of Chemistry, (39): 4939-4947 2015.

Gao, X. Z.; Li, N.; King, R. B.
Binuclear cyclopentadienyliridium hydride chemistry: Terminal versus bridging hydride and cyclopentadienyl ligands

Inorganica Chimica Acta, (436): 94-102 2015.

Gao, X. Z.; Li, N.; King, R. B.; Schaefer, H. F.
Binuclear cyclopentadienylrhenium hydride chemistry: terminal versus bridging hydride and cyclopentadienyl ligands
Journal of Molecular Modeling, (21) 2015.

Gao, Y.; Wu, H. Q.; Sun, S. L.; Xu, H. L.; Su, Z. M.
One lithium atom binding with P-nitroaniline: lithium salts or lithium electrides?
Journal of Molecular Modeling, (21) 2015.

Garcia, G.; Atilhan, M.; Aparicio, S.
The impact of charges in force field parameterization for molecular dynamics simulations of deep eutectic solvents
Journal of Molecular Liquids, (211): 506-514 2015.

Garcias-Morales, C.; Ortegon-Reyna, D.; Ariza-Castolo, A.
Investigation of the role of stereoelectronic effects in the conformation of piperidones by NMR spectroscopy and X-ray diffraction
Beilstein Journal of Organic Chemistry, (11): 1973-1984 2015.

Gaus, M.; Jin, H. Y.; Demapan, D.; Christensen, A. S.; Goyal, P.; Elstner, M.; Cui, Q.
DFTB3 Parametrization for Copper: The Importance of Orbital Angular Momentum Dependence of Hubbard Parameters
Journal of Chemical Theory and Computation, (11): 4205-4219 2015.

Gazitua, M.; Fuentealba, P.; Contreras, R.; Ormazabal-Toledo, R.
Lewis Acidity/Basicity Changes in Imidazolium Based Ionic Liquids Brought About by Impurities
Journal of Physical Chemistry B, (119): 13160-13166 2015.

Geidl, S.; Bouchal, T.; Racek, T.; Varekova, R. S.; Hejret, V.; Krenek, A.; Abagyan, R.; Koca, J.
High-quality and universal empirical atomic charges for chemoinformatics applications
Journal of Cheminformatics, (7) 2015.

Geiss, D.; Arz, M. I.; Strassmann, M.; Schnakenburg, G.; Filippou, A. C.
Si=P Double Bonds: Experimental and Theoretical Study of an NHCStabilized Phosphasilenylidene
Angewandte Chemie-International Edition, (54): 2739-2744 2015.

Genc, Z. K.; Tekin, S.; Sandal, S.; Genc, M.
Theoretical calculations, cytotoxic evaluation, and molecular docking studies of 4-(1-adamantyl)-5- 2-(3-hydroxynapthyl) -2H-1,2,4-triazole-3(4H)-thione as a novel chemotherapeutic agent
Research on Chemical Intermediates, (41): 6229-6244 2015.

Georgiou, D. C.; Stringer, B. D.; Hogan, C. F.; Barnard, P. J.; Wilson, D. J. D.; Holzmann, N.; Frenking, G.; Dutton, J. L.
The Fate of NHC-Stabilized Dicarbon
Chemistry-a European Journal, (21): 3377-3386 2015.

Gerasimova, T. P.; Katsyuba, S. A.
Infrared and Raman bands of cyclopentadienyl ligands as indicators of electronic configuration of metal centers in metallocenes
Journal of Organometallic Chemistry, (776): 30-34 2015.

Gerhards, F.; Griebel, N.; Runsink, J.; Raabe, G.; Gais, H. J.
Chiral Lithiated Allylic alpha-Sulfonyl Carbanions: Experimental and Computational Study of Their Structure, Configurational Stability, and Enantioselective Synthesis
Chemistry-a European Journal, (21): 17904-17920 2015.

Gerosa, G. G.; Spanevello, R. A.; Suarez, A. G.; Sarotti, A. M.
Joint Experimental, in Silico, and NMR Studies toward the Rational Design of Iminium-Based Organocatalyst Derived from Renewable Sources

Journal of Organic Chemistry, (80): 7626-7634 2015.

Gershoni-Poranne, R.; Stanger, A.
Magnetic criteria of aromaticity
Chemical Society Reviews, (44): 6597-6615 2015.

Geudtner, G.; Dominguez-Soria, V. D.; Calaminici, P.; Koster, A. M.
Molecular graphs of Li-n, Na-n and Cu-n (n=6-9) clusters from the density and the molecular electrostatic potential
Computational and Theoretical Chemistry, (1053): 337-342 2015.

Ghadwal, R. S.; Schurmann, C. J.; Andrada, D. M.; Frenking, G.
Mono- and di-cationic hydrido boron compounds
Dalton Transactions, (44): 14359-14367 2015.

Ghafari, S.; Gholipour, A.
Simultaneous interactions of pyrimidine ring with BeF2 and BF3 in BeF2 center dot center dot center dot X-Pyr center dot center dot center dot BF3 complexes: non-cooperativity
Journal of Molecular Modeling, (21) 2015.

Ghafouri, R.; Anafcheh, M.
A Computational Investigation of the Electronic Properties of Partially Hydrogenated Fullerenes C60Hn (n=18, 20, 24, 36 and 48)
Fullerenes Nanotubes and Carbon Nanostructures, (23): 40-48 2015.

Ghafouri, R.; Ektefa, F.
X24Y24 fullerene-like cages with the group III and V elements X = B, Al, and Ga; Y = N, P, and As: a DFT prediction
Monatshefte fur Chemie, (146): 1241-1247 2015.

Ghafouri, R.; Ektefa, F.; Zahedi, M.
Characterization of Hydrogen Bonds in the End-Functionalized Single-Wall Carbon Nanotubes: A DFT Study
Nano, (10) 2015.

Ghalla, H.; Govindarajan, M.; Flakus, H. T.; Issaoui, N.; Yaghmour, S. J.; Oujia, B.
Molecular structure and vibrational spectroscopic studies on 2-furanacetic acid monomer and dimer
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (136): 579-593 2015.

Ghasemi, A. S.; Deilam, M.; Sharifi-Rad, J.; Ashrafi, F.; Hoseini-Alfatemi, S. M.
Molecular structure, spectroscopic assignments and other quantum chemical calculations of anticancer drugs - A review
Cellular and Molecular Biology, (61): 110-118 2015.

Ghasemi, A. S.; Mashhadban, F.; Hoseini-Alfatemi, S. M.; Sharifi-Rad, J.
Conformational stability, spectroscopic and computational studies, highest occupied molecular orbital, lowest unoccupied molecular orbital, natural bond orbital analysis and thermodynamic parameters of anticancer drugs on nanotube - A review
Cellular and Molecular Biology, (61): 74-78 2015.

Ghasemi, K.; Rezvani, A. R.; Habibi-Khorassani, S. M.; Shahraki, M.; Shokrollahi, A.; Moghimi, A.; Tamandani, H. K.; Gavahi, S.
An experimental and theoretical study of a hydrogen-bonded complex: O-phenylenediamine with 2,6-pyridinedicarboxylic acid
Journal of Molecular Structure, (1100): 597-604 2015.

Ghiasi, R.
A chromium carbene (OC)(5)Cr=C(OEt)(-C C-Ph): Quantum mechanical study of molecular structure, HOMO-LUMO analysis, IR spectroscopy, natural bond orbital analysis
Journal of Theoretical & Computational Chemistry, (14) 2015.

Ghiasi, R.; Amini, E.

Substituent and solvent effects on geometric and electronic structure of C5H5Ir(PH3)(3) iridabenzene: A theoretical insight
Journal of Structural Chemistry, (56): 1483-1494 2015.

Ghiasi, R.; Amini, E.
Theoretical view on structure, chemical reactivity, aromaticity and N-14 NQR parameters of iridapyridine isomers
Journal of Structural Chemistry, (56): 1458-1467 2015.

Ghiassi, H.; Raissi, H.
Comprehensive study of the structural and electronic properties of complexes formed by Mz+ (Li+, Na+, K+, Be2+, Mg2+, Ca2+) cation and thiophene and its derivatives
Journal of Sulfur Chemistry, (36): 48-66 2015.

Ghiassi, H.; Raissi, H.
Investigation of adsorption properties of CS2 on interior and exterior surfaces of single-walled silicon-carbide nanotubes and effect of applied electric field: electronic structure, charge density and NMR studies
Rsc Advances, (5): 84022-84037 2015.

Gholivand, K.; Gholami, A.; Ebrahimi, A. A. V.; Abolghasemi, S. T.; Esrafili, M. D.; Fadaei, F. T.; Schenk, K. J.
Triphenyltin(IV) adducts of diphosphoryl ligands: structural, electronic and energy aspects from X-ray crystallography and theoretical calculations
Rsc Advances, (5): 17482-17492 2015.

Gholivand, K.; Molaei, F.
Synthesis and structural study of some new phosphorus(v) hydrazide compounds: spectroscopic evidence and a theoretical approach
New Journal of Chemistry, (39): 3747-3757 2015.

Gholivand, K.; Molaei, F.; Hosseini, M.
Phosphoramides bearing isoxazole derivative: spectroscopic and structural characterization, study of hydrogen-bonding interactions and two lanthanide complexes (Ln(III) = Ce and Eu)
Acta Crystallographica Section B-Structural Science Crystal Engineering and Materials, (71): 176-185 2015.

Gholivand, K.; Molaei, F.; Thibonnet, J.
A novel Zn(II) complex of N-nicotinyl phosphoramide: Combined experimental and computational studies
Journal of Molecular Structure, (1092): 130-136 2015.

Ghosh, S.; Holt, K. B.; Kabir, S. E.; Richmond, M. G.; Hogarth, G.
Electrocatalytic proton reduction catalysed by the low-valent tetrairon-oxo cluster Fe-4(CO)(10)(kappa(2)-dppn)(mu(4)-O) (2-) dppn=1,1 '- bis(diphenylphosphino)naphthalene
Dalton Transactions, (44): 5160-5169 2015.

Gil, A.; Melle-Franco, M.; Branchadell, V.; Calhorda, M. J.
How the Intercalation of Phenanthroline Affects the Structure, Energetics, and Bond Properties of DNA Base Pairs: Theoretical Study Applied to Adenine-hymine and Guanine-ytosine Tetramers
Journal of Chemical Theory and Computation, (11): 2714-2728 2015.

Gil, D. M.; Lestard, M. E. D.; Estevez-Hernandez, O.; Duque, J.; Reguera, E.
Quantum chemical studies on molecular structure, spectroscopic (IR, Raman, UV-Vis), NBO and Homo-Lumo analysis of 1-benzyl-3-(2-furoyl) thiourea
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (145): 553-562 2015.

Gil, D. M.; Tuttolomondo, M. E.; Ben Altabef, A.
Vibrational studies (FTIR and Raman), conformational analysis, NBO, HOMO-LUMO and reactivity descriptors of S-methyl thiobutanoate, CH3CH2CH2C(O)SCH3
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (149): 408-418 2015.

Gilday, L. C.; Robinson, S. W.; Barendt, T. A.; Langton, M. J.; Mullaney, B. R.; Beer, P. D.

Halogen Bonding in Supramolecular Chemistry
Chemical Reviews, (115): 7118-7195 2015.

Giri, G. F.; Sarotti, A. M.; Spanevello, R. A.
Understanding reactivity and regioselectivity in Diels-Alder reactions of a sugar-derived dienophile bearing two competing EWGs. An experimental and computational study
Carbohydrate Research, (415): 54-59 2015.

Giricheva, N. I.; Fedorov, M. S.; Girichev, G. V.
Conformations of methylbenzenesulfonate and its substituted derivatives: gas-phase electron diffraction versus vibrational spectroscopy
Structural Chemistry, (26): 1543-1553 2015.

Giricheva, N. I.; Lapykina, E. A.; Fedorov, M. S.; Petrova, D. A.
Fluorescent tags. dansyl amide (CH3)(2)N-D(10)De(6)-SO2NH2: Reflection of the conformational properties of a free molecule in crystal structures
Journal of Structural Chemistry, (56): 619-627 2015.

Gish, J. T.; Popov, I. A.; Boldyrev, A. I.
Homocatenation of Aluminum: Alkane-like Structures of Li2Al2H6 and Li3Al3H8
Chemistry-a European Journal, (21): 5307-5310 2015.

Gladich, I.; Francisco, J. S.; Buszek, R. J.; Vazdar, M.; Carignano, M. A.; Shepson, P. B.
Ab Initio Study of the Reaction of Ozone with Bromide Ion
Journal of Physical Chemistry A, (119): 4482-4488 2015.

Glatz, M.; Bichler, B.; Mastalir, M.; Stoger, B.; Weil, M.; Mereiter, K.; Pittenauer, E.; Allmaier, G.; Veiros, L. F.; Kirchner, K.
Iron(II) complexes featuring kappa(3)- and kappa(2)-bound PNP pincer ligands - the significance of sterics
Dalton Transactions, (44): 281-294 2015.

Goh, M. S.; Rintoul, L.; Pfrunder, M. C.; McMurtrie, J. C.; Arnold, D. P.
Azo dicarboxylates are not conjugated: X-ray crystal structure and theoretical calculations on di-t-butylazodicarboxylate
Journal of Molecular Structure, (1098): 298-305 2015.

Golchoubian, H.; Moayyedi, G.
Experimental and DFT studies on solvatochromism behavior of a synthesized mixed chelate copper(II) complex
Polyhedron, (100): 303-312 2015.

Goli, M.; Shahbazian, S.
Hidden aspects of the Structural theory of chemistry: MC-QTAIM analysis reveals "alchemical'' transformation from a triatomic to a diatomic structure
Physical Chemistry Chemical Physics, (17): 245-255 2015.

Gomes, G. D.; Vil, V.; Terent'ev, A.; Alabugin, I. V.
Stereoelectronic source of the anomalous stability of bis-peroxides
Chemical Science, (6): 6783-6791 2015.

Gomez, S.; Restrepo, A.; Hadad, C. Z.
Theoretical tools to distinguish O-ylides from O-ylidic complexes in carbene-solvent interactions
Physical Chemistry Chemical Physics, (17): 31917-31930 2015.

Gondzik, S.; Wolper, C.; Haack, R.; Jansen, G.; Schulz, S.
(L2Zn2)-L-Me(mu-1,6-Ph-2-N-6) - a building block for new hexazene complexes
Dalton Transactions, (44): 15703-15711 2015.

Gong, S. D.; Luo, Q.; Dou, N.; Chi, Q. K.; Peng, B.; Xie, Y. M.; King, R. B.; Schaefer, H. F.
Homoleptic Tetranuclear Rhodium Carbonyls: Comparison with Their Iridium Analogues

Journal of Physical Chemistry A, (119): 1177-1189 2015.

Gong, S. D.; Luo, Q.; Li, Q. S.; Xie, Y. M.; King, R. B.; Schaefer, H. F.
Major differences between trifluorophosphine and carbonyl ligands in binuclear cyclopentadienyliron complexes
New Journal of Chemistry, (39): 3708-3718 2015.

Gong, Y.; Andrews, L.; Liebov, B. K.; Fang, Z. T.; Garner, E. B.; Dixon, D. A.
Reactions of laser-ablated U atoms with (CN)(2): infrared spectra and electronic structure calculations of UNC, U(NC)(2), and U(NC)(4) in solid argon
Chemical Communications, (51): 3899-3902 2015.

Gong, Y.; de Jong, W. A.; Gibson, J. K.
Gas Phase Uranyl Activation: Formation of a Uranium Nitrosyl Complex from Uranyl Azide
Journal of the American Chemical Society, (137): 5911-5915 2015.

Gonzalez, M. M.; Bravo-Rodriguez, K.; Suardiaz, R.; de la Vega, J. M. G.; Montero, L. A.; Sanchez-Garcia, E.; Crespo-Otero, R.
Complexes of nitric oxide with water and imidazole
Theoretical Chemistry Accounts, (134) 2015.

Gonzalez-Santana, S.; Morera-Boado, C.; Montero-Cabrera, L. A.; Trueba, M.; Trasatti, S. P.
Pyrrolyl-Silicon Compounds as Precursors for Donor-Acceptor Systems Stabilized by Noncovalent Interactions
Journal of Physical Chemistry A, (119): 7038-7051 2015.

Gopi, R.; Ramanathan, N.; Sundararajan, K.
Acetonitrile-water hydrogen-bonded interaction: Matrix-isolation infrared and ab initio computation
Journal of Molecular Structure, (1094): 118-129 2015.

Gopi, R.; Ramanathan, N.; Sundararajan, K.
Hydrogen-bonded complexes of acetylene and acetonitrile: A matrix isolation infrared and computational study
Journal of Molecular Structure, (1083): 364-373 2015.

Govindarasu, K.; Kavitha, E.
Structural, vibrational spectroscopic studies and quantum chemical calculations of n-(2,4-dinitrophenyl)-L-alanine methyl ester by density functional theory
Journal of Molecular Structure, (1088): 70-84 2015.

Govindarasu, K.; Kavitha, E.; Sundaraganesan, N.; Suresh, M.; Padusha, M. S. A.
Synthesis, structural and spectral analysis of (E)-N '-(4-Methoxybenzylidene)pyridine-3-carbohydrazide dihydrate by density functional theory
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (135): 1123-1136 2015.

Govindasamy, P.; Gunasekaran, S.
Experimental and theoretical studies of (FT-IR, FT-Raman, UV-Visible and DFT) 4-(6-methoxynaphthalen-2-yl) butan-2-one
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (149): 800-811 2015.

Govindasamy, P.; Gunasekaran, S.
Quantum mechanical calculations and spectroscopic (FT-IR, FT-Raman and UV) investigations, molecular orbital, NLO, NBO, NLMO and MESP analysis of 4- 5-(4-methylphenyl)-3-(trifluoromethyl)-1H-pyrazol-1-yl benzene-1-sulfonamide
Journal of Molecular Structure, (1081): 96-109 2015.

Govindasamy, P.; Gunasekaran, S.
Spectroscopic (FT-IR, FT-Raman and UV) investigation, NLO, NBO, molecular orbital and MESP analysis of 2-{2- (2,6-dichlorophenyl)amino phenyl}acetic acid
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (136): 1543-1556 2015.

Grabowski, S. J.
Cleavage of hydrogen by activation at a single non-metal centre - towards new hydrogen storage materials

Physical Chemistry Chemical Physics, (17): 13539-13546 2015.

Grabowski, S. J.
Lewis acid-Lewis base interactions: From NFH3+center dot center dot center dot NCH and NF4+center dot center dot center dot NCH complexes to NFH3+center dot center dot center dot dot(NCH)(n) and NF4+center dot center dot center dot dot(NCH)(n) clusters
Computational and Theoretical Chemistry, (1053): 289-297 2015.

Grabowski, S. J.
pi-Hole Bonds: Boron and Aluminum Lewis Acid Centers
Chemphyschem, (16): 1470-1479 2015.

Grabowski, S. J.
Triel Bonds, pi-Hole-pi-Electrons Interactions in Complexes of Boron and Aluminium Trihalides and Trihydrides with Acetylene and Ethylene
Molecules, (20): 11297-11316 2015.

Grande-Aztatzi, R.; Cabellos, J. L.; Islas, R.; Infante, I.; Mercero, J. M.; Restrepo, A.; Merino, G.
Planar pentacoordinate carbons in CBe54- derivatives
Physical Chemistry Chemical Physics, (17): 4620-4624 2015.

Greif, A. H.; Hrobarik, P.; Hrobarikova, V.; Arbuznikov, A. V.; Autschbach, J.; Kaupp, M.
A Relativistic Quantum-Chemical Analysis of the trans Influence on H-1 NMR Hydride Shifts in Square-Planar Platinum(II) Complexes
Inorganic Chemistry, (54): 7199-7208 2015.

Gronowski, M.; Kofos, R.
An ab initio study of structure, stability, and spectroscopic parameters of 5-atomic C, C, H, N, S isomers
Journal of Molecular Structure, (1090): 76-85 2015.

Grossekappenberg, H.; Luhmann, N.; Saak, W.; Muller, T.
A Molecular Hexacoordinated Triorganoaluminum Compound with Trifold Si-H center dot center dot center dot Al Coordination
Zeitschrift fur Anorganische und Allgemeine Chemie, (641): 2543-2548 2015.

Gualco, P.; Mallet-Ladeira, S.; Kameo, H.; Nakazawa, H.; Mercy, M.; Maron, L.; Amgoune, A.; Bourissou, D.
Coordination of a Triphosphine-Silane to Gold: Formation of a Trigonal Pyramidal Complex Featuring Au+-> Si Interaction
Organometallics, (34): 1449-1453 2015.

Guha, A. K.; Borthakur, B.; Phukan, A. K.
Spectroscopic Distinction of Different Carbon Bases: An Insight from Theory
Journal of Organic Chemistry, (80): 7301-7304 2015.

Guidara, S.; Feki, H.; Abid, Y.
Structural, vibrational, NLO, MEP, NBO analysis and DFT calculation of bis 2,5-dimethylaniliniurn sulfate
Journal of Molecular Structure, (1080): 176-187 2015.

Gumus, H. P.; Tamer, O.; Avci, D.; Atalay, Y.
A theoretical study on 2-chloro-5-(2-hydroxyethyl)-4-methoxy-6-methylpyrimidine by DFT/ab initio calculations
Materials Science-Poland, (33): 369-380 2015.

Gunay, N.; Tamer, O.; Kuzalic, D.; Avci, D.; Atalay, Y.
Theoretical Investigation of N-Methyl-N '-(4-nitrobenzylidene) pyrazine-2-carbohydrazide: Conformational Study, NBO Analysis, Molecular Structure and NMR Spectra
Acta Physica Polonica A, (127): 701-710 2015.

Guo, J. C.; Ren, G. M.; Miao, C. Q.; Tian, W. J.; Wu, Y. B.; Wang, X. T.

CBe(5)H(n)n-4 (n=2-5): Hydrogen-Stabilized CBe5 Pentagons Containing Planar or Quasi-Planar Pentacoordinate Carbons
Journal of Physical Chemistry A, (119): 13101-13106 2015.

Guo, W. L.; Lian, X.; Xiao, P.; Liu, F. L.; Yang, Y.; Zhang, Y. H.; Zhang, X. X.
DFT studies on the interaction of PtxRuyMz (M = Fe, Ni, Cu, Mo, Sn, x + y + z = 4, x >= 1, y >= 1) alloy clusters with O-2
Molecular Physics, (113): 854-865 2015.

Guo, X.; An, X. L.; Li, Q. Z.
Se center dot center dot center dot N Chalcogen Bond and Se center dot center dot center dot X Halogen Bond Involving F2C=Se: Influence of Hybridization, Substitution, and Cooperativity
Journal of Physical Chemistry A, (119): 3518-3527 2015.

Guo, X.; Li, Q. Z.
Dual functions of Lewis acid and base of Se in F2C=Se and their interplay in F2CSe center dot center dot center dot NH3 center dot center dot center dot HX
Journal of Molecular Modeling, (21) 2015.

Guo, X.; Li, Q. Z.; Xiao, B.; Yang, X.; Li, W. Z.; Cheng, J. B.
Influence of F and Se substitution on the structures, stabilities and nature of the complexes between F2CSe and HOX (X = F, Cl, Br, and I)
Rsc Advances, (5): 52667-52675 2015.

Guo, X.; Liu, Y. W.; Li, Q. Z.; Li, W. Z.; Cheng, J. B.
Competition and cooperativity between tetrel bond and chalcogen bond in complexes involving F2CX (X = Se and Te)
Chemical Physics Letters, (620): 7-12 2015.

Gupta, R.; Yehl, J.; Li, M. Y.; Polenova, T.
V-51 magic angle spinning NMR spectroscopy and quantum chemical calculations in vanadium bio-inorganic systems: current perspective
Canadian Journal of Chemistry, (93): 929-937 2015.

Gupta, U.; Kumar, V.; Singh, V. K.; Kant, R.; Khajuria, Y.
Spectroscopic studies and quantum chemical investigations of (3,4-dimethoxybenzylidene) propanedinitrile
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (140): 65-73 2015.

Gutsev, G. L.; Belay, K. G.; Weatherford, C. A.; Ramachandran, B. R.; Gutsev, L. G.; Jena, P.
Structure and Properties of Polyfluoride F-n(-) Clusters (n=3-29)
Journal of Physical Chemistry A, (119): 6483-6492 2015.

Gutsev, G. L.; Weatherford, C. A.; Ramachandran, B. R.; Gutsev, L. G.; Zheng, W. J.; Thomas, O. C.; Bowen, K. H.
Photoelectron spectra and structure of the Mn-n(-) anions (n=2-16)
Journal of Chemical Physics, (143) 2015.

Gutsev, L. G.; Dalal, N. S.; Gutsev, G. L.
Structure and Properties of a (CdSe)(6)@(CdSe)(30) Cluster Doped with Mn Atoms
Journal of Physical Chemistry C, (119): 6261-6277 2015.

Hadad, C. Z.; Jenkins, S.; Florez, E.
Unusual solvation through both p-orbital lobes of a carbene carbon
Journal of Chemical Physics, (142) 2015.

Haghdadi, M.; Asghari, S.; Ramezani, S.
Computational study on the mechanism of the three-component reaction of dimethylacetylene dicarboxylate and triphenylphosphine with 2-acetylbutyrolactone
Canadian Journal of Chemistry, (93): 666-672 2015.

Haider, A.; Bhattacharya, S.; Datta, A.; Bhattacharyya, D.; Mitra, A.

The role of N7 protonation of guanine in determining the structure, stability and function of RNA base pairs
Physical Chemistry Chemical Physics, (17): 26249-26263 2015.

Haines, B. E.; Musaev, D. G.
Factors Impacting the Mechanism of the Mono-N-Protected Amino Acid Ligand-Assisted and Directing-Group-Mediated C-H Activation Catalyzed by Pd(II) Complex
Acs Catalysis, (5): 830-840 2015.

Hajipour, A. R.; Chermahini, A. N.; Karimzadeh, M.; Rezapour, M.
Tautomerism and mechanism of intramolecular proton transfer under the gas phase and micro-hydrated solvent conditions: biuret as a case study
Structural Chemistry, (26): 159-169 2015.

Halbert, S.; Gerard, H.
A computational study of the effects of ancillary ligands on copper(I)-ethylene interaction
New Journal of Chemistry, (39): 5410-5419 2015.

Hamad, S.; Balestra, S. R. G.; Bueno-Perez, R.; Calero, S.; Ruiz-Salvador, A. R.
Atomic charges for modeling metal-organic frameworks: Why and how
Journal of Solid State Chemistry, (223): 144-151 2015.

Hamedani, S.; Aghaie, H.
Molecular Structure and Theoretical Thermodynamic Study of Folic Acid Based on the Computational Approach
Chinese Journal of Structural Chemistry, (34): 1307-1316 2015.

Hamedani, S.; Moradi, S.; Aghaie, H.
Adsorption of Folic Acid on the Single-walled Carbon Nanotubes: AIM and NBO Analyses via DFT
Chinese Journal of Structural Chemistry, (34): 1161-1169 2015.

Hamid, A.; Kanan, S.; Tahat, Z. A.
DFT analysis of substituent effects on electron-donating efficacy of pyridine
Research on Chemical Intermediates, (41): 6859-6875 2015.

Hammami, F.; Ghalla, H.; Chebaane, A.; Nasr, S.
Structural and spectroscopic investigation of the N-methylformamide-water (NMF center dot center dot center dot 3H(2)O) complex
Molecular Physics, (113): 149-159 2015.

Hammami, F.; Ghalla, H.; Nasr, S.
Intermolecular hydrogen bonds in urea-water complexes: DEL NBO, and AIM analysis
Computational and Theoretical Chemistry, (1070): 40-47 2015.

Hamzehloueian, M.; Sarrafi, Y.; Aghaei, Z.
An experimental and theoretical study on the regioselective synthesis of a new class of spiropyrrolothiazoles with quinoxaline motifs via a 1,3-dipolar cycloaddition reaction. An evaluation of DFT methods
Rsc Advances, (5): 76368-76376 2015.

Han, L.; Lei, Y.; Xing, P.; Zhao, X. L.; Jiang, B.
2.2 Paracyclophane-Derived Monodentate Phosphoramidite Ligands for Copper-Catalyzed Asymmetric Conjugate Addition of Diethylzinc to Substituted Chalcones
Journal of Organic Chemistry, (80): 3752-3757 2015.

Han, Y. X.; Kong, C.; Hou, L. J.; Wu, B. W.; Chen, D. P.; Gao, L. G.
Theoretical Research on the Multi-channel Reaction Mechanism of CHF Radical with HNCO by Density Functional Theory
Chinese Journal of Structural Chemistry, (34): 1151-1160 2015.

Hapka, M.; Dranka, M.; Orlowska, K.; Chalasinski, G.; Szczesniak, M. M.; Zachara, J.

Noncovalent interactions determine the conformation of aurophilic complexes with 2-mercapto-4-methyl-5-thiazoleacetic acid ligands
Dalton Transactions, (44): 13641-13650 2015.

Haque, M. R.; Ghosh, S.; Hogarth, G.; Richmond, M. G.; Kabir, S. E.
Synthesis, structure and bonding of new mono- and dinuclear molybdenum complexes containing pyridine-2-thiolate (pyS) and different P-donors
Inorganica Chimica Acta, (434): 150-157 2015.

Haress, N. G.; El-Emam, A. A.; Al-Deeb, O. A.; Panicker, C. Y.; Al-Saadi, A. A.; Van Alsenoy, C.; War, J. A.; Srivastava, S. K.
Vibrational spectroscopic and molecular docking study of 2-Benzylsulfanyl-4- (4-methylphenyl)-sulfanyl -6-pentylpyrimidine-5-carb onitrile, a potential chemotherapeutic agent
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (137): 569-580 2015.

Harper, L. K.; Bayse, C. A.
Modeling the chelation of As(III) in lewisite by dithiols using density functional theory and solvent-assisted proton exchange
Journal of Inorganic Biochemistry, (153): 60-67 2015.

Harper, L. K.; Shoaf, A. L.; Bayse, C. A.
Predicting Trigger Bonds in Explosive Materials through Wiberg Bond Index Analysis
Chemphyschem, (16): 3886-3892 2015.

Harrath, K.; Boughdiri, S.; Linguerri, R.; Hochlaf, M.
Mechanistic study of bismuth-catalyzed direct benzylation of 2,4-pentanediones: the case of BiCl3 and generalization
Theoretical Chemistry Accounts, (135) 2015.

Hasanzadeh, N.; Nori-Shargh, D.
Correlations between hardness, electronegativity, anomeric effect associated with electron delocalizations and electrostatic interactions in 1,4,5,8-tetraoxadecalin and its analogs containing S and Se atoms
Computational and Theoretical Chemistry, (1051): 1-9 2015.

Hasanzadeh, N.; Nori-Shargh, D.; Farzipour, M.; Ahmadi, B.
The origin of the anomeric effect: probing the impacts of stereoelectronic interactions
Organic & Biomolecular Chemistry, (13): 6965-6976 2015.

Haschka, T.; Henon, E.; Jaillet, C.; Martiny, L.; Etchebest, C.; Dauchez, M.
Direct minimization: Alternative to the traditional L-2 norm to derive partial atomic charges
Computational and Theoretical Chemistry, (1074): 50-57 2015.

Hasebe, M.; Musumeci, D.; Yu, L.
Fast Surface Crystallization of Molecular Glasses: Creation of Depletion Zones by Surface Diffusion and Crystallization Flux
Journal of Physical Chemistry B, (119): 3304-3311 2015.

Hassan, B.; Muraleedharan, K.; Mujeeb, V. M. A.
Density functional theory studies of Pb (II) interaction with chitosan and its derivatives
International Journal of Biological Macromolecules, (74): 483-488 2015.

He, H. Y.; Chen, H.; Zheng, Y. Z.; Zhang, S. J.; Yu, Z. W.
Hydrogen-bonding interactions between a pyridinium-based ionic liquid C4Py SCN and dimethyl sulfoxide
Chemical Engineering Science, (121): 169-179 2015.

He, P. A.; Zhang, J. G.; Wang, K.; Yin, X.; Zhang, T. L.
Combination Multinitrogen with Good Oxygen Balance: Molecule and Synthesis Design of Polynitro-Substituted Tetrazolotriazine-Based Energetic Compounds
Journal of Organic Chemistry, (80): 5643-5651 2015.

Heidamezhad, Z.; Vahedpour, M.; Razavizadeh, S. A.
A theoretical DFT study on the stability of imidazopyridine and its derivatives considering the solvent effects and NBO analysis
Bulgarian Chemical Communications, (47): 578-586 2015.

Heinz, N.; Dolg, M.; Berkessel, A.
A Theoretical Study of Imine Hydrocyanation Catalyzed by Halogen-Bonding
Journal of Computational Chemistry, (36): 1812-1817 2015.

Hemmateenejad, B.; Shojaeifard, Z.; Shamsipur, M.; Neymeyr, K.; Sawall, M.; Mohajeri, A.
Solute-induced perturbation of methanol-water association
Rsc Advances, (5): 71102-71108 2015.

Hernandez-Soto, H.; Jaffer, E.; Chen, S. M.; Pesch, M. J.
Theoretical study of CH3SO3-Na+center dot H2O (n) clusters: Implications for sea-salt methanesulfonate aerosols
Computational and Theoretical Chemistry, (1065): 7-11 2015.

Herres-Pawlis, S.; Haase, R.; Verma, P.; Hoffmann, A.; Kang, P.; Stack, T. D. P.
Formation of Hybrid Guanidine-Stabilized Bis(mu-oxo)-dicopper Cores in Solution: Electronic and Steric Perturbations
European Journal of Inorganic Chemistry: 5426-5436 2015.

Herve, A.; Bouzidi, Y.; Berthet, J. C.; Belkhiri, L.; Thuery, P.; Boucekkine, A.; Ephritikhine, M.
U-III-CN versus U-IV-NC Coordination in Tris(silylamide) Complexes
Inorganic Chemistry, (54): 2474-2490 2015.

Herve, M.; Lefevre, G.; Mitchell, E. A.; Maes, B. U. W.; Jutand, A.
On the Triple Role of Fluoride Ions in Palladium-Catalyzed Stille Reactions
Chemistry-a European Journal, (21): 18401-18406 2015.

Heydari, H.; Raissi, H.; Mollania, F.
Quantum chemical study on influence of the substitution effect on the structural and electronic properties and intramolecular hydrogen bonding of 2-nitrophenyl hydrosulfide in ground and electronic excited state
Structural Chemistry, (26): 971-987 2015.

Hiberty, P. C.; Danovich, D.; Shaik, S.
Comment on "Rabbit-ears hybrids, VSEPR sterics, and other orbital anachronisms''. A reply to a criticism
Chemistry Education Research and Practice, (16): 689-693 2015.

Hickox, H. P.; Wang, Y. Z.; Xie, Y. M.; Chen, M.; Wei, P.; Schaefer, H. F.; Robinson, G. H.
Transition-Metal-Mediated Cleavage of a Si=Si Double Bond
Angewandte Chemie-International Edition, (54): 10267-10270 2015.

Hien, N. K.; Bao, N. C.; Nhung, N. T. A.; Trung, N. T.; Nam, P. C.; Duong, T.; Kim, J. S.; Quang, D. T.
A highly sensitive fluorescent chemosensor for simultaneous determination of Ag(I), Hg(II), and Cu(II) ions: Design, synthesis, characterization and application
Dyes and Pigments, (116): 89-96 2015.

Higashino, T.; Imahori, H.
Hybrid 5 Radialenes with Bispyrroloheteroles: New Electron-Donating Units
Chemistry-a European Journal, (21): 13375-13381 2015.

Hilal, R.; Aziz, S. G.; Alyoubi, A. O.; Elroby, S. A.
Ultrafast radiationless decay mechanisms through conical intersections in cytosine: Computational insight and topological analysis of the charge density distributions
Indian Journal of Chemistry Section a-Inorganic Bio-Inorganic Physical Theoretical & Analytical Chemistry, (54): 27-34 2015.

Hinz, A.; Schulz, A.; Villinger, A.

A Mixed Arsenic-Phosphorus Centered Biradicaloid
Angewandte Chemie-International Edition, (54): 668-672 2015.

Hinz, A.; Schulz, A.; Villinger, A.; Wolter, J. M.
Cyclo-Pnicta-triazanes: Biradicaloids or Zwitterions?
Journal of the American Chemical Society, (137): 3975-3980 2015.

Ho, M. H.; O'Hagan, M.; Dupuis, M.; DuBois, D. L.; Bullock, R. M.; Shaw, W. J.; Raugei, S.
Water-assisted proton delivery and removal in bio-inspired hydrogen production catalysts
Dalton Transactions, (44): 10969-10979 2015.

Holligan, K.; Rogler, P.; Rehe, D.; Pamula, M.; Kornienko, A. Y.; Emge, T. J.; Krogh-Jespersen, K.; Brennan, J. G.
Copper, Indium, Tin, and Lead Complexes with Fluorinated Selenolate Ligands: Precursors to MSex
Inorganic Chemistry, (54): 8896-8904 2015.

Holtomo, O.; Nsangou, M.; Fifen, J. J.; Motapon, O.
Antioxidative Potency and UV-Vis spectra features of the compounds resulting from the chelation of Fe2+ by Caffeic Acid Phenethyl Ester and two of its derivatives
Computational and Theoretical Chemistry, (1067): 135-147 2015.

Holzmann, N.; Andrada, D. M.; Frenking, G.
Bonding situation in silicon complexes (L)(2)(Si-2) and (L)(2)(Si) with NHC and cAAC ligands
Journal of Organometallic Chemistry, (792): 139-148 2015.

Honarparvar, B.; Pawar, S. A.; Alves, C. N.; Lameira, J.; Maguire, G. E. M.; Silva, J. R. A.; Govender, T.; Kruger, H. G.
Pentacycloundecane lactam vs lactone norstatine type protease HIV inhibitors: binding energy calculations and DFT study
Journal of Biomedical Science, (22) 2015.

Horacek, M.; Gyepes, R.; Cisarova, I.; Pinkas, J.; Kubista, J.; Lamac, M.
Intramolecular activation of a pendant nitrile group in Ti and Zr metallocene complexes
Journal of Organometallic Chemistry, (787): 56-64 2015.

Horn, P. R.; Head-Gordon, M.
Polarization contributions to intermolecular interactions revisited with fragment electric-field response functions
Journal of Chemical Physics, (143) 2015.

Hou, D.; Wu, D.; Sun, W. M.; Li, Y.; Li, Z. R.
Evolution of structure, stability, and nonlinear optical properties of the heterodinuclear CNLin (n=1-10) clusters
Journal of Molecular Graphics and Modelling, (59): 92-99 2015.

Hou, J. H.; Duan, Q.; Qin, J. M.; Shen, X. D.; Zhao, J. X.; Liang, Q. C.; Jiang, D. Y.; Gao, S.
Unconventional charge distribution in the planar wheel-type M (c) B6H6-/0/+ (M = Mn, Fe and Co): central M with negative charges and peripheral boron ring with positive charges
Physical Chemistry Chemical Physics, (17): 9644-9650 2015.

Hou, S. L.; Bernath, P. F.
Relationship between Dipole Moments and Harmonic Vibrational Frequencies in Diatomic Molecules
Journal of Physical Chemistry A, (119): 1435-1438 2015.

Hruszkewycz, D. P.; Guard, L. M.; Balcells, D.; Feldman, N.; Hazari, N.; Tilset, M.
Effect of 2-Substituents on Allyl-Supported Precatalysts for the Suzuki-Miyaura Reaction: Relating Catalytic Efficiency to the Stability of Palladium(I) Bridging Allyl Dimers
Organometallics, (34): 381-394 2015.

Hsu, Y. C.; Shen, J. S.; Lin, B. C.; Chen, W. C.; Chan, Y. T.; Ching, W. M.; Yap, G. P. A.; Hsu, C. P.; Ong, T. G.
Synthesis and Isolation of an Acyclic Tridentate Bis(pyridine)carbodicarbene and Studies on Its Structural Implications and Reactivities

Angewandte Chemie-International Edition, (54): 2420-2424 2015.

Hu, D. D.; Sun, S. J.; Yuan, P. Q.; Zhao, L.; Liu, T.
Evaluation of CO2-Philicity of Poly(vinyl acetate) and Poly(vinyl acetate-alt-maleate) Copolymers through Molecular Modeling and Dissolution Behavior Measurement
Journal of Physical Chemistry B, (119): 3194-3204 2015.

Hu, Y. Q.; Zhu, N.; Han, L. M.
Channel of Electronic Interactions in Diferrocenyl Pyrrole Derivatives
Acta Physico-Chimica Sinica, (31): 227-236 2015.

Huang, C.; He, R. X.; Shen, W.; Li, M.
Mechanisms for the synthesis of conjugated enynes from diphenylacetylene and trimethylsilylacetylene catalyzed by a nickel(0) complex: DFT study of ligand-controlled selectivity
Journal of Molecular Modeling, (21) 2015.

Huang, K. M.; Ke, X. N.; Wang, H. K.; Wang, J. Y.; Zhou, C. C.; Xu, X. F.; Liu, L. Y.; Li, J.
PtI2-catalyzed cyclization of 3-acyloxy-1,5-enynes with the elimination of HOAc and a benzyl shift: synthesis of unsymmetrical m-terphenyls
Organic & Biomolecular Chemistry, (13): 4486-4493 2015.

Huang, N. N.; Xu, J. Z.; Zhang, H.; Xu, Z.
The origin of the decreasing basicity from monofunctional alkoxysilane to tetrafunctional alkoxysilane: A combined IR and theoretical study
Journal of Molecular Structure, (1089): 216-221 2015.

Huang, P. Q.; Lai, C. H.
Computational study of unsaturated and saturated cyclic (alkyl) (amino) carbene borane complexes
Computational and Theoretical Chemistry, (1051): 17-23 2015.

Huang, X. Q.; Wang, M.; Wang, L. S.; Wang, J. Y.
How rhodium (III) complexes catalyze alkenylation of C(sp(3))-H bond of 8-methyquinolines
Journal of Organometallic Chemistry, (787): 1-7 2015.

Huang, Y. J.; Zhu, Q. J.
Computational Modeling and Theoretical Calculations on the Interactions between Spermidine and Functional Monomer (Methacrylic Acid) in a Molecularly Imprinted Polymer
Journal of Chemistry, 2015.

Hubner, A.; Kaese, T.; Diefenbach, M.; Endeward, B.; Bolte, M.; Lerner, H. W.; Holthausen, M. C.; Wagner, M.
A Preorganized Ditopic Borane as Highly Efficient One- or Two-Electron Trap
Journal of the American Chemical Society, (137): 3705-3714 2015.

Hughes, Z. E.; Walsh, T. R.
Computational chemistry for graphene-based energy applications: progress and challenges
Nanoscale, (7): 6883-6908 2015.

Hunt, P. A.; Ashworth, C. R.; Matthews, R. P.
Hydrogen bonding in ionic liquids
Chemical Society Reviews, (44): 1257-1288 2015.

Hupf, E.; Lork, E.; Mebs, S.; Beckmann, J.
Sterically Congested 5-Diphenylphosphinoacenaphth-6-yl-silanes and -silanols
Organometallics, (34): 3873-3887 2015.

Hussain, M. A.; Mahadevi, A. S.; Sastry, G. N.
Estimating the binding ability of onium ions with CO2 and pi systems: a computational investigation
Physical Chemistry Chemical Physics, (17): 1763-1775 2015.

Hwang, L.; Ayaz-Guner, S.; Gregorich, Z. R.; Cai, W. X.; Valeja, S. G.; Jin, S.; Ge, Y.
Specific Enrichment of Phosphoproteins Using Functionalized Multivalent Nanoparticles
Journal of the American Chemical Society, (137): 2432-2435 2015.

Ibad, M. F.; Schuz, A.; Villinger, A.
Pentafluorophenyl Silver: Structure and Bonding of Arene Solvates
Organometallics, (34): 3893-3901 2015.

Ikawa, T.; Kaneko, H.; Masuda, S.; Ishitsubo, E.; Tokiwa, H.; Akai, S.
Trifluoromethanesulfonyloxy-group-directed regioselective (3+2) cycloadditions of benzynes for the synthesis of functionalized benzo-fused heterocycles
Organic & Biomolecular Chemistry, (13): 520-526 2015.

Improta, R.; Vitagliano, L.; Esposito, L.
Bond distances in polypeptide backbones depend on the local conformation
Acta Crystallographica Section D-Biological Crystallography, (71): 1272-1283 2015.

Ince, A.; Carstensen, H. H.; Reyniers, M. F.; Marin, G. B.
First-principles based group additivity values for thermochemical properties of substituted aromatic compounds
AIChE Journal, (61): 3858-3870 2015.

Ince, H. H.; Konuklar, F. A. S.; Ugur, I.; Ozcan, O. A.; Sayadi, M.; Feig, M.; Aviyente, V.
Role of the n+1 amino acid residue on the deamidation of asparagine in pentapeptides
Molecular Physics, (113): 3839-3848 2015.

Ioannidis, E. I.; Kulik, H. J.
Towards quantifying the role of exact exchange in predictions of transition metal complex properties
Journal of Chemical Physics, (143) 2015.

Iriarte, A. G.; Pelaez, W. J.; Fulop, F.; Arguello, G. A.
Vibrational spectra of solid cis- and trans-2-thioxohexahydroquinazolin-4(1H)-one and theoretical calculations towards the interpretation of its thermal reactivity
Rsc Advances, (5): 43345-43352 2015.

Ishikawa, H.; Kawasaki, T.; Inomata, R.
Infrared Spectroscopy of Phenol-Triethylsilane Dihydrogen-Bonded Cluster and its Cationic Analogues: Intrinsic Strength of the Si-H center dot center dot center dot H-O Dihydrogen Bond
Journal of Physical Chemistry A, (119): 601-609 2015.

Issaoui, N.; Ghalla, H.; Muthu, S.; Flakus, H. T.; Oujia, B.
Molecular structure, vibrational spectra, AIM, HOMO-LUMO, NBO, UV, first order hyperpolarizability, analysis of 3-thiophenecarboxylic acid monomer and dimer by Hartree-Fock and density functional theory
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (136): 1227-1242 2015.

Ivanov, A. S.; Miller, E.; Boldyrev, A. I.; Kameoka, Y.; Sato, T.; Tanaka, K.
Pseudo Jahn-Teller Origin of Buckling Distortions in Two-Dimensional Triazine-Based Graphitic Carbon Nitride (g-C3N4) Sheets
Journal of Physical Chemistry C, (119): 12008-12015 2015.

Ivanov, A. S.; Zhang, X.; Wang, H.; Boldyrev, A. I.; Gantefoer, G.; Bowen, K. H.; Cernusak, I.
Anion Photoelectron Spectroscopy and CASSCF/CASPT2/RASSI Study of La-n(-) (n=1, 3-7)
Journal of Physical Chemistry A, (119): 11293-11303 2015.

Izadyar, M.; Balgerdi, R.; Pourayoubi, M.
A combined quantum mechanics and molecular mechanics study on nitrogen oxide adsorption/dissociation on a tungsten oxide surface
Progress in Reaction Kinetics and Mechanism, (40): 128-142 2015.

Izadyar, M.; Khavani, M.; Housaindokht, M. R.
A combined molecular dynamic and quantum mechanic study of the solvent and guest molecule effect on the stability and length of heterocyclic peptide nanotubes
Physical Chemistry Chemical Physics, (17): 11382-11391 2015.

Izquierdo-Ruiz, F.; Menendez, J. M.; Recio, J. M.
Theoretical analysis of vibrational modes in uranyl aquo chloro complexes
Theoretical Chemistry Accounts, (134) 2015.

Jagadeesan, R.; Velmurugan, G.; Venuvanalingam, P.
The nature of Pd-carbene and Pd-halogen bonds in (bisNHC)PdX2 type catalysts: insights from density functional theory
Rsc Advances, (5): 80661-80667 2015.

Jager, M.; Freitag, L.; Gonzalez, L.
Using computational chemistry to design Ru photosensitizers with directional charge transfer
Coordination Chemistry Reviews, (304): 146-165 2015.

Jaladanki, C. K.; Taxak, N.; Varikoti, R. A.; Bharatam, P. V.
Toxicity Originating from Thiophene Containing Drugs: Exploring the Mechanism using Quantum Chemical Methods
Chemical Research in Toxicology, (28): 2364-2376 2015.

Jalali, E.; Nori-Shargh, D.
Symmetry breaking in the axial symmetrical configurations of enolic propanedial, propanedithial, and propanediselenal: pseudo Jahn-Teller effect versus the resonance-assisted hydrogen bond theory
Canadian Journal of Chemistry, (93): 673-684 2015.

Jalife, S.; Wu, J. I. C.; Martinez-Guajardo, G.; Schleyer, P. V.; Fernandez-Herrera, M. A.; Merino, G.
The 9-homocubyl cation rearrangement revisited
Chemical Communications, (51): 5391-5393 2015.

Jana, S.; Harms, K.; Bauza, A.; Frontera, A.; Chattopadhyay, S.
Synthesis, Structures, and DFT Study of CuBr Based Coordination Polymers via in Situ Reduction of Copper(II)
Crystal Growth & Design, (15): 257-267 2015.

Janciene, R.; Javorskis, T.; Mikulskiene, G.; Vektariene, A.; Vektaris, G.; Klimavicius, K. A.
Novel synthesis of quinazolino 3,2-a 1,5 benzodiazepines: an experimental and computational study
Arkivoc: 366-382 2015.

Janesko, B. G.; Scalmani, G.; Frisch, M. J.
Quantifying solvated electrons' delocalization
Physical Chemistry Chemical Physics, (17): 18305-18317 2015.

Jankovic, N.; Bugarcic, Z.; Markovic, S.
Double catalytic effect of (PhNH3)(2)CuCl4 in a novel, highly efficient synthesis of 2-oxo- and thioxo-1,2,3,4-tetrahydropyrimidines
Journal of the Serbian Chemical Society, (80): 595-604 2015.

Jasmine, N. J.; Muthiah, P. T.; Arunagiri, C.; Subashini, A.
Vibrational spectra (experimental and theoretical), molecular structure, natural bond orbital, HOMO-LUMO energy, Mulliken charge and thermodynamic analysis of N '-hydroxy-pyrimidine-2-carboximidamide by DFT approach
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (144): 215-225 2015.

Jastrzebska, I.; Morawiak, M.; Rode, J. E.; Seroka, B.; Siergiejczyk, L.; Morzycki, J. W.
Oxidation of Olefins with Benzeneseleninic Anhydride in the Presence of TMSOTf
Journal of Organic Chemistry, (80): 6052-6061 2015.

Javadian, S.; Ektefa, F.
An efficient approach to explore the adsorption of benzene and phenol on nanostructured catalysts: a DFT analysis
Rsc Advances, (5): 100799-100808 2015.

Jeilani, Y. A.; Duncan, K. A.; Newallo, D. S.; Thompson, A. N.; Bose, N. K.
Tandem mass spectrometry and density functional theory of RDX fragmentation pathways: Role of ion-molecule complexes in loss of NO3 and lack of molecular ion peak
Rapid Communications in Mass Spectrometry, (29): 802-810 2015.

Jerez, A. L. P.; Antognini, A. F.; Cutin, E. H.; Robles, N. L.
Synthesis, characterization and vibrational properties of p-fluorosulfinylaniline
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (137): 300-305 2015.

Jerez, A. L. P.; Chemes, D. M.; Cutin, E. H.; Oberhammer, H.; Robles, N. L.
Synthesis and experimental and theoretical characterization of m-fluorosulfinylaniline
New Journal of Chemistry, (39): 4445-4451 2015.

Jerez, A. L. P.; de Armino, D. J. A.; Robles, N. L.
Synthesis and characterization of o-fluorosulfinylaniline. A comparative vibrational study of fluorinated sulfinylaniline series
New Journal of Chemistry, (39): 9894-9902 2015.

Jesus, A. J. L.; Jarmelo, S.; Fausto, R.; Reva, I.
Conformational preferences of 3,4-dihydroxyphenylacetic acid (DOPAC)
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (140): 54-64 2015.

Jesus, A. J. L.; Redinha, J. S.
Methoxyindoles: stability and pi-electron delocalization
Structural Chemistry, (26): 655-666 2015.

Jeyavijayan, S.
Molecular structure, spectroscopic (FTIR, FT-Raman, C-13 and H-1 NMR, UV), polarizability and first-order hyperpolarizability, HOMO-LUMO analysis of 2,4-difluoroacetophenone
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (136): 553-566 2015.

Jeyavijayan, S.
Molecular structure, vibrational spectra, NBO analysis, first hyperpolarizability, and HOMO-LUMO studies of 2-amino-4-hydroxypyrimidine by density functional method
Journal of Molecular Structure, (1085): 137-146 2015.

Jeyavijayan, S.
Spectroscopic (FTIR, FT-Raman), molecular electrostatic potential, NBO and HOMO-LUMO analysis of P-bromobenzene sulfonyl chloride based on DFT calculations
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (136): 890-899 2015.

Ji, L. F.; Li, A. Y.; Li, Z. Z.
Structures and stabilities of asymmetrical dimer radical cation systems (AH(3)-H2O)(+) (A=N, P, As)
Structural Chemistry, (26): 109-119 2015.

Ji, L. F.; Li, A. Y.; Li, Z. Z.
Structures and stabilities of hemi-bonded vs proton-transferred isomers of dimer radical cation systems (XH3-YH3)(+) (X,Y = N,P,As)
Chemical Physics Letters, (619): 115-121 2015.

Jiang, H. Y.; Zhang, G. B.; Liu, Y.; Guo, X. Y.; Liu, Z.; Yan, H.; Liu, H. L.; Huang, X. R.
Theoretical insights into the reaction mechanism and solvation effect of conjugate addition of dimethyl propanedioate to 1-nitroprop-1-ene catalyzed by cinchona alkaloids
Structural Chemistry, (26): 951-959 2015.

Jiang, N.; Schwarz, W. H. E.; Li, J.
Theoretical Studies on Hexanuclear Oxometalates M6L19 (q-) (M = Cr, Mo, W, Sg, Nd, U). Electronic Structures, Oxidation States, Aromaticity, and Stability
Inorganic Chemistry, (54): 7171-7180 2015.

Jiang, Y. X.; Peng, Y. J.
Excited-State Intramolecular Proton Transfer Reaction of 3-Hydroxyflavone
Journal of Cluster Science, (26): 1983-1992 2015.

Jiao, Y.; Zheng, Y.; Jaroniec, M. T.; Qiao, S. Z.
Design of electrocatalysts for oxygen- and hydrogen-involving energy conversion reactions
Chemical Society Reviews, (44): 2060-2086 2015.

Jin, L.; Wu, Y.; Zhao, X.
Theoretical Insight into the Mechanism of Gold(I)-Catalyzed Rearrangement of 2-Propargyl 2H-Azirines to Pyridines
Journal of Organic Chemistry, (80): 3547-3555 2015.

Jin, L. X.; Zhao, C. B.; Zhang, T. L.; Wang, Z. Y.; Min, S. T.; Wang, W. L.; Wei, Y. W.
Effects of an acid-alkaline environment on the reactivity of 5-carboxycytosine with hydroxyl radicals
Rsc Advances, (5): 87364-87376 2015.

Jin, R. F.; Chang, Y. F.
A theoretical study on photophysical properties of triphenylamine-cored molecules with naphthalimide arms and different pi-conjugated bridges as organic solar cell materials
Physical Chemistry Chemical Physics, (17): 2094-2103 2015.

Jin, X.; Willeke, M.; Lucchesi, R.; Daniliuc, C. G.; Frohlich, R.; Wibbeling, B.; Uhl, W.; Wurthwein, E. U.
Hydroalumination of Ketenimines and Subsequent Reactions with Heterocumulenes: Synthesis of Unsaturated Amide Derivatives and 1,3-Diimines
Journal of Organic Chemistry, (80): 6062-6075 2015.

Jin, X. L.; Hao, L. K.; She, M. Y.; Obst, M.; Kappler, A.; Yin, B.; Liu, P.; Li, J. L.; Wang, L. Y.; Shi, Z.
Visualizing tributyltin (TBT) in bacterial aggregates by specific rhodamine-based fluorescent probes
Analytica Chimica Acta, (853): 514-520 2015.

John, J. S.; Sajan, D.; Umadevi, T.; Chaitanya, K.; Sankar, P.; Philip, R.
Synthesis, crystal structure, vibrational spectral analysis and Z-scan studies of a new organic crystal N,N ' dimethylurea ninhydrin: A scaled quantum mechanical force field study
Optical Materials, (48): 233-242 2015.

Johnston, S. B.; Raines, R. T.
Conformational Stability and Catalytic Activity of PTEN Variants Linked to Cancers and Autism Spectrum Disorders
Biochemistry, (54): 1576-1582 2015.

Jones, J. S.; Wade, C. R.; Gabbai, F. P.
Guilty on Two Counts: Stepwise Coordination of Two Fluoride Anions to the Antimony Atom of a Noninnocent Stibine Ligand
Organometallics, (34): 2647-2654 2015.

Joo, B.; Kim, E. G.
Model-independent determination of the degree of charge transfer in molecular and metal complexes
Chemical Communications, (51): 15071-15074 2015.

Joohari, S.; Monajjemi, M.
NMR and NBO study of vinblastine as a biological inhibitor
Bulgarian Chemical Communications, (47): 631-646 2015.

Joseph, J. A.; McDowell, S. A. C.
Comparative Computational Study of Model Halogen-Bonded Complexes of FKrCl
Journal of Physical Chemistry A, (119): 2568-2577 2015.

Joshi, P. R.; Ramanathan, N.; Sundararajan, K.; Sankaran, K.
Evidence for Phosphorus Bonding in Phosphorus Trichloride-Methanol Adduct: A Matrix Isolation Infrared and ab Initio Computational Study
Journal of Physical Chemistry A, (119): 3440-3451 2015.

Jothi, M.; Kumaradhas, P.
Probing the effect of electric field in 9,10-dimethoxy-2,6-bis(2-p-tolylethynyl)anthracene molecular nanowire using quantum chemical and charge density analysis
Molecular Simulation, (41): 315-324 2015.

Juaristi, E.; Notario, R.
Theoretical Examination of the S-C-P Anomeric Effect
Journal of Organic Chemistry, (80): 2879-2883 2015.

Kabanda, M. M.
A theoretical study of the antioxidant properties of phenolic acid amides investigated through the radical-scavenging and metal chelation mechanisms
European Food Research and Technology, (241): 553-572 2015.

Kabanda, M. M.; Tran, V. T.; Seema, K. M.; Serobatse, K. R. N.; Tsiepe, T. J.; Tran, Q. T.; Ebenso, E. E.
Conformational, electronic and antioxidant properties of lucidone, linderone and methyllinderone: DFT, QTAIM and NBO studies
Molecular Physics, (113): 683-697 2015.

Kahlfuss, C.; Metay, E.; Duclos, M. C.; Lemaire, M.; Milet, A.; Saint-Aman, E.; Bucher, C.
Chemically and Electrochemically Triggered Assembly of Viologen Radicals: Towards Multiaddressable Molecular Switches
Chemistry-a European Journal, (21): 2090-2106 2015.

Kakanejadifard, A.; Japelaghi, S.; Ghasemian, M.; Zabardasti, A.
Theoretical study of molecular interactions of sulfoximine with hypohalous acids HOF, HOCl, and HOBr
Structural Chemistry, (26): 23-33 2015.

Kalpana, A.; Akilandeswari, L.
The effect of fluorine substitution on the conformation and aromaticity of eta 6(-)fluoro arene chromium tricarbonyl complexes - Density functional insights
Computational and Theoretical Chemistry, (1069): 125-131 2015.

Kalyva, M.; Zografos, A. L.; Kapourani, E.; Giambazolias, E.; Devel, L.; Papakyriakou, A.; Dive, V.; Lazarou, Y. G.; Georgiadis, D.
Probing the Mechanism of Allylic Substitution of Morita-Baylis-Hillman Acetates (MBHAs) by using the Silyl Phosphonite Paradigm: Scope and Applications of a Versatile Transformation
Chemistry-a European Journal, (21): 3278-3289 2015.

Kamaee, M.; Sun, M.; Luong, H.; van Wijngaarden, J.
Investigation of Structural Trends in Mono-, Di-, and Pentafluorobenzonitriles Using Fourier Transform Microwave Spectroscopy
Journal of Physical Chemistry A, (119): 10279-10292 2015.

Kamalian, M.; Jalili, Y. S.; Abbasi, A.
Density functional theory calculations of the carbon nanotube based P-N junction by substitution of carbon atoms with B, N, Ge and Sn
Indian Journal of Physics, (89): 663-669 2015.

Kan, M.; Nam, H. G.; Lee, Y. H.; Sun, Q.

Phase stability and Raman vibration of the molybdenum ditelluride (MoTe2) monolayer
Physical Chemistry Chemical Physics, (17): 14866-14971 2015.

Kanagathara, N.; Marchewka, M. K.; Drozd, M.; Gunasekaran, S.; Rajakunnar, P. R.; Anbalagan, G.
Structural and vibrational spectroscopic studies on charge transfer and ionic hydrogen bonding interactions of melaminium benzoate dihydrate
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (145): 394-409 2015.

Kandasamy, M.; Velraj, G.; Kalaichelvan, S.; Mariappan, G.
Characterization of 1,5-dimethoxynaphthalene by vibrational spectroscopy (FT-IR and FT-Raman) and density functional theory calculations
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (134): 191-199 2015.

Kang, Y. K.; Park, H. S.
Hairpin formation promoted by the heterochiral dinipecotic acid segment: A DFT study
Biopolymers, (103): 609-617 2015.

Karakus, N.; Demirel, M.
The trans-cis and the azide-tetrazole ring-chain isomerization of 2-azido-1,3-azoles: Quantum chemical study
Journal of Molecular Structure, (1093): 65-76 2015.

Karczmarzyk, Z.; Wysocki, W.; Urbanczyk-Lipkowska, Z.; Kalicki, P.; Bielawska, A.; Bielawski, K.; Laweckea, J.
Synthetic Approaches for Sulfur Derivatives Containing 1,2,4-Triazine Moiety: Their Activity for in Vitro Screening towards Two Human Cancer Cell Lines
Chemical and Pharmaceutical Bulletin, (63): 531-537 2015.

Kariev, A. M.; Green, M. E.
Quantum Effects in a Simple Ring with Hydrogen Bonds
Journal of Physical Chemistry B, (119): 5962-5969 2015.

Karpfen, A.
On the potential energy surfaces of dimers formed between trans-glyoxal, trans-acrolein and formaldehyde
Computational and Theoretical Chemistry, (1061): 60-71 2015.

Karpinska, G.; Dobrowolski, J. C.
On tautomerism of 1,2,4-triazol-3-ones
Computational and Theoretical Chemistry, (1052): 58-67 2015.

Karpinska, G.; Dobrowolski, J. C.
On the 6-and 7-substituted chromone system. A computational study
Computational and Theoretical Chemistry, (1067): 158-163 2015.

Karthick, T.; Balachandran, V.; Perumal, S.
Spectroscopic investigations, molecular interactions, and molecular docking studies on the potential inhibitor "thiophene-2-carboxylicacid"
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (141): 104-112 2015.

Kasavajhala, K.; Bikkina, S.; Patil, I.; MacKerell, A. D.; Priyakumar, U. D.
Dispersion Interactions between Urea and Nucleobases Contribute to the Destabilization of RNA by Urea in Aqueous Solution
Journal of Physical Chemistry B, (119): 3755-3761 2015.

Katari, M.; Rajaraman, G.; Ghosh, P.
An insight into a base-free Michael addition reaction as catalyzed by a bifunctional nickel N-heterocyclic carbene complex using density functional theory studies
Journal of Organometallic Chemistry, (775): 109-116 2015.

Kato, K.; Fukuzawa, K.; Mochizuki, Y.

Modeling of hydroxyapatite-peptide interaction based on fragment molecular orbital method
Chemical Physics Letters, (629): 58-64 2015.

Kaur, D.; Kaur, R.
Theoretical Characterization of Hydrogen Bonding Interactions between RCHO (R = H, CN, CF3, OCH3, NH2) and HOR'(R' = H, Cl, CH3, NH2, C(O)H, C6H5)
Journal of Chemical Sciences, (127): 1299-1313 2015.

Kaur, G.; Vikas
Exploring the mechanism of isomerisation and water-migration in the water-complexes of amino-acid L-proline: electrostatic potential and vibrational analysis
Rsc Advances, (5): 82587-82604 2015.

Kaur, J.; Singla, P.; Goel, N.
Adsorption of oxazole and isoxazole on BNNT surface: A DFT study
Applied Surface Science, (328): 632-640 2015.

Kaur, R. P.; Kaur, D.; Sharma, R.
Substituent effect on N-H bond dissociation enthalpies of carbamates: a theoretical study
Canadian Journal of Chemistry, (93): 279-288 2015.

Kavipriya, R.; Kavitha, H. P.; Karthikeyan, B.; Nataraj, A.
Molecular structure, spectroscopic (FT-IR, FT-Raman), NBO analysis of N,N '-diphenyl-6-piperidin-1-yl- 1,3,5 -triazine-2,4-diamine
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (150): 476-487 2015.

Kavousi, H.; Raissi, H.; Rezaeifard, A.; Jafarpour, M.
Stereoelectronic effects of porphyrin ligand on the oxygen transfer efficiency of high valent manganese-oxo porphyrin species: A DFT study
Journal of Porphyrins and Phthalocyanines, (19): 1130-1139 2015.

Kavousi, H.; Rezaeifard, A.; Raissi, H.; Jafarpour, M.
A DFT investigation of axial N-donor ligands effects on the high valent manganese-oxo meso-tetraphenyl porphyrin
Journal of Porphyrins and Phthalocyanines, (19): 651-662 2015.

Kawauchi, S.; Hayashi, Y.; Tomita, Y.; Hashimoto, R.; Honda, K.; Itoh, Y.; Mikami, K.
THEORETICAL STUDY ON RADICAL TRIFLUOROMETHYLATION OF SILYL ENOL ETHERS ACCELERATED VIA COMPLEXATION WITH DIALICYLZINC
Heterocycles, (90): 907-917 2015.

Keaveney, S. T.; Harper, J. B.; Croft, A. K.
Computational approaches to understanding reaction outcomes of organic processes in ionic liquids
Rsc Advances, (5): 35709-35729 2015.

Kecel-Gunduz, S.; Celik, S.; Ozel, A. E.; Akyuz, S.
Structural and vibrational spectroscopic elucidation of sulpiride in solid state
Journal of Biomolecular Structure and Dynamics, (33): 322-343 2015.

Keddie, N. S.; Slawin, A. M. Z.; Lebl, T.; Philp, D.; O'Hagan, D.
All-cis 1,2,3,4,5,6-hexafluorocyclohexane is a facially polarized cyclohexane
Nature Chemistry, (7): 483-488 2015.

Kee, C. L.; Zhou, F.; Su, H. B.; Yan, Y. K.
Formation of "A-frame" dirhenium(I) hexacarbonyl complexes by trans-1,2-bis(diphenylphosphino)ethylene and bis(bidentate) ligands
Journal of Organometallic Chemistry, (792): 211-219 2015.

Keerthana, S. P.; Kolandaivel, P.

Interaction between dimer interface residues of native and mutated SOD1 protein: a theoretical study
Journal of Biological Inorganic Chemistry, (20): 509-522 2015.

Kegl, T.
Computational aspects of hydroformylation
Rsc Advances, (5): 4304-4327 2015.

Kelemen, Z.; Streubel, R.; Nyulaszi, L.
Zwitterionic carbene adducts and their carbene isomers
Rsc Advances, (5): 41795-41802 2015.

Khalili, B.; Rimaz, M.; Tondro, T.
DFT study on foscarnet as an antiviral drug: Conformer analysis, gas phase acidity, metal ion affinity and influence of metal complexation on gas phase acidity
Journal of Molecular Structure, (1080): 80-87 2015.

Khan, E.; Shukla, A.; Srivastava, A.; Shweta; Tandon, P.
Molecular structure, spectral analysis and hydrogen bonding analysis of ampicillin trihydrate: a combined DFT and AIM approach
New Journal of Chemistry, (39): 9800-9812 2015.

Khan, M. S.; Pal, S.; Krupadam, R. J.
Computational strategies for understanding the nature of interaction in dioxin imprinted nanoporous trappers
Journal of Molecular Recognition, (28): 427-437 2015.

Khatilian, M. H.; Mirzaei, S.; Taherpour, A.
Comprehensive insights into the structure and coordination behavior of thiosemicarbazone ligands: a computational assessment of the E-Z interconversion mechanism during coordination
New Journal of Chemistry, (39): 9313-9324 2015.

Khavani, M.; Izadyar, M.
A Comprehensive Study of the Solvent Effects on the Cycloaddition Reaction of Diethyl Azodicarboxylate and Ethyl Vinyl Ether: Efficient Implementation of QM and TD-DFT Study
International Journal of Quantum Chemistry, (115): 381-388 2015.

Khavani, M.; Izadyar, M.
Implicit and explicit solvent effects on the selectivity of the cycloaddition reaction of cyclopentadiene and methyl acrylate; a theoretical study
Progress in Reaction Kinetics and Mechanism, (40): 303-312 2015.

Khavani, M.; Izadyar, M.; Housaindokht, M. R.
DFT investigation and molecular dynamic simulation on the selective complexation of cis-cyclic nanopeptides with alkaline earth metal ions
Sensors and Actuators B-Chemical, (221): 1120-1129 2015.

Khavani, M.; Izadyar, M.; Housaindokht, M. R.
Theoretical design of the cyclic lipopeptide nanotube as a molecular channel in the lipid bilayer, molecular dynamics and quantum mechanics approach
Physical Chemistry Chemical Physics, (17): 25536-25549 2015.

Kilina, S.; Kilin, D.; Tretiak, S.
Light-Driven and Phonon-Assisted Dynamics in Organic and Semiconductor Nanostructures
Chemical Reviews, (115): 5929-5978 2015.

Kim, K. C.; Moghadam, P. Z.; Fairen-Jimenez, D.; Snurr, R. Q.
Computational Screening of Metal Catecholates for Ammonia Capture in Metal-Organic Frameworks
Industrial & Engineering Chemistry Research, (54): 3257-3267 2015.

Kirilchuk, A. A.; Yurchenko, A. A.; Kostyuk, A. N.; Rozhenko, A. B.
1,2-Migration in N-Phosphano Functionalized N-Heterocyclic Carbenes
Journal of Computational Chemistry, (36): 42-48 2015.

Kisan, H. K.; Sunoj, R. B.
Axial Coordination Dichotomy in Dirhodium Carbenoid Catalysis: A Curious Case of Cooperative Asymmetric Dual-Catalytic Approach toward Amino Esters
Journal of Organic Chemistry, (80): 2192-2197 2015.

Kishida, R.; Saputro, A. G.; Kasai, H.
Mechanism of dopachrome tautomerization into 5,6-dihydroxyindole-2-carboxylic acid catalyzed by Cu(II) based on quantum chemical calculations
Biochimica Et Biophysica Acta-General Subjects, (1850): 281-286 2015.

Knizia, G.; Klein, J.
Electron Flow in Reaction Mechanisms-Revealed from First Principles
Angewandte Chemie-International Edition, (54): 5518-5522 2015.

Knorr, A.; Fumino, K.; Bonsa, A. M.; Ludwig, R.
Spectroscopic evidence of 'jumping and pecking' of cholinium and H-bond enhanced cation-cation interaction in ionic liquids
Physical Chemistry Chemical Physics, (17): 30978-30982 2015.

Knorr, A.; Ludwig, R.
Cation-cation clusters in ionic liquids: Cooperative hydrogen bonding overcomes like-charge repulsion
Scientific Reports, (5) 2015.

Knurr, B. J.; Weber, J. M.
Structures of CoO(CO2)(n) (-) and NiO(CO2)(n) (-) Clusters Studied by Infrared Spectroscopy
Journal of Physical Chemistry A, (119): 843-850 2015.

Kobayashi, H.; Teranishi, M.; Naya, S.; Tada, H.
Mechanism of the Multiple-Electron Oxygen Reduction Reaction in the Presence of the Binuclear Cu(acac)(2) Complex
Chemphyschem, (16): 3392-3396 2015.

Kochanek, S. E.; Clymer, T. M.; Pakkala, V. S.; Hebert, S. P.; Reeping, K.; Firestine, S. M.; Evanseck, J. D.
Intramolecular Charge-Assisted Hydrogen Bond Strength in Pseudochair Carboxyphosphate
Journal of Physical Chemistry B, (119): 1184-1191 2015.

Koleva, G.; Galabov, B.; Hadjieva, B.; Schaefer, H. F.; Schleyer, P. V.
An Experimentally Established Key Intermediate in Benzene Nitration with Mixed Acid
Angewandte Chemie-International Edition, (54): 14123-14127 2015.

Kolocouris, A.; Koch, A.; Kleinpeter, E.; Stylianakis, I.
2-Substituted and 2,2-disubstituted adamantane derivatives as models for studying substituent chemical shifts and C-H-ax center dot center dot center dot Y-ax cyclohexane contacts-results from experimental and theoretical NMR spectroscopic chemical shifts and DFT structures
Tetrahedron, (71): 2463-2481 2015.

Kondo, M.; Kobayashi, N.; Hatanaka, T.; Funahashi, Y.; Nakamura, S.
Catalytic Enantioselective Reaction of -Phenylthioacetonitriles with Imines Using Chiral Bis(imidazoline)-Palladium Catalysts
Chemistry-a European Journal, (21): 9066-9070 2015.

Kong, L. B.; Ganguly, R.; Li, Y. X.; Kinjo, R.
Diverse reactivity of a tricoordinate organoboron L2PhB: (L = oxazol-2-ylidene) towards alkali metal, group 9 metal, and coinage metal precursors
Chemical Science, (6): 2893-2902 2015.

Kong, M. M.; Wang, K.; Dong, R. N.; Gao, H. J.
Enzyme catalytic nitration of aromatic compounds
Enzyme and Microbial Technology, (73-74): 34-43 2015.

Kong, Z. G.; Wang, W.; Zhang, S. Q.; Zhao, F. W.; Wang, X. Y.
Synthesis, Crystal Structure, Physical Properties and Theoretical Calculations of a New One-Dimensional Ni(II) Coordination Polymer Constructed by 1,10-Phenanthroline Derivative Ligand and Sulfate
Journal of Inorganic and Organometallic Polymers and Materials, (25): 1441-1447 2015.

Koohi, M.; Kassaee, M. Z.; Haerizade, B. N.; Ghavami, M.; Ashenagar, S.
Substituent effects on cyclonona-3,5,7-trienylidenes: a quest for stable carbenes at density functional theory level
Journal of Physical Organic Chemistry, (28): 514-526 2015.

Korenaga, T.; Suzuki, N.; Sueda, M.; Shimada, K.
Ligand effect on direct arylation by CMD process
Journal of Organometallic Chemistry, (780): 63-69 2015.

Korlyukov, A. A.
Coordination compounds of tetravalent silicon, germanium and tin: the structure, chemical bonding and intermolecular interactions in them
Russian Chemical Reviews, (84): 422-440 2015.

Kotyk, C. M.; Fieser, M. E.; Palumbo, C. T.; Ziller, J. W.; Darago, L. E.; Long, J. R.; Furche, F.; Evans, W. J.
Isolation of+2 rare earth metal ions with three anionic carbocyclic rings: bimetallic bis(cyclopentadienyl) reduced arene complexes of La(2+)and Ce2+ are four electron reductants
Chemical Science, (6): 7267-7273 2015.

Kovac, B.; Ljubic, I.; Kivimaki, A.; Corenoc, M.; Novak, I.
The study of the electronic structure of some N-heterocyclic carbenes (NHCs) by variable energy photoelectron spectroscopy
Physical Chemistry Chemical Physics, (17): 10656-10667 2015.

Kovacs, A.; Apostolidis, C.; Walter, O.; Lindqvist-Reis, P.
'Lanthanide contraction' in Ln(BTP)(3) (CF3SO3)(3) complexes
Structural Chemistry, (26): 1287-1295 2015.

Koyama, K.; Kudoh, S.; Miyajima, K.; Mafune, F.
Dissociation energy for O-2 release from gas-phase iron oxide clusters measured by temperature-programmed desorption experiments
Chemical Physics Letters, (625): 104-109 2015.

Koyama, K.; Kudoh, S.; Miyajima, K.; Mafune, F.
Stable Stoichiometry of Gas-Phase Manganese Oxide Cluster Ions Revealed by Temperature-Programmed Desorption
Journal of Physical Chemistry A, (119): 8433-8442 2015.

Kroutil, O.; Chval, Z.; Skelton, A. A.; Predota, M.
Computer Simulations of Quartz (101)-Water Interface over a Range of pH Values
Journal of Physical Chemistry C, (119): 9274-9286 2015.

Kumar, A.; Bheeter, L. P.; Gangwar, M. K.; Sortais, J. B.; Darcel, C.; Ghosh, P.
Nickel complexes of 1,2,4-triazole derived amido-functionalized N-heterocyclic carbene ligands: Synthesis, theoretical studies and catalytic application
Journal of Organometallic Chemistry, (786): 63-70 2015.

Kumar, C. S. C.; Balachandran, V.; Fun, H. K.; Chandraju, S.; Quah, C. K.
Synthesis, crystal growth, single crystal X-ray analysis and vibrational spectral studies of (2E)-3-(2-chloro-4-fluorophenyl)-1-(3,4-dimethoxyphenyl)prop-2-en-1-one: A combined DFT study

Journal of Molecular Structure, (1100): 299-310 2015.

Kumar, C. S. C.; Govindarasu, K.; Fun, H. K.; Kavitha, E.; Chandraju, S.; Quah, C. K.
Synthesis, molecular structure, spectroscopic characterization and quantum chemical calculation studies of (2E)-1-(5-chlorothiophen-2-yl)-3-(2,3,4-trimethoxyphenyl)prop-2-en-1-one
Journal of Molecular Structure, (1085): 63-77 2015.

Kumar, J. S.; Jeyavijayan, S.; Arivazhagan, M.
Vibrational spectral investigation, NBO, first hyperpolarizability and UV-Vis spectral analysis of 3,5-dichlorobenzonitrile and m-bromobenzonitrile by ab initio and density functional theory methods
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (136): 234-246 2015.

Kumar, K. A.; Kannaboina, P.; Dhaked, D. K.; Vishwakarma, R. A.; Bharatam, P. V.; Das, P.
Cu-catalyzed arylation of the amino group in the indazole ring: regioselective synthesis of pyrazolo-carbazoles
Organic & Biomolecular Chemistry, (13): 1481-1491 2015.

Kumar, N.; Sandi, G.; Kaminski, M.; Bobadilla, A.; Mertz, C.; Seminario, J. M.
Electron Transport in Graphene-Based Nanosensors for Eu(III) Detection
Journal of Physical Chemistry C, (119): 12037-12046 2015.

Kumar, S. S.; Athimoolam, S.; Sridhar, B.
Hydrogen bonding motifs, spectral characterization, theoretical computations and anticancer studies on chloride salt of 6-mercaptopurine: An assembly of corrugated lamina shows enhanced solubility
Journal of Molecular Structure, (1098): 332-341 2015.

Kumar, S. S.; Athimoolam, S.; Sridhar, B.
XRD, vibrational spectra and quantum chemical studies of an anticancer drug: 6-Mercaptopurine
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (146): 204-213 2015.

Kumar, V. R.; Rajkumar, N.; Umapathy, S.
Solvatochromism of 9,10-phenanthrenequinone: An electronic and resonance Raman spectroscopic study
Journal of Chemical Physics, (142) 2015.

Kumar, V. R. S.; Binoy, J.; Roy, S. D. D.; Marchewka, M. K.; Jayakumar, V. S.
Evans hole and non linear optical activity in Bis(melaminium) sulphate dihydrate: A vibrational spectral study
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (151): 292-301 2015.

Kurnia, K. A.; Quental, M. V.; Santos, L.; Freire, M. G.; Coutinho, J. A. P.
Mutual solubilities between water and non-aromatic sulfonium-, ammonium- and phosphonium-hydrophobic ionic liquids
Physical Chemistry Chemical Physics, (17): 4569-4577 2015.

Kus, N.; Sagdinc, S.; Fausto, R.
Infrared Spectrum and UV-Induced Photochemistry of Matrix-Isolated 5-Hydroxyquinoline
Journal of Physical Chemistry A, (119): 6296-6308 2015.

Kusama, H.; Sayama, K.
A comparative computational study on the interactions of N719 and N749 dyes with iodine in dye-sensitized solar cells
Physical Chemistry Chemical Physics, (17): 4379-4387 2015.

Kutateladze, A. G.; Mukhina, O. A.
Minimalist Relativistic Force Field: Prediction of Proton-Proton Coupling Constants in H-1 NMR Spectra Is Perfected with NBO Hybridization Parameters
Journal of Organic Chemistry, (80): 5218-5225 2015.

Kuznetsov, A. E.
Metalloporphyrins with all the pyrrole nitrogens replaced with phosphorus atoms, MP(P)(4) (M = Sc, Ti, Fe, Ni, Cu, Zn)
Chemical Physics, (447): 36-45 2015.

Kuznetsov, M. L.; Rocha, B. G. M.; Pombeiro, A. J. L.; Shul'pin, G. B.
Oxidation of Olefins with Hydrogen Peroxide Catalyzed by Bismuth Salts: A Mechanistic Study
Acs Catalysis, (5): 3823-3835 2015.

Lai, C. H.
A Comparison of the Lewis Basicity of Diamidocarbenes and Diaminocarbenes
Australian Journal of Chemistry, (68): 1084-1090 2015.

Lakshmipriya, A.; Chaudhari, S. R.; Shahi, A.; Arunan, E.; Suryaprakash, N.
Three centered hydrogen bonds of the type C=O...H(N)...X-C in diphenyloxamide derivatives involving halogens and a rotating CF3 group: NMR, QTAIM, NCI and NBO studies
Physical Chemistry Chemical Physics, (17): 7528-7536 2015.

Lan, J. H.; Wang, C. Z.; Wu, Q. Y.; Wang, S. A.; Feng, Y. X.; Zhao, Y. L.; Chai, Z. F.; Shi, W. Q.
A Quasi-relativistic Density Functional Theory Study of the Actinyl(VI, V) (An = U, Np, Pu) Complexes with a Six-Membered Macrocycle Containing Pyrrole, Pyridine, and Furan Subunits
Journal of Physical Chemistry A, (119): 9178-9188 2015.

Landis, C. R.; Hughes, R. P.; Weinhold, F.
Bonding Analysis of TM(cAAC)(2) (TM = Cu, Ag, and Au) and the Importance of Reference State
Organometallics, (34): 3442-3449 2015.

Landman, M.; Conradie, J.
E versus Z isomers of Fischer aminocarbene complex Mo(CO)(4)(PPh3){C(NHCy)(2-furyl)} : N-H center dot center dot center dot O versus C-H center dot center dot center dot O intramolecular hydrogen bonds
Journal of Molecular Structure, (1094): 36-45 2015.

Landman, M.; Levell, T. J.; Conradie, M. M.; van Rooyen, P. H.; Conradie, J.
Structural and conformational study of pentacarbonyl and phosphine substituted Fischer alkoxy- and aminocarbene complexes of molybdenum
Journal of Molecular Structure, (1086): 190-200 2015.

Lankelma, M.; de Boer, J.; Ferbinteanu, M.; Ramos, A. L. D.; Tanasa, R.; Rothenberg, G.; Tanase, S.
A novel one-dimensional chain built of vanadyl ions and pyrazine-2,5-dicarboxylate
Dalton Transactions, (44): 11380-11387 2015.

Lasri, J.; Soliman, S. M.; Charmier, M. A. J.; Rios-Gutierrez, M.; Domingo, L. R.
Synthesis, molecular structure and stability of fused bicyclic Delta(4)-1,2,4-oxadiazoline Pt(II) complexes
Polyhedron, (98): 55-63 2015.

Lassagne, F.; Chevallier, F.; Roisnel, T.; Dorcet, V.; Mongin, F.; Domingo, L. R.
A Combined Experimental and Theoretical Study of the Ammonium Bifluoride Catalyzed Regioselective Synthesis of Quinoxalines and Pyrido 2,3-b pyrazines
Synthesis-Stuttgart, (47): 2680-2689 2015.

Laurence, C.; Legros, J.; Chantzis, A.; Planchat, A.; Jacquemin, D.
A Database of Dispersion-Induction DI, Electrostatic ES, and Hydrogen Bonding alpha 1 and beta 1 Solvent Parameters and Some Applications to the Multiparameter Correlation Analysis of Solvent Effects
Journal of Physical Chemistry B, (119): 3174-3184 2015.

Layeb, H.; Nacereddine, A. K.; Djerourou, A.; Rios-Gutierrez, M.; Domingo, L. R.
Understanding the role of the trifluoromethyl group in reactivity and regioselectivity in 3+2 cycloaddition reactions of enol acetates with nitrones. A DFT study
Journal of Molecular Modeling, (21) 2015.

LeBlanc, L. M.; Boyd, R. J.; Burnell, D. J.

Density Functional Theory Study of BF3-Mediated Additions of Enols and (Trimethylsilyl)oxy alkenes to an Oxyallyl Cation: Homologous Mukaiyama Reactions
Journal of Physical Chemistry A, (119): 6714-6722 2015.

Lee, J. H.; Park, H. S.; Kang, Y. K.
Conformational preferences of beta-sheet structures in cyclopropane-containing gamma-peptides
New Journal of Chemistry, (39): 4640-4646 2015.

Lee, M.; Zimmermann-Steffens, S. G.; Arey, J. S.; Fenner, K.; von Gunten, U.
Development of Prediction Models for the Reactivity of Organic Compounds with Ozone in Aqueous Solution by Quantum Chemical Calculations: The Role of Delocalized and Localized Molecular Orbitals
Environmental Science & Technology, (49): 9925-9935 2015.

Leela, J.; Hemamalini, R.; Muthu, S.; Al-Saadi, A. A.
Spectroscopic investigation (FTIR spectrum), NBO, HOMO-LUMO energies, NLO and thermodynamic properties of 8-Methyl-N-vanillyl-6-nonenamideby DFT methods
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (146): 177-186 2015.

Legnani, L.; Porta, A.; Caramella, P.; Toma, L.; Zanoni, G.; Vidari, G.
Computational Mechanistic Study of the Julia-Kocienski Reaction
Journal of Organic Chemistry, (80): 3092-3100 2015.

Lenormand, H.; Corce, V.; Sorin, G.; Chhun, C.; Chamoreau, L. M.; Krim, L.; Zins, E. L.; Goddard, J. P.; Fensterbank, L.
Versatile Access to Martin's Spirosilanes and Their Hypervalent Derivatives
Journal of Organic Chemistry, (80): 3280-3288 2015.

Lestard, M. E. D.; Tuttolomondo, M. E.; Ben Altabef, A.
Vibrational spectroscopy and conformation of S-ethyl thioacetate: CH3COSCH2CH3 and comparison with -C(O)S- and -C(O)O- compounds
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (135): 907-914 2015.

Leth, R.; Rydberg, P.; Jorgensen, F. S.; Olsen, L.
Density Functional Theory Study on the Formation of Reactive Benzoquinone Imines by Hydrogen Abstraction
Journal of Chemical Information and Modeling, (55): 660-666 2015.

Li, B.; Liu, B. G.; Li, J. Q.; Xiao, H. Z.; Wang, J. Y.; Liang, G. Z.
Experimental and Theoretical Investigations on the Supermolecular Structure of Isoliquiritigenin and 6-O-alpha-D-Maltosyl-beta-cyclodextrin Inclusion Complex
International Journal of Molecular Sciences, (16): 17999-18017 2015.

Li, C.; Dinoi, C.; Coppel, Y.; Etienne, M.
CH Bond Activation of Methane by a Transient eta(2)-Cyclopropene/Metallabicyclobutane Complex of Niobium
Journal of the American Chemical Society, (137): 12450-12453 2015.

Li, C. Y.; Agarwal, J.; Wu, C. H.; Allen, W. D.; Schaefer, H. F.
Intricate Internal Rotation Surface and Fundamental Infrared Transitions of the n-Propyl Radical
Journal of Physical Chemistry B, (119): 728-735 2015.

Li, F. X.; Xu, D. G.
Functional role of R462 in the degradation of hyaluronan catalyzed by hyaluronate lyase from Streptococcus pneumoniae
Journal of Molecular Modeling, (21) 2015.

Li, G. F.; Qi, X. F.; Li, X. M.; Ji, J. Y.; Niu, Y. L.; Wang, Q. W.
Synthesis, Crystal Structure and Theoretical Calculations of a Zinc(II) Coordination Polymer Assembled by 4,4'-Oxydibenzoic acid and 1,3-Bis(imidazol-1-ylmethyl)-benzene Ligands
Journal of Inorganic and Organometallic Polymers and Materials, (25): 576-582 2015.

Li, H. F.; Zhang, L. S.; Fan, X. L.; Zhao, Y.
Theoretical Studies on the Redox-Stimulated Isomerization in Electrochromic Osmium Sulfoxide Complexes
Journal of Physical Chemistry A, (119): 4244-4251 2015.

Li, H. F.; Zhang, L. S.; Wang, Y. F.; Fan, X. L.
Theoretical studies on the photoisomerization mechanism of osmium(II) sulfoxide complexes
Rsc Advances, (5): 58580-58586 2015.

Li, H. J.; Yi, H. B.; Xu, J. J.
High-order Cu(II) chloro-complexes in LiCl brines: Insights from density function theory and molecular dynamics
Geochimica et Cosmochimica Acta, (165): 1-13 2015.

Li, J.; Morrison, C. N.; Molenda, M. A.; Suvarna, T.; Tyminska, N.; Brennessel, W. W.; Sevilla, M. D.; Chavez, F. A.
Synthesis, structure and properties of tris(1-ethyl-4-isopropyl-imidazolyl-kappa N)phosphine copper(II)
Inorganica Chimica Acta, (434): 79-84 2015.

Li, J. B.; Rogachev, A. Y.
SO2 - yet another two-faced ligand
Physical Chemistry Chemical Physics, (17): 1987-2000 2015.

Li, J. C.; Li, Y.; Purushothaman, I.; De, S.; Li, B.; Zhu, H. P.; Parameswaran, P.; Ye, Q. S.; Liu, W. P.
Fine Tuning of the Substituents on the N-Geminal Phosphorus/Silicon-Based Lewis Pairs for the Synthesis of Z-Type Silyliminophosphoranylalkenes
Organometallics, (34): 4209-4217 2015.

Li, J. H.; Zuehlsdorff, T. J.; Payne, M. C.; Hine, N. D. M.
Identifying and tracing potential energy surfaces of electronic excitations with specific character via their transition origins: application to oxirane
Physical Chemistry Chemical Physics, (17): 12065-12079 2015.

Li, J. J.; Li, J. H.; Zhang, D. J.; Liu, C. B.
Theoretical Explanation for How SO3H-Functionalized Ionic Liquids Promote the Conversion of Cellulose to Glucose
Chemphyschem, (16): 3044-3048 2015.

Li, L.; Zhang, X. H.; Gong, S. D.; Zhao, H. X.; Bai, Y.; Li, Q. S.; Ji, L.
The discussion of descriptors for the QSAR model and molecular dynamics simulation of benzimidazole derivatives as corrosion inhibitors
Corrosion Science, (99): 76-88 2015.

Li, L. C.; Matsuo, T.; Hashizume, D.; Fueno, H.; Tanaka, K.; Tamao, K.
Coplanar Oligo(p-phenylenedisilenylene)s as Si=Si Analogues of Oligo(p-phenylenevinylene)s: Evidence for Extended pi-Conjugation through the Carbon and Silicon,pi-Frameworks
Journal of the American Chemical Society, (137): 15026-15035 2015.

Li, L. C.; Wang, W.; Peng, D.; Pan, R.; Tian, A. M.
Investigation on the photodriven catalytic coupling reaction mechanism of p-aminothiophenol on the silver cluster
Journal of Theoretical & Computational Chemistry, (14) 2015.

Li, L. W.; Wu, C. J.; Wang, Z. Q.; Zhao, L. X.; Li, Z.; Sun, C. S.; Sun, T. M.
Density functional theory (DFT) and natural bond orbital (NBO) study of vibrational spectra and intramolecular hydrogen bond interaction of L-ornithine-L-aspartate
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (136): 338-346 2015.

Li, M. C.; Shih, T. W.; Li, Y. C.; Ma, J. Y.; Su, M. D.
A Model Study on Molecular Properties and Mechanistic Investigations of P=C=E-14 Molecules
European Journal of Inorganic Chemistry: 1795-1803 2015.

Li, M. J.; Diao, L.; Liao, X. F.; Kou, L.; Lu, W. C.

DFT study on addition reaction mechanism of guanine-cytosine base pair with OH radical
Journal of Physical Organic Chemistry, (28): 437-444 2015.

Li, P.; Niu, W. X.; Gao, T.
Systematic analysis of structural and spectroscopic properties of neptunimine (HN=NpH2) and plutonimine (HN=PuH2)
Journal of Molecular Modeling, (21) 2015.

Li, Q. Z.; Zheng, J. J.; Zhao, X.
Azide addition to Sc-2@C-66: favorable activity on unsaturated linear triquinanes and dramatic reactivity difference compared with the free C-66 cage
Physical Chemistry Chemical Physics, (17): 20485-20489 2015.

Li, Q. Z.; Zheng, J. J.; Zhao, X.
Bingel-Hirsch Reaction on Sc-2@C-66: A Highly Regioselective Bond Neighboring to Unsaturated Linear Triquinanes
Journal of Physical Chemistry C, (119): 26196-26201 2015.

Li, Q. Z.; Zhuo, H. Y.; Li, H. B.; Liu, Z. B.; Li, W. Z.; Cheng, J. B.
Tetrel-Hydride Interaction between XH3F (X = C, Si, Ge, Sn) and HM (M = Li, Na, BeH, MgH)
Journal of Physical Chemistry A, (119): 2217-2224 2015.

Li, S. J.; Tang, H. B.; Wang, Y.; Zhu, Y. Y.; Fang, D. C.; Wei, D. H.; Tang, M. S.
A DFT study on the competing mechanisms of PPh3-catalyzed 3+3 and 3+2 annulations between 5-acetoxypenta-2,3-dienoate and 1C,3O-bisnucleophiles
Journal of Molecular Catalysis a-Chemical, (407): 137-146 2015.

Li, S. T.; Chen, L. P.; Ning, X. J.; Guo, M.; Zhang, M.
(1-x)Bi0.5Na0.5TiO3-xK(0.5)Na(0.5)NbO(3) ceramics with low coercive field: Preparation from hydrothermally synthesized precursor powders
Ceramics International, (41): 195-204 2015.

Li, S. W.; Yuan, D. W.; Yu, A.; Czap, G.; Wu, R. Q.; Ho, W.
Rotational Spectromicroscopy: Imaging the Orbital Interaction between Molecular Hydrogen and an Adsorbed Molecule
Physical Review Letters, (114) 2015.

Li, T. P.; Taylor-Edinbyrd, K.; Kumar, R.
A computational study of the effect of the metal organic framework environment on the release of chemically stored nitric oxide
Physical Chemistry Chemical Physics, (17): 23403-23412 2015.

Li, W.; Chen, C. H.; Zhao, D. B.; Li, S. H.
LSQC: Low Scaling Quantum Chemistry Program
International Journal of Quantum Chemistry, (115): 641-646 2015.

Li, W. L.; Li, Y.; Xu, C. Q.; Wang, X. B.; Vorpagel, E.; Li, J.
Periodicity, Electronic Structures, and Bonding of Gold Tetrahalides AuX4 (-) (X = F, Cl, Br, I, At, Uus)
Inorganic Chemistry, (54): 11157-11167 2015.

Li, X. H.; Cui, H. L.; Zhang, R. Z.; Zhang, X. Z.
Theoretical investigation on the non-linear optical properties, vibrational spectroscopy and frontier molecular orbital of (E)-2-cyano-3-(3-hydroxyphenyl)acrylamide molecule
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (137): 321-327 2015.

Li, X. H.; Yong, Y. L.; Cui, H. L.; Zhang, R. Z.; Zhang, X. Z.
Theoretical investigation on vibrational spectra, first order hyperpolarizability and NBO analysis of 4-Phenylpyridinium hydrogen squarate
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (147): 14-19 2015.

Li, X. M.; Pan, Y. R.; Ji, J. Y.; Niu, Y. L.; Wang, Q. W.
Synthesis, Crystal Structure and Theoretical Calculations of a Cadmium(II) Coordination Polymer Assembled by 5-Nitroisophthalic Acid and 1,3-Bis(imidazol-1-ylmethyl)-benzene Ligands
Journal of Inorganic and Organometallic Polymers and Materials, (25): 1069-1076 2015.

Li, X. P.; He, A. Q.; Huang, K.; Liu, H. Z.; Zhao, Y.; Wei, Y. J.; Xu, Y. Z.; Noda, I.; Wu, J. G.
Two-dimensional asynchronous spectrum with auxiliary cross peaks in probing intermolecular interactions
Rsc Advances, (5): 87739-87749 2015.

Li, X. Y.; Geng, Z. D.
Investigation into the metallophilic interaction in coinage-metal halides: an ab initio study of CMX (CM = Cu and Ag, X = F - I)
Journal of Molecular Modeling, (21) 2015.

Li, Y.; Wang, L.; Huang, T. F.; Zhang, J. L.; He, H. Q.
Catalytic Activity of a Series of Synthesized and Newly Designed Pyridinium-Based Ionic Liquids on the Fixation of Carbon Dioxide: A DFT Investigation
Industrial & Engineering Chemistry Research, (54): 8093-8099 2015.

Li, Y. Q.; Feng, Y. T.; Sun, M. T.
Photoinduced Charge Transport in a BHJ Solar Cell Controlled by an External Electric Field
Scientific Reports, (5) 2015.

Li, Y. W.; Zhang, S. H.; Yu, J. B.; Wang, Q.; Sun, Q.; Jena, P. R.
A new C=C embedded porphyrin sheet with superior oxygen reduction performance
Nano Research, (8): 2901-2912 2015.

Li, Z. J.; Wang, J.; Yu, Y. Q.; Li, G. X.; Ni, M. Y.; Zhang, J.
Theoretical study of conformational effect on electronic structure and charge transfer in silabiphenyl system
Computational and Theoretical Chemistry, (1052): 6-11 2015.

Li, Z. Z.; Li, A. Y.; Ji, L. F.
Theoretical Predictions of C-3v Symmetric Three-H-Bridged Noble Gas Compounds NgBeH(3)BeR, NgBeH(3)BR(+), and NgBH(3)BR(2+)
Journal of Physical Chemistry A, (119): 8400-8413 2015.

Lian, X.; Guo, W. L.; Liu, F. L.; Yang, Y.; Xiao, P.; Zhang, Y. H.; Tian, W. Q.
DFT studies on Pt3M (M = Pt, Ni, Mo, Ru, Pd, Rh) clusters for CO oxidation
Computational Materials Science, (96): 237-245 2015.

Liang, H. L.; Chai, B. J.; Chen, G. H.; Chen, W.; Chen, S.; Xiao, H. L.; Lin, S. J.
Electric Field-driven Acid-base Transformation: Proton Transfer from Acid(HBr/HF) to Base(NH3/H2O)
Chemical Research in Chinese Universities, (31): 418-426 2015.

Liang, J. X.; Su, Q.; Wang, Y. B.; Geng, Z. Y.
S(N)2 Reaction of IO- + CH3Cl: An Ab Initio and DFT Benchmark Study
Bulletin of the Chemical Society of Japan, (88): 110-116 2015.

Liang, J. X.; Su, Q.; Zheng, S. J.; Yu, J.; Geng, Z. Y.
Computational comparison of reactions of CS2 with CHX center dot- (X = F, Cl, and Br). Do F, Cl, and Br substitutions effect differently?
Journal of Theoretical & Computational Chemistry, (14) 2015.

Liang, X. Q.; Zhou, J. J.; Zheng, Y.; Ma, F.
Theoretical Studies on the Mechanism of the Azido-Tetrazole of Azido-s-triazine
Natural Product Communications, (10): 269-272 2015.

Liao, J. H.; Wu, T. H.; Chen, M. Y.; Chen, W. T.; Lu, S. Y.; Wang, Y. H.; Wang, S. P.; Hsu, Y. M.; Huang, Y. S.; Huang, Z. Y.; Lin, Y. C.; Chang, C. M.; Huang, F. Y.; Wu, S. H.
The Comparative Studies of Binding Activity of Curcumin and Didemethylated Curcumin with Selenite: Hydrogen Bonding vs Acid-Base Interactions
Scientific Reports, (5) 2015.

Lin, C. H.; Pursley, D.; Klein, J.; Teske, J.; Allen, J. A.; Rami, F.; Kohn, A.; Plietker, B.
Non-decarbonylative photochemical versus thermal activation of Bu4N Fe(CO)(3)(NO) - the Fe-catalyzed Cloke-Wilson rearrangement of vinyl and arylcyclopropanes
Chemical Science, (6): 7034-7043 2015.

Lin, H. S.; Lu, S. Y.; Huang, F. Y.; Wu, Y.; Su, W. L.; Wang, S. P.
An Insight of the Results Provided by Color-Tuning Studies Made on Ir(III) Complexes: A pi-Neutral CF3 Group Viewed by Adjusting Energies of pi-type Molecular Orbitals
Journal of the Chinese Chemical Society, (62): 939-943 2015.

Lin, T. J.; Lin, S. T.
Theoretical study on the torsional potential of alkyl, donor, and acceptor substituted bithiophene: the hidden role of noncovalent interaction and backbone conjugation
Physical Chemistry Chemical Physics, (17): 4127-4136 2015.

Linclau, B.; Peron, F.; Bogdan, E.; Wells, N.; Wang, Z.; Compain, G.; Fontenelle, C. Q.; Galland, N.; Le Questel, J. Y.; Graton, J.
Intramolecular OH center dot center dot center dot Fluorine Hydrogen Bonding in Saturated, Acyclic Fluorohydrins: The gamma-Fluoropropanol Motif
Chemistry-a European Journal, (21): 17808-17816 2015.

Ling, L.; Liu, K.; Li, X. Q.; Li, Y. X.
General Reaction Mode of Hypervalent Iodine Trifluoromethylation Reagent: A Density Functional Theory Study
Acs Catalysis, (5): 2458-2468 2015.

Ling, Y. F.; Ren, X. L.; Lai, W. P.; Luo, J.
4,4,8,8-Tetranitroadamantane-2,6-diyl Dinitrate: A High-Density Energetic Material
European Journal of Organic Chemistry: 1541-1547 2015.

Liu, C. C.; Liu, Q. L.; Wu, Z. Y.; Chen, Y. C.; Xie, H. J.; Lei, Q. F.; Fang, W. J.
Mechanistic insights into small molecule activation induced by ligand cooperativity in PCcarbeneP nickel pincer complexes: a quantumchemistry study
Journal of Molecular Modeling, (21) 2015.

Liu, C. C.; Zeng, Y. L.; Li, X. Y.; Meng, L. P.; Zhang, X. Y.
A comprehensive analysis of P center dot center dot center dot pi pnicogen bonds: substitution effects and comparison with Br center dot center dot center dot pi halogen bonds
Journal of Molecular Modeling, (21) 2015.

Liu, J. B.; Shi, Y.; Tang, S. S.; Jin, R. F.
Theoretical and experimental research on the self-assembled system of molecularly imprinted polymers formed by salbutamol and methacrylic acid
Journal of Separation Science, (38): 1065-1071 2015.

Liu, K.; Korchowiec, J.; Aoki, Y.
Intermediate Electrostatic Field for the Generalized Elongation Method
Chemphyschem, (16): 1551-1556 2015.

Liu, M. X.; Cai, M. Y.; Li, Q. Z.; Li, W. Z.; Cheng, J. B.
Synergistic and diminutive effects between halogen bond and lithium bond in complexes involving aromatic compounds
Journal of Molecular Modeling, (21) 2015.

Liu, R. H.; Chen, X. Y.; Falk, S. P.; Masters, K. S.; Weisblum, B.; Gellman, S. H.
Nylon-3 Polymers Active against Drug-Resistant Candida albicans Biofilms
Journal of the American Chemical Society, (137): 2183-2186 2015.

Liu, X. J.; Sun, X.; Xu, X. J.; Sun, P.
Growth mechanism, electronic spectral investigation and molecular orbital studies of L-prolinium phosphate
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (150): 470-475 2015.

Liu, X. J.; Xu, X. J.; Zhang, C. W.
Interface morphology and DFT computation of L-valinium fumarate
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (136): 162-167 2015.

Liu, Y. M.; Junk, T.; Liu, Y. C.; Tzeng, N. F.; Perkins, R.
Benchmarking quantum mechanical calculations with experimental NMR chemical shifts of 2-HADNT
Journal of Molecular Structure, (1086): 43-48 2015.

Liu, Y. Z.; Yuan, K.; Lv, L. L.; Zhu, Y. C.; Yuan, Z.
Designation and Exploration of Halide-Anion Recognition Based on Cooperative Noncovalent Interactions Including Hydrogen Bonds and Anion-pi
Journal of Physical Chemistry A, (119): 5842-5852 2015.

Liu, Y. Z.; Yuan, K.; Yuan, Z.; Zhu, Y. C.; Zhao, X.
Theoretical exploration of pnicogen bond noncovalent interactions in HCHO...PH2X (X=CH3, H, C6H5, F, Cl, Br, and NO2) complexes
Journal of Chemical Sciences, (127): 1729-1738 2015.

Lodowski, P.; Jaworska, M.; Garabato, B. D.; Kozowski, P. M.
Mechanism of Co-C Bond Photolysis in Methylcobalamin: Influence of Axial Base
Journal of Physical Chemistry A, (119): 3913-3928 2015.

Long, S. H.; Zhou, P. P.; Theiss, K. L.; Siegler, M. A.; Li, T. L.
Solid-state identity of 2-hydroxynicotinic acid and its polymorphism
Crystengcomm, (17): 5195-5205 2015.

Lopez, L.; Ruiz, P.; Castro, M.; Quijano, J.; Duque-Norena, M.; Perez, P.; Chamorro, E.
Understanding the thermal dehydrochlorination reaction of 1-chlorohexane. Revealing the driving bonding pattern at the planar catalytic reaction center
Rsc Advances, (5): 62946-62956 2015.

Lopez, R. V.; Faza, O. N.; Lopez, C. S.
Diradical ring closing reactions displaying Woodward-Hoffmann behaviour and torquoselectivity
Rsc Advances, (5): 30405-30408 2015.

Lopez-Berganza, J. A.; Diao, Y. J.; Pamidighantam, S.; Espinosa-Marzal, R. M.
Ab Initio Studies of Calcium Carbonate Hydration
Journal of Physical Chemistry A, (119): 11591-11600 2015.

Lopez-Cabana, Z. E.; Valdes, O.; Vergara, C. E.; Camarada, M. B.; Nachtigall, F. M.; Gonzalez-Nilo, F. D.; Santos, L. S.
Photophysical studies of the interactions of poly(amidoamine) generation zero (PAMAM G0) with copper and zinc ions
Journal of Luminescence, (164): 23-30 2015.

Lu, D. M.; Tang, H. R.
Theoretical survey of the ligand tunability of poly(azolyl)borates
Physical Chemistry Chemical Physics, (17): 17027-17033 2015.

Lu, F. F.; Li, X. Y.; Sun, Z.; Zeng, Y. L.; Meng, L. P.
Influences of the substituents on the M-M bonding in Cp4Al4 and Cp2M2X2 (M = B, Al, Ga; Cp = C5H5, X = halogen)
Dalton Transactions, (44): 14092-14100 2015.

Lu, J.; Zhang, Z. Y.; Ni, Z.; Shen, H. J.; Tu, Z. G.; Liu, H. Q.; Lu, R. Z.; Shi, H. F.
The non-additive contribution of hydroxyl substituents to Akt kinase-apigenin affinity
Molecular Simulation, (41): 653-662 2015.

Lu, N.; Wang, H. T.
A Theoretical Investigation on Palladium-Catalyzed One-Pot Coupling of Aryl Iodides, Alkynes, and Amines Through C-N Bond Cleavage for the Synthesis of Indole Derivatives
International Journal of Quantum Chemistry, (115): 361-368 2015.

Lu, W. J.; Wang, C. Y.; Luo, Q.; Li, Q. S.; Xie, Y. M.; King, R. B.; Schaefer, H. F.
Carbonyl migration from phosphorus to the metal in binuclear phosphaketenyl metal carbonyl complexes to give bridging diphosphido complexes
New Journal of Chemistry, (39): 1390-1403 2015.

Lucas, L. J.; Tellez, C.; Castilho, M. L.; Lee, C. L. D.; Hupman, M. A.; Vieira, L. S.; Ferreira, I.; Raniero, L.; Hewitt, K. C.
Development of a sensitive, stable and EGFR-specific molecular imaging agent for surface enhanced Raman spectroscopy
Journal of Raman Spectroscopy, (46): 434-446 2015.

Lugo, G.; Schwanen, V.; Fresch, B.; Remacle, F.
Charge Redistribution Effects on the UV-Vis Spectra of Small Ligated Gold Clusters: a Computational Study
Journal of Physical Chemistry C, (119): 10969-10980 2015.

Lukomska, M.; Rybarczyk-Pirek, A. J.; Jablonski, M.; Palusiak, M.
The nature of NO-bonding in N-oxide group
Physical Chemistry Chemical Physics, (17): 16375-16387 2015.

Lumbroso, A.; Catak, S.; Sulzer-Mosse, S.; De Mesmaeker, A.
Efficient access to functionalized cyclobutanone derivatives using cyclobuteniminium salts as highly reactive Michael acceptors
Tetrahedron Letters, (56): 2397-2401 2015.

Luo, J.; Wang, C. Z.; Lan, J. H.; Wu, Q. Y.; Zhao, Y. L.; Chai, Z. F.; Nie, C. M.; Shi, W. Q.
Theoretical studies on the AnO(2)(n+) (An = U, Np; n=1, 2) complexes with di-(2-ethylhexyl) phosphoric acid
Dalton Transactions, (44): 3227-3236 2015.

Luo, Y. H.; Chang, Z. D.; Blamo, B. J.; Wu, X.; Hussain, M.; Uslu, H.; Li, W. J.; Liu, S. X.; Sun, C. Y.; Hua, C.
Efficiency of fluorinated alcohol for extraction of organic acid from its dilute aqueous solution: A molecular optimization study of extractant
Journal of Fluorine Chemistry, (180): 234-239 2015.

Luzanov, A. V.; Casanova, D.; Feng, X. T.; Krylov, A. I.
Quantifying charge resonance and multiexciton character in coupled chromophores by charge and spin cumulant analysis
Journal of Chemical Physics, (142) 2015.

Lyczko, K.; Lyczko, M.; Wozniak, K.; Stachowicz, M.; Oziminski, W. P.; Kubo, K.
Influence of pH and type of counterion on the formation of bismuth(III) complexes with tropolonato and 5-methyltropolonato ligands: Synthesis, structure, spectroscopic characterization and calculation studies
Inorganica Chimica Acta, (436): 57-68 2015.

Lymperopoulou, S.; Dokorou, V. N.; Tsipis, A. C.; Weidler, P. G.; Plakatouras, J. C.; Powell, A. K.; Kostakis, G. E.
Influence of the metal salt on the self-assembly of isophthaloylbis-beta-alanine and Cu(II) ion
Polyhedron, (89): 313-321 2015.

Ma, J.; Li, R.; Ma, X. L.; Zhu, K. L.; Geng, Z. Y.

Study of the competitive mechanisms of cyclohexane dehydrogenation by gas-phase Ni-2(+) cationic dimer: one-face dehydrogenation versus flip dehydrogenation
Journal of Molecular Modeling, (21) 2015.

Ma, L. J.; Jia, J. F.; Wu, H. S.
Computational investigation of hydrogen storage on scandium-acetylene system
International Journal of Hydrogen Energy, (40): 420-428 2015.

Ma, Y.; Wang, L. S.; Liu, Z.; Cheng, R. H.; Zhong, L.; Yang, Y.; He, X. L.; Fang, Y. W.; Terano, M. R.; Liu, B. P.
High-resolution XPS and DFT investigations into Al-modified Phillips CrOx/SiO2 catalysts
Journal of Molecular Catalysis a-Chemical, (401): 1-12 2015.

Maes, B. U. W.; Verbeeck, S.; Verhelst, T.; Ekomie, A.; von Wolff, N.; Lefevre, G.; Mitchell, E. A.; Jutand, A.
Oxidative Addition of Haloheteroarenes to Palladium(0): Concerted versus SNAr-Type Mechanism
Chemistry-a European Journal, (21): 7858-7865 2015.

Mahalakshmi, G.; Balachandran, V.
NBO, HOMO, LUMO analysis and vibrational spectra (FTIR and FT Raman) of 1-Amino 4-methylpiperazine using ab initio HF and DFT methods
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (135): 321-334 2015.

Mahdavifar, Z.; Abbasi, N.; Shakerzadeh, E.
Carbon monoxide monitoring using pristine and Cu-functionalized aluminum nitride and silicon carbide nanotubes; DFT study
Journal of Molecular Liquids, (204): 147-155 2015.

Maheswari, J. U.; Muthu, S.; Sundius, T.
QM/MM methodology, docking and spectroscopic (FT-IR/FT-Raman, NMR, UV) and Fukui function analysis on adrenergic agonist
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (137): 841-855 2015.

Mahmood, A.; Teixeira, E. S.; Longo, R. L.
Understanding the Reactivity and Regioselectivity of Methylation of Nitronates (RRCNO2)-R-1-C-2 (-) by CH3I in the Gas Phase
Journal of Organic Chemistry, (80): 8198-8205 2015.

Mai, B. K.; Kim, Y.
The Kinetic Isotope Effect as a Probe of Spin Crossover in the C-H Activation of Methane by the FeO+ Cation
Angewandte Chemie-International Edition, (54): 3946-3951 2015.

Mai, B. K.; Kim, Y.
Long-range proton relay shows an inverse linear free energy relationship depending on the pK(a) of the hydrogen-bonded wire
Rsc Advances, (5): 2669-2676 2015.

Maiore, L.; Aragoni, M. C.; Carcangiu, G.; Cocco, O.; Isaia, F.; Lippolis, V.; Meloni, P.; Murru, A.; Tuveri, E.; Arca, M.
Synthesis, characterization and DFT-modeling of novel agents for the protection and restoration of historical calcareous stone substrates
Journal of Colloid and Interface Science, (448): 320-330 2015.

Maity, A.; Stanek, R. J.; Anderson, B. L.; Zeller, M.; Hunter, A. D.; Moore, C. E.; Rheingold, A. L.; Gray, T. G.
Fluoride Complexes of Cyclometalated Iridium(III)
Organometallics, (34): 109-120 2015.

Maity, B.; Goosen, L. J.; Koley, D.
Computational study of the mechanism and selectivity of ruthenium-catalyzed hydroamidations of terminal alkynes
Chemical Science, (6): 2532-2552 2015.

Maity, B.; Mondal, T.; Dey, K.; Biswas, S.; Koley, D.
Role of ligands in controlling the regioselectivity in ruthenium-catalysed addition of carboxylic acids to terminal alkynes: A DFT study
Journal of Chemical Sciences, (127): 281-293 2015.

Majerz, I.; Gutmann, M. J.
Intermolecular OHN hydrogen bond with a proton moving in 3-methylpyridinium 2,6-dichloro-4-nitrophenolate
Rsc Advances, (5): 95576-95584 2015.

Makarova, M. V.; Semenov, S. G.
Quantum-chemical study of barbaralone in singlet and triplet states
Russian Journal of General Chemistry, (85): 589-594 2015.

Makiabadi, B.; Kian, H.
The hydrogen bond interactions in glycine-nitrosamine complexes: a DFT study
Monatshefte fur Chemie, (146): 69-78 2015.

Makiabadi, B.; Tajaddini, Z. A.
Theoretical Investigation of Proton Transfer in Thiazolidine-2-thione and Oxazolidine-2-thione via Direct Transition and Self-Assisted and Water-Assisted Tautomerization
Chemistry of Heterocyclic Compounds, (51): 361-369 2015.

Maldonado, A.; Rosas, F.; Mora, J. R.; Brusco, Y.; Cordova-Sintjago, T. C.; Chuchani, G.
Homogeneous catalysis on the gas-phase dehydration reaction of tertiary alcohols by hydrogen bromide. Density functional theory calculation
Molecular Physics, (113): 282-293 2015.

Manceau, A.; Lemouchi, C.; Rovezzi, M.; Lanson, M.; Gatzel, P.; Nagy, K. L.; Gautier-Luneau, I.; Joly, Y.; Enescu, M.
Structure, Bonding, and Stability of Mercury Complexes with Thiolate and Thioether Ligands from High-Resolution XANES Spectroscopy and First-Principles Calculations
Inorganic Chemistry, (54): 11776-11791 2015.

Mandal, B.; Mondal, M.; Srivastava, B.; Barman, M. K.; Ghosh, C.; Chatterjee, M.
Chromatographic method for pre-concentration and separation of Zn(II) with microalgae and density functional optimization of the extracted species
Rsc Advances, (5): 31205-31218 2015.

Mandal, S.; Pan, S.; Deb, D.; Giri, S.; Duley, S.; Radenkovic, S.; Cooper, D. L.; Bultinck, P.; Anoop, A.; Bhattacharjee, M.; Chattaraj, P. K.
Three-dimensional networks containing rectangular Sr-4 and Ba-4 units: Synthesis, structure, bonding, and potential application for Ne gas separation
International Journal of Quantum Chemistry, (115): 1501-1509 2015.

Mandegani, Z.; Asadi, M.; Asadi, Z.; Mohajeri, A.; Iranpoor, N.; Omidvar, A.
A nano tetraimine Pd(0) complex: synthesis, characterization, computational studies and catalytic applications in the Heck-Mizoroki reaction in water
Green Chemistry, (17): 3326-3337 2015.

Manna, D.; Mondal, S.; Mugesh, G.
Halogen Bonding Controls the Regioselectivity of the Deiodination of Thyroid Hormones and their Sulfate Analogues
Chemistry-a European Journal, (21): 2409-2416 2015.

Mansour, A. M.
Photocatalytic degradation of methylene blue with hematite nanoparticles synthesized by thermal decomposition of fluoroquinolones oxalato-iron(III) complexes
Rsc Advances, (5): 62052-62061 2015.

Mansour, A. M.; Mohamed, R. R.

Sulfamethazine copper(II) complexes as antimicrobial thermal stabilizers and co-stabilizers for rigid PVC: spectroscopic, thermal, and DFT studies
Rsc Advances, (5): 5415-5423 2015.

Mao, J. X.; Damodaran, K.
Spectroscopic and computational analysis of the molecular interactions in the ionic liquid Emim (+) FAP (-)
Ionics, (21): 1605-1613 2015.

Mariappan, G.; Sundaraganesan, N.
Structural and vibrational spectroscopic analysis of anticancer drug mitotane using DFT method; a comparative study of its parent structure
Journal of Molecular Structure, (1086): 73-85 2015.

Marin-Luna, M.; Alkorta, I.; Elguero, J.
The influence of halogen bonds on tautomerism: the case of 3-mercapto-1,2-azoles (pyrazoles, isoxazoles, isothiazoles)
Structural Chemistry, (26): 639-645 2015.

Marin-Luna, M.; Alkorta, I.; Elguero, J.
The influence of intermolecular halogen bonds on the tautomerism of nucleobases. I. Guanine
Tetrahedron, (71): 5260-5266 2015.

Marin-Luna, M.; Alkorta, I.; Elguero, J.; Mo, O.; Yanez, M.
Interplay between Beryllium Bonds and Anion-pi Interactions in BeR2:C6X6:Y- Complexes R = H, F and Cl, X = H and F, and Y = Cl and Br)
Molecules, (20): 9961-9976 2015.

Markovic, S.; Tosovic, J.
Application of Time-Dependent Density Functional and Natural Bond Orbital Theories to the UV-vis Absorption Spectra of Some Phenolic Compounds
Journal of Physical Chemistry A, (119): 9352-9362 2015.

Marmitt, S.; Goncalves, P. F. B.
A DFT study on the insertion of CO2 into styrene oxide catalyzed by 1-butyl-3-methyl-Imidazolium bromide ionic liquid
Journal of Computational Chemistry, (36): 1322-1333 2015.

Marquez, M. J.; Brizuela, A. B.; Davies, L.; Brandan, S. A.
Spectroscopic and structural studies on lactose species in aqueous solution combining the HATR and Raman spectra with SCRF calculations
Carbohydrate Research, (407): 34-41 2015.

Marsh, B. M.; Zhou, J.; Garand, E.
Charge transfer in MOH(H2O)(+) (M = Mn, Fe, Co, Ni, Cu, Zn) complexes revealed by vibrational spectroscopy of mass-selected ions
Physical Chemistry Chemical Physics, (17): 25786-25792 2015.

Martinez, Y. B.; Pirani, L. S. R.; Erben, M. F.; Reuter, C. G.; Vishnevskiy, Y. V.; Stammler, H. G.; Mitzel, N. W.; Della Vedova, C. O.
The structure of chloromethyl thiocyanate, CH2ClSCN, in gas and crystalline phases
Physical Chemistry Chemical Physics, (17): 15805-15812 2015.

Martinez-Cifuentes, M.; Salazar, R.; Escobar, C. A.; Weiss-Lopez, B. E.; Santos, L. S.; Araya-Maturana, R.
Correlating experimental electrochemistry and theoretical calculations in 2 '-hydroxy chalcones: the role of the intramolecular hydrogen bond
Rsc Advances, (5): 50929-50937 2015.

Martin-Somer, A.; Mo, O.; Yanez, M.; Guillemin, J. C.
Acidity enhancement of unsaturated bases of group 15 by association with borane and beryllium dihydride. Unexpected boron and beryllium Bronsted acids
Dalton Transactions, (44): 1193-1202 2015.

Mary, Y. S.; Panicker, C. Y.; Sapnakumari, M.; Narayana, B.; Sarojini, B. K.; Al-Saadi, A. A.; Van Alsenoy, C.; War, J. A.; Fun, H. K.
Infrared spectrum, structural and optical properties and molecular docking study of 3-(4-fluorophenyl)-5-phenyl-4,5-dihydro-1H-pyrazole-1-carbaldehyde
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (138): 529-538 2015.

Mary, Y. S.; Panicker, C. Y.; Thiemann, B. T.; Al-Azani, M.; Al-Saadi, A. A.; Van Alsenoy, C.; Raju, K.; War, J. A.; Srivastava, S. K.
Molecular conformational analysis, vibrational spectra, NBO, NLO analysis and molecular docking study of bis (E)-anthranyl-9-acrylic anhydride based on density functional theory calculations
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (151): 350-359 2015.

Mary, Y. S.; Panicker, C. Y.; Thiemann, T.; Al-Azani, M.; Al-Saadi, A. A.; Van Alsenoy, C.; Raju, K.; War, J. A.; Srivastava, S. K.
Molecular conformational analysis, vibrational spectra, NBO, NLO analysis and molecular docking study of bis (E)-anthranyl-9-acrylic anhydride based on density functional theory calculations
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (151): 350-359 2015.

Mary, Y. S.; Varghese, H. T.; Panicker, C. Y.; Girisha, M.; Sagar, B. K.; Yathirajan, H. S.; Al-Saadi, A. A.; Van Alsenoy, C.
Vibrational spectra, HOMO, LUMO, NBO, MEP analysis and molecular docking study of 2,2-diphenyl-4-(piperidin-1-yl)butanamide
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (150): 543-556 2015.

Mary, Y. S.; Varghese, H. T.; Panicker, C. Y.; Thiemann, T.; Al-Saadi, A. A.; Popoola, S. A.; Van Alsenoy, C.; Al Jasem, Y.
Molecular conformational analysis, vibrational spectra, NBO, NLO, HOMO-LUMO and molecular docking studies of ethyl 3-(E)-(anthracen-9-yl)prop-2-enoate based on density functional theory calculations
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (150): 533-542 2015.

Mary, Y. S.; Yamuna, T. S.; Panicker, C. Y.; Yathirajan, H. S.; Siddegowda, M. S.; Al-Saadi, A. A.; Van Alsenoy, C.; War, J. A.
Vibrational spectroscopic studies and molecular docking of 10,10-Dimethylanthrone
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (135): 652-661 2015.

Masoodi, H. R.; Bagheri, S.
The influence of carbon hybridization on coupling constants across C-X center dot center dot center dot Cl-F dihalogen bond: A computational study
Chemical Physics Letters, (637): 153-158 2015.

Masoodi, H. R.; Ebrahimi, A.; Bagheri, S.
The influence of cations and anions on some structural and electronic properties of single-walled zigzag boron nitride and aluminum nitride nanotubes: a computational study
Structural Chemistry, (26): 1013-1024 2015.

Matczak, P.
Theoretical investigation of the N -> Sn coordination in (Me3SnCN)(2)
Structural Chemistry, (26): 301-318 2015.

Mathammal, R.; Sudha, N.; Prasad, L. G.; Ganga, N.; Krishnakumar, V.
Spectroscopic (FTIR, FT-Raman, UV and NMR) investigation and NLO, HOMO-LUMO, NBO analysis of 2-Benzylpyridine based on quantum chemical calculations
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (137): 740-748 2015.

Matin, M. A.; Chitumalla, R. K.; Lim, M.; Gao, X. F.; Jang, J.
Density Functional Theory Study on the Cross-Linking of Mussel Adhesive Proteins
Journal of Physical Chemistry B, (119): 5496-5504 2015.

Matsuda, Y.; Endo, T.; Mikami, N.; Fujii, A.; Morita, M.; Takahashi, K.
The Large Variation in Acidity of Diethyl Ether Cation Induced by Internal Rotation about a Single Covalent Bond
Journal of Physical Chemistry A, (119): 4885-4890 2015.

Matsuoka, A.; Sandoval, C. A.; Uchiyama, M.; Noyori, R.; Naka, H.

Why p-Cymene? Conformational Effect in Asymmetric Hydrogenation of Aromatic Ketones with a eta(6)-Arene/Ruthenium(II) Catalyst
Chemistry-an Asian Journal, (10): 112-115 2015.

Matthews, R. P.; Welton, T.; Hunt, P. A.
Hydrogen bonding and pi-pi interactions in imidazolium-chloride ionic liquid clusters
Physical Chemistry Chemical Physics, (17): 14437-14453 2015.

Mavrandonakis, A.; Vogiatzis, K. D.; Boese, A. D.; Fink, K.; Heine, T.; Klopper, W.
Ab Initio Study of the Adsorption of Small Molecules on Metal-Organic Frameworks with Oxo-centered Trimetallic Building Units: The Role of the Undercoordinated Metal Ion
Inorganic Chemistry, (54): 8251-8263 2015.

Mavrova, A. T.; Yancheva, D.; Anastassova, N.; Anichina, K.; Zvezdanovic, J.; Djordjevic, A.; Markovic, D.; Smelcerovic, A.
Synthesis, electronic properties, antioxidant and antibacterial activity of some new benzimidazoles
Bioorganic & Medicinal Chemistry, (23): 6317-6326 2015.

Mayes, H. B.; Nolte, M. W.; Beckham, G. T.; Shanks, B. H.; Broadbelt, L. J.
The Alpha-Bet(a) of Salty Glucose Pyrolysis: Computational Investigations Reveal Carbohydrate Pyrolysis Catalytic Action by Sodium Ions
Acs Catalysis, (5): 192-202 2015.

Mazurek, A.; Dobrowolski, J. C.
On the incorporation effect of the ring-junction heteroatom. The sEDA(III) and pEDA(III) Descriptors
Journal of Physical Organic Chemistry, (28): 290-297 2015.

McDowell, S. A. C.; Holder, Z. L.
Computational study of non-covalent interactions in oxirane center dot center dot center dot XF complexes (X = H, F, Cl, Br, Li) and their F-/Li-substituted analoguesy
Molecular Physics, (113): 3757-3766 2015.

McDowell, S. A. C.; Maynard, S. J.
A computational study of model beryllium-bonded complexes of oxirane and F-substituted oxiranes with BeX2 (X = H, Cl)
Chemical Physics Letters, (630): 91-95 2015.

Mebs, S.; Braun, B.; Kositzki, R.; Limberg, C.; Haumann, M.
Abrupt versus Gradual Spin-Crossover in Fe-ll(phen)(2)(NCS)(2) and Fe(III)dedtc)(3) Compared by X-ray Absorption and Emission Spectroscopy and Quantum-Chemical Calculations
Inorganic Chemistry, (54): 11606-11624 2015.

Medved, M.; Budzak, S.; Pluta, T.
Electric properties of the low-lying excited states of benzonitrile: geometry relaxation and solvent effects
Theoretical Chemistry Accounts, (134) 2015.

Meenatchi, V.; Meenakshisundaram, S. P.
Synthesis, growth, spectral studies, first-order molecular hyperpolarizability and Hirshfeld surface analysis of isonicotinohydrazide single crystals
Rsc Advances, (5): 64180-64191 2015.

Mehandzhiyski, A. Y.; Riccardi, E.; van Erp, T. S.; Koch, H.; Astrand, P. O.; Trinh, T. T.; Grimes, B. A.
Density Functional Theory Study on the Interactions of Metal Ions with Long Chain Deprotonated Carboxylic Acids
Journal of Physical Chemistry A, (119): 10195-10203 2015.

Mehranfar, A.; Izadyar, M.; Esmaeili, A. A.
Hydrogen storage by N-ethylcarbazol as a new liquid organic hydrogen carrier: A DFT study on the mechanism
International Journal of Hydrogen Energy, (40): 5797-5806 2015.

Mei, Y.; Simmonett, A. C.; Pickard, F. C.; DiStasio, R. A.; Brooks, B. R.; Shao, Y. H.
Numerical Study on the Partitioning of the Molecular Polarizability into Fluctuating Charge and Induced Atomic Dipole Contributions
Journal of Physical Chemistry A, (119): 5865-5882 2015.

Melekhova, A. A.; Novikov, A. S.; Luzyanin, K. V.; Bokach, N. A.; Starova, G. L.; Gurzhiy, V. V.; Kukushkin, V. Y.
Tris-isocyanide copper(I) complexes: Synthetic, structural, and theoretical study
Inorganica Chimica Acta, (434): 31-36 2015.

Melis, M.; Arca, M.; Aragoni, M. C.; Cabras, T.; Caltagirone, C.; Castagnola, M.; Crnjar, R.; Messana; Tepper, B. J.; Barbarossa, I. T.
Dose-Dependent Effects of L-Arginine on PROP Bitterness Intensity and Latency and Characteristics of the Chemical Interaction between PROP and L-Arginine
Plos One, (10) 2015.

Menendez, M.; Boto, R. A.; Francisco, E.; Pendas, A. M.
One-Electron Images in Real Space: Natural Adaptive Orbitals
Journal of Computational Chemistry, (36): 833-843 2015.

Meng, Q. X.; Wang, F.; Yin, H. Z.
Theoretical studies of cobalt(I)-catalyzed hydroacylation of vinylsilanes and alkyl aldehydes
Journal of Physical Organic Chemistry, (28): 431-436 2015.

Messersmith, R. E.; Tovar, J. D.
Assessment of the aromaticity of borepin rings by spectroscopic, crystallographic and computational methods: a historical overview
Journal of Physical Organic Chemistry, (28): 378-387 2015.

Meyer, J.; Gonzalez-Gallardo, S.; Hohnstein, S.; Garnier, D.; Armbruster, M. K.; Fink, K.; Klopper, W.; Breher, F.
Tris(3,5-dimethylpyrazolyl)methane-Based Heterobimetallic Complexes that Contain Zn- and Cd-Transition-Metal Bonds: Synthesis, Structures, and Quantum Chemical Calculations
Chemistry-a European Journal, (21): 2905-2914 2015.

Meza-Morales, P. J.; Santana-Vargas, A.; Curet-Arana, M. C.
DFT analysis of coordination polymer ligands: unraveling the electrostatic properties and their effect on CO2 interaction
Adsorption-Journal of the International Adsorption Society, (21): 533-546 2015.

Minyaev, R. M.; Popov, I. A.; Koval, V. V.; Boldyrev, A. I.; Minkin, V. I.
Supertetrahedral B80H20, C80H20, and Al80H20 analogs of dodecahedrane and their substituted molecules
Structural Chemistry, (26): 223-229 2015.

Miranda-Rojas, S.; Toro-Labbe, A.
Mechanistic insights into the dehalogenation reaction of fluoroacetate/fluoroacetic acid
Journal of Chemical Physics, (142) 2015.

Mirzadeh, N.; Bennett, M. A.; Wachtler, E.; Zhechkov, L.; Heine, T.; Bhargava, S. K.
Formation of heterobinuclear Pt-Au complexes by chelate ring-opening of cis- Pt(kappa(2)-C6R4PPh2)(2) (R = H, F)
Journal of Organometallic Chemistry, (783): 130-134 2015.

Mirzaei, S.; Khalilian, M. H.; Taherpour, A. A.
Mechanistic study of the hydrolytic degradation and protonation of temozolomide
Rsc Advances, (5): 41112-41119 2015.

Mirzaeva, I. V.; Kozlova, S. G.; Anyushin, A. V.
Relativistic Effects in NMR of New Prospective Water-Soluble Ligands SeP(CH2OH)(3) and H Se2P(CH2OH)(2)
Applied Magnetic Resonance, (46): 1147-1157 2015.

Mishima, K.; Kinoshita, T.; Hayashi, M.; Jono, R.; Segawa, H.; Yamashita, K.; Lin, S. H.
Theoretical studies on the absorption spectra of cis- Ru(4,4 '-COO-2,2 '-bpy)(2)(X)(2) (4-), (X = NCS, Cl) and panchromatic trans-terpyridyl Ru complexes including strong spin-orbit coupling
Physical Chemistry Chemical Physics, (17): 12317-12327 2015.

Mishra, R.; Srivastava, A.; Tandon, P.; Jain, S.
Spectroscopic and quantum chemical analysis of a natural product - Hayatin hydrochloride
Journal of Molecular Structure, (1093): 101-112 2015.

Mishra, S. K.; Suryaprakash, N.
Intramolecular hydrogen bonds involving organic fluorine in the derivatives of hydrazides: an NMR investigation substantiated by DFT based theoretical calculations
Physical Chemistry Chemical Physics, (17): 15226-15235 2015.

Mishra, S. K.; Suryaprakash, N.
Organic fluorine involved intramolecular hydrogen bonds in the derivatives of imides: NMR evidence corroborated by DFT based theoretical calculations
Rsc Advances, (5): 86013-86022 2015.

Miyazaki, J.; Sudo, N.; Yamada, Y.
Infrared spectroscopic and density functional theoretical study of tris(cyclopentadienyl)ytterbium (YbCp3) and acetone adduct molecules of YbCp3 in low-temperature matrices
Journal of Molecular Spectroscopy, (314): 26-34 2015.

Moc, J.
Theoretical Investigation of the Reaction Paths of the Aluminum Cluster Cation with Water Molecule in the Gas Phase: A Facile Route for Dihydrogen Release
Journal of Physical Chemistry A, (119): 8683-8691 2015.

Modak, S.; Gangwar, M. K.; Rao, M. N.; Madasu, M.; Kalita, A. C.; Dorcet, V.; Shejale, M. A.; Butcher, R. J.; Ghosh, P.
Fluoride-free Hiyama coupling by palladium abnormal N-heterocyclic carbene complexes
Dalton Transactions, (44): 17617-17628 2015.

Mohajeri, A.; Bitaab, N.
Investigating the Nature of Intermolecular and Intramolecular Bonds in Noble Gas Containing Molecules
International Journal of Quantum Chemistry, (115): 165-171 2015.

Mohajeri, A.; Fallahzadeh, R.
Tuning the halogen-hydride interaction: the role of halogen and metal environments
Molecular Physics, (113): 463-472 2015.

Mohamed, R. K.; Mondal, S.; Gold, B.; Evoniuk, C. J.; Banerjee, T.; Hanson, K.; Alabugin, I. V.
Alkenes as Alkyne Equivalents in Radical Cascades Terminated by Fragmentations: Overcoming Stereoelectronic Restrictions on Ring Expansions for the Preparation of Expanded Polyaromatics
Journal of the American Chemical Society, (137): 6335-6349 2015.

Mohamed, T. A.; Soliman, U. A.; Shaaban, I. A.; Zoghaib, W. M.; Wilson, L. D.
Raman, infrared and NMR spectral analysis, normal coordinate analysis and theoretical calculations of 5-(methylthio)-1,3,4-thiadiazole-2(3H)-thione and its thiol tautomer
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (150): 339-349 2015.

Mohammadnezhad, G.; Amini, M. M.; Langer, V.; Adineh, M.
Formation of R-4(4) (8) ring in chloride salts of 8-hydroxyquinolinium derivatives: synthesis, structural, and theoretical studies
Zeitschrift Fur Kristallographie-Crystalline Materials, (230): 157-165 2015.

Moller, K. H.; Hansen, A. S.; Kjaergaard, H. G.
Gas Phase Detection of the NH-P Hydrogen Bond and Importance of Secondary Interactions

Journal of Physical Chemistry A, (119): 10988-10998 2015.

Momeni, M. R.; Shulman, L.; Rivard, E.; Brown, A.
Interplay of donor-acceptor interactions in stabilizing boron nitride compounds: insights from theory
Physical Chemistry Chemical Physics, (17): 16525-16535 2015.

Monascal, Y.; Maldonado, A.; Mora, J. R.; Cordova, T.; Chuchani, G.
Homogeneous and unimolecular gas-phase thermal decomposition kinetics of methyl benzoylformate: experimental and theoretical study
Journal of Physical Organic Chemistry, (28): 40-46 2015.

Mondal, S.; Mandal, S.; Carrella, L.; Jana, A.; Fleck, M.; Kohn, A.; Rentschler, E.; Mohanta, S.
A Series of (MCu3II)-Cu-II Stars (M = Mn, Ni, Cu, Zn) Exhibiting Unusual Magnetic Properties
Inorganic Chemistry, (54): 117-131 2015.

Monicka, J. C.; James, C.
FT-Raman and FTIR spectra, DFT investigation of the structure and vibrational assignment of mefenacet
Journal of Molecular Structure, (1095): 1-7 2015.

Montejo-Valencia, B. D.; Curet-Arana, M. C.
DFT Study of the Lewis Acidities and Relative Hydrothermal Stabilities of BEC and BEA Zeolites Substituted with Ti, Sn, and Ge
Journal of Physical Chemistry C, (119): 4148-4157 2015.

Montero-Campillo, M. M.; Bruna, S.; Cuadrado, I.; Mo, O.
Intervalence charge transfer across noncovalent interactions on vinyl silyl bridged biferrocenyl compounds
Computational and Theoretical Chemistry, (1053): 281-288 2015.

Montoro, T.; Tardajos, G.; Guerrero, A.; Torres, M. D.; Salgado, C.; Fernandez, I.; Barcina, J. O.
sigma-Hole center dot center dot center dot pi and lone pair center dot center dot center dot pi interactions in benzylic halides
Organic & Biomolecular Chemistry, (13): 6194-6202 2015.

Moore, C. M.; Szymczak, N. K.
Redox-induced fluoride ligand dissociation stabilized by intramolecular hydrogen bonding
Chemical Communications, (51): 5490-5492 2015.

Moorthi, P. P.; Gunasekaran, S.; Swaminathan, S.; Ramkumaar, G. R.
Quantum chemical density functional theory studies on the molecular structure and vibrational spectra of mannitol
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (137): 412-422 2015.

Moosavi-Tekyeh, Z.; Tayyari, S. F.
Theoretical and spectroscopic studies on molecular structure and hydrogen bonding of 2-trifluoroacetylphenol
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (135): 820-827 2015.

Moquist, P.; Chen, G. Q.; Muck-Lichtenfeld, C.; Bussmann, K.; Daniliuc, C. G.; Kehr, G.; Erker, G.
alpha-CH acidity of alkyl-B(C6F5)(2) compounds - the role of stabilized borata-alkene formation in frustrated Lewis pair chemistry
Chemical Science, (6): 816-825 2015.

Morais, S. F. D.; Mundim, K. C.; Ferreira, D. A. C.
An alternative interpretation of the ultracold methylhydroxycarbene rearrangement mechanism: cooperative effects
Physical Chemistry Chemical Physics, (17): 7443-7448 2015.

Moreira, D. N.; Fresno, N.; Perez-Fernandez, R.; Frizzo, C. P.; Goya, P.; Marco, C.; Martins, M. A. P.; Elguero, J.
Bronsted acid-base pairs of drugs as dual ionic liquids: NMR ionicity studies
Tetrahedron, (71): 676-685 2015.

Morita, M.; Matsuda, Y.; Endo, T.; Mikami, N.; Fujii, A.; Takahashi, K.
Hyperconjugation in diethyl ether cation versus diethyl sulfide cation
Physical Chemistry Chemical Physics, (17): 23602-23612 2015.

Morzyk-Ociepa, B.; Dysz, K.; Turowska-Tyrk, I.; Michalska, D.
Reinvestigation of the crystal structure, vibrational spectroscopic studies and DFT calculations of 5-bromo-7-azaindole with dual N-H center dot center dot center dot N hydrogen bonds in dimers
Journal of Molecular Structure, (1101): 91-100 2015.

Mos, A.; Castro, C.; Indris, S.; Strobele, M.; Fink, R. F.; Meyer, H. J.
From WCl6 to WCl2: Properties of Intermediate Fe-W-Cl Phases
Inorganic Chemistry, (54): 9826-9832 2015.

Mottishaw, J. D.; Erck, A. R.; Kramer, J. H.; Sun, H. R.; Koppang, M.
Electrostatic Potential Maps and Natural Bond Orbital Analysis: Visualization and Conceptualization of Reactivity in Sanger's Reagent
Journal of Chemical Education, (92): 1846-1852 2015.

Mougel, V.; Santiago, C. B.; Zhizhko, P. A.; Bess, E. N.; Varga, J.; Frater, G.; Sigman, M. S.; Coperet, C.
Quantitatively Analyzing Metathesis Catalyst Activity and Structural Features in Silica-Supported Tungsten Imido-Alkylidene Complexes
Journal of the American Chemical Society, (137): 6699-6704 2015.

Mukherjee, S.; Reddy, B. V. P.; Mitra, I.; Saha, R.; Bose, K. J. C.; Dodda, S. R.; Linert, W.; Moi, S. C.
In vitro model reaction of sulfur containing bio-relevant ligands with Pt(II) complex: kinetics, mechanism, bioactivity and computational studies
Rsc Advances, (5): 76987-76999 2015.

Mundlapati, V. R.; Ghosh, S.; Bhattacherjee, A.; Tiwari, P.; Biswal, H. S.
Critical Assessment of the Strength of Hydrogen Bonds between the Sulfur Atom of Methionine/Cysteine and Backbone Amides in Proteins
Journal of Physical Chemistry Letters, (6): 1385-1389 2015.

Murugan, V.; Parasuraman, P.; Selvin, J. F. A.; Priyadarzini, T. R. K.; Gromiha, M. M.; Fukui, K.; Veluraja, K.
Geometry Optimization of Carbohydrate Binding Sites of Influenza: A Quantum Mechanical Approach
Journal of Carbohydrate Chemistry, (34): 409-429 2015.

Murugesan, S.; Stoger, B.; Weil, M.; Veiros, L. F.; Kirchner, K.
Synthesis, Structure, and Reactivity of Co(II) and Ni(II) PCP Pincer Borohydride Complexes
Organometallics, (34): 1364-1372 2015.

Musavi, S. M.; Amani, J.; Noruzi, P.
Reaching for Two New Stable Ambiphilic Quinoline-Derived N-Heterocyclic Carbenes at DFT Level
International Journal of Quantum Chemistry, (115): 224-230 2015.

Muthu, K.; Meenatchi, V.; Rajasekar, M.; Prasad, A. A.; Meena, K.; Agilandeshwari, R.; Kanagarajan, V.; Meenakshisundaram, S. P.
Combined theoretical and experimental studies on the molecular structure, spectral and Hirshfeld surface studies of NLO tris(thiourea)zinc(II) sulfate crystals
Journal of Molecular Structure, (1091): 210-221 2015.

Muthu, S.; Elamuruguporchelvi, E.; Varghese, A.
DFT electronic structure calculations, spectroscopic studies, and normal coordinate analysis of 2- (5-nitro-1,3-thiazol-2-yl)carbamoyl phenyl acetate
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (138): 743-752 2015.

Muthu, S.; Porchelvi, E. E.; Karabacak, M.; Asiri, A. M.; Swathi, S. S.

Synthesis, structure, spectroscopic studies (FT-IR, FT-Raman and UV), normal coordinate, NBO and NLO analysis of salicylaldehyde p-chlorophenylthiosemicarbazone
Journal of Molecular Structure, (1081): 400-412 2015.

Muthu, S.; Prabakaran, A.
Scaled Quantum Chemical Studies of the Molecular Structure and Vibrational Spectra of Minoxidil
Spectroscopy Letters, (48): 63-73 2015.

Muthunatesan, S.; Ragavendran, V.
A study of vibrational spectra and investigations of charge transfer and chemical bonding features of 2-chloro benzimidazole based on DFT computations
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (134): 148-154 2015.

Nacereddine, A. K.; Layeb, H.; Chafaa, F.; Yahia, W.; Djerourou, A.; Domingo, L. R.
A DFT study of the role of the Lewis acid catalysts in the 3+2 cycloaddition reaction of the electrophilic nitrone isomer of methyl glyoxylate oxime with nucleophilic cyclopentene
Rsc Advances, (5): 64098-64105 2015.

Nacereddine, A. K.; Sobhi, C.; Djerourou, A.; Rios-Gutierrez, M.; Domingo, L. R.
Non-classical CH center dot center dot center dot O hydrogen-bond determining the regio- and stereoselectivity in the 3+2 cycloaddition reaction of (Z)-C-phenyl-N-methylnitrone with dimethyl 2-benzylidenecyclopropane-1,1-dicarboxylate. A topological electron-density study
Rsc Advances, (5): 99299-99311 2015.

Nagabalasubramanian, P. B.; Periandy, S.; Karabacak, M.; Govindarajan, M.
Molecular structure, vibrational, electronic and thermal properties of 4-vinylcyclohexene by quantum chemical calculations
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (145): 340-352 2015.

Naito, Y.; Murakami, W.; Eda, K.; Yamamoto, M.; Osakai, T.
Coextraction of Water into Nitrobenzene with Organic Ions
Journal of Physical Chemistry B, (119): 6010-6017 2015.

Nakamae, K.; Takemura, Y.; Kure, B.; Nakajima, T.; Kitagawa, Y.; Tanase, T.
Self-Alignment of Low-Valent Octanuclear Palladium Atoms
Angewandte Chemie-International Edition, (54): 1016-1021 2015.

Nakamura, T.; Suzuki, K.; Yamashita, M.
An Isolable Anionic Gallabenzene: Synthesis and Characterization
Organometallics, (34): 1806-1808 2015.

Nakano, H.; Noguchi, J.; Mochida, T.; Sato, H.
Theoretical Studies on the Electronic States and Liquid Structures of Ferrocenium-Based Ionic Liquids
Journal of Physical Chemistry A, (119): 5181-5188 2015.

Naktode, K.; Das Gupta, S.; Kundu, A.; Jana, S. K.; Nayek, H. P.; Mallik, B. S.; Panda, T. K.
Functionalisation of Imidazolin-2-imine to Corresponding Phosphinamine, Chalcogenide (O, S, Se, Te), and Borane Compounds
Australian Journal of Chemistry, (68): 127-136 2015.

Narbutt, J.; Wodynski, A.; Pecul, M.
The selectivity of diglycolamide (TODGA) and bis-triazine-bipyridine (BTBP) ligands in actinide/lanthanide complexation and solvent extraction separation - a theoretical hpproach
Dalton Transactions, (44): 2657-2666 2015.

Nazarparvar, E.; Zahedi, M.; Klein, E.
Theoretical study of the substituent effects on O-H BDE of trans-resveratrol derivatives in water and benzene: NBO analysis of intramolecular hydrogen bonds

Structural Chemistry, (26): 47-59 2015.

Nechaev, I. V.; Samofalova, T. V.; Naumov, A. V.; Semenov, V. N.
Structure and IR spectra of bis(thiourea)cadmium sulfate according to quantum-chemical calculation data
Russian Journal of Inorganic Chemistry, (60): 180-186 2015.

Nedd, S.; Alexandrova, A. N.
The mechanism of the Pd-catalyzed formation of coumarins: a theoretical study
Physical Chemistry Chemical Physics, (17): 1347-1353 2015.

Neela, Y. I.; Sastry, G. N.
Theoretical investigation of anion (F-, Cl-) and cation (Na+) interactions with substituted benzene C6H6 - nYn (Y = -F, -CN, -NO2; n = 1-6)
Molecular Physics, (113): 137-148 2015.

Nekoei, A. R.; Haghgoo, S.
Introduction and theoretical investigation of new azafullerene structures with nitrogen belts
Computational and Theoretical Chemistry, (1067): 148-157 2015.

Nepal, B.; Scheiner, S.
Angular dependence of hydrogen bond energy in neutral and charged systems containing CH and NH proton donors
Chemical Physics Letters, (630): 6-11 2015.

Nepal, B.; Scheiner, S.
Competitive Halide Binding by Halogen Versus Hydrogen Bonding: Bis-triazole Pyridinium
Chemistry-a European Journal, (21): 13330-13335 2015.

Neri, G.; Scala, A.; Fazio, E.; Mineo, P. G.; Rescifina, A.; Piperno, A.; Grassi, G.
Repurposing of oxazolone chemistry: gaining access to functionalized graphene nanosheets in a top-down approach from graphite
Chemical Science, (6): 6961-6970 2015.

Neuba, A.; Rohrmuller, M.; Holscher, R.; Schmidt, W. G.; Henkel, G.
A panel of peralkylated sulfur-guanidine type bases: Novel pro-ligands for use in biomimetic coordination chemistry
Inorganica Chimica Acta, (430): 225-238 2015.

Nguyen, A. L.; Bobadova-Parvanova, P.; Hopfinger, M.; Fronczek, F. R.; Smith, K. M.; Vicente, M. G. H.
Synthesis and Reactivity of 4,4-Dialkoxy-BODIPYs: An Experimental and Computational Study
Inorganic Chemistry, (54): 3228-3236 2015.

Ni, F. W.; Zhang, Y.; Zhang, F.; Zhao, J. Y.; Wu, L. B.; Chu, X. Z.
Synthesis, structural characterization and theoretical approach of 3-(2,6-dichlorobenzyl)-5-methyl-N-nitro-1,3,5-oxadiazinan-4-imine
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (138): 648-659 2015.

Nie, B. L.; Yan, S. H.; Sun, L. X.
Geometry, vibrational frequency, and isomerization of neutral and cation Cu-CN complex
Journal of Theoretical & Computational Chemistry, (14) 2015.

Nijesh, K.; Rojisha, V. C.; De, S.; Parameswaran, P.
2-Adamantylidene and its heavier analogues: hyperconjugation versus lone pair stability and electrophilicity versus nucleophilicity
Dalton Transactions, (44): 4693-4706 2015.

Nikolova, V.; Galabov, B.
EFFECTS OF STRUCTURAL VARIATIONS ON THE HYDROGEN BOND PAIRING BETWEEN ADENINE DERIVATIVES AND THYMINE
Macedonian Journal of Chemistry and Chemical Engineering, (34): 159-167 2015.

Niu, D. F.; Wang, H. Y.; Li, H. C.; Wu, Z. J.; Zhang, X. S.
Roles of ion pairing on electroreduction of carbon dioxide based on imidazolium-based salts
Electrochimica Acta, (158): 138-142 2015.

Niu, D. F.; Wang, H. Y.; Li, H. C.; Zhang, X. S.
The effect of the alkyl chain length of the tetraalkylammoniumcation on CO2 electroreduction in an aprotic medium
Electrochemistry Communications, (52): 58-62 2015.

Niu, W. X.; Zhang, H.; Li, P.; Gao, T.
Gas-Phase Ammonia Activation by Th, Th+, and Th2+ : Reaction Mechanisms, Bonding Analysis, and Rate Constant Calculations
International Journal of Quantum Chemistry, (115): 6-18 2015.

Nizovtsev, A. S.; Ivanov, A. S.; Boldyrev, A. I.; Konchenko, S. N.
Li4E8 (E = P, As, Sb, Bi) Clusters: The Quest for Realgar-Type E-8 (4-) Zintl Anions
European Journal of Inorganic Chemistry: 5801-5807 2015.

Noorjahan, A.; Choi, P.
Effect of partial atomic charges on the calculated free energy of solvation of poly(vinyl alcohol) in selected solvents
Journal of Molecular Modeling, (21) 2015.

Nordheider, A.; Hupf, E.; Chalmers, B. A.; Knight, F. R.; Buhl, M.; Mebs, S.; Checinska, L.; Lork, E.; Camacho, P. S.; Ashbrook, S. E.; Arachchige, K. S. A.; Cordes, D. B.; Slawin, A. M. Z.; Beckmann, J.; Woollins, J. D.
Peri-Substituted Phosphorus-Tellurium Systems-An Experimental and Theoretical Investigation of the P center dot center dot center dot Te through-Space Interaction
Inorganic Chemistry, (54): 2435-2446 2015.

Nouri, A.; Zahedi, E.; Jafari, F. J.; Nouri, A.
Diels-Alder reactions of a-cyano alpha,beta-unsaturated ketones with 2-methyl-1,3-butadiene: DFT study of mechanism, reactivity and regioselectivity
Progress in Reaction Kinetics and Mechanism, (40): 177-189 2015.

Novak, M.; Foroutan-Nejad, C.; Marek, R.
Asymmetric bifurcated halogen bonds
Physical Chemistry Chemical Physics, (17): 6440-6450 2015.

Nunes, C. M.; Reva, I.; Rosado, M. T. S.; Fausto, R.
The Quest for Carbenic Nitrile Imines: Experimental and Computational Characterization of C-Amino Nitrile Imine
European Journal of Organic Chemistry: 7484-7493 2015.

Nunez-Zarur, F.; Comas-Vives, A.
The Effect of the Electronic Nature of Spectator Ligands in the C-H Bond Activation of Ethylene by Cr(III) Silicates: An ab initio Study
Chimia, (69): 225-229 2015.

Nurazar, R.; Ebrahimi, Z. F.; Esrafili, M. D.; Vessally, E.
Sensing and Catalytic Decomposition of Hydrogen Peroxide by Silicon Carbide Nanotubes: A DFT Study
International Journal of Quantum Chemistry, (115): 471-476 2015.

Nziko, V. D. N.; Scheiner, S.
Interactions between Thiourea and Imines. Prelude to Catalysis
Journal of Organic Chemistry, (18): 10334-10341 2015.

Nziko, V. D. N.; Scheiner, S.
Intramolecular S center dot center dot center dot O Chalcogen Bond as Stabilizing Factor in Geometry of Substituted Phenyl-SF3 Molecules
Journal of Organic Chemistry, (80): 2356-2363 2015.

Nziko, V. D. N.; Scheiner, S.
S center dot center dot center dot pi Chalcogen Bonds between SF2 or SF4 and C-C Multiple Bonds
Journal of Physical Chemistry A, (119): 5889-5897 2015.

Ochi, N.; Matsumoto, T.; Dei, T.; Nakao, Y.; Sato, H.; Tatsumi, K.; Sakaki, S.
Heterolytic Activation of Dihydrogen Molecule by Hydroxo-/Sulfido-Bridged Ruthenium-Germanium Dinuclear Complex. Theoretical Insights
Inorganic Chemistry, (54): 576-585 2015.

Odoh, S. O.; Cramer, C. J.; Truhlar, D. G.; Gagliardi, L.
Quantum-Chemical Characterization of the Properties and Reactivities of Metal-Organic Frameworks
Chemical Reviews, (115): 6051-6111 2015.

Ojha, M.; Maheshwari, P.; Gurjar, A.; Bansal, R. K.
EFFECT OF (CRR2)-R-1/(P+RR2)-R-1 EXCHANGE ON THE DEGENERATE COPE REARRANGEMENT OF BARBARALANE
Phosphorus Sulfur and Silicon and the Related Elements, (190): 2255-2266 2015.

Olech, K.; Gutkowski, R.; Kuznetsov, V.; Roszak, S.; Soloducho, J.; Schuhmann, W.
Synthesis and Electrochromic Properties of Conducting Polymers Based on Highly Planar 2,7-Disubstituted Xanthene Derivatives
Chempluschem, (80): 679-687 2015.

Oliveira, B. G.; Zabardasti, A.; Goudarziafshar, H.; Salehnassaj, M.
The electronic mechanism ruling the dihydrogen bonds and halogen bonds in weakly bound systems of H3SiH center dot center dot center dot HOX and H3SiH center dot center dot center dot XOH (X = F, Cl, and Br)
Journal of Molecular Modeling, (21) 2015.

Omidvar, A.; Mohajeri, A.
Promotional effect of the electron donating functional groups on the gas sensing properties of graphene nanofakes
Rsc Advances, (5): 54535-54543 2015.

Ona, O. B.; Torres-Vega, J. J.; Torre, A.; Lain, L.; Alcoba, D. R.; Vasquez-Espinal, A.; Tiznado, W.
Chemical bonding analysis in boron clusters by means of localized orbitals according to the electron localization function topology
Theoretical Chemistry Accounts, (134) 2015.

Ootani, Y.; Sodeyama, K.; Han, L. Y.; Tateyama, Y.
Possibility of NCS Group Anchor for Ru Dye Adsorption to Anatase TiO2(101) Surface: A Density Functional Theory Investigation
Journal of Physical Chemistry C, (119): 234-241 2015.

Orbach, M.; Shankar, S.; Zenkina, O. V.; Milko, P.; Diskin-Posner, Y.; van der Boom, M. E.
Generation of Mono- and Bimetallic Palladium Complexes and Mechanistic Insight into an Operative Metal Ring-Walking Process
Organometallics, (34): 1098-1106 2015.

Orekhov, D. V.; Kamorin, D. M.; Rumyantsev, M.; Kazantsev, O. A.; Sivokhin, A. P.; Gushchin, A. V.; Savinova, M. V.
Assembly of oligo(ethylene glycol)- and amine-containing methacrylic esters in water and water-hexane mixtures
Colloids and Surfaces a-Physicochemical and Engineering Aspects, (481): 20-30 2015.

Ortega, D. E.; Gutierrez-Oliva, S.; Tantillo, D. J.; Toro-Labbe, A.
A detailed analysis of the mechanism of a carbocationic triple shift rearrangement
Physical Chemistry Chemical Physics, (17): 9771-9779 2015.

Ortega, P. G. R.; Montejo, M.; Gonzalez, J. J. L.
Vibrational Circular Dichroism and Theoretical Study of the Conformational Equilibrium in (-)-S-Nicotine
Chemphyschem, (16): 342-352 2015.

Ortega, P. G. R.; Montejo, M.; Marquez, F.; Gonzalez, J. J. L.
DFT-Aided Vibrational Circular Dichroism Spectroscopy Study of (-)-S-cotinine
Chemphyschem, (16): 1416-1427 2015.

Osakai, T.; Naito, Y.; Eda, K.; Yamamoto, M.
Prediction of the Standard Gibbs Energy of Transfer of Organic Ions Across the Interface between Two Immiscible Liquids
Journal of Physical Chemistry B, (119): 13167-13176 2015.

Ostojic, B. D.; Dordevic, D. S.
Two nitro derivatives of azabenzo a pyrene N-oxide: Electronic properties and their relation to mutagenic activity
Journal of Hazardous materials, (285): 94-102 2015.

Otsuka, M.; Tsuchida, N.; Ikeda, Y.; Lambert, N.; Nakamura, R.; Mutoh, Y.; Ishii, Y.; Takano, K.
Theoretical Study on Internal Alkyne/Vinylidene Isomerization in Group 8 Transition-Metal Complexes
Organometallics, (34): 3934-3943 2015.

Ou, Z. W.; Liu, Z. H.; Deng, Z. P.; Xie, Y. M.; Schaefer, H. F.; King, R. B.
New Titanium Carbonyls: Ti-2(CO)(10), Ti-2(CO)(11), and Ti-2(CO)(12)
Journal of Physical Chemistry A, (119): 5224-5232 2015.

Oziminski, W. P.; Ramsden, C. A.
A DFT and ab initio study of conjugated and semi-conjugated mesoionic rings and their covalent isomers
Tetrahedron, (71): 7191-7198 2015.

Pahan, S.; Boda, A.; Ali, S. M.
Density functional theoretical analysis of structure, bonding, interaction and thermodynamic selectivity of hexavalent uranium (UO22+) and tetravalent plutonium (Pu4+) ion complexes of tetramethyl diglycolamide (TMDGA)
Theoretical Chemistry Accounts, (134) 2015.

Pal, S.; Kundu, T. K.
Design of Methane Hydrate Inhibitor Molecule Using Density Functional Theory
Journal of Cluster Science, (26): 551-563 2015.

Palma-Goyes, R. E.; Vazquez-Arenas, J.; Torres-Palma, R. A.; Ostos, C.; Ferraro, F.; Gonzalez, I.
The abatement of indigo carmine using active chlorine electrogenerated on ternary Sb2O5-doped Ti/RuO2-ZrO2 anodes in a filter-press FM01-LC reactor
Electrochimica Acta, (174): 735-744 2015.

Pan, Y. R.; Sun, M.; Li, X. M.
Synthesis, Crystal Structure and Theoretical Calculations of a Nickel(II) Coordination Polymer Assembled by 4,4 '-Oxydibenzoic Acid and 1,3-Bis(imidazol-1-ylmethyl)-benzene Ligands
Chinese Journal of Structural Chemistry, (34): 710-718 2015.

Pandey, K. K.; Vishwakarma, R.; Patidar, S. K.; Bariya, P. K.
Structure and bonding analysis of intermediate model heme-imidazole and heme-thiolate enzymes complexed with formate, acetate and nitrate: A theoretical study
Computational and Theoretical Chemistry, (1051): 137-143 2015.

Pandey, P.; Pant, C. K.; Gururani, K.; Arora, P.; Pandey, N.; Bhatt, P.; Sharma, Y.; Negi, J. S.; Mehata, M. S.
Affinity of Smectite and Divalent Metal Ions (Mg2+, Ca2+, Cu2+) with L-leucine: An Experimental and Theoretical Approach Relevant to Astrobiology
Origins of Life and Evolution of Biospheres, (45): 411-426 2015.

Pandiyan, B. V.; Deepa, P.; Kolandaivel, P.
Do resonance-assisted intramolecular halogen bonds exist without a charge transfer and a sigma-hole?
Physical Chemistry Chemical Physics, (17): 27496-27508 2015.

Papadopoulos, A. G.; Charistos, N. D.; Kyriakidou, K.; Sigalas, M. P.
Study of Electron Delocalization in 1,2-, 1,3-, and 1,4-Azaborines Based on the Canonical Molecular Orbital Contributions to the Induced Magnetic Field and Polyelectron Population Analysis
Journal of Physical Chemistry A, (119): 10091-10100 2015.

Parameswari, A. R.; Rajalakshmi, G.; Kumaradhas, P.
A combined molecular docking and charge density analysis is a new approach for medicinal research to understand drug-receptor interaction: Curcumin-AChE model
Chemico-Biological Interactions, (225): 21-31 2015.

Pardillo, A. D.; Morozov, A. N.; Chatfield, D. C.
Proximal Pocket Hydrogen Bonds Significantly Influence the Mechanism of Chloroperoxidase Compound I Formation
Journal of Physical Chemistry B, (119): 12590-12602 2015.

Paredes-Gil, K.; Jaque, P.
Initiation stage of alkene metathesis: Insights from natural bond orbital and charge decomposition analyses
Chemical Physics Letters, (618): 174-181 2015.

Parlak, C.; Ramasami, P.; Kumar, C. S. C.; Tursun, M.; Quah, C. K.; Rhyman, L.; Bilge, M.; Fun, H. K.; Chandraju, S.
(2E)-1-(5-Chlorothiophen-2-yl)-3-{4- (E)-2-phenylethenyl phenyl} prop-2-en-1-one: Synthesis, XRD, FT-IR, Raman and DFT studies
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (149): 385-395 2015.

Parra, R. D.
Cooperative effects and energy barriers to bromonium ion transfer in cyclic (BrX)(n) halogen-bonded clusters (X = F, OH, or NH2; n=3-5): An ab initio study
Computational and Theoretical Chemistry, (1066): 47-54 2015.

Pastor, M. B.; Zhao, Q. L.
A DFT investigation on the electronic properties of octahaloditechnetate anions: Correlation between charge and bond strength
Inorganica Chimica Acta, (424): 308-315 2015.

Pathak, S. K.; Srivastava, R.; Sachan, A. K.; Prasad, O.; Sinha, L.; Asiri, A. M.; Karabacak, M.
Experimental (FT-IR, FT-Raman, UV and NMR) and quantum chemical studies on molecular structure, spectroscopic analysis, NLO, NBO and reactivity descriptors of 3,5-Difluoroaniline
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (135): 283-295 2015.

Pati, K.; Gomes, G. D.; Harris, T.; Hughes, A.; Phan, H.; Banerjee, T.; Hanson, K.; Alabugin, I. V.
Traceless Directing Groups in Radical Cascades: From Oligoalkynes to Fused Helicenes without Tethered Initiators
Journal of the American Chemical Society, (137): 1165-1180 2015.

Pati, K.; Michas, C.; Allenger, D.; Piskun, I.; Coutros, P. S.; Gomes, G. D.; Alabugin, I. V.
Synthesis of Functionalized Phenanthrenes via Regioselective Oxidative Radical Cyclization
Journal of Organic Chemistry, (80): 11706-11717 2015.

Paul, B. K.; Ghosh, N.; Mondal, R.; Mukherjee, S.
A critical approach toward resonance-assistance in the intramolecular hydrogen bond interaction of 3,5-diiodosalicylic acid: a spectroscopic and computational investigation
Photochemical & Photobiological Sciences, (14): 1147-1162 2015.

Pavelka, L. C.; Hanson, M. A.; Staroverov, V. N.; Baines, K. M.
Mechanism of the addition of alkynes to silenes and germenes: A density functional study
Canadian Journal of Chemistry, (93): 134-142 2015.

Pazos, M.; Martinez, S.; Vila, M. A.; Rodriguez, P.; Veiga, N.; Seoane, G.; Carrera, I.

Aza and oxo Diels-Alder reactions using cis-cyclohexadienediols of microbial origin: chemoenzymatic preparation of synthetically valuable heterocyclic scaffolds
Tetrahedron-Asymmetry, (26): 1436-1447 2015.

Pelzer, A. W.; Jellinek, J.; Jackson, K. A.
H-2 Saturation on Palladium Clusters
Journal of Physical Chemistry A, (119): 3594-3603 2015.

Perez, C.; Neill, J. L.; Muckle, M. T.; Zaleski, D. P.; Pena, I.; Lopez, J. C.; Alonso, J. L.; Pate, B. H.
Water-Water and Water-Solute Interactions in Microsolvated Organic Complexes
Angewandte Chemie-International Edition, (54): 979-982 2015.

Perez, P.; Domingo, L. R.
A DFT Study of Inter- and Intramolecular Aryne Ene Reactions
European Journal of Organic Chemistry: 2826-2834 2015.

Perez-Gallegos, A.; Garcia-Viloca, M.; Gonzalez-Lafont, A.; Lluch, J. M.
A QM/MM study of Kemptide phosphorylation catalyzed by protein kinase A. The role of Asp166 as a general acid/base catalyst
Physical Chemistry Chemical Physics, (17): 3497-3511 2015.

Perotto, C. U.; Marshall, G.; Jones, G. J.; Davies, E. S.; Lewis, W.; McMaster, J.; Schroder, M.
A Ni(I)Fe(II) analogue of the Ni-L state of the active site of the NiFe hydrogenases
Chemical Communications, (51): 16988-16991 2015.

Petrovic, Z. D.; Dorovic, J.; Simijonovic, D.; Petrovic, V. P.; Markovic, Z.
Experimental and theoretical study of antioxidative properties of some salicylaldehyde and vanillic Schiff bases
Rsc Advances, (5): 24094-24100 2015.

Petukhov, A. N.; Shablykin, D. N.; Vorotyntsev, A. V.; Vorotyntsev, I. V.; Vorotyntsev, V. M.
Effects of association with impurities in ammonia purification
Fluid Phase Equilibria, (406): 163-167 2015.

Peyghan, A. A.; Soleymanabadi, H.
Computational study on ammonia adsorption on the X12Y12 nano-clusters (X = B, Al and Y = N, P)
Current Science, (108): 1910-1914 2015.

Pham, H. V.; Karns, A. S.; Vanderwal, C. D.; Houk, K. N.
Computational and Experimental Investigations of the Formal Dyotropic Rearrangements of Himbert Arene/Allene Cycloadducts
Journal of the American Chemical Society, (137): 6956-6964 2015.

Phipps, M. J. S.; Fox, T.; Tautermann, C. S.; Skylaris, C. K.
Energy decomposition analysis approaches and their evaluation on prototypical protein-drug interaction patterns
Chemical Society Reviews, (44): 3177-3211 2015.

Pienko, T.; Taciak, P. P.; Mazurek, A. P.
On the Basicity of 8-Phenylsulfanyl Quipazine Derivatives: New Potential Serotonergic Agents
Journal of Physical Chemistry A, (119): 6989-6999 2015.

Pierpont, A. W.; Batista, E. R.; Martin, R. L.; Chen, W. Z.; Kim, J. K.; Hoyt, C. B.; Gordon, J. C.; Michalczyk, R.; Silks, L. A.; Wu, R. L.
Origins of the Regioselectivity in the Lutetium Inflate Catalyzed Ketalization of Acetone with Glycerol: A DFT Study
Acs Catalysis, (5): 1013-1019 2015.

Pillai, R. S.; Jorge, M.; Gomes, J. R. B.
A density functional theory study on the interaction of paraffins, olefins, and acetylenes with Na-ETS-10
Theoretical Chemistry Accounts, (134) 2015.

Pinto, G. P.; Bras, N. F.; Perez, M. A. S.; Fernandes, P. A.; Russo, N.; Ramos, M. J.; Toscano, M.
Establishing the Catalytic Mechanism of Human Pancreatic alpha-Amylase with QM/MM Methods
Journal of Chemical Theory and Computation, (11): 2508-2516 2015.

Plech, T.; Kapron, B.; Paneth, A.; Wujec, M.; Czarnomysy, R.; Bielawska, A.; Bielawski, K.; Trotsko, N.; Kusmierz, E.; Paneth, P.
Search for human DNA topoisomerase II poisons in the group of 2,5-disubstituted-1,3,4-thiadiazoles
Journal of Enzyme Inhibition and Medicinal Chemistry, (30): 1021-1026 2015.

Pluhackoya, K.; Morhenn, H.; Lautner, L.; Lohstroh, W.; Nemkovski, K. S.; Unruh, T.; Bockmann, R. A.
Extension of the LOPLS-AA Force Field for Alcohols, Esters, and Monoolein Bilayers and its Validation by Neutron Scattering Experiments
Journal of Physical Chemistry B, (119): 15287-15299 2015.

Pogany, P.; Kovacs, A.
Theoretical investigation of NpC, NpC2 and NpC4 molecules
Structural Chemistry, (26): 1309-1322 2015.

Polat, T.; Bulut, F.; Arican, I.; Kandemirli, F.; Yildirim, G.
Vibrational assignments, spectroscopic investigation (FT-IR and FT-Raman), NBO, MEP, HOMO-LUMO analysis and intermolecular hydrogen bonding interactions of 7-fluoroisatin, 7-bromoisatin and 1-methylisatin - A comparative study
Journal of Molecular Structure, (1101): 189-211 2015.

Politzer, P.; Murray, J. S.
Quantitative Analyses of Molecular Surface Electrostatic Potentials in Relation to Hydrogen Bonding and Co-Crystallization
Crystal Growth & Design, (15): 3767-3774 2015.

Politzer, P.; Murray, J. S.; Clark, T.
Mathematical modeling and physical reality in noncovalent interactions
Journal of Molecular Modeling, (21) 2015.

Politzer, P.; Murray, J. S.; Clark, T.
sigma-Hole Bonding: A Physical Interpretation
Halogen Bonding I: Impact on Materials Chemistry and Life Sciences, (358): 19-42 2015.

Popescu, A. R.; Rojo, I.; Teixidor, F.; Sillanpaa, R.; Vinas, C.
Intramolecular Communication in Anionic Oxidized Phosphanes through a Chelated Proton
Chemistry-a European Journal, (21): 8613-8625 2015.

Popov, I. A.; Averkiev, B. B.; Starikova, A. A.; Boldyrev, A. I.; Minyaev, R. M.; Minkin, V. I.
Assessing the Viability of Extended Nonmetal Atom Chains in MnF4n+2 (M = S and Se)
Angewandte Chemie-International Edition, (54): 1476-1480 2015.

Popov, I. A.; Zhang, X. X.; Eichhorn, B. W.; Boldyrev, A. I.; Bowen, K. H.
Aluminum chain in Li2Al3H8- as suggested by photoelectron spectroscopy and ab initio calculations
Physical Chemistry Chemical Physics, (17): 26079-26083 2015.

Porchelvi, E. E.; Muthu, S.
Vibrational spectra, molecular structure, natural bond orbital, first order hyperpolarizability, thermodynamic analysis and normal coordinate analysis of Salicylaldehyde p-methylphenylthiosemicarbazone by density functional method
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (134): 453-464 2015.

Portnyagin, A. S.; Bratskaya, S. Y.; Pestov, A. V.; Voit, A. V.
Binding Ni(II) ions to chitosan and its N-heterocyclic derivatives: Density functional theory investigation
Computational and Theoretical Chemistry, (1069): 4-10 2015.

Prabavathi, N.; Nayaki, N. S.; Reddy, B. V.

Molecular structure, vibrational spectra, natural bond orbital and thermodynamic analysis of 3,6-dichloro-4-methylpyridazine and 3,6-dichloropyridazine-4-carboxylic acid by dft approach
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (136): 1134-1148 2015.

Prabavathi, N.; Nilufer, A.
Quantum chemical calculations on elucidation of molecular structure and spectroscopic insights on 2-amino-4-methoxy-6-methylpyrimidine and 2-amino-5-bromo-6-methyl-4-pyrimidinol - A comparative study
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (136): 192-204 2015.

Prabhaharan, M.; Prabakaran, A. R.; Gunasekaran, S.; Srinivasan, S.
DFT studies on vibrational spectra, HOMO-LUMO, NBO and thermodynamic function analysis of cyanuric fluoride
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (136): 494-503 2015.

Pradeepa, S. J.; Sundaraganesan, N.
Spectroscopic and molecular structure investigations of 9-vinylcarbazole by DFT and ab initio method
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (136): 690-699 2015.

Prakash, G. K. S.; Olah, G. A.; Rasul, G.
Ab Initio/GIAO-CCSD(T) investigation of B-11-C-13 NMR chemical shift relationships in trifluoro- and trihydridoborate anions and their isoelectronic neutral alkane derivatives
Journal of Organometallic Chemistry, (798): 229-233 2015.

Prasad, A. A.; Meenakshisundaram, S. P.
Crystal growth, characterization and Density functional theory computations of supramolecular N-carbamothioyl acetamide
Crystal Research and Technology, (50): 395-404 2015.

Prasad, A. A.; Muthu, K.; Meenatchi, V.; Rajasekar, M.; Agilandeshwari, R.; Meena, K.; Manonmoni, J. V.; Meenakshisundaram, S. P.
Optical, vibrational, NBO, first-order molecular hyperpolarizability and Hirshfeld surface analysis of a nonlinear optical chalcone
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (140): 311-327 2015.

Prasad, A. A.; Muthu, K.; Rajasekar, M.; Meenatchi, V.; Meenakshisundaram, S. P.
Synthesis, crystal growth, characterization and theoretical studies of 4-aminobenzophenonium picrate
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (135): 46-54 2015.

Prasad, K. V.; Samatha, K.; Rao, D. J.; Santhamma, C.; Muthu, S.; Heron, B. M.
Spectroscopic studies (FT-IR, FT-Raman, UV-Visible), normal co-ordinate analysis, first-order hyperpolarizability and HOMO, LUMO studies of 3,4-dichlorobenzophenone by using Density Functional Methods
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (151): 644-654 2015.

Prasad, M. V. S.; Sri, N. U.; Veeraiah, V.
A combined experimental and theoretical studies on FT-IR, FT-Raman and UV-vis spectra of 2-chloro-3-quinolinecarboxaldehyde
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (148): 163-174 2015.

Premkumar, S.; Jawahar, A.; Mathavan, T.; Dhas, M. K.; Benial, A. M. F.
Vibrational spectroscopic and DFT calculation studies of 2-amino-7-bromo-5-oxo- 1 benzopyrano 2,3-b pyridine-3 carbonitrile
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (138): 252-263 2015.

Proud, A. J.; Mackenzie, D.; Pearson, J. K.
Exploring electron pair behaviour in chemical bonds using the extracule density
Physical Chemistry Chemical Physics, (17): 20194-20204 2015.

Pruitt, C. J. M.; Goebbert, D. J.
Experimental and Theoretical Study of the Decomposition of Copper Nitrate Cluster Anions

Journal of Physical Chemistry A, (119): 4755-4762 2015.

Qiao, Y. M.; Fan, Z. L.; Jiang, Y. J.; Li, N.; Dong, H.; He, N.; Zhou, D. H.
Structures and vibrational spectra of Ti-MWW zeolite upon adsorption of H2O and NH3: A density functional theory study
Chinese Journal of Catalysis, (36): 1733-1741 2015.

Quinonero, D.
Anion Recognition by Pyrylium Cations and Thio-, Seleno- and Telluro-Analogues: A Combined Theoretical and Cambridge Structural Database Study
Molecules, (20): 11632-11659 2015.

Rabanal-Leon, W. A.; Murillo-Lopez, J. A.; Paez-Hernandez, D.; Arratia-Perez, R.
Aromatic Lateral Substituents Influence the Excitation Energies of Hexaaza Lanthanide Macrocyclic Complexes: A Wave Function Theory and Density Functional Study
Journal of Physical Chemistry A, (119): 9931-9940 2015.

Rad, A. S.; Nasimi, N.; Jafari, M.; Shabestari, D. S.; Gerami, E.
Ab-initio study of interaction of some atmospheric gases (SO2, NH3, H2O, CO, CH4 and CO2) with polypyrrole (3PPy) gas sensor: DFT calculations
Sensors and Actuators B-Chemical, (220): 641-651 2015.

Rad, A. S.; Shadravan, A.; Soleymani, A. A.; Motaghedi, N.
Lewis acid-base surface interaction of some boron compounds with N-doped graphene; first principles study
Current Applied Physics, (15): 1271-1277 2015.

Rai, S.; Singh, H.; Priyakumar, U. D.
Binding to gold nanoclusters alters the hydrogen bonding interactions and electronic properties of canonical and size-expanded DNA base pairs
Rsc Advances, (5): 49408-49419 2015.

Raj, R. K.; Gunasekaran, S.; Gnanasambandan, T.; Seshadri, S.
Combined spectroscopic and DFT studies on 6-bromo-4-chloro-3-formyl coumarin
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (139): 505-514 2015.

Raja, B.; Balachandran, V.; Revathi, B.
Structural study, NCA, FT-IR, FT-Raman spectral investigations, NBO analysis, thermodynamic functions of N-acetyl-L-phenylalanine
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (138): 283-295 2015.

Raja, K.; Mugesh, G.
Remarkable Effect of Chalcogen Substitution on an Enzyme Mimetic for Deiodination of Thyroid Hormones
Angewandte Chemie-International Edition, (54): 7674-7678 2015.

Raja, R.; Seshadri, S.; Gnanasambandan, T.; Saravanan, R. R.
Crystal growth and properties of NLO optical crystal - Butylated Hydroxy Toluene (BHT)
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (138): 13-20 2015.

Rajabi, M.; Gholivand, K.; Salami, R.; Molaei, F.; Thibonnet, J.; Zare, K.; Tirani, F. F.; Schenk, K. J.
Synthesis, structural determination, theoretical studies and catalytic activity of Mn(II) complex of N-isonicotinyl phosphoric triamide ligand
Inorganica Chimica Acta, (432): 149-157 2015.

Rajaei, I.; Mirsattari, S. N.
Synthesis and spectroscopic properties of a copper(II) binuclear complex of a novel tetradentate asymmetrical Schiff base ligand and its DFT study
Polyhedron, (102): 479-489 2015.

Rajaraman, D.; Sundararajan, G.; Kamaraj, A.; Saleem, H.; Krishnasamy, K.
Synthesis, computational and spectroscopic analysis on (E)-(4-(2-(benzo d thiazol-2-yl)hydrazono)-3-methyl-2,6-diphenylpiperidi ne-1-yl)(phenyl)methanone using DFT approach
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (151): 480-489 2015.

Rajesh, P.; Gunasekaran, S.; Gnanasambandan, T.; Seshadri, S.
Experimental, quantum chemical and NBO/NLMO investigations of pantoprazole
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (136): 247-255 2015.

Rajesh, P.; Gunasekaran, S.; Gnanasambandan, T.; Seshadri, S.
Molecular structure and vibrational analysis of Trifluoperazine by FT-IR, FT-Raman and UV-Vis spectroscopies combined with DFT calculations
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (137): 1184-1193 2015.

Rajkumar, R.; Kamaraj, A.; Bharanidharan, S.; Saleem, H.; Krishnasamy, K.
Synthesis, spectral characterization, single crystal X-ray diffraction and DFT studies of 4-((2,4,5-triphenyl-1H-imidazol-1-yl)methyl)pyridine derivatives
Journal of Molecular Structure, (1084): 74-81 2015.

Ramakrishnan, A.; Chourasiya, S. S.; Bharatam, P. V.
Azine or hydrazone? The dilemma in amidinohydrazones
Rsc Advances, (5): 55938-55947 2015.

Ramalakshmi, R.; Bhattacharyya, M.; Rao, C. E.; Ghosh, S.
*Synthesis, structure and chemistry of low-boron containing molybdaborane: Arachno- Cp*Mo(CO)(2)B3H8*
Journal of Organometallic Chemistry, (792): 31-36 2015.

Ramanathan, N.; Rao, C.; Sankaran, K.; Sundararajan, K.
Unraveling the Conformational Landscape of Triallyl Phosphate: Matrix Isolation Infrared Spectroscopy and Density Functional Theory Computations
Journal of Physical Chemistry A, (119): 4017-4031 2015.

Ramanathan, N.; Sundararajan, K.; Sankaran, K.
Conformations of n-butyl imidazole: Matrix isolation infrared and DFT studies
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (139): 75-85 2015.

Ramasami, P.; Ford, T. A.
Chalcogen-bonded complexes. Selenium-bound adducts of NH3, H2O, PH3, and H2S with OCSe, SCSe, and CSe2
Journal of Molecular Modeling, (21) 2015.

Ramirez, B.; Cordova-Sintjago, T. C.; Ruette, F.; Chuchani, G.
Assessment in the competition between steric and electronic effects in the elimination kinetic of hydrogen in 1,4-cyclohexadienes in the gas phase. Quantum chemical theory calculations
Molecular Physics, (113): 237-248 2015.

Ramos-Berdullas, N.; Lopez-Carballeira, D.; Mandado, M.; Perez-Juste, I.
Revisiting the mechanism and the influence of the excitation wavelength on the surface-enhanced Raman scattering of the pyridine-Ag-20 system
Theoretical Chemistry Accounts, (134) 2015.

Ramos-Cordoba, E.; Postils, V.; Salvador, P.
Oxidation States from Wave Function Analysis
Journal of Chemical Theory and Computation, (11): 1501-1508 2015.

Ramya, K.; Joseph, A.
Synergistic effects and hydrogen bonded interaction of alkyl benzimadazoles and thiourea pair on mild steel in hydrochloric acid
Journal of the Taiwan Institute of Chemical Engineers, (52): 127-139 2015.

Ramya, K.; Mohan, R.; Anupama, K. K.; Joseph, A.
Electrochemical and theoretical studies on the synergistic interaction and corrosion inhibition of alkyl benzimidazoles and thiosemicarbazide pair on mild steel in hydrochloric acid
Materials Chemistry and Physics, (149): 632-647 2015.

Ranlalakshmi, R.; Saha, K.; Roy, D. K.; Varghese, B.; Phukan, A. K.; Ghosh, S.
New Routes to a Series of sigma-Borane/Borate Complexes of Molybdenum and Ruthenium
Chemistry-a European Journal, (21): 17191-17195 2015.

Rao, M. N.; Haridas, M.; Gangwar, M. K.; Rajakannu, P.; Kalita, A. C.; Ghosh, P.
Asymmetric Base-Free Michael Addition at Room Temperature with Nickel-Based Bifunctional Amido-Functionalized N-Heterocyclic Carbene Catalysts
European Journal of Inorganic Chemistry: 1604-1615 2015.

Rao, N. Z.; Larkin, J. D.; Bock, C. W.
A computational investigation of monosubstituted boroxines(RH2B3O3): structure and formation
Structural Chemistry, (26): 1151-1162 2015.

Rao, S. S.; Bejoy, N. B.; Gejji, S. P.
Hydrogen Bonding, H-1 NMR, and Molecular Electron Density Topographical Characteristics of Ionic Liquids Based on Amino Acid Cations and Their Ester Derivatives
Journal of Physical Chemistry A, (119): 8752-8764 2015.

Rao, S. S.; Gejji, S. P.
Molecular insights accompanying aggregation in amino acid ionic liquids
Computational and Theoretical Chemistry, (1057): 24-38 2015.

Rasheed, T.; Siddiqui, S. A.
Chemical Differentiation of Electronically Equivalent Tautomers of Adenine Base Using GaN Modified Fullerene (C-60) as a Nanoscale Sensor
Journal of Computational and Theoretical Nanoscience, (12): 2545-2551 2015.

Rauf, S. M. A.; Arvidsson, P. I.; Albericio, F.; Govender, T.; Maguire, G. E. M.; Kruger, H. G.; Honarparvar, B.
The effect of N-methylation of amino acids (Ac-X-OMe) on solubility and conformation: a DFT study
Organic & Biomolecular Chemistry, (13): 9993-10006 2015.

Rawat, P.; Singh, R. N.
Experimental and DFT study on a newly synthesized ethyl 2-cyano-3- 5-(phenyl-hydrazonomethyl)-1H-pyrrol-2-yl - acrylate
Journal of Molecular Structure, (1081): 293-303 2015.

Rawat, P.; Singh, R. N.
Experimental and theoretical study of 4-formyl pyrrole derived aroylhydrazones
Journal of Molecular Structure, (1084): 326-339 2015.

Rawat, P.; Singh, R. N.
Synthesis, conformational, spectroscopic and chemical reactivity analysis of 2-cyano-3-(1H-pyrrol-2-yl)acrylohydrazide using experimental and quantum chemical approaches
Journal of Molecular Structure, (1082): 118-130 2015.

Rawat, P.; Singh, R. N.
Synthesis, spectral and chemical reactivity analysis of 2,4-dinitrophenyl hydrazone having pyrrole moiety
Journal of Molecular Structure, (1097): 214-225 2015.

Ray, A.; Bagani, K.; Banerjee, S.; Bhattacharyya, D.
Oxidative Tearing of Graphene Sheets: Insights into the Probable Situations by Computational and Experimental Studies

Journal of Physical Chemistry C, (119): 951-959 2015.

Ray, A.; Panigrahi, S.; Bhattacharyya, D.
A Comparison of Four Different Conformations Adopted by Human Telomeric G-Quadruplex Using Computer Simulations
Biopolymers, (105): 83-99 2015.

Reddi, Y.; Sunoj, R. B.
Mechanistic Studies on Stereoselective Organocatalytic Direct beta-C-H Activation in an Aliphatic Chain by Chiral N-Heterocyclic Carbenes
Acs Catalysis, (5): 5794-5802 2015.

Reen, G. K.; Dudhe, P.; Ahuja, M.; Kumar, A.; Sharma, P.
Acid-Catalyzed, Silica-Supported, One-Pot Benzoylation Route to Synthesize 2-(Substituted Phenyl)oxazolo 4,5-b pyridines Under Ambient Conditions
Synthetic Communications, (45): 1986-1994 2015.

Reid, D. M.; Collins, M. A.
Calculating nuclear magnetic resonance shieldings using systematic molecular fragmentation by annihilation
Physical Chemistry Chemical Physics, (17): 5314-5320 2015.

Reimers, J. R.; McKemmish, L. K.; McKenzie, R. H.; Hush, N. S.
Bond angle variations in XH3 X = N, P, As, Sb, Bi : the critical role of Rydberg orbitals exposed using a diabatic state model
Physical Chemistry Chemical Physics, (17): 24618-24640 2015.

Reimers, J. R.; McKemmish, L. K.; McKenzie, R. H.; Hush, N. S.
A unified diabatic description for electron transfer reactions, isomerization reactions, proton transfer reactions, and aromaticity
Physical Chemistry Chemical Physics, (17): 24598-24617 2015.

Rekha, T. N.; Umadevi, M.; Rajkumar, B. J. M.
Structural and spectroscopic study of adsorption of anthracene on silver
Molecular Physics, (113): 3673-3682 2015.

Rekha, T. N.; Umadevi, M.; Rajkumar, B. J. M.
Structural and spectroscopic study of adsorption of naphthalene on silver
Journal of Molecular Structure, (1079): 155-162 2015.

Rekik, N.; Flakus, H. T.; Jarczyk-Jedryka, A.; Al-Age, F. A.; Daouahi, M.; Jones, P. G.; Kusz, J.; Nowak, M.
Elucidating the Davydov-coupling mechanism in hydrogen bond dimers: Experimental and theoretical investigation of the polarized IR spectra of 3-thiopheneacetic and 3-thiopheneacrylic acid crystals
Journal of Physics and Chemistry of Solids, (77): 68-84 2015.

Remya, K.; Suresh, C. H.
Intermolecular carbon-carbon, nitrogen-nitrogen and oxygen-oxygen non-covalent bonding in dipolar molecules
Physical Chemistry Chemical Physics, (17): 18380-18392 2015.

Ren, C.; Wang, W. H.; Guo, C.; Li, P.; Liu, Y. X.; Bi, S. W.; Li, Z.; Sun, Q.
Strong chemisorption of CO on M@B-n(-) (M = Co, Ir, Rh, Ru, Ta, Nb, n=8-10) clusters: an implication for wheel boron clusters as CO gas detectors
Rsc Advances, (5): 82524-82530 2015.

Ren, F. D.; Cao, D. L.; Shi, W. J.; You, M.; Li, M.
A theoretical prediction of the possible trigger linkage of CH3NO2 and NH2NO2 in an external electric field
Journal of Molecular Modeling, (21) 2015.

Rezac, J.; de la Lande, A.

Robust, Basis-Set Independent Method for the Evaluation of Charge-Transfer Energy in Noncovalent Complexes
Journal of Chemical Theory and Computation, (11): 528-537 2015.

Rezaeifard, A.; Kavousi, H.; Raissi, H.; Jafarpour, M.
Significant hydrogen-bonding effect on the reactivity of high-valent manganese(V)-oxo porphyrins in C-H bond activation: A DFT study
Journal of Porphyrins and Phthalocyanines, (19): 1197-1203 2015.

Rilak, A.; Puchta, R.; Bugarcic, Z. D.
Mechanism of the reactions of ruthenium(II) polypyridyl complexes with thiourea, sulfur-containing amino acids and nitrogen-containing heterocycles
Polyhedron, (91): 73-83 2015.

Rimola, A.; Ugliengo, P.; Sodupe, M.
Strained ring motif at silica surfaces: A quantum mechanical study of their reactivity towards protic molecules
Computational and Theoretical Chemistry, (1074): 168-177 2015.

Rios-Gutierrez, M.; Domingo, L. R.; Perez, P.
Understanding the high reactivity of carbonyl compounds towards nucleophilic carbenoid intermediates generated from carbene isocyanides
Rsc Advances, (5): 84797-84809 2015.

Rios-Gutierrez, M.; Layeb, H.; Domingo, L. R.
A DFT study of the mechanism of Bronsted acid catalysed Povarov reactions
Tetrahedron, (71): 9339-9345 2015.

Rios-Gutierrez, M.; Perez, P.; Domingo, L. R.
A bonding evolution theory study of the mechanism of 3+2 cycloaddition reactions of nitrones with electron-deficient ethylenes
Rsc Advances, (5): 58464-58477 2015.

Rivera, A.; Uribe, J. M.; Rios-Motta, J.; Osorio, H. J.; Bolte, M.
Evidence for stereoelectronic effects in the N-C-N group of 8,10,12-triaza-1-azoniatetracyclo 8.3.1.1(8,12).0(2,7) pentadecane 4-nitrophenolate 4-nitrophenol monosolvate from the protonation of aminal (2R,7R)-1,8,10,12-tetraazatetracyclo 8.3.1.1(8,12).0(2,7) pentadecane: X-ray and natural bond orbital analysis
Acta Crystallographica Section C-Structural Chemistry, (71): 284-+ 2015.

Robertson, M. J.; Jorgensen, W. L.
Illustrating Concepts in Physical Organic Chemistry with 3D Printed Orbitals
Journal of Chemical Education, (92): 2113-2116 2015.

Robles, N. L.; Chemes, D. M.; Oberhammer, H.; Cutin, E. H.
Structural, conformational and vibrational properties of 1,1,1-Trifluoro-N-(1,1,2,2,2-pentafluoroethyl) methanesulfinimidoyl chloride, CF3CF2-N=S(Cl)CF3
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (145): 139-144 2015.

Rojas-Valencia, N.; Ibarguen, C.; Restrepo, A.
Molecular interactions in the microsolvation of dimethylphosphate
Chemical Physics Letters, (635): 301-305 2015.

Romani, D.; Brandan, S. A.
Structural and spectroscopic studies of two 1,3-benzothiazole tautomers with potential antimicrobial activity in different media. Prediction of their reactivities
Computational and Theoretical Chemistry, (1061): 89-99 2015.

Romani, D.; Marquez, M. J.; Marquez, M. B.; Brandan, S. A.
Structural, topological and vibrational properties of an isothiazole derivatives series with antiviral activities
Journal of Molecular Structure, (1100): 279-289 2015.

Roohi, H.; Abdollahinezhad, N.
Photo-induced proton transfer in fluorene- and carbazole-based compounds as red- and orange-light-emitting molecules: A TD-DFT study
Organic Electronics, (25): 121-130 2015.

Roohi, H.; Ghauri, K.
Exploring physicochemical properties of the nanostructured Tunable Aryl Alkyl Ionic Liquids (TAAILs)
Journal of Molecular Liquids, (209): 14-24 2015.

Roohi, H.; Jahantab, M.
Adsorption sensitivity of nanocrystalline B-substituted H-ZSM-5 and alkali metal-exchanged M-ZSM-5 zeolites towards parent nitrosamine: A B97D study
Computational and Theoretical Chemistry, (1066): 76-87 2015.

Roohi, H.; Jahantab, M.; Delcheh, S. R.; Khoshakhlagh, B. P.
Chemical functionalization of boron nitride nanotube via the 1,3-dipolar cycloaddition reaction of azomethine ylide: a quantum chemical study
Structural Chemistry, (26): 749-759 2015.

Roohi, H.; Jahantab, M.; Yakta, M.
Effect of the Stone-Wales (SW) defect on the response of BNNT to axial tension and compression: a quantum chemical study
Structural Chemistry, (26): 11-22 2015.

Roohi, H.; Khyrkhah, S.
Quantum chemical studies on nanostructures of the hydrated methylimidazolium-based ionic liquids
Journal of Molecular Modeling, (21) 2015.

Rosenberg, R. E.; Kelly, W. J.
Felkin-Anh is not enough
Journal of Physical Organic Chemistry, (28): 47-56 2015.

Rosokha, S. V.; Loboda, E. A.
Interplay of Halogen and pi-pi Charge-Transfer Bondings in Intermolecular Associates of Bromo- or Iododinitrobenzene with Tetramethyl-p-phenylenediamine
Journal of Physical Chemistry A, (119): 3833-3842 2015.

Rosokha, S. V.; Traversa, A.
From charge transfer to electron transfer in halogen-bonded complexes of electrophilic bromocarbons with halide anions
Physical Chemistry Chemical Physics, (17): 4989-4999 2015.

Roth, T.; Vasilenko, V.; Wadepohl, H.; Wright, D. S.; Gade, L. H.
Structures, Electronics, and Reactivity of Strained Phosphazane Cages: A Combined Experimental and Computational Study
Inorganic Chemistry, (54): 7636-7644 2015.

Roy, D. K.; Mondal, B.; Anju, R. S.; Ghosh, S.
Chemistry of Diruthenium and Dirhodium Analogues of Pentaborane(9): Synthesis and Characterization of Metal N,S-Heterocyclic Carbene and B-Agostic Complexes
Chemistry-a European Journal, (21): 3640-3648 2015.

Roy, D. K.; Mondal, B.; De, A.; Panda, S.; Ghosh, S.
Novel Neutral Zirconaborane (Cp2Zr)(2)B5H11 : An arachno-B3H9 Analogue (Cp = eta(5)-C5H5)
Organometallics, (34): 908-912 2015.

Rozada, T. C.; Gauze, G. F.; Rosa, F. A.; Favaro, D. C.; Rittner, R.; Pontes, R. M.; Basso, E. A.

The conformational analysis of 2-halocyclooctanones
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (137): 176-184 2015.

Rumyantsev, M.; Sitnikov, N. S.; Somov, N. V.
Hydrogen-Bond-Assisted Organocatalytic Acetalization of Secondary Alcohols: Experimental and Theoretical Studies
Journal of Physical Chemistry A, (119): 4108-4117 2015.

Rybarczyk-Pirek, A. J.; Lukomska-Rogala, M.; Wojtulewski, S.; Palusiak, M.
N-Oxide as a Proton Accepting Group in Multicomponent Crystals: X-ray and Theoretical Studies on New p-Nitropyridine-N-oxide Co-Crystals
Crystal Growth & Design, (15): 5802-5815 2015.

Saavedra-Torres, M.; Jaque, P.; Tielens, F.; Santos, J. C.
Theoretical study of dibenzyl disulfide adsorption on Cu-7 cluster as a first approximation to sulfur-induced copper corrosion process
Theoretical Chemistry Accounts, (134) 2015.

Sabate, C. M.; Delalu, H.
Synthesis and Characterization of Secondary Nitrosamines from Secondary Amines Using Sodium Nitrite and p-Toluenesulfonic Acid
Chemistry-an Asian Journal, (10): 674-678 2015.

Sabet-Sarvestani, H.; Eshghi, H.; Izadyar, M.; Bakavoli, M.; Noroozi-Shad, N.; Ziaee, F.
Stereoelectronic effects: a powerful concept in explaning kinetic and thermodynamic aspects of retro cheletropic reactions
Journal of Chemical Research: 635-639 2015.

Sadaf, H.; Isab, A. A.; Ahmad, S.; Espinosa, A.; Mas-Montoya, M.; Khan, I. U.; Ejaz; Rehman, S. U.; Ali, M. A. J.; Saleem, M.; Ruiz, J.; Janiak, C.
Synthesis, crystal structure, theoretical calculations and antimicrobial properties of Pt(tetramethylthiourea)(4) Pt(CN)(4) center dot 4H(2)O
Journal of Molecular Structure, (1085): 155-161 2015.

Sadeghian, Z.
Theoretical studies on the structural properties of 2,3-bis(furan-2-yl)pyrazino- 2,3-f 1,10 phenanthroline
Journal of Structural Chemistry, (56): 1295-1298 2015.

Sadeghzade, Z.; Beyramabadi, S. A.; Morsali, A.
A DFT investigation of structure, spectroscopic properties and tautomerism of the anticonvulsant drug Lyrica
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (138): 637-642 2015.

Sadhu, B.; Sundararajan, M.; Bandyopadhyay, T.
Selectivity of a Singly Permeating Ion in Nonselective NaK Channel: Combined QM and MD Based Investigations
Journal of Physical Chemistry B, (119): 12783-12797 2015.

Sadhu, B.; Sundararajan, M.; Bandyopadhyay, T.
Water-Mediated Differential Binding of Strontium and Cesium Cations in Fulvic Acid
Journal of Physical Chemistry B, (119): 10989-10997 2015.

Saeed, A.; Khurshid, A.; Bolte, M.; Fantoni, A. C.; Erben, M. F.
Intra- and intermolecular hydrogen bonding and conformation in 1-acyl thioureas: An experimental and theoretical approach on 1-(2-chlorobenzoyl)thiourea
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (143): 59-66 2015.

Saeed, A.; Perveen, F.; Abbas, N.; Jamal, S.; Florke, U.
Synthesis, Structure and Quantum Mechanical Calculations of Methyl 2-(5-((Quinolin-8-yloxy)-methyl)-1,3,4-oxadiazol-2-ylthio)-acetate
Chinese Journal of Structural Chemistry, (34): 858-870 2015.

Saeed, A.; Qasim, M.; Hussain, M.; Florke, U.; Erben, M. F.
A combined experimental and theoretical study of the tautomeric and conformational properties of (5-phenyl-tetrazol-2-yl)-acetic acid methyl ester
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (150): 1-8 2015.

Saes, B. W. H.; Verhoeven, D. G. A.; Lutz, M.; Gebbink, R.; Moret, M. E.
Coordination of a Diphosphine-Ketone Ligand to Ni(0), Ni(I), and Ni(II): Reduction-Induced Coordination
Organometallics, (34): 2710-2713 2015.

Saftic, D.; Vianello, R.; Zinic, B.
5-Triazolyluracils and Their N-1-Sulfonyl Derivatives: Intriguing Reactivity Differences in the Sulfonation of Triazole N-1-Substituted and N-1-Unsubstituted Uracil Molecules
European Journal of Organic Chemistry: 7695-7704 2015.

Saglam, E. G.; Ebinc, A.; Zeyrek, C. T.; Unver, H.; Hokelek, T.
Structural studies on some dithiophosphonato complexes of Ni(II), Cd(II), Hg(II) and theoretical studies on a dithiophosphonato Ni(II) complex using density functional theory
Journal of Molecular Structure, (1099): 490-501 2015.

Sahra, K.; Dinar, K.; Seridi, A.; Kadri, M.
Investigation on the inclusion of diclofenac with beta-cyclodextrin: a molecular modeling approach
Structural Chemistry, (26): 61-69 2015.

Sahu, C.; Ghosh, D.; Sen, K.; Das, A. K.
Decomposition of O,S-dimethyl methylphosphonothiolate by ammonia on magnesium oxide: a theoretical study of catalytic detoxification of a chemical warfare agent
Physical Chemistry Chemical Physics, (17): 20231-20249 2015.

Saiad, A.; Zouchoune, B.
Electronic structure and bonding analysis of transition metal sandwich and half-sandwich complexes of the triphenylene ligand
Canadian Journal of Chemistry, (93): 1096-1108 2015.

Sainna, M. A.; Singh, D.; Kumar, D.; de Visser, S. P.
A Trimetal Carbene with Reactivity Reminiscent of Fischer-Tropsch Catalysis
Organometallics, (34): 1651-1660 2015.

Sakai, H.; Tokumasu, T.
Quantum chemical analysis of the deprotonation of sulfonic acid in a hydrocarbon membrane model at low hydration levels
Solid State Ionics, (274): 94-99 2015.

Salavati-Fard, T.; Caratzoulas, S.; Doren, D. J.
DFT Study of Solvent Effects in Acid-Catalyzed Diels-Alder Cycloadditions of 2,5-Dimethylfuran and Maleic Anhydride
Journal of Physical Chemistry A, (119): 9834-9843 2015.

Salazar, R.; Vidal, J.; Martinez-Cifuentes, M.; Araya-Maturana, R.; Ramirez-Rodriguez, O.
Electrochemical characterization of hydroquinone derivatives with different substituents in acetonitrile
New Journal of Chemistry, (39): 1237-1246 2015.

Saleem, H.; Subashchandrabose, S.; Babu, N. R.; Padusha, M. S. A.
Vibrational spectroscopy investigation and density functional theory calculations on (E)-N '-(4-methoxybenzylidene) benzohydrazide
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (143): 230-241 2015.

Salvatore, P.; Nazmutdinov, R. R.; Ulstrup, J.; Zhang, J. D.
DNA Bases Assembled on the Au(110)/Electrolyte Interface: A Combined Experimental and Theoretical Study

Journal of Physical Chemistry B, (119): 3123-3134 2015.

Sambathkumar, K.
Vibrational spectra, NBO, HOMO-LUMO and conformational stability studies of 4-hydroxythiobenzamide
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (147): 51-66 2015.

Samimi, H. A.; Esrafili, M. D.; Mohammadian-Sabet, F.; Haddadi, H.
Theoretical study on cooperative interplay between anion-pi and chalcogen-bonding interactions
Molecular Physics, (113): 1442-1450 2015.

Samuilov, A. Y.; Balabanova, F. B.; Samuilov, Y. D.
Computational study of the reaction of dimethyl carbonate with methyl amine on Zn4O4 cluster
Computational and Theoretical Chemistry, (1067): 33-39 2015.

Sanchez-Eguia, B. N.; Flores-Alamo, M.; Orio, M.; Castillo, I.
Side-on cupric-superoxo triplet complexes as competent agents for H-abstraction relevant to the active site of PHM
Chemical Communications, (51): 11134-11137 2015.

Sanchez-Marquez, J.
Reactivity indices for natural bond orbitals: a new methodology
Journal of Molecular Modeling, (21) 2015.

Sanchez-Sanz, G.
Aromatic behaviour of benzene and naphthalene upon pnictogen substitution
Tetrahedron, (71): 826-839 2015.

Sanchez-Sanz, G.; Trujillo, C.; Alkorta, I.; Elguero, J.
Theoretical study of cyanophosphines: Pnicogen vs. dipole-dipole interactions
Computational and Theoretical Chemistry, (1053): 305-314 2015.

Sancho, M. I.; Russo, M. G.; Moreno, M. S.; Gasull, E.; Blanco, S. E.; Narda, G. E.
Physicochemical Characterization of 2-Hydroxybenzophenone with beta-Cyclodextrin in Solution and Solid State
Journal of Physical Chemistry B, (119): 5918-5925 2015.

Sangilipandi, S.; Nagarajaprakash, R.; Sutradhar, D.; Kaminsky, W.; Chandra, A. K.; Rao, K. M.
Synthesis, molecular structural studies and DFT calculations of tricarbonylrhenium(I) metal complexes containing nitrogen based N boolean AND N donor polypyridyl ligands
Inorganica Chimica Acta, (437): 177-187 2015.

Santiago-Rodriguez, Y.; Curest-Arana, M. C.
Quantum mechanical study of the reaction of CO2 and ethylene oxide catalyzed by metal-salen complexes: effect of the metal center and the axial ligand
Reaction Kinetics Mechanisms and Catalysis, (116): 351-370 2015.

Santolini, V.; Malhado, J. P.; Robb, M. A.; Garavelli, M.; Bearpark, M. J.
Photochemical reaction paths of cis-dienes studied with RASSCF: the changing balance between ionic and covalent excited states
Molecular Physics, (113): 1978-1990 2015.

Santra, P. K.; Palmstrom, A. F.; Tanskanen, J. T.; Yang, N.; Bent, S. F.
Improving Performance in Colloidal Quantum Dot Solar Cells by Tuning Band Alignment through Surface Dipole Moments
Journal of Physical Chemistry C, (119): 2996-3005 2015.

Saravanan, S.; Balachandran, V.
Conformational stability, spectroscopic (FT-IR, FT-Raman and UV-Vis) analysis, NLO, NBO, FMO and Fukui function analysis of 4-hexylacetophenone by density functional theory
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (138): 406-423 2015.

Sargolzaei, M.; Afshar, M.
The Effect of Solvent on Tautomerization of 4-bromo Substituted 1H-Pyrazoles: Density Functional Theory Study
Letters in Organic Chemistry, (12): 344-351 2015.

Sarish, S. P.; Samuel, P. P.; Roesky, H. W.; Schulzke, C.; Nijesh, K.; De, S.; Parameswaran, P.
Multiple Cycloaddition Reactions of Ketones with a beta-Diketiminate Al Compound
Chemistry-a European Journal, (21): 19041-19047 2015.

Sarkar, S.; Pavan, M. S.; Row, T. N. G.
Experimental validation of 'pnicogen bonding' in nitrogen by charge density analysis
Physical Chemistry Chemical Physics, (17): 2330-2334 2015.

Sas, E. B.; Kose, E.; Kurt, M.; Karabacak, M.
FT-IR, FT-Raman, NMR and UV-Vis spectra and DFT calculations of 5-bromo-2-ethoxyphenylboronic acid (monomer and dimer structures)
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (137): 1315-1333 2015.

Sas, E. B.; Kurt, M.; Karabacak, M.; Poiyamozhi, A.; Sundaraganesan, N.
FT-IR, FT-Raman, dispersive Raman, NMR spectroscopic studies and NBO analysis of 2-Bromo-1H-Benzimidazol by density functional method
Journal of Molecular Structure, (1081): 506-518 2015.

Sasaki, S.; Hattori, K.; Igawa, K.; Konishi, G.
Directional Control of pi-Conjugation Enabled by Distortion of the Donor Plane in Diarylaminoanthracenes: A Photophysical Study
Journal of Physical Chemistry A, (119): 4898-4906 2015.

Sasikala, V.; Sajan, D.; Sabu, K. J.; Arumanayagam, T.; Murugakoothan, P.
Electronic structure, vibrational spectral and intervening orbital interactions studies of NLO material: Guanidinium 4-nitrobenzoate
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (139): 555-572 2015.

Savithiri, S.; Doss, M. A.; Rajarajana, G.; Thanikachalam, V.; Bharanidharan, S.; Saleem, H.
Spectroscopic (FT-IR, FT-Raman) and quantum mechanical studies of 3t-pentyl-2r,6c-diphenylpiperidin-4-one thiosemicarbazone
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (136): 782-792 2015.

Saxena, A.; Agrawal, M.; Gupta, A.
Vibrational study, molecular properties and first-order molecular hyperpolarizability of Methyl 2-amino 5-bromobenzoate using DFT method
Optical Materials, (46): 154-167 2015.

Sayin, K.; Karaka, D.; Karakus, N.; Sayin, T. A.; Zaim, Z.; Kariper, S. E.
Spectroscopic investigation, FMOs and NLO analyses of Zn(II) and Ni(II) phenanthroline complexes: A DFT approach
Polyhedron, (90): 139-146 2015.

Scarbath-Evers, L. K.; Hunt, P. A.; Kirchner, B.; MacFarlane, D. R.; Zahn, S.
Molecular features contributing to the lower viscosity of phosphonium ionic liquids compared to their ammonium analogues
Physical Chemistry Chemical Physics, (17): 20205-20216 2015.

Scarpi, D.; Begliomini, S.; Prandi, C.; Oppedisano, A.; Deagostino, A.; Gomez-Bengoa, E.; Fiser, B.; Occhiato, E. G.
Gold-Catalysed Synthesis of Exocyclic Vinylogous Amides and -Amino Ketones: A Detailed Study on the 5-exo/6-endo-dig Selectivity, Methodology and Scope
European Journal of Organic Chemistry: 3251-3265 2015.

Schamnad, S.; Chakraborty, S.

Substituent effect in O-H center dot center dot center dot Se hydrogen bond-Density Functional Theory study of para-substituted phenol-SeH2 complexes
Chemical Physics Letters, (622): 28-33 2015.

Scheiner, S.
Comparison of CH center dot center dot center dot O, SH center dot center dot center dot O, Chalcogen, and Tetrel Bonds Formed by Neutral and Cationic Sulfur-Containing Compounds
Journal of Physical Chemistry A, (119): 9189-9199 2015.

Scheiner, S.
Dissection of the Factors Affecting Formation of a CH center dot center dot center dot O H-Bond. A Case Study
Crystals, (5): 327-345 2015.

Scheiner, S.
The Interplay between Charge Transfer, Rehybridization, and Atomic Charges in the Internal Geometry of Subunits in Noncovalent Interactions
International Journal of Quantum Chemistry, (115): 28-33 2015.

Schmidt, M. W.; Hull, E. A.; Windus, T. L.
Valence Virtual Orbitals: An Unambiguous ab Initio Quantification of the LUMO Concept
Journal of Physical Chemistry A, (119): 10408-10427 2015.

Schroder, S. D.; Wallberg, J. H.; Kroll, J. A.; Maroun, Z.; Vaida, V.; Kjaergaard, H. G.
Intramolecular Hydrogen Bonding in Methyl Lactate
Journal of Physical Chemistry A, (119): 9692-9702 2015.

Schulz, A.; Villinger, A.
Binary Polyazides of Cadmium and Mercury
Chemistry-a European Journal, (21): 3649-3663 2015.

Schutz, M.; Sakota, K.; Moritz, R.; Schmies, M.; Ikeda, T.; Sekiya, H.; Dopfer, O.
Simultaneous Interaction of Hydrophilic and Hydrophobic Solvents with Ethylamino Neurotransmitter Radical Cations: Infrared Spectra of Tryptamine(+)-(H2O)(m)-(N-2)(n), Clusters (m,n <= 3)
Journal of Physical Chemistry A, (119): 10035-10051 2015.

Sebastian, S.; Al-Tamimi, A. M. S.; El-Brollosy, N. R.; El-Emam, A. A.; Panicker, C. Y.; Van Alsenoy, C.
Vibrational spectroscopic (FT-IR and FT-Raman) studies, HOMO-LUMO, NBO analysis and MEP of 6-methyl-1-{{ (2E)-2-methyl-3-phenyl-prop-2-en-l-yl oxy}methyl)-1,2,3,4- tetra-hydroquinazoline-2,4-dione, a potential chemotherapeutic agent, using density functional methods
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (134): 316-325 2015.

Sebastian, S.; Sylvestre, S.; Jayabharathi, J.; Ayyapan, S.; Amalanathan, M.; Oudayakumar, K.; Herman, I. A.
Study on conformational stability, molecular structure, vibrational spectra, NBO, TD-DFT, HOMO and LUMO analysis of 3,5-dinitrosalicylic acid by DFT techniques
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (136): 1107-1118 2015.

Seeburrun, N.; Alswaidan, I. A.; Fun, H. K.; Archibong, E. F.; Ramasami, P.
A comparative ab initio study to investigate the rich structural variety and electronic properties of GamTen (m=1, 2 and n=1-4) with analogous oxides, sulfides and selenides
Rsc Advances, (5): 68076-68084 2015.

Seeburrun, N.; Alswaidan, I. A.; Fun, H. K.; Archibong, E. F.; Ramasami, P.
Probing the structural and electronic properties of doped gallium oxide and sulfide, M(GaX2)(2) where M = alkali or coinage metal; X = O, S
Rsc Advances, (5): 106141-106150 2015.

Seeburrun, N.; Archibong, E. F.; Ramasami, P.
Mono and digallium selenide clusters as potential superhalogens

Journal of Molecular Modeling, (21) 2015.

Seidler, T.; Champagne, B.
Which charge definition for describing the crystal polarizing field and the chi((1)) and chi((2)) of organic crystals?
Physical Chemistry Chemical Physics, (17): 19546-19556 2015.

Seipp, C. A.; Williams, N. J.; Bryantsev, V. S.; Custelcean, R.; Moyer, B. A.
A conformationally persistent pseudo-bicyclic guanidinium for anion coordination as stabilized by dual intramolecular hydrogen bonds
Rsc Advances, (5): 107266-107269 2015.

Sekhar, M. C.; Sankar, M. G.; Venkatesulu, A.
Thermodynamic and theoretical study on hydrogen bonded binary mixtures of isomeric butanols with o-toluidine at T = (303.15 to 318.15) K
Journal of Molecular Liquids, (209): 428-439 2015.

Selikhov, A. N.; Cherkasov, A. V.; Fukin, G. K.; Trifonov, A. A.; del Rosal, I.; Maron, L.
Amido Analogues of Nonbent Lanthanide (II) and Calcium Metallocenes. Heterolytic Cleavage of pi-Bond Ln-Carbazolyl Ligand Promoted by Lewis Base Coordination
Organometallics, (34): 555-562 2015.

Semenov, N. A.; Lonchakov, A. V.; Gritsan, N. P.; Zibarev, A. V.
Donor-acceptor coordination of anions by chalcogen atoms of 1,2,5-chalcogenadiazoles
Russian Chemical Bulletin, (64): 499-510 2015.

Semenov, S. G.; Makarova, M. V.
Quantum chemical study Ca@C-60 and Sc+@C-60 endo complexes in the gas phase and pyridine
Russian Journal of General Chemistry, (85): 889-893 2015.

Semenov, S. G.; Shakhova, V. M.; Makarova, M. V.
Quantum chemical study of structure of ionic complexes of I and II groups metals with xenon or krypton
Russian Journal of General Chemistry, (85): 790-795 2015.

Semenov, V. A.; Samultsev, D. O.; Krivdin, L. B.
Theoretical and experimental study of N-15 NMR protonation shifts
Magnetic Resonance in Chemistry, (53): 433-441 2015.

Sengupta, T.; Das, S.; Pal, S.
Oxidative addition of the C-I bond on aluminum nanoclusters
Nanoscale, (7): 12109-12125 2015.

Seth, S. K.; Lee, V. S.; Yana, J.; Zain, S. M.; Cunha, A. C.; Ferreira, V. F.; Jordao, A. K.; de Souza, M.; Wardell, S.; Wardell, J. L.; Tiekink, E. R. T.
Crystallographic and computational study of 1-(arylamino)-1,2,3-triazole-4-carbohydrazides
Crystengcomm, (17): 2255-2266 2015.

Sethi, A.; Prakash, R.
Novel synthetic ester of Brassicasterol, DFT investigation including NBO, NLO response, reactivity descriptor and its intramolecular interactions analyzed by AIM theory
Journal of Molecular Structure, (1083): 72-81 2015.

Setiawan, D.; Kraka, E.; Cremer, D.
Hidden Bond Anomalies: The Peculiar Case of the Fluorinated Amine Chalcogenides
Journal of Physical Chemistry A, (119): 9541-9556 2015.

Setiawan, D.; Kraka, E.; Cremer, D.
Strength of the Pnicogen Bond in Complexes Involving Group Va Elements N, P, and As
Journal of Physical Chemistry A, (119): 1642-1656 2015.

Seyedhosseini, B.; Izadyar, M.; Housaindokht, M. R.
Thermal decomposition mechanisms of the ionic liquids based on alpha-amino acid anion and N-7,N-9-dimethyladeninium cation: Quantum chemistry approach
Journal of Molecular Liquids, (209): 779-784 2015.

Shahabi, M.; Raissi, H.; Mollania, F.
Electronic structures, intramolecular hydrogen bond interaction, and aromaticity of substituted 4-amino-3-penten-2-one in ground and electronic excited state
Structural Chemistry, (26): 491-506 2015.

Shahangi, F.; Chermahini, A. N.; Farrokhpour, H.; Teimouri, A.
Selective complexation of alkaline earth metal ions with nanotubular cyclopeptides: DFT theoretical study
Rsc Advances, (5): 2305-2317 2015.

Shahi, A.; Arunan, E.
Microwave spectroscopic and theoretical investigations of the strongly hydrogen bonded hexafluoroisopropanol...water complex
Physical Chemistry Chemical Physics, (17): 24774-24782 2015.

Shahi, A.; Arunan, E.
Microwave Spectrum of Hexafluoroisopropanol and Torsional Behavior of Molecules with a CF3-C-CF3 Group
Journal of Physical Chemistry A, (119): 5650-5657 2015.

Shakhova, V. M.; Semenov, S. G.; Titov, A. V.
Quantum Chemical Study of Pentafluorophenylxenonium Pentafluorobenzoate in the Gas Phase and Acetonitrile Solution
Russian Journal of General Chemistry, (85): 2816-2817 2015.

Shakhova, V. M.; Semenov, S. G.; Titov, A. V.
Quantum-chemical estimation of the relaxation of equilibrium structure upon radiochemical reactions of iodine-containing molecules and ions
Russian Journal of General Chemistry, (85): 2262-2267 2015.

Shakourian-Fard, M.; Kamath, G.; Sankaranarayanan, S.
Electronic Structure Insights into the Solvation of Magnesium Ions with Cyclic and Acyclic Carbonates
Chemphyschem, (16): 3607-3617 2015.

Shakourian-Fard, M.; Kamath, G.; Smith, K.; Xiong, H.; Sankaranarayanan, S.
Trends in Na-Ion Solvation with Alkyl-Carbonate Electrolytes for Sodium-Ion Batteries: Insights from First-Principles Calculations
Journal of Physical Chemistry C, (119): 22747-22759 2015.

Shankar, R.; Radhika, R.; Thangamani, D.; Kumar, L. S.; Kolandaivel, P.
Theoretical studies on interaction of anticancer drugs (dacarbazine, procarbazine and triethylenemelamine) with normal (AT and GC) and mismatch (GG, CC, AA and TT) base pairs
Molecular Simulation, (41): 633-652 2015.

Shao, Y. H.; Gan, Z. T.; Epifanovsky, E.; Gilbert, A. T. B.; Wormit, M.; Kussmann, J.; Lange, A. W.; Behn, A.; Deng, J.; Feng, X. T.; Ghosh, D.; Goldey, M.; Horn, P. R.; Jacobson, L. D.; Kaliman, I.; Khaliullin, R. Z.; Kus, T.; Landau, A.; Liu, J.; Proynov, E. I.; Rhee, Y. M.; Richard, R. M.; Rohrdanz, M. A.; Steele, R. P.; Sundstrom, E. J.; Woodcock, H. L.; Zimmerman, P. M.; Zuev, D.; Albrecht, B.; Alguire, E.; Austin, B.; Beran, G. J. O.; Bernard, Y. A.; Berquist, E.; Brandhorst, K.; Bravaya, K. B.; Brown, S. T.; Casanova, D.; Chang, C. M.; Chen, Y. Q.; Chien, S. H.; Closser, K. D.; Crittenden, D. L.; Diedenhofen, M.; DiStasio, R. A.; Do, H.; Dutoi, A. D.; Edgar, R. G.; Fatehi, S.; Fusti-Molnar, L.; Ghysels, A.; Golubeva-Zadorozhnaya, A.; Gomes, J.; Hanson-Heine, M. W. D.; Harbach, P. H. P.; Hauser, A. W.; Hohenstein, E. G.; Holden, Z. C.; Jagau, T. C.; Ji, H. J.; Kaduk, B.; Khistyaev, K.; Kim, J.; Kim, J.; King, R. A.; Klunzinger, P.; Kosenkov, D.; Kowalczyk, T.; Krauter, C. M.; Lao, K. U.; Laurent, A. D.; Lawler, K. V.; Levchenko, S. V.; Lin, C. Y.; Liu, F.; Livshits, E.; Lochan, R. C.; Luenser, A.; Manohar, P.; Manzer, S. F.; Mao, S. P.; Mardirossian, N.; Marenich, A. V.; Maurer, S. A.; Mayhall, N. J.; Neuscamman, E.; Oana, C. M.; Olivares-Amaya, R.; O'Neill, D. P.; Parkhill, J. A.; Perrine, T. M.; Peverati, R.;

Prociuk, A.; Rehn, D. R.; Rosta, E.; Russ, N. J.; Sharada, S. M.; Sharma, S.; Small, D. W.; Sodt, A.; Stein, T.; Stuck, D.; Su, Y. C.; Thom, A. J. W.; Tsuchimochi, T.; Vanovschi, V.; Vogt, L.; Vydrov, O.; Wang, T.; Watson, M. A.; Wenzel, J.; White, A.; Williams, C. F.; Yang, J.; Yeganeh, S.; Yost, S. R.; You, Z. Q.; Zhang, I. Y.; Zhang, X.; Zhao, Y.; Brooks, B. R.; Chan, G. K. L.; Chipman, D. M.; Cramer, C. J.; Goddard, W. A.; Gordon, M. S.; Hehre, W. J.; Klamt, A.; Schaefer, H. F.; Schmidt, M. W.; Sherrill, C. D.; Truhlar, D. G.; Warshel, A.; Xu, X.; Aspuru-Guzik, A.; Baer, R.; Bell, A. T.; Besley, N. A.; Chai, J. D.; Dreuw, A.; Dunietz, B. D.; Furlani, T. R.; Gwaltney, S. R.; Hsu, C. P.; Jung, Y. S.; Kong, J.; Lambrecht, D. S.; Liang, W. Z.; Ochsenfeld, C.; Rassolov, V. A.; Slipchenko, L. V.; Subotnik, J. E.; Van Voorhis, T.; Herbert, J. M.; Krylov, A. I.; Gill, P. M. W.; Head-Gordon, M.
Advances in molecular quantum chemistry contained in the Q-Chem 4 program package
Molecular Physics, (113): 184-215 2015.

Sharma, P.; Ahuja, M.; Kumar, A.; Sahu, V.
Contribution of reactivity indexes in the formation of beta-lactams through 2+2 cycloaddition between substituted ketenes and imines
Chemical Physics Letters, (628): 85-90 2015.

Sharmila, D.; Mondal, B.; Ramalakshmi, R.; Kundu, S.; Varghese, B.; Ghosh, S.
First-Row Transition-Metal-Diborane and -Borylene Complexes
Chemistry-a European Journal, (21): 5074-5083 2015.

Sheela, G. E.; Manimaran, D.; Joe, I. H.; Rahim, S.; Jothy, V. B.
Structure and nonlinear optical property analysis of L-Methioninium Oxalate: A DFT approach
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (143): 40-48 2015.

Shehab, O. R.; Mansour, A. M.
Sparfloxacin charge transfer complexes with 2,3-dichloro-5,6-dicyano-1,4-benzoquinone and tetracyanoquinodimethane: Molecular structures, spectral, and DFT studies
Journal of Molecular Structure, (1093): 186-194 2015.

Shen, D.; Kong, C. P.; Jia, R.; Fu, P.; Zhang, H. X.
Investigation of Properties of Mg-n Clusters and Their Hydrogen Storage Mechanism: A Study Based on DFT and a Global Minimum Optimization Method
Journal of Physical Chemistry A, (119): 3636-3643 2015.

Shevchenko, I. V.; Turcheniuk, K. V.; Kirilchuk, A. A.; Leszczynski, J.; Rozhenko, A. B.
On the Reaction of Diaminocarbenes with Aroylimines
Journal of Organic Chemistry, (80): 1387-1394 2015.

Shi, Y.; Suguri, T.; Kojima, S.; Yamamoto, Y.
7-6-7 Ring-based transition-metal catalysts for the transfer dehydrogenation of isopropanol
Journal of Organometallic Chemistry, (799-800): 7-12 2015.

Shi, Y. X.; Liang, R. Z.; Martin, K. A.; Weston, N.; Gonzalez-Calera, S.; Ganguly, R.; Li, Y. X.; Lu, Y. P.; Ribeiro, A. J. M.; Ramos, M. J.; Fernandes, P. A.; Garcia, F.
Synthesis and Hydrolytic Studies on the Air-Stable (4-CN-PhO)(E)P(mu-(NBu)-Bu-t) (2) (E = O, S, and Se) Cyclodiphosphazanes
Inorganic Chemistry, (54): 6423-6432 2015.

Shih, T. W.; Li, M. C.; Su, M. D.
Doubly Bonded E-13=P and B=E-15 Molecules and Their Reactions with H-2, Acetonitrile, Benzophenone, and 2,3-Dimethylbutadiene
Inorganic Chemistry, (54): 5154-5161 2015.

Shiroudi, A.; Deleuze, M. S.
Reaction mechanisms and kinetics of the isomerization processes of naphthalene peroxy radicals
Computational and Theoretical Chemistry, (1074): 26-35 2015.

Shiroudi, A.; Deleuze, M. S.; Canneaux, S.

Theoretical study of the oxidation mechanisms of naphthalene initiated by hydroxyl radicals: the O-2 addition reaction pathways
Physical Chemistry Chemical Physics, (17): 13719-13732 2015.

Shoji, Y.; Tanaka, N.; Hashizume, D.; Fukushima, T.
The molecular and electronic structures of a thioaroyl cation formed by borinium ion-mediated C=S double bond cleavage of CS2
Chemical Communications, (51): 13342-13345 2015.

Shugurov, S. M.; Panin, A. I.; Lopatin, S. I.; Emelyanova, K. A.
Formation and thermodynamics of gaseous germanium and tin vanadates: a mass spectrometric and quantum chemical study
Dalton Transactions, (44): 10014-10021 2015.

Shukla, R.; Chopra, D.
Exploring the Role of Substitution on the Formation of Se center dot center dot center dot O/N Noncovalent Bonds
Journal of Physical Chemistry B, (119): 14857-14870 2015.

Siadati, S. A.
Effect of steric congestion on the stepwise character and synchronicity of a 1,3-dipolar reaction of a nitrile ylide and an olefin
Journal of Chemical Research: 640-644 2015.

Siadati, S. A.
An example of a stepwise mechanism for the catalyst-free 1,3-dipolar cycloaddition between a nitrile oxide and an electron rich alkene
Tetrahedron Letters, (56): 4857-4863 2015.

Siadati, S. A.; Alinezhad, M.
A theoretical study on the functionalisation process of C18NB fullerene through its open 5,5 cycloaddition with 4-pyridine nitrile oxide
Progress in Reaction Kinetics and Mechanism, (40): 169-176 2015.

Siadati, S. A.; Mirabi, A.
Diels-Alder versus 1,3-dipolar cycloaddition pathways in the reaction of C-20 fullerene and 2-furan nitrile oxide
Progress in Reaction Kinetics and Mechanism, (40): 383-390 2015.

Siddiqui, S. A.; Rasheed, T.; Bouarissa, N.; Al-hajry, A.
Possible use of BN-modified fullerene as a nano-biosensor to detect adenine-thymine Watson-Crick base pair in mutagenic tautomeric form: Theoretical approach
Journal of Theoretical & Computational Chemistry, (14) 2015.

Sidir, Y. G.; Sidir, I.; Demiray, F.
Structural and electronic properties of heptachlor
Journal of Structural Chemistry, (56): 1275-1289 2015.

Sidorkin, V. F.; Belogolova, E. F.; Doronina, E. P.
Assignment of photoelectron spectra of silatranes: first ionization energies and the nature of the dative Si <- N contact
Physical Chemistry Chemical Physics, (17): 26225-26237 2015.

Signorelli, S.; Dans, P. D.; Coitino, E. L.; Borsani, O.; Monza, J.
Connecting Proline and gamma-Aminobutyric Acid in Stressed Plants through Non-Enzymatic Reactions
Plos One, (10) 2015.

Sikdar, Y.; Modak, R.; Bose, D.; Banerjee, S.; Bienko, D.; Zierkiewicz, W.; Bienko, A.; Das Saha, K.; Goswami, S.
Doubly chloro bridged dimeric copper(II) complex: magneto-structural correlation and anticancer activity
Dalton Transactions, (44): 8876-8888 2015.

Simon, L.; Paton, R. S.
Origins of Asymmetric Phosphazene Organocatalysis: Computations Reveal a Common Mechanism for Nitro- and Phospho-Aldol Additions
Journal of Organic Chemistry, (80): 2756-2766 2015.

Singh, R. K.; Singh, A. K.
Synthesis, molecular structure, spectral analysis, natural bond order and intramolecular interactions of 2-acetylpyridine thiosemicarbazone: A combined DFT and AIM approach
Journal of Molecular Structure, (1094): 61-72 2015.

Singh, R. N.; Rawat, P.; Kumar, A.; Kant, P.; Srivastava, A.
Spectral Analysis, Chemical Reactivity and First Hyperpolarizability Evaluation of a Novel 1,9-bis(2-Cyano-2-Ethoxycarbonylvinyl)-5-(2-Furyl)-Dipyrromethane: Experimental and Theoretical Approaches
Spectroscopy Letters, (48): 235-250 2015.

Singh, R. N.; Rawat, P.; Sahu, S.
Vibrational spectra, electronic absorption, nonlinear optical properties, evaluation of bonding, chemical reactivity and thermodynamic properties of ethyl 4-(1-(2-(hydrazinecarbonothioyl)hydrazono)ethyl)-3,5-dimethyl-1H-pyrrole -2-carboxylate molecule by ab initio HF and density functional methods
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (135): 1162-1168 2015.

Singh, V. P.; Poon, J. F.; Butcher, R. J.; Lu, X.; Mestres, G.; Ott, M. K.; Engman, L.
Effect of a Bromo Substituent on the Glutathione Peroxidase Activity of a Pyridoxine-like Diselenide
Journal of Organic Chemistry, (80): 7385-7395 2015.

Sirijaraensre, J.; Limtrakul, J.
Modification of the catalytic properties of the Au-4 nanocluster for the conversion of methane-to-methanol: synergistic effects of metallic adatoms and a defective graphene support
Physical Chemistry Chemical Physics, (17): 9706-9715 2015.

Siskos, M. G.; Tzakos, A. G.; Gerothanassis, I. P.
Accurate ab initio calculations of O-H center dot center dot center dot O and O-H center dot center dot center dot O-proton chemical shifts: towards elucidation of the nature of the hydrogen bond and prediction of hydrogen bond distances
Organic & Biomolecular Chemistry, (13): 8852-8868 2015.

Skelton, A. A.; Agrawal, N.; Fried, J. R.
Quantum mechanical calculations of the interactions between diazacrowns and the sodium cation: an insight into Na+ complexation in diazacrown-based synthetic ion channels
Rsc Advances, (5): 55033-55047 2015.

Skelton, J. M.; Crespo-Otero, R.; Hatcher, L. E.; Parker, S. C.; Raithby, P. R.; Walsh, A.
Energetics, thermal isomerisation and photochemistry of the linkage-isomer system Ni(Et(4)dien)(eta(2)-O,ON)(eta(1)-NO2)
Crystengcomm, (17): 383-394 2015.

Smiles, D. E.; Wu, G.; Kaltsoyannis, N.; Hayton, T. W.
Thorium-ligand multiple bonds via reductive deprotection of a trityl group
Chemical Science, (6): 3891-3899 2015.

Smit, B. M.; Pavlovic, R. Z.; Milenkovic, D. A.; Markovic, Z. S.
Mechanism, kinetics and selectivity of selenocyclization of 5-alkenylhydantoins: an experimental and computational study
Beilstein Journal of Organic Chemistry, (11): 1865-1875 2015.

Smith, J. M.; Rowley, C. N.
Automated computational screening of the thiol reactivity of substituted alkenes
Journal of Computer-Aided Molecular Design, (29): 725-735 2015.

Solans-Monfort, X.; Coperet, C.; Eisenstein, O.
Metallacyclobutanes from Schrock-Type d(0) Metal Alkylidene Catalysts: Structural Preferences and Consequences in Alkene Metathesis
Organometallics, (34): 1668-1680 2015.

Sole, D.; Mariani, F.; Fernandez, I.
A Joint Experimental-Computational Comparative Study of the Pd-0-Catalysed Reactions of Aryl Iodides and Aldehydes with N, O, and S Tethers
European Journal of Organic Chemistry: 3935-3942 2015.

Soliman, S. M.; Abu-Youssef, M. A. M.; Albering, J.; El-Faham, A.
Molecular structure and DFT investigations on new cobalt(II) chloride complex with superbase guanidine type ligand
Journal of Chemical Sciences, (127): 2137-2149 2015.

Soliman, S. M.; Abu-Youssef, M. A. M.; Kassem, T. S.; Assem, R.
Synthesis of two new silver(I) complexes with 3-bromoquinoline: Molecular structure, spectroscopic characterizations and DFT studies
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (149): 352-362 2015.

Soliman, S. M.; Assem, R.; Abu-Youssef, M. A. M.; Kassem, T. S.
Synthesis, characterization and DFT studies of two new silver(I) complexes with 3,4-lutidine
Journal of Molecular Structure, (1085): 126-136 2015.

Soliman, S. M.; Hagar, M.; Ibid, F.; El Ashry, E. H.
Experimental and theoretical spectroscopic studies, HOMO-LUMO, NBO analyses and thione-thiol tautomerism of a new hybrid of 1,3,4-oxadiazole-thione with quinazolin-4-one
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (145): 270-279 2015.

Song, X. H.; Zhang, C. Y.
Density Functional Study on the Geometries and Magnetic Properties of Bimetallic Clusters: AunM- (1 <= n <= 8; M = In, Tl)
Chinese Journal of Structural Chemistry, (34): 1633-1640 2015.

Song, X. H.; Zhang, C. Y.; Zhang, L.; Zhang, J.; Wang, B. Q.
Density-functional investigation of gold cluster anions doped with gallium: Au (n) Ga- (1 a (c) 1/2 n a (c) 1/2 8)
Russian Journal of Physical Chemistry A, (89): 1853-1862 2015.

Sorella, S.; Devaux, N.; Dagrada, M.; Mazzola, G.; Casula, M.
Geminal embedding scheme for optimal atomic basis set construction in correlated calculations
Journal of Chemical Physics, (143) 2015.

Soto, C. A. T.; Costa, A. C.; Versiane, O.; Lemma, T.; Machado, N. C. F.; Mondragon, M. A.; Martin, A. A.
Surface enhanced Raman scattering, natural bond orbitals and Mulliken atomic charge distribution in the normal modes of diethyldithiocarbamate cadmium (II) complex, Cd(DDTC)(2)
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (146): 192-203 2015.

Spinney, H. A.; Clough, C. R.; Cummins, C. C.
The titanium tris-anilide cation Ti(N Bu-t Ar)(3) (+) stabilized as its perfluoro-tetra-phenylborate salt: structural characterization and synthesis in connection with redox activity of 4,4 '-bipyridine dititanium complexes
Dalton Transactions, (44): 6784-6796 2015.

Sproviero, E. M.
Opsin Effect on the Electronic Structure of the Retinylidene Chromophore in Rhodopsin
Journal of Chemical Theory and Computation, (11): 1206-1219 2015.

Sriana, T.; Leggesse, E. G.; Jiang, J. C.
Novel benzimidazole salts for lithium ion battery electrolytes: effects of substituents

Physical Chemistry Chemical Physics, (17): 16462-16468 2015.

Srinivasaraghavan, R.; Thamaraikannan, S.; Seshadri, S.; Gnanasambandan, T.
Molecular conformational stability and Spectroscopic analysis of Parared with experimental techniques and quantum chemical calculations
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (137): 1194-1205 2015.

Srivastava, A.; Mishra, R.; Kumar, S.; Dev, K.; Tandon, P.; Maurya, R.
Molecular structure, spectral investigation (H-1 NMR, C-13 NMR, UV-Visible, FT-IR, FT-Raman), NBO, intramolecular hydrogen bonding, chemical reactivity and first hyperpolarizability analysis of formononetin 7-hydroxy-3(4-methoxyphenyl)chromone : A quantum chemical study
Journal of Molecular Structure, (1084): 55-73 2015.

Srivastava, A. K.; Misra, N.
Ab initio investigations on lithium-superhalogen (Li-X) complexes (X = LiF2, BeF3, BF4 and PF6): competition between s-block and p-block anions
Molecular Physics, (113): 866-870 2015.

Srivastava, A. K.; Misra, N.
Can Li2F2 cluster be formed by LiF2/Li2F-Li/F interactions? An ab initio investigation
Molecular Simulation, (41): 1278-1282 2015.

Srivastava, A. K.; Misra, N.
Fluorinated ferromagnetic metal clusters and their superhalogen behaviour
Molecular Physics, (113): 36-44 2015.

Srivastava, A. K.; Misra, N.
Gold oxyfluorides, Au(OF)(n) (n=1-6): novel superhalogens with oxyfluoride ligands
New Journal of Chemistry, (39): 9543-9549 2015.

Srivastava, A. K.; Misra, N.
Structures, stability, and electronic properties of novel superalkali-halogen clusters
Journal of Molecular Modeling, (21) 2015.

Srivastava, A. K.; Misra, N.
Superhalogen properties of CoOn (n >= 3) species revealed by density functional theory
Theoretical Chemistry Accounts, (134) 2015.

Srivastava, A. K.; Pandey, A. K.; Misra, N.
Quantum chemical investigation on structures and energetics of Tungsten Fluoride (WFnq) species (q=0, +/- 1; n < 6)
Journal of Chemical Sciences, (127): 1853-1858 2015.

Srivastava, A. K.; Pandey, S. K.; Misra, N.
Superhalogen properties of ReFn (n >= 6) species
Chemical Physics Letters, (624): 15-18 2015.

Srivastava, R.; Sinha, L.; Karabacak, M.; Prasad, O.; Pathak, S. K.; Asiri, A. M.; Cinar, M.
Spectral features, electric properties, NBO analysis and reactivity descriptors of 2-(2-Benzothiazolylthio)-Ethanol: Combined experimental and DFT studies
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (136): 1205-1215 2015.

Stadelmann, B.; Bender, J.; Forster, D.; Frey, W.; Nieger, M.; Gudat, D.
An anionic phosphenium complex as an ambident nucleophile
Dalton Transactions, (44): 6023-6031 2015.

Stasyuk, O. A.; Szatylowicz, H.; Guerra, C. F.; Krygowski, T. M.
Theoretical study of electron-attracting ability of the nitro group: classical and reverse substituent effects
Structural Chemistry, (26): 905-913 2015.

Steciuk, I.; Durka, K.; Gontarczyk, K.; Dabrowski, M.; Lulinski, S.; Wozniak, K.
Nitrogen-boron coordination versus OH center dot center dot center dot N hydrogen bonding in pyridoxaboroles - aza analogues of benzoxaboroles
Dalton Transactions, (44): 16534-16546 2015.

Steglenko, D. V.; Shevelev, S. A.; Kletskii, M. E.; Burov, O. N.; Lisovin, A. V.; Starosotnikov, A. M.; Morozov, P. G.; Kurbatov, S. V.; Minkin, V. I.; Bastrakov, M. A.
Quantum-chemical and NMR study of nitrofuroxanoquinoline cycloaddition
Chemistry of Heterocyclic Compounds, (51): 845-857 2015.

Stegmuller, A.; Tonner, R.
beta-Hydrogen Elimination Mechanism in the Absence of Low-Lying Acceptor Orbitals in EH2(t-C4H9) (E = N-Bi)
Inorganic Chemistry, (54): 6363-6372 2015.

Stegmuller, A.; Tonner, R.
A Quantum Chemical Descriptor for CVD Precursor Design: Predicting Decomposition Rates of TBP and TBAs Isomers and Derivatives
Chemical Vapor Deposition, (21): 161-165 2015.

Sterkhova, I. V.; Nikonov, A. Y.; Lazarev, I. M.; Moskalik, M. Y.; Lazareva, N. F.
Stereoelectronic structure and self-association of N-trimethylsilylsulfonamides RSO2NHSiMe3 (R = Me, CF3, Ph)
Russian Journal of General Chemistry, (85): 1661-1667 2015.

Sterkhova, I. V.; Nikonov, A. Y.; Lazarev, I. M.; Smirnov, V. I.; Lazareva, N. F.
N-trimetylsilyl carboxamides RC(0)NHSiMe3 (R = Me, CF3, Ph): X-ray, DFT and FTIR study
Journal of Molecular Structure, (1098): 408-415 2015.

Stock, R. I.; Nandi, L. G.; Nicoleti, C. R.; Schramm, A. D. S.; Meller, S. L.; Heying, R. S.; Coimbra, D. F.; Andriani, K. F.; Caramori, G. F.; Bortoluzzi, A. J.; Machado, V. G.
Synthesis and Solvatochromism of Substituted 4-(Nitrostyryl)phenolate Dyes
Journal of Organic Chemistry, (80): 7971-7983 2015.

Stockton, K. P.; Glover, S. A.; Greatrex, B. W.
Nucleophilic Trapping of Alkoxy-Stabilized Oxyallyl Systems Generated from Inosose 2-O-Mesylates
Synlett, (26): 111-115 2015.

Stojanovic, M.; Baranac-Stojanovic, M.
A theoretical study on borenium ion affinities toward ammonia, formaldehyde and chloride anions
Rsc Advances, (5): 75895-75910 2015.

Streubel, R.; Murcia-Garcia, C.; Schnakenburg, G.; Ferao, A. E.
Evidence for Terminal Phosphinidene Oxide Complexes in O,P,C-Cage Complex Formation: Rearrangement of Oxaphosphirane Complexes
Organometallics, (34): 2676-2682 2015.

Strieter, E. R.; Andrew, T. L.
Restricting the psi Torsion Angle Has Stereoelectronic Consequences on a Scissile Bond: An Electronic Structure Analysis
Biochemistry, (54): 5748-5756 2015.

Su, B. F.; Fu, H. Q.; Yang, H. Q.; Hu, C. W.
Catalytic reduction of NO by CO on Rh-4(+) clusters: a density functional theory study
Catalysis Science & Technology, (5): 3203-3215 2015.

Su, J.; Dau, P. D.; Liu, H. T.; Huang, D. L.; Wei, F.; Schwarz, W. H. E.; Li, J.; Wang, L. S.
Photoelectron spectroscopy and theoretical studies of gaseous uranium hexachlorides in different oxidation states: UCl6q- (q=0-2)

Journal of Chemical Physics, (142) 2015.

Su, P. F.; Chen, Z. C.; Wu, W.
An energy decomposition analysis study for intramolecular non-covalent interaction
Chemical Physics Letters, (635): 250-256 2015.

Su, Z.; Kim, C. K.
Trienamine catalysis for asymmetric Diels-Alder reactions of 2,4-dienones: a theoretical investigation
Organic & Biomolecular Chemistry, (13): 6313-6324 2015.

Subashchandrabose, S.; Babu, N. R.; Saleem, H.; Padusha, M. S. A.
Vibrational studies on (E)-1-((pyridine-2-yl)methylene)semicarbazide using experimental and theoretical method
Journal of Molecular Structure, (1094): 254-263 2015.

Subhapriya, G.; Kalyanaraman, S.; Surumbarkuzhali, N.; Vijayalakshmi, S.; Krishnakumar, V.
Investigation of intermolecular hydrogen bonding in 2,3,4,5,6 pentafluorobenzoic acid through molecular structure and vibrational analysis - A DFT approach
Journal of Molecular Structure, (1083): 48-56 2015.

Suhasini, M.; Sailatha, E.; Gunasekaran, S.; Ramkumaar, G. R.
Vibrational and electronic investigations, thermodynamic parameters, HOMO and LUMO analysis on Lornoxicam by density functional theory
Journal of Molecular Structure, (1100): 116-128 2015.

Sui, H. G.; Zhang, F. Y.; Hou, F.; Zhao, L. M.; Guo, W. Y.; Yao, J.
Theoretical Investigation of the Methanol Decomposition by Fe+ and Fe(C2H4)(+): A pi-Type Ligand Effect
Journal of Physical Chemistry A, (119): 10204-10211 2015.

Sun, C. Z.; Liu, M. S.; Sun, H. T.; Hang, F.; Sun, N.; Chen, D. Z.
Theoretical Mechanism for Selective Catalysis of Ruthenium Complex Catalyzed Hydroboration of Terminal Alkynes to Z-Vinylboronates
International Journal of Quantum Chemistry, (115): 59-67 2015.

Sun, W. M.; Hou, D.; Wu, D.; Li, X. H.; Li, Y.; Chen, J. H.; Li, C. Y.; Li, Z. R.
Theoretical characterization of a series of N-5-based aromatic hyperhalogen anions
Dalton Transactions, (44): 19901-19908 2015.

Sun, Z.; Schaefer, H. F.; Xie, Y. M.; Liu, Y. D.; Zhong, R. G.
Prototypical metal-oxo bonds: the reactions of Cr(PF3)(6), Fe(PF3)(5), and Ni(PF3)(4) with oxygen
Theoretical Chemistry Accounts, (134) 2015.

Sundaram, R.; Scheiner, S.; Roy, A. K.; Kar, T.
Site and chirality selective chemical modifications of boron nitride nanotubes (BNNTs) via Lewis acid-base interactions
Physical Chemistry Chemical Physics, (17): 3850-3866 2015.

Surajbali, P.; Ramanah, D. K.; Rhyman, L.; Alswaidan, I. A.; Fun, H. K.; Somanah, R.; Ramasami, P.
Density Functional Theory Study of Cyanoetheneselenol: A Molecule of Astrobiological Interest
Origins of Life and Evolution of Biospheres, (45): 455-468 2015.

Suresh, M.; Padusha, M. S. A.; Bharanidharan, S.; Saleem, H.; Dhandapani, A.; Manivarman, S.
Synthesis, spectral characterization and density functional theory exploration of 1-(quinolin-3-yl)piperidin-2-ol
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (144): 243-257 2015.

Suresh, M.; Padusha, M. S. A.; Govindarasu, K.; Kavitha, E.
Synthesis, structural and spectral analysis of 1-(pyrazin-2-yl) piperidin-2-ol by density functional theory
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (138): 271-282 2015.

Suresh, S.; Gunasekaran, S.; Srinivasan, S.

Vibrational spectra (FT-IR, FT-Raman), frontier molecular orbital, first hyperpolarizability, NBO analysis and thermodynamics properties of Piroxicam by HF and DFT methods
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (138): 447-459 2015.

Sutter, K.; Aucar, G. A.; Autschbach, J.
Analysis of Proton NMR in Hydrogen Bonds in Terms of Lone-Pair and Bond Orbital Contributions
Chemistry-a European Journal, (21): 18138-18155 2015.

Suveges, B. D.; Podlech, J.
Dependence of Stereoelectronic and Charge Effects on pK(a) Values of 1,3-Dithiane-Derived Sulfides, Sulfoxides, and Sulfones: An Experimental and Computational Investigation
European Journal of Organic Chemistry: 987-994 2015.

Suvitha, A.; Periandy, S.; Gayathri, P.
NBO, HOMO-LUMO, UV, NLO, NMR and vibrational analysis of veratrole using FT-IR, FT-Raman, FT-NMR spectra and HF-DFT computational methods
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (138): 357-369 2015.

Suvitha, A.; Periandy, S.; Govindarajan, M.; Gayathri, P.
Vibrational analysis using FT-IR, FT-Raman spectra and HF-DFT methods and NBO, NLO, NMR, HOMO-LUMO, UV and electronic transitions studies on 2,2,4-trimethyl pentane
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (138): 900-912 2015.

Suzuki, T.; Wasada-Tsutsui, Y.; Ogawa, T.; Inomata, T.; Ozawa, T.; Sakai, Y.; Fryzuk, M. D.; Masuda, H.
N-2 Activation by an Iron Complex with a Strong Electron-Donating Iminophosphorane Ligand
Inorganic Chemistry, (54): 9271-9281 2015.

Swarnalatha, N.; Gunasekaran, S.; Muthu, S.; Nagarajan, M.
Molecular structure analysis and spectroscopic characterization of 9-methoxy-2H-furo 3,2-g chromen-2-one with experimental (FT-IR and FT-Raman) techniques and quantum chemical calculations
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (137): 721-729 2015.

Swarnalatha, N.; Gunasekaran, S.; Nagarajan, M.; Srinivasan, S.; Sankari, G.; Ramkumaar, G. R.
Vibrational, UV spectra, NBO, first order hyperpolarizability and HOMO-LUMO analysis of carvedilol
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (136): 567-578 2015.

Swiderski, G.; Kalinowska, M.; Wojtulewski, S.; Lewandowski, W.
The experimental and theoretical study on the influence of alkali metals on the electronic charge distribution in five-membered aromatic acids (2-thiophenecarboxylic, 2-furanecarboxylic and 2-pyrrolecarboxylic acids)
Polyhedron, (97): 118-139 2015.

Szatylowicz, H.; Stasyuk, O. A.; Krygowski, T. M.
Substituent Effects in Heterocyclic Systems
Advances in Heterocyclic Chemistry, Vol 116, (116): 137-192 2015.

Szczepaniak, M.; Moc, J.
Tautomers of Gas-Phase Erythrose and Their Interconversion Reactions: Insights from High-Level ab Initio Study
Journal of Physical Chemistry A, (119): 10946-10958 2015.

Szostak, R.; Aube, J.; Szostak, M.
Determination of Structures and Energetics of Small- and Medium-Sized One-Carbon-Bridged Twisted Amides using ab Initio Molecular Orbital Methods: Implications for Amidic Resonance along the C-N Rotational Pathway
Journal of Organic Chemistry, (80): 7905-7927 2015.

Tabassum, S.; Gilani, M. A.; Ayub, K.; Wilhelm, R.
First examples of carbene-catalyzed allylation of benzaldehyde with allyltrichlorosilane
Journal of the Iranian Chemical Society, (12): 1199-1205 2015.

Tabayashi, K.; Takahashi, O.
Substituent Electron Push-Pull Interaction in Intermolecular Resonance-Assisted Hydrogen Bonds: Thymine/Adenine Base Pair and Their Complexes with Carboxylic Acids
Bulletin of the Chemical Society of Japan, (88): 1466-1478 2015.

Tabrizi, L.; Chiniforoshan, H.; Tavakol, H.
New mixed ligand palladium(II) complexes based on the antiepileptic drug sodium valproate and bioactive nitrogen-donor ligands: Synthesis, structural characterization, binding interactions with DNA and BSA, in vitro cytotoxicity studies and DFT calculations
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (141): 16-26 2015.

Taherpour, A. A.; Mozafai, A.; Ranjbar, S.; Taban, S.
A study of the effects of solvent on structural and conformational properties of ranitidine tautomer forms by DFT method
Structural Chemistry, (26): 517-529 2015.

Taherpour, A. A.; Rezaei, O.; Shahri, Z.; Jalilian, J.; Jamshidi, M.; Zolfaghar, N.
First principles studies of electronic and optical properties of helium adsorption on Sc-doped BN monolayer
Journal of the Iranian Chemical Society, (12): 1983-1990 2015.

Tainter, C. J.; Shi, L.; Skinner, J. L.
Reparametrized E3B (Explicit Three-Body). Water Model Using the TIP4P/2005 Model as a Reference
Journal of Chemical Theory and Computation, (11): 2268-2277 2015.

Tamer, O.; Avci, D.; Arioglu, C.; Basoslu, A.; Atalay, Y.
A theoretical study on structural, spectroscopic, electronic and electric properties of 4-chloro 4-nitrostilbene
Indian Journal of Physics, (89): 1-11 2015.

Tamer, O.; Avci, D.; Atalay, Y.
Geometry Optimization, Spectral Analysis, Molecular Electrostatic Potential Surface, and Nonlinear Optical Activity of 4-Methyl Anilinium Phenolsulfonate: a DFT Study
Journal of Applied Spectroscopy, (82): 687-699 2015.

Tamer, O.; Avci, D.; Atalay, Y.
Synthesis, crystal structure, spectroscopic characterization and nonlinear optical properties of Co(II)- picolinate complex
Materials Chemistry and Physics, (168): 138-146 2015.

Tamer, O.; Avci, D.; Atalay, Y.
Synthesis, X-ray structure, spectroscopic characterization and nonlinear optical properties of Nickel (II) complex with picolinate: A combined experimental and theoretical study
Journal of Molecular Structure, (1098): 12-20 2015.

Tanabe, M.; Omine, S.; Ishikawa, N.; Osakada, K.; Hayashi, Y.; Kawauchi, S.
Bond Formation and Coupling between Germyl and Bridging Germylene Ligands in Dinuclear Palladium(I) Complexes
Angewandte Chemie-International Edition, (54): 2679-2683 2015.

Tanaka, H.; Hiraide, S.; Kondo, A.; Miyahara, M. T.
Modeling and Visualization of CO2 Adsorption on Elastic Layer-Structured Metal-Organic Framework-11: Toward a Better Understanding of Gate Adsorption Behavior
Journal of Physical Chemistry C, (119): 11533-11543 2015.

Tang, C. M.; Kang, J.; Zhang, Z. J.; Zou, J. F.; He, X.; Xu, Y.
The study of the hydrogen storage capacity of the Ti atoms coated Si@Ga-12 clusters
International Journal of Hydrogen Energy, (40): 16278-16287 2015.

Tang, H. R.; Lu, D. M.; Wu, C.
Cation-assisted interactions between N-heterocycles and CO2

Physical Chemistry Chemical Physics, (17): 15725-15731 2015.

Tang, L. H.; Bao, S. Y.; Peng, J. H.; Li, K.; Ning, P.; Guo, H. B.; Zhu, T. T.; Gu, J. J.; Li, Q. S.
Structure, energetics, and bonding of novel potential high energy density materials Rh-2(N-5)(4): A DFT study
Chemical Physics Letters, (639): 166-171 2015.

Tang, Q. J.; Li, Q. Z.
Abnormal synergistic effects between Lewis acid- base interaction and halogen bond in F3B center dot center dot center dot NCX center dot center dot center dot NCM
Molecular Physics, (113): 3809-3814 2015.

Tang, Q. J.; Li, Q. Z.
Non-additivity of F substituent in enhancing the halogen bond in C6H5I center dot center dot center dot NCH
Computational and Theoretical Chemistry, (1070): 21-26 2015.

Tao, Y. P.; Han, L. G.; Han, Y. X.; Liu, Z. J.
Experimental and theoretical studies on the vibrational spectra of trans-3-phenylacryloyl
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (137): 892-898 2015.

Tavakol, H.; Khedri, N.
DFT Study of the effects of counter ions on bonding, molecular and spectral properties of pentaflourophenyl xenonium diflouride cation
Journal of Chemical Sciences, (127): 1675-1685 2015.

Teimouri, A.; Najari, B.; Chermahini, A. N.; Farrokhpour, H.
Selective Complexation of S-block Cations with Nanotubular Silk Type Cyclopeptides: A DFT Study
Journal of the Chinese Chemical Society, (62): 1105-1113 2015.

Teixeira, F.; Natalia, M.; Cordeiro, D. S.
Simple descriptors for assessing the outcome of aza-Diels-Alder reactions
Rsc Advances, (5): 50729-50740 2015.

Testa, C.; Roger, J.; Scheib, S.; Fleurat-Lessard, P.; Hierso, J. C.
Palladium-Catalysed C-H Bond Electrophilic Fluorination of Highly Substituted Arylpyrazoles: Experimental and DFT Mechanistic Insights
Advanced Synthesis & Catalysis, (357): 2913-2923 2015.

Thanigaimani, K.; Khalib, N. C.; Temel, E.; Arshad, S.; Razak, I. A.
New supramolecular cocrystal of 2-amino-5-chloropyridine with 3-methylbenzoic acids: Syntheses, structural characterization, Hirshfeld surfaces and quantum chemical investigations
Journal of Molecular Structure, (1099): 246-256 2015.

Thanthiriwatte, K. S.; Vasiliu, M.; Battey, S. R.; Lu, Q.; Peterson, K. A.; Andrews, L.; Dixon, D. A.
Gas Phase Properties of MX2 and MX4 (X = F, Cl) for M = Group 4, Group 14, Cerium, and Thorium
Journal of Physical Chemistry A, (119): 5790-5803 2015.

Thapa, B.; Schlegel, H. B.
Calculations of pK(a)'s and Redox Potentials of Nucleobases with Explicit Waters and Polarizable Continuum Solvation
Journal of Physical Chemistry A, (119): 5134-5144 2015.

Thirman, J.; Head-Gordon, M.
An energy decomposition analysis for second-order Moller-Plesset perturbation theory based on absolutely localized molecular orbitals
Journal of Chemical Physics, (143) 2015.

Thomas, M.; Brehm, M.; Kirchner, B.
Voronoi dipole moments for the simulation of bulk phase vibrational spectra
Physical Chemistry Chemical Physics, (17): 3207-3213 2015.

Tian, H. W.; Feng, W.; Wang, R.; Liu, H. L.; Huang, X. R.
Theoretical study of stabilities, electronic, and catalytic performance of supported platinum on modified graphene
Molecular Physics, (113): 3514-3523 2015.

Tian, Q. Q.; Li, R. S.; Sun, H. T.; Xue, Z. M.; Mu, T. C.
Theoretical and experimental study on the interaction between 1-butyl-3-methylimidazolium acetate and CO2
Journal of Molecular Liquids, (208): 259-268 2015.

Tian, Q. Q.; Liu, S. Y.; Sun, X. F.; Sun, H. T.; Xue, Z. M.; Mu, T. C.
Theoretical studies on the dissolution of chitosan in 1-butyl-3-methylimidazolium acetate ionic liquid
Carbohydrate Research, (408): 107-113 2015.

Tian, W. J.; You, X. R.; Li, D. Z.; Ou, T.; Chen, Q.; Zhai, H. J.; Li, S. D.
A first-principles study on the B5O5+/0 and B5O5- clusters: The boron oxide analogs of C6H5+/0 and CH3Cl
Journal of Chemical Physics, (143) 2015.

Tian, W. J.; Zhao, L. J.; Chen, Q.; Ou, T.; Xu, H. G.; Zheng, W. J.; Zhai, H. J.; Li, S. D.
Photoelectron spectroscopy of B4O4-: Dual 3c-4e pi hyperbonds and rhombic 4c-4e o-bond in boron oxide clusters
Journal of Chemical Physics, (142) 2015.

Tian, Y.; Fu, J.; Zhang, Y.; Cao, K. C.; Bai, C. Y.; Wang, D. Q.; Li, S. J.; Xue, Y.; Ma, L. L.; Zheng, C.
Ligand-exchange mechanism: new insight into solid-phase extraction of uranium based on a combined experimental and theoretical study
Physical Chemistry Chemical Physics, (17): 7214-7223 2015.

Tognetti, V.; Morell, C.; Joubert, L.
Quantifying Electro/Nucleophilicity by Partitioning the Dual Descriptor
Journal of Computational Chemistry, (36): 649-659 2015.

Tong, Y. C.; Zhang, X. Y.; Wang, Q. Y.; Xu, X. J.; Wang, Y. C.
A theoretical view on CrO2+-mediated C-H bond activation in ethane
Journal of Molecular Structure, (1089): 129-134 2015.

Torii, H.
Electronic Structural Basis for the Atomic Partial Charges of Planar Molecular Systems Derived from Out-of-Plane Dipole Derivatives
Journal of Physical Chemistry A, (119): 3277-3284 2015.

Toure, M.; Chuzel, O.; Parrain, J. L.
Synthesis and structure of Ag(I), Pd(II), Rh(I), Ru(II) and Au(I) NHC-complexes with a pendant Lewis acidic boronic ester moiety
Dalton Transactions, (44): 7139-7143 2015.

Toy, M.; Tanak, H.; Senoz, H.
Identification of structural and spectral properties of synthesized 3-(p-isopropylphenyl)-5-(o,m,p-nitrophenyl)-1-phenylformazans: A combined experimental and DFT study
Dyes and Pigments, (113): 510-521 2015.

Trogolo, D.; Mishra, B. K.; Heeb, M. B.; von Gunten, U.; Arey, J. S.
Molecular Mechanism of NDMA Formation from N,N-Dimethylsulfamide During Ozonation: Quantum Chemical Insights into a Bromide-Catalyzed Pathway
Environmental Science & Technology, (49): 4163-4175 2015.

Troyano, J.; Corral, I.; Castillo, O.; Zamora, F.; Mas-Balleste, R.; Delgado, S.
S-S Bond Activation in Multi-Copper Aggregates Containing Perthiocarboxylato Ligands
European Journal of Inorganic Chemistry: 4044-4054 2015.

Trujillo, C.; Rodriguez-Sanz, A. A.; Rozas, I.
Aromatic Amino Acids-Guanidinium Complexes through Cation-pi Interactions
Molecules, (20): 9214-9228 2015.

Trujillo, C.; Saanchez-Sanz, G.; Alkorta, I.; Elguero, J.
Halogen, chalcogen and pnictogen interactions in (XNO2)(2) homodimers (X = F, Cl, Br, I)
New Journal of Chemistry, (39): 6791-6802 2015.

Tsiepe, T. J.; Kabanda, M. M.; Serobatse, K. R. N.
Antioxidant Properties of Kanakugiol Revealed Through the Hydrogen Atom Transfer, Electron Transfer and M2+ (M2+ = Cu(II) or Co(II) Ion) Coordination Ability Mechanisms. A DFT Study In Vacuo and in Solution
Food Biophysics, (10): 342-359 2015.

Tsipis, A. C.; Gkarbounis, D. N.
Sequential metalation of benzene: electronic, bonding, magnetotropic and spectroscopic properties of coinage metalated benzenes studied by DFT
Journal of Molecular Modeling, (21) 2015.

Tsipis, A. C.; Gkarmpounis, D. N.
The hydrogen storage capacity of coinage metalated benzenes studied by DFT
Journal of Coordination Chemistry, (68): 2653-2665 2015.

Tsipis, A. C.; Stalikas, A. V.
Electronic, bonding, and optical properties of 1d CuCN (n) (n=1-10) chains, 2d CuCN (n) (n=2-10) nanorings, and 3d Cu-n(CN)(n) (m) (n=4, m=2, 3; n=10, m=2) tubes studied by DFT/TD-DFT methods
Journal of Computational Chemistry, (36): 1334-1347 2015.

Tsuchido, Y.; Ide, T.; Suzaki, Y.; Osakada, K.
1,4-Selective Diels-Alder Reaction of 9,10-Diethynylanthracene with 3,6-Difluorobenzyne
Bulletin of the Chemical Society of Japan, (88): 821-823 2015.

Tumminakatti, S.; Khatri, B.; Krishnamurti, V.; Athavale, V.; Prabhakaran, E. N.
Solution structural features of N-acyl homoserine lactones
Tetrahedron Letters, (56): 5771-5775 2015.

Turner, W. E.; Agarwal, J.; Schaefer, H. F.
Structures, Bonding, and Energetics of Potential Triatomic Circumstellar Molecules Containing Group 15 and 16 Elements
Journal of Physical Chemistry A, (119): 11693-11700 2015.

Tyagi, P.; Chandra, S.; Saraswat, B. S.
Ni(II) and Zn(II) complexes of 2-((thiophen-2-ylmethylene)amino)benzamide: Synthesis, spectroscopic characterization, thermal, DFT and anticancer activities
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (134): 200-209 2015.

Tyagi, P.; Chandra, S.; Saraswat, B. S.; Sharma, D.
Design, spectral characterization, DFT and biological studies of transition metal complexes of Schiff base derived from 2-aminobenzamide, pyrrole and furan aldehyde
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (143): 1-11 2015.

Ucar, I.; Vural, H.; Kucuk, E.
Two new chelidamate complexes with the 4-methoxypyridine: A combined theoretical and experimental study
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (151): 667-672 2015.

Udagawa, T.
Theoretical analysis on the aromaticity of uracil: Important electronic configurations and solvent effect on the aromaticity
Chemical Physics Letters, (637): 115-119 2015.

Uddin, N.; Choi, C. H.
Comparative Atomic Charges on Na+-(H2O)(n) (n=1-6) Clusters
Bulletin of the Korean Chemical Society, (36): 827-831 2015.

Ukrainets, I. V.; Petrushova, L. A.; Shishkina, S. V.; Sim, G.
2,1-Benzothiazine 2,2-Dioxides. 9(*). Alkylation of Methyl 4-Hydroxy-1-Methyl-2,2-Dioxo-1De-2 lambda(6),1-Benzothiazine-3-Carboxylate with Ethyl Iodide
Chemistry of Heterocyclic Compounds, (50): 1741-1747 2015.

Ulahannan, R. T.; Panicker, C. Y.; Varghese, H. T.; Musiol, R.; Jampilek, J.; Van Alsenoy, C.; War, J. A.; Manojkumar, T. K.
Vibrational spectroscopic studies and molecular docking study of 2- (E)-2-phenylethenyl quinoline-5-carboxylic acid
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (150): 190-199 2015.

Umadevi, P.; Aiswarya, T.; Senthilkumar, L.
Encapsulation of fluoroethanols in pristine and Stone-Wales defect boron nitride nanotube - A DFT study
Applied Surface Science, (345): 369-378 2015.

Unsalan, O.; Kus, N.; Jarmelo, S.; Faust, R.
Trans- and cis-stilbene isolated in cryogenic argon and xenon matrices
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (136): 81-94 2015.

Upadhyay, M. K.; Sengupta, S. K.; Singh, H. J.
Nitro and dinitroamino N-oxides of octaazaanthracene as high energy materials
Journal of Molecular Modeling, (21) 2015.

Usui, K.; Ando, M.; Yokogawa, D.; Irle, S.
Understanding the On-Off Switching Mechanism in Cationic Tetravalent Group-V-Based Fluoride Molecular Sensors Using Orbital Analysis
Journal of Physical Chemistry A, (119): 12693-12698 2015.

Uzunova, E. L.; Seriani, N.; Mikosch, H.
CO2 conversion to methanol on Cu(I) oxide nanolayers and clusters: an electronic structure insight into the reaction mechanism
Physical Chemistry Chemical Physics, (17): 11088-11094 2015.

Vafaeezadeh, M.; Hashemi, M. M.
Investigations for gas-phase deprotonation of the silica-propyl-SO3H catalyst using cage-like nanocluster modeling technique
Journal of the Iranian Chemical Society, (12): 1991-1997 2015.

Vakili, M.; Tayyari, S. F.; Afzali, R.
Conformation, molecular structure, and vibrational assignment of bis(2,2,6,6-tetramethylheptane-3,5-dionato)copper(II)
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (136): 1827-1833 2015.

Valdes, O.; Vergara, C. E.; Camarada, M. B.; Carrasco-Sanchez, V.; Nachtigall, F. M.; Tapia, J.; Fischer, R.; Gonzalez-Nilo, F. D.; Santos, L. S.
Synthesis and characterization of an insoluble polymer based on polyamidoamine: Applications for the decontamination of metals in aqueous systems
Journal of Environmental Management, (147): 321-329 2015.

Valencia, I.; Avila-Torres, Y.; Barba-Behrens, N.; Garzon, I. L.
Circular dichroism and optical absorption spectra of mononuclear and trinuclear chiral Cu(II) amino-alcohol coordinated compounds: A combined theoretical and experimental study
Journal of Molecular Structure, (1085): 52-62 2015.

Vallet, V.; Masella, M.

Benchmark binding energies of ammonium and alkyl-ammonium ions interacting with water. Are ammonium-water hydrogen bonds strong?
Chemical Physics Letters, (618): 168-173 2015.

Vanpoucke, D. E. P.; Olah, J.; De Proft, F.; Van Speybroeck, V.; Roos, G.
Convergence of Atomic Charges with the Size of the Enzymatic Environment
Journal of Chemical Information and Modeling, (55): 564-571 2015.

Vaquer, A. F.; Frongia, A.; Secci, F.; Tuveri, E.
Disulfide-based metal-free alpha-sulfanylation of ketones
Rsc Advances, (5): 96695-96704 2015.

Varadwaj, A.; Varadwaj, P. R.; Jin, B. Y.
Fluorines in Tetrafluoromethane as Halogen Bond Donors: Revisiting Address the Nature of the Fluorine's sigma(hole)
International Journal of Quantum Chemistry, (115): 453-470 2015.

Vasiliu, M.; Peterson, K. A.; Gibson, J. K.; Dixon, D. A.
Reliable Potential Energy Surfaces for the Reactions of H2O with ThO2, PaO2+, UO22+, and UO2+
Journal of Physical Chemistry A, (119): 11422-11431 2015.

Vatanparast, M.; Nekoei, A. R.
RAHB concept and sigma-skeleton in some oximes of 3-hydroxy fulvene; DFT, AIM, ELF and NBO studies
Structural Chemistry, (26): 1039-1048 2015.

Vatanparast, M.; Taghizadeh, M. T.; Parvini, E.
Theoretical insight into the interplay between lithium and halogen-hydride bonds: An ab initio study
Journal of Theoretical & Computational Chemistry, (14) 2015.

Velian, A.; Cummins, C. C.
INORGANIC CHEMISTRY Synthesis and characterization of P2N3-: An aromatic ion composed of phosphorus and nitrogen
Science, (348): 1001-1004 2015.

Velmurugan, G.; Venuvanalingam, P.
Luminescent Re(I) terpyridine complexes for OLEDs: what does the DFT/TD-DFT probe reveal?
Dalton Transactions, (44): 8529-8542 2015.

Velraj, G.; Soundharam, S.; Sridevi, C.
Investigation of structure, vibrational, electronic, NBO and NMR analyses of 2-chloro-4-nitropyridine (CNP), 2-chloro-4-methyl-5-nitropyridine (CMNP) and 3-amino-2-chloro-4-methylpyridine (ACMP) by experimental and theoretical approach
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (137): 790-803 2015.

Venkataramanan, N. S.
Effect of oxygen content and charge on the structure, stability and optoelectronic properties of yttrium oxide clusters
Journal of Physics and Chemistry of Solids, (82): 91-100 2015.

Vent-Schmidt, T.; Andrews, L.; Thanthiriwatte, K. S.; Dixon, D. A.; Riedel, S.
Reaction of Laser-Ablated Uranium and Thorium Atoms with H2Se: A Rare Example of Selenium Multiple Bonding
Inorganic Chemistry, (54): 9761-9769 2015.

Vent-Schmidt, T.; Metzger, J.; Andrews, L.; Riedel, S.
Investigation of thorium hydride fluorides by matrix-isolation spectroscopy
Journal of Fluorine Chemistry, (174): 2-7 2015.

Verma, K.; Dave, K.; Viswanathan, K. S.
Hydrogen-Bonded Complexes of Phenylacetylene-Acetylene: Who is the Proton Donor?
Journal of Physical Chemistry A, (119): 12656-12664 2015.

Verma, P.; Maurice, R.; Truhlar, D. G.
Identifying the Interactions That Allow Separation of O-2 from N-2 on the Open Iron Sites of Fe-2(dobdc)
Journal of Physical Chemistry C, (119): 28499-28511 2015.

Verma, P. L.; Rao, S. S.; Gejji, S. P.
Probing molecular interactions underlying imidazolium and pyridinium based ionic liquids
Journal of Molecular Liquids, (212): 885-899 2015.

Viana, R. B.; da Silva, A. B. F.
Electronic properties of the AsCO, AsSiO and AsGeO radicals: Linear or cyclic?
Polyhedron, (89): 160-167 2015.

Viana, R. B.; da Silva, A. B. F.
Interaction between PH3 and small water clusters: Understanding the electronic and spectroscopic properties
Computational and Theoretical Chemistry, (1059): 35-44 2015.

Vijayachamundeeswari, S. P.; Narayana, B. Y.; Pradeepa, S. J.; Sundaraganesan, N.
Vibrational analysis, NBO analysis, NMR, UV-VIS, hyperpolarizability analysis of Trimethadione by density functional theory
Journal of Molecular Structure, (1099): 633-643 2015.

Vijayan, P.; Viswanathamurthi, P.; Velmurugan, K.; Nandhakumar, R.; Balakumaran, M. D.; Kalaichelvan, P. T.; Malecki, J. G.
Nickel(II) and copper(II) complexes constructed with N2S2 hybrid benzamidine-thiosemicarbazone ligand: synthesis, X-ray crystal structure, DFT, kinetico-catalytic and in vitro biological applications
Rsc Advances, (5): 103321-103342 2015.

Villegas-Escobar, N.; Gutierrez-Oliva, S.; Toro-Labbe, A.
Catalytic Mechanism of H-2 Activation by a Carbenoid Aluminum Complex
Journal of Physical Chemistry C, (119): 26598-26604 2015.

Vishnevskiy, Y. V.; Schwabedissen, J.; Rykov, A. N.; Kuznetsov, V. V.; Makhova, N. N.
Conformational and Bonding Properties of 3,3-Dimethyl- and 6,6-Dimethyl-1,5-diazabicyclo 3.1.0 hexane: A Case Study Employing the Monte Carlo Method in Gas Electron Diffraction
Journal of Physical Chemistry A, (119): 10871-10881 2015.

Vitnik, V. D.; Vitnik, Z. J.
The spectroscopic (FT-IR, FT-Raman, C-13, H-1 NMR and UV) and NBO analyses of 4-bromo-1-(ethoxycarbonyl)piperidine-4-carboxylic acid
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (138): 1-12 2015.

Vlassa, M.; Bende, A.
Theoretical investigation of polymer chain stability in the metal coordinated azorubine and cyclam complex
Chemical Physics, (457): 152-159 2015.

Vogt-Geisse, S.; Wu, J. I. C.; Schleyer, P. V.; Schaefer, H. F.
Bonding, aromaticity, and planar tetracoordinated carbon in Si2CH2 and Ge2CH2
Journal of Molecular Modeling, (21) 2015.

Vojta, D.; Kovacevic, G.; Vazdar, M.
The exploration of hydrogen bonding properties of 2,6- and 3,5-diethynylpyridine by IR spectroscopy
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (136): 1912-1923 2015.

Volcker, F.; Muck, F. M.; Vogiatzis, K. D.; Fink, K.; Roesky, P. W.
Bi- and trimetallic rare-earth-palladium complexes ligated by phosphinoamides
Chemical Communications, (51): 11761-11764 2015.

Vollmer, G. Y.; Wallasch, M. W.; Saurenz, D.; Eger, T. R.; Bauer, H.; Wolmershauser, G.; Prosenc, M. H.; Sitzmann, H.

Benzylidyne Bridges from Diphenylacetylene and a Methylidyne Bridge from Methylmagnesium Chloride
Organometallics, (34): 644-652 2015.

Vovusha, H.; Sanyal, B.
DFT and TD-DFT studies on the electronic and optical properties of explosive molecules adsorbed on boron nitride and graphene nano flakes
Rsc Advances, (5): 4599-4608 2015.

Vranova, I.; Alonso, M.; Lo, R.; Sedlak, R.; Jambor, R.; Ruzicka, A.; De Proft, F.; Hobza, P.; Dostal, L.
From Dibismuthenes to Three- and Two-Coordinated Bismuthinidenes by Fine Ligand Tuning: Evidence for Aromatic BiC3N Rings through a Combined Experimental and Theoretical Study
Chemistry-a European Journal, (21): 16917-16928 2015.

Vural, H.; Ucar, I.
A combined theoretical and experimental study of chelidamate cadmium (II) complex, Cd-2(dpa)(2)(chel)(2) center dot 2 Cd(dpa)(chel) center dot 6H(2)O
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (136): 1298-1307 2015.

Wada, T.; Enami, K.; Kojima, R.; Okada, T.; Ishikawa, Y.; Miyazato, Y.; Horn, E.; Mochizuki, Y.
Reversible Structural Changes Accompanying the Two-Electron Redox Reaction of Pt(tacn) (tacn: 1,4,7-triazacyclononane) Complexes
Bulletin of the Chemical Society of Japan, (88): 1230-1237 2015.

Waerder, B.; Steinhauer, S.; Bader, J.; Neumann, B.; Stammler, H. G.; Vishnevskiy, Y. V.; Hoge, B.; Mitzel, N. W.
Pentafluoroethyl-substituted alpha-silanes: model compounds for new insights
Dalton Transactions, (44): 13347-13358 2015.

Wagner, M.; Lutter, M.; Dietz, C.; Prosenc, M. H.; Jurkschat, K.
On the Reactivity of RSnCl and RSiMe3 {R=4-tBu-2,6- P(O)(OiPr)(2) (2)C6H2} towards BF3 center dot OEt2: Competing Lewis Acidities
European Journal of Inorganic Chemistry: 2152-2158 2015.

Wan, Y. L.; Wang, X. Y.; Liu, N.
The reactivity of phenancyl bromide under beta-cyclodextrin as supramolecular catalyst: a computational survey
Journal of Molecular Modeling, (21) 2015.

Wang, C. W.; Mo, Y. R.; Wagner, J. P.; Schreiner, P. R.; Jemmis, E. D.; Danovich, D.; Shaik, S.
The Self-Association of Graphane Is Driven by London Dispersion and Enhanced Orbital Interactions
Journal of Chemical Theory and Computation, (11): 1621-1630 2015.

Wang, C. Y.; Cheng, C.; Su, J.; Huai, P.
Bonding nature of the actinide tetrafluorides AnF(4) (An = Th-Cm)
Molecular Physics, (113): 3450-3458 2015.

Wang, C. Y.; Xie, X.; Liu, J.; Liu, Y. H.; Li, Y. X.
Gold(I)-Catalyzed 1,4-and/or 1,5-Heteroaryl Migration Reactions through Regiocontrolled Cyclizations
Chemistry-a European Journal, (21): 559-564 2015.

Wang, C. Z.; Gibson, J. K.; Lan, J. H.; Wu, Q. Y.; Zhao, Y. L.; Li, J.; Chai, Z. F.; Shi, W. Q.
Actinide (An = Th-Pu) dimetallocenes: promising candidates for metal-metal multiple bonds
Dalton Transactions, (44): 17045-17053 2015.

Wang, F.; Islam, S.; Vasilyev, V.
Ferrocene Orientation Determined Intramolecular Interactions Using Energy Decomposition Analysis
Materials, (8): 7723-7737 2015.

Wang, F.; Zhu, S. H.; Meng, Q. X.; Yin, H. Z.
Theoretical studies of nickel-catalyzed ring-opening hydroacylation of methylenecyclopropanes and benzaldehydes

Journal of Molecular Modeling, (21) 2015.

Wang, H.; Li, C.; Wang, W. Z.; Jin, W. J.
Strength order and nature of the pi-hole bond of cyanuric chloride and 1,3,5-triazine with halide
Physical Chemistry Chemical Physics, (17): 20636-20646 2015.

Wang, H. F.; Zhao, L. M.; Xu, W. B.; Wang, S. P.; Ding, Q. Y.; Lu, X. Q.; Guo, W. Y.
The properties of the bonding between CO and ZIF-8 structures: a density functional theory study
Theoretical Chemistry Accounts, (134) 2015.

Wang, H. Y.; Wang, H.; King, R. B.
The binuclear cyclooctatetraene sandwich compounds (C8H8)(2)M-2 of the first row transition metals: Analogues of the perpendicular dimetallocenes
Polyhedron, (97): 47-54 2015.

Wang, J. C.; Yao, E. D.; Chen, Z. T.; Ma, Y. G.
Fluorinated Nickel(II) Phenoxyiminato Catalysts: Exploring the Role of Fluorine Atoms in Controlling Polyethylene Productivities and Microstructures
Macromolecules, (48): 5504-5510 2015.

Wang, J. H.; Li, Z. P.; Guo, L. Y.
Electronic Properties and Stability of Graphene Oxyradical Systems
Materials Transactions, (56): 1102-1106 2015.

Wang, J. J.; Zhou, Z. J.; Bai, Y.; He, H. M.; Wu, D.; Li, Y.; Li, Z. R.; Zhang, H. X.
A new strategy for simultaneously enhancing nonlinear optical response and electron stability in novel cup-saucer(+)-cage(-)-shaped sandwich electride molecules with an excess electron protected inside the cage
Dalton Transactions, (44): 4207-4214 2015.

Wang, J. R.; Su, D. P.; Wang, D. Q.; Ding, S. D.; Huang, C.; Huang, H.; Hu, X. Y.; Wang, Z. P.; Li, S. M.
Selective Extraction of Americium(III) over Europium(III) with the Pyridylpyrazole Based Tetradentate Ligands: Experimental and Theoretical Study
Inorganic Chemistry, (54): 10648-10655 2015.

Wang, L.; Die, D.; Wang, S. J.; Zhao, Z. Q.
Geometrical, electronic, and magnetic properties of CunFe (n=1-12) clusters: A density functional study
Journal of Physics and Chemistry of Solids, (76): 10-16 2015.

Wang, L.; Jin, X. F.; Li, Y.; Li, P.; Zhang, J. L.; He, H. Y.; Zhang, S. J.
Insight into the activity of efficient acid-base bifunctional catalysts for the coupling reaction of CO2
Molecular Physics, (113): 3524-3530 2015.

Wang, L.; Li, P.; Li, Y.; He, H. Q.; Zhang, J. L.
Insight into the catalytic activity for a series of synthesized and newly designed phosphonium-based ionic liquids on the fixation of carbon dioxide
Theoretical Chemistry Accounts, (134) 2015.

Wang, M.; Luo, H.; Wang, L. S.; Wang, J. Y.
What factors cause the complete substrate-controlled selectivity in Rh-2(Piv)(4)-catalyzed cycloadditions of 1,2,3-triazoles with isocyanates or isothiocyanates
Journal of Organometallic Chemistry, (788): 58-67 2015.

Wang, M.; Zhao, J.; Zhang, L. B.; Su, X. Y.; Su, H. L.; Bu, Y. X.
Intriguing radical-radical interactions among double-electron oxidized adenine-thymine base pairs
Chemical Physics Letters, (619): 223-229 2015.

Wang, M. A.; Luo, H.; Zhang, M.; Wang, J. Y.
Why trans- or cis-Dimethyl Fumarate Addition to 2,5-Dimethylpyrrole Gives Exclusively trans-7-Azanorbornane

Journal of Physical Chemistry A, (119): 6563-6573 2015.

Wang, Q.; Guo, C. H.; Jia, J. F.; Wu, H. S.
Theoretical investigation of the mechanism for the cycloaddition of CO2 to epoxides catalyzed by a magnesium(II) porphyrin complex
Journal of Molecular Modeling, (21) 2015.

Wang, Q. N.; Dong, H.; Yu, H.; Yu, H. B.
Enhanced performance of gas diffusion electrode for electrochemical reduction of carbon dioxide to formate by adding polytetrafluoroethylene into catalyst layer
Journal of Power Sources, (279): 1-47 2015.

Wang, Q. W.; Sun, M.; Wang, Y. N.; Qi, X. F.; Li, X. M.; Liu, B.
Synthesis, Crystal Structure and Theoretical Calculations of a New Two-dimensional Co(II) Coordination Polymer Based on Oxalic Acid and Bis(imidazol) Ligands
Chinese Journal of Structural Chemistry, (34): 393-400 2015.

Wang, S. F.; Wang, J. J.; Cheng, W. W.; Yang, X. W.; Zhang, Z. Y.; Xu, Y.; Liu, H. K.; Wu, Y.; Fang, M.
A Zr metal-organic framework based on tetrakis(4-carboxyphenyl) silane and factors affecting the hydrothermal stability of Zr-MOFs
Dalton Transactions, (44): 8049-8061 2015.

Wang, W. H.; Zhang, X. X.; Li, P.; Sun, Q.; Li, Z.; Ren, C.; Guo, C.
CO2 Capture and Separation from N-2/CH4 Mixtures by Co@B-8/Co@B-8(-) and M@B-9/M@B-9(-) (M = Ir, Rh, Ru) Clusters: A Theoretical Study
Journal of Physical Chemistry A, (119): 796-805 2015.

Wang, Y.; Gao, X. Z.; Li, N.; King, R. B.
Binuclear cyclopentadienylosmium hydride chemistry: A stable quadruply bridged structure
Inorganica Chimica Acta, (434): 60-66 2015.

Wang, Y.; Guo, X. K.; Tang, M. S.; Wei, D. H.
Theoretical Investigations toward the Asymmetric Insertion Reaction of Diazoester with Aldehyde Catalyzed by N-Protonated Chiral Oxazaborolidine: Mechanisms and Stereoselectivity
Journal of Physical Chemistry A, (119): 8422-8431 2015.

Wang, Y.; Guo, X. K.; Wu, B. H.; Wei, D. H.; Tang, M. S.
Mechanistic and stereoselectivity study for the reaction of trifluoropyruvates with arylpropenes catalyzed by a cationic Lewis acid rhodium complex
Rsc Advances, (5): 100147-100158 2015.

Wang, Y. F.; Li, B.; Huang, J. G.; Li, J.; Li, Z. R.
Effect of alkaline earth metal atom on the large static first hyperpolarizabilities of alkaline earth-based alkalides Be(NH3)(n)M (M = Be and Ca) in comparison with alkalides Li(NH3)(n)Na (n=1-3)
Computational and Theoretical Chemistry, (1051): 10-16 2015.

Wang, Y. X.; Zheng, W. R.
A comparison of the C-H bond dissociation enthalpies of sulfur-containing fused heterocyclic compounds to the C-H bond dissociation enthalpies in other heterocycles
Journal of Sulfur Chemistry, (36): 155-169 2015.

Wang, Y. X.; Zheng, W. R.
A theoretical study on C-H bond dissociation enthalpies of oxygen-containing fused heterocyclic compounds
Research on Chemical Intermediates, (41): 7207-7225 2015.

Wang, Y. Y.; Wang, Y.; Zhang, W. J.; Zhu, Y. Y.; Wei, D. H.; Tang, M. S.
Mechanisms and stereoselectivities of the Rh(I)catalyzed carbenoid carbon insertion reaction of benzocyclobutenol with diazoester

Organic & Biomolecular Chemistry, (13): 6587-6597 2015.

Wang, Z. B.; Sezen, H.; Liu, J. X.; Yang, C. W.; Roggenbuck, S. E.; Peikert, K.; Froba, M.; Mavrantonakis, A.; Supronowicz, B.; Heine, T.; Gliemann, H.; Woll, C.
Tunable coordinative defects in UHM-3 surface-mounted MOFs for gas adsorption and separation: A combined experimental and theoretical study
Microporous and Mesoporous Materials, (207): 53-60 2015.

Wang, Z. X.; Liu, Q. Q.; Chen, T.; Wang, Y.; Yuan, J.; Zheng, C.; Chen, R. F.; Huang, W.
Molecular rearrangement at charged states: Intrinsic effects upon photo and electroluminescence
Dyes and Pigments, (113): 529-535 2015.

Wei, L.; Yang, X.; Gao, Z. Q.; Wang, D. Q.; Xue, J. Q.; Yang, W. J.; Wang, J. J.; Zhang, Y. H.; Fang, G. L.; Liu, Y.
Oxovanadium(IV) Schiff Base Complex Derived From Phenylalanine Analogue Containing 2,3-Diaminopropionic Acid (DAP): Synthesis, Computational Study, and Biological Evaluation
Synthesis and Reactivity in Inorganic Metal-Organic and Nano-Metal Chemistry, (45): 455-467 2015.

Weinhold, F.; Klein, R. A.
Improved General Understanding of the Hydrogen-Bonding Phenomena: A Reply
Angewandte Chemie-International Edition, (54): 2600-2602 2015.

Wen, J.; Havlas, Z.; Michl, J.
Captodatively Stabilized Biradicaloids as Chromophores for Singlet Fission
Journal of the American Chemical Society, (137): 165-172 2015.

Werle, C.; Karmazin, L.; Bailly, C.; Ricard, L.; Djukic, J. P.
Stabilization of an Electron-Unsaturated Pd(I)-Pd(I) Unit by Double Hemichelation
Organometallics, (34): 3055-3064 2015.

West, A. C.; Schmidt, M. W.; Gordon, M. S.; Ruedenberg, K.
A Comprehensive Analysis in Terms of Molecule-Intrinsic, Quasi-Atomic Orbitals. III. The Covalent Bonding Structure of Urea
Journal of Physical Chemistry A, (119): 10368-10375 2015.

West, A. H. C.; Yoder, B. L.; Luckhaus, D.; Signorell, R.
Solvated Electrons in Clusters: Magic Numbers for the Photoelectron Anisotropy
Journal of Physical Chemistry A, (119): 12376-12382 2015.

Weststrate, N. A.; Fernandez, I.; Liles, D. C.; van Jaarsveld, N.; Lotz, S.
Fischer-Type Carbene Complexes of Tris(1,4-phenylene)amines and Tri(2-furyl)phosphine
Organometallics, (34): 696-710 2015.

Wielinska, J.; Liberek, B.; Nowacki, A.
DFT studies of the formation of furanoid derivatives of ammonium chlorides
Journal of Molecular Graphics and Modelling, (56): 74-83 2015.

Wilfer, C.; Liebhauser, P.; Erdmann, H.; Hoffmann, A.; Herres-Pawlis, S.
Biomimetic Hydroxylation Catalysis Through Self-Assembly of a Bis(pyrazolyl)methane Copper-Peroxo Complex
European Journal of Inorganic Chemistry: 494-502 2015.

Wilfer, C.; Liebhauser, P.; Hoffmann, A.; Erdmann, H.; Grossmann, O.; Runtsch, L.; Paffenholz, E.; Schepper, R.; Dick, R.; Bauer, M.; Durr, M.; Ivanovic-Burmazovic, I.; Herres-Pawlis, S.
Efficient Biomimetic Hydroxylation Catalysis with a Bis(pyrazolyl)imidazolylmethane Copper Peroxide Complex
Chemistry-a European Journal, (21): 17639-17649 2015.

Willmann, K.; Vent-Schmidt, T.; Rasanen, M.; Riedel, S.; Khriachtchev, L.
Matrix-isolation and computational study of the HKrCCH center dot center dot center dot HCCH complex
Rsc Advances, (5): 35783-35791 2015.

Woidy, P.; Buhl, M.; Kraus, F.
UO2(NH3)(5) Br-2 center dot NH3: synthesis, crystal structure, and speciation in liquid ammonia solution by first-principles molecular dynamics simulations
Dalton Transactions, (44): 7332-7337 2015.

Wojciechowska, A.; Gagor, A.; Zierkiewicz, W.; Jarzab, A.; Dylong, A.; Duczmal, M.
Metal-organic framework in an L-arginine copper(II) ion polymer: structure, properties, theoretical studies and microbiological activity
Rsc Advances, (5): 36295-36306 2015.

Wojciechowska, A.; Janczak, J.; Zierkiewicz, W.; Dylong, A.; Matczak-Jon, E.
Structural and spectroscopic properties and density functional theory (DFT) calculations of a linearly bridged zinc(II) L-tyrosinato complex
Polyhedron, (85): 665-674 2015.

Wolf, S.; Reiter, K.; Weigend, F.; Klopper, W.; Feldmann, C.
(Pb6I8){Mn(CO)(5)}(6)}(2-): An Octahedral (M6X8)-like Cluster with Inverted Bonding
Inorganic Chemistry, (54): 3989-3994 2015.

Wollenhaupt, M.; Krupicka, M.; Marx, D.
Should the Woodward-Hoffmann Rules be Applied to Mechanochemical Reactions?
Chemphyschem, (16): 1593-1597 2015.

Wolters, L. P.; Bickelhaupt, F. M.
The activation strain model and molecular orbital theory
Wiley Interdisciplinary Reviews-Computational Molecular Science, (5): 324-343 2015.

Word, T. A.; Whittington, C. L.; Karolak, A.; Kemp, M. T.; Woodcock, H. L.; van der Vaart, A.; Larsen, R. W.
Photoacoustic calorimetry study of ligand photorelease from the Ru(II)bis(2,2 '-bipyridine)(6,6 '-dimethyl-2,2 '-bipyridine) complex in aqueous solution
Chemical Physics Letters, (619): 214-218 2015.

Wu, D. H.; Xie, Z. J.; Zhou, Z.; Shen, P. W.; Chen, Z. F.
Designing high-voltage carbonyl-containing polycyclic aromatic hydrocarbon cathode materials for Li-ion batteries guided by Clar's theory
Journal of Materials Chemistry A, (3): 19137-19143 2015.

Wu, Q. Y.; Lan, J. H.; Wang, C. Z.; Zhao, Y. L.; Chai, Z. F.; Shi, W. Q.
Terminal U E (E = N, P, As, Sb, and Bi) Bonds in Uranium Complexes: A Theoretical Perspective
Journal of Physical Chemistry A, (119): 922-930 2015.

Wu, S. X.; Kan, Y. H.; Li, H. B.; Zhao, L.; Wu, Y.; Su, Z. M.
Quantum Chemical Insight into the LiF Interlayer Effects in Organic Electronics: Reactions between Al Atom and LiF Clusters
Journal of Physical Chemistry Letters, (6): 2950-2958 2015.

Wu, W. H.; Lu, Y. X.; Ding, H. R.; Peng, C. J.; Liu, H. L.
The acidity/basicity of metal-containing ionic liquids: insights from surface analysis and the Fukui function
Physical Chemistry Chemical Physics, (17): 1339-1346 2015.

Xavier, R. J.; Dinesh, P.
A study of the molecular, vibrational, electronic and quantum chemical investigation of 2-methyl-1-vinylimidazole
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (136): 1569-1581 2015.

Xavier, R. J.; Prabaharan, A.
Vibrational spectroscopic investigations of 4,4-dimethyl-2-oxazoline: A density functional theory approach
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (136): 1530-1542 2015.

Xavier, T. S.; Kenny, P. T. M.; Manimaran, D.; Joe, I. H.
FT-IR and Raman spectroscopic and DFT studies of anti-cancer active molecule N-{(meta-ferrocenyl) Benzoyl} - L-Alanine - Glycine ethyl ester
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (145): 523-530 2015.

Xia, Y.; Miao, Z. H.; Wang, F.; Yao, H. T.; Cui, M. F.; Ma, Y.; Qi, Z. J.; Sun, Y. M.
Theoretical investigation on electronic structures and stability of the dinuclear palladium and platinum complexes
Journal of Organometallic Chemistry, (779): 81-85 2015.

Xiao, C. L.; Wang, C. Z.; Mei, L.; Zhang, X. R.; Wall, N.; Zhao, Y. L.; Chai, Z. F.; Shi, W. Q.
Europium, uranyl, and thorium-phenanthroline amide complexes in acetonitrile solution: an ESI-MS and DFT combined investigation
Dalton Transactions, (44): 14376-14387 2015.

Xie, J. B.; Li, Q. L.; Shi, W. J.; Ren, F. D.; Song, H.
Theoretical studies on H-M center dot center dot center dot pi (M=H, Li, Na, K) interactions involving the pi-electron donors, C2H2, C2H4 and C6H6
Indian Journal of Chemistry Section a-Inorganic Bio-Inorganic Physical Theoretical & Analytical Chemistry, (54): 709-719 2015.

Xie, L. M.; Bai, F. Q.; Li, W.; Zhang, Z. X.; Zhang, H. X.
Theoretical research on the effect of regulated pi-conjugation on the photophysical properties of Ir(III) complexes
Physical Chemistry Chemical Physics, (17): 10014-10021 2015.

Xing, Y. M.; Zhang, L.; Fang, D. C.
DFT Studies on the Mechanism of Palladium(IV)-Mediated C-H Activation Reactions: Oxidant Effect and Regioselectivity
Organometallics, (34): 770-777 2015.

Xiong, X. G.; Wang, Y. L.; Xu, C. Q.; Qiu, Y. H.; Wang, L. S.; Li, J.
On the gold-ligand covalency in linear AuX2 (-) complexes
Dalton Transactions, (44): 5535-5546 2015.

Xiong, Y.; Yao, S. L.; Muller, R.; Kaupp, M.; Driess, M.
From Silylone to an Isolable Monomeric Silicon Disulfide Complex
Angewandte Chemie-International Edition, (54): 10254-10257 2015.

Xu, K. M.; Huang, T.; Liu, Y. R.; Jiang, S.; Zhang, Y.; Lv, Y. Z.; Gai, Y. B.; Huang, W.
Probing the structures and electronic properties of dual-phosphorus-doped gold cluster anions (AunP2-, n=1-8): A density functional theory investigation
Chemical Physics, (456): 13-21 2015.

Xu, K. M.; Jiang, S.; Zhu, Y. P.; Huang, T.; Liu, Y. R.; Zhang, Y.; Lv, Y. Z.; Huang, W.
On the properties of Au2P3z (z =-1, 0,+1): analysis of geometry, interaction, and electron density
Rsc Advances, (5): 26071-26080 2015.

Xu, Q. H.; Li, D. Z.; Zhang, S. G.
A Density-Functional Study on the Adsorption of C2H Radical onto Small Silver Clusters
Journal of Cluster Science, (26): 529-539 2015.

Xu, S. H.; Wang, Z. C.; Wang, C. L.; Wang, Z. Y.; Cui, Y. P.
Investigation of a naked Ag-7 cluster: configurations and spectral characteristics
New Journal of Chemistry, (39): 3105-3108 2015.

Xu, Y. J.; Viger-Gravel, J.; Korobkov, I.; Bryce, D. L.
Mechanochemical Production of Halogen-Bonded Solids Featuring P=O center dot center dot center dot I-C Motifs and Characterization via X-ray Diffraction, Solid-State Multinuclear Magnetic Resonance, and Density Functional Theory

Journal of Physical Chemistry C, (119): 27104-27117 2015.

Xue, Y. S.; Cai, Y. P.; Chen, Z. X.
Mechanism and stereoselectivity of the Rh(II)-catalyzed cyclopropanation of diazooxindole: a density functional theory study
Rsc Advances, (5): 57781-57791 2015.

Yablokov, A. S.; Steglenko, D. V.; Ruchko, E. A.; Nawrozkij, M. B.; Brunilina, L. L.; Novakov, I. A.; Minkin, V. I.
Experimental and quantum chemical study of the reactions of 2-methyloxirane with 5-alkyl-6-(2,6-dihalobenzyl)-2-thioxo-1,2-dihydropyrimidine-4(3H)-one derivatives
Russian Chemical Bulletin, (64): 525-533 2015.

Yadav, D.; Siwatch, R. K.; Sinhababu, S.; Karwasara, S.; Singh, D.; Rajaraman, G.; Nagendran, S.
Digermylene Oxide Stabilized Group 11 Metal Iodide Complexes
Inorganic Chemistry, (54): 11067-11076 2015.

Yahia, W.; Khorief Nacereddine, A.; Seddiki, K.; Liacha, M.
EXPERIMENTAL AND THEORETICAL INVESTIGATION OF THE INTRAMOLECULAR CYCLISATION OF N-(BENZOXAZOLINON-6-YL)MALEIMIDE DERIVATIVES
Revue Roumaine de Chimie, (60): 853-859 2015.

Yalcin, S. P.; Ceylan, U.; Sarioglu, A. O.; Sonmez, M.; Aygun, M.
Synthesis, structural, spectral (FT-IR, H-1 and C-13 NMR and UV-Vis), NBO and first order hyperpolarizability analysis of N-(4-nitrophenyl)-2, 2-dibenzoylacetamide by density functional theory
Journal of Molecular Structure, (1098): 400-407 2015.

Yamaguchi, E.; Wang, C. G.; Fukazawa, A.; Taki, M.; Sato, Y.; Sasaki, T.; Ueda, M.; Sasaki, N.; Higashiyama, T.; Yamaguchi, S.
Environment-Sensitive Fluorescent Probe: A Benzophosphole Oxide with an Electron-Donating Substituent
Angewandte Chemie-International Edition, (54): 4539-4543 2015.

Yan, B. F.; Li, W. Z.; Xiao, C. P.; Li, Q. Z.; Cheng, J. B.
Insight into the substitution reactions of silylenoid H2SiLiF with GeH3X (X=F, Cl, Br): a theoretical study
Journal of Molecular Modeling, (21) 2015.

Yan, B. F.; Li, W. Z.; Xiao, C. P.; Liu, Z. B.; Li, Q. Z.; Cheng, J. B.
New insights into the insertion reactions of germylenoid H2GeLiF with RH (R=F, OH, NH2)
Journal of Molecular Modeling, (21) 2015.

Yang, C. T.; Wood, B. C.; Bhethanabotla, V. R.; Joseph, B.
The effect of the morphology of supported subnanometer Pt clusters on the first and key step of CO2 photoreduction
Physical Chemistry Chemical Physics, (17): 25379-25392 2015.

Yang, D. P.; Zhao, F.; Zheng, R.; Wang, Y. S.; Lv, J.
A detailed theoretical investigation on the excited-state intramolecular proton-transfer mechanism of 3-BTHPB chemosensor
Theoretical Chemistry Accounts, (134) 2015.

Yang, D. P.; Zhao, J. F.; Zheng, R.; Wang, Y. S.; Lv, J.
A DFT/TDDFT investigation of the excited state proton transfer reaction of fisetin chromophore
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (151): 368-374 2015.

Yang, F.; Yu, P. Y.; Zhao, J.; Zhao, Y.; Wang, J. P.
Intermolecular Hydrogen Bonding Structural Dynamics in Ethylene Glycol by Femtosecond Nonlinear Infrared Spectroscopy
Acta Physico-Chimica Sinica, (31): 1275-1282 2015.

Yang, H. Q.; Fu, H. Q.; Su, B. F.; Xiang, B.; Xu, Q. Q.; Hu, C. W.
Theoretical Study on the Catalytic Reduction Mechanism of NO by CO on Tetrahedral Rh-4 Subnanocluster

Journal of Physical Chemistry A, (119): 11548-11564 2015.

Yang, L.; Nesterov, V. N.; Wang, X. P.; Richmond, M. G.
Synthesis of the Stereoisomeric Clusters 1,2-Os-3(CO)(10)(trans-dpmn) and 1,2-Os-3(CO)(10)(cis-dpmn) where dpmn=2,3-bis(diphenylphosphinomethyl)-5-norbornene : DFT Evaluation of the Isomeric Clusters 1,2-Os-3(CO)(10)(dpmn) and Isomer-Dependent Diphosphine Ligand Activation
Journal of Cluster Science, (26): 93-109 2015.

Yang, L. M.; Bacic, V.; Popov, I. A.; Boldyrev, A. I.; Heine, T.; Frauenheim, T.; Ganz, E.
Two-Dimensional Cu2Si Monolayer with Planar Hexacoordinate Copper and Silicon Bonding
Journal of the American Chemical Society, (137): 2757-2762 2015.

Yang, L. M.; Popov, I. A.; Boldyrev, A. I.; Heine, T.; Frauenheim, T.; Ganz, E.
Post-anti-van't Hoff-Le Bel motif in atomically thin germanium-copper alloy film
Physical Chemistry Chemical Physics, (17): 17545-17551 2015.

Yang, L. M.; Popov, I. A.; Frauenheim, T.; Boldyrev, A. I.; Heine, T.; Baciac, V.; Ganz, E.
Revealing unusual chemical bonding in planar hyper-coordinate Ni2Ge and quasi-planar Ni2Si two-dimensional crystals
Physical Chemistry Chemical Physics, (17): 26043-26048 2015.

Yang, N.; Su, Z. S.; Feng, X. M.; Hu, C. W.
Theoretical Studies on the Asymmetric Baeyer-Villiger Oxidation Reaction of 4-Phenylcyclohexanone with m-Chloroperoxobenzoic Acid Catalyzed by Chiral Scandium(III)-N,N '-Dioxide Complexes
Chemistry-a European Journal, (21): 7264-7277 2015.

Yang, S. N.; Zhang, C. J.
Theoretical Investigation of Obtaining Compounds with Planar Tetracoordinate Carbons by Frustrated Lewis Pairs
Journal of Physical Chemistry A, (119): 8950-8957 2015.

Yang, Y. G.; Liu, Y. F.; Yang, D. P.; Li, H.; Jiang, K.; Sun, J. F.
Photoinduced excited state intramolecular proton transfer and spectral behaviors of Aloesaponarin 1
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (151): 814-820 2015.

Yang, Y. Q.; Fang, Y.; Liu, J.; Hu, S. Y.; Hu, S.; Yang, L.; Wang, D. W.; Zhang, H. B.; Luo, S. Z.
Complexation behavior of Eu(III), Tb(III), Tm(III), and Am(III) with three 1,10-phenanthroline-type ligands: insights from density functional theory
Journal of Molecular Modeling, (21) 2015.

Yang, Y. Q.; Hu, S. Y.; Fang, Y.; Wei, H. Y.; Hu, S.; Wang, D. W.; Yang, L.; Zhang, H. B.; Luo, S. Z.
Density functional theory study of the Eu(III) and Am(III) complexes with two 1,10-phenanthroline-type ligands
Polyhedron, (95): 86-90 2015.

Yang, Y. Q.; Liu, J.; Yang, L.; Li, K.; Zhang, H. B.; Luo, S. Z.; Rao, L. F.
Probing the difference in covalence by enthalpy measurements: a new heterocyclic N-donor ligand for actinide/lanthanide separation
Dalton Transactions, (44): 8959-8970 2015.

Ye, F.; Qu, S. L.; Zhou, L.; Peng, C.; Wang, C. P.; Cheng, J. J.; Hossain, M. L.; Liu, Y. Z.; Zhang, Y.; Wang, Z. X.; Wang, J. B.
Palladium-Catalyzed C-H Functionalization of Acyldiazomethane and Tandem Cross-Coupling Reactions
Journal of the American Chemical Society, (137): 4435-4444 2015.

Yildirim, M. H.; Pasaoglu, H.; Odabasoglu, H. Y.; Odabasoglu, M.; Yildirim, A. O.
Synthesis, structural and computational characterization of 2-amino-3,5-diiodobenzoic acid and 2-amino-3,5-dibromobenzoic acid
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (146): 50-60 2015.

Yildiz, C. B.; Azizoglu, A.

Substituent and Solvent Effects on the Electronic and Structural Properties of Silacyclopropylidenoids
Journal of the Mexican Chemical Society, (59): 24-28 2015.

Yin, J.; Chaitanya, K.; Ju, X. H.
Theoretical study of the fluorination effect on charge transport properties in fused thiophene derivatives
Rsc Advances, (5): 65192-65202 2015.

Yin, Y. P.; Dong, C. Z.; Ding, X. B.
Theoretical Study on Structures and Bond Properties of NpO Ions and NpO Complexes in the Gas Phase and Aqueous Solution
Journal of Physical Chemistry A, (119): 3253-3260 2015.

Yoosefian, M.; Karimi-Maleh, H.; Sanati, A. L.
A theoretical study of solvent effects on the characteristics of the intramolecular hydrogen bond in Droxidopa
Journal of Chemical Sciences, (127): 1007-1013 2015.

Yoosefian, M.; Mola, A.
Solvent effects on binding energy, stability order and hydrogen bonding of guanine-cytosine base pair
Journal of Molecular Liquids, (209): 526-530 2015.

Yoosefian, M.; Raissi, H.; Mola, A.
The hybrid of Pd and SWCNT (Pd loaded on SWCNT) as an efficient sensor for the formaldehyde molecule detection: A DFT study
Sensors and Actuators B-Chemical, (212): 55-62 2015.

Yoosefian, M.; Raissi, H.; Soheili, S.
A comprehensive study of the structure, tautomeric properties, and conformational flexibility of 3-Hydroxy-propeneselenal
Journal of Chemical Sciences, (127): 999-1006 2015.

You, X.; Xie, X.; Chen, H. Y.; Li, Y. X.; Liu, Y. H.
Cyano-Schmittel Cyclization through Base-Induced Propargyl-Allenyl Isomerization: Highly Modular Synthesis of Pyridine-Fused Aromatic Derivatives
Chemistry-a European Journal, (21): 18699-18705 2015.

You, Z. Q.; Mewes, J. M.; Dreuw, A.; Herbert, J. M.
Comparison of the Marcus and Pekar partitions in the context of non-equilibrium, polarizable-continuum solvation models
Journal of Chemical Physics, (143) 2015.

Yourdkhani, S.; Korona, T.; Hadipour, N. L.
Structure and Energetics of Complexes of B12N12 with Hydrogen Halides-SAPT(DFT) and MP2 Study
Journal of Physical Chemistry A, (119): 6446-6467 2015.

Yu, W.; Guggolz, L.; Fuhr, O.; Fenske, D.; Dehnen, S.
Syntheses, structures and theoretical investigations of Au10S2(PPh2)(2)(dppma(2))(4)-(dppma(3)) center dot Au6S2(dppma2)(2)(dppma3)
Dalton Transactions, (44): 9363-9366 2015.

Yu, Z. N.; Xu, X.; Xia, S. W.; Yu, L. M.
Density Functional Theoretical Study on the Reaction Mechanism of HOCO and Its Radical
Chinese Journal of Structural Chemistry, (34): 985-994 2015.

Yuan, H. Y.; Zhang, J. P.
DBU-H (+) and H(2)o as effective catalyst form for 2,3-dihydropyrido 2,3-d pyrimidin-4(1H)-ones: A DFT Study
Journal of Computational Chemistry, (36): 1295-1303 2015.

Yuan, J. N.; Cheng, Y.; Zhang, X. Q.; Chen, X. R.; Cai, L. C.

First-Principles Study of Electronic and Elastic Properties of Hexagonal Layered Crystal MoS2 Under Pressure
Zeitschrift Fur Naturforschung Section a-a Journal of Physical Sciences, (70): 529-537 2015.

Yuan, J. Y.; Yang, B. C.; Li, G. W.; Si, Y. B.; Wang, S. W.; Zhang, S. R.; Chen, H. Y.
Geometries and electronic properties of bimetallic CuVn (n=1-5) clusters and their cations: Insight from density functional calculations
Computational Materials Science, (102): 213-219 2015.

Yuan, K.; Dang, J. S.; Guo, Y. J.; Zhao, X.
Theoretical Prediction of the Host-Guest Interactions Between Novel Photoresponsive Nanorings and C-60: A Strategy for Facile Encapsulation and Release of Fullerene
Journal of Computational Chemistry, (36): 518-528 2015.

Yuan, K.; Zhou, C. H.; Zhu, Y. C.; Zhao, X.
Theoretical exploration of the nanoscale host-guest interactions between n cycloparaphenylenes (n=10, 8 and 9) and fullerene C-60: from single- to three-potential well
Physical Chemistry Chemical Physics, (17): 18802-18812 2015.

Yuan, R. M.; Lin, Z. Y.
Mechanistic Insight into the Gold-Catalyzed Carboxylative Cyclization of Propargylamines
Acs Catalysis, (5): 2866-2872 2015.

Yuan, X. G.; Zhang, W. W.; Xie, L. H.; Ma, J.; Huang, W.; Liu, W. J.
Role of Planar Conformations in Aggregation Induced Spectral Shifts of Supermolecular Oligofluorenols in Solutions and Films: A Combined Experimental and MD/TD-DFT Study
Journal of Physical Chemistry B, (119): 10316-10333 2015.

Yuki, M.; Sakata, K.; Hirao, Y.; Nonoyama, N.; Nakajima, K.; Nishibayashi, Y.
Thiolate-Bridged Dinuclear Ruthenium and Iron Complexes as Robust and Efficient Catalysts toward Oxidation of Molecular Dihydrogen in Protic Solvents
Journal of the American Chemical Society, (137): 4173-4182 2015.

Yumura, T.; Yamashita, H.
Key factors in determining the arrangement of pi-conjugated oligomers inside carbon nanotubes
Physical Chemistry Chemical Physics, (17): 22668-22677 2015.

Yurdakul, S.; Badoglu, S.; Gulesci, Y.
Experimental and theoretical study on free 5-nitroquinoline, 5-nitroisoquinoline, and their zinc(II) halide complexes
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (137): 945-956 2015.

Yuvaraj, K.; Roy, D. K.; Mondal, B.; Varghese, B.; Ghosh, S.
Homometallic Cubane Clusters: Participation of Three-Coordinated Hydrogen in 60-Valence Electron Cubane Core
Inorganic Chemistry, (54): 8673-8678 2015.

Zabardasti, A.; Sharifi-Rad, A.; Kakanejadifard, A.
Interplay between H center dot center dot center dot O, H center dot center dot center dot X, X center dot center dot center dot O and X center dot center dot center dot X interactions in the complex pairing of formyl halides with hypohalous acids
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (151): 746-759 2015.

Zaboli, M.; Raissi, H.
The analysis of electronic structures, adsorption properties, NBO, QTAIM and NMR parameters of the adsorbed hydrogen sulfide on various sites of the outer surface of aluminum phosphide nanotube: a DFT study
Structural Chemistry, (26): 1059-1075 2015.

Zaboli, M.; Raissi, H.
Structural, QTAIM, thermodynamic properties, bonding, aromaticity and NMR analyses of cation-pi interactions of mono and divalent metal cations (Li+, Na+, K+, Be2+, Mg2+, and Ca2+) with substituted pyrazine derivatives

Journal of Theoretical & Computational Chemistry, (14) 2015.

Zahedi, E.; Pangh, A.; Ghorbanpour, H.
DFT STUDY OF CO AND NO ADSORPTION ON BORON NITRIDE (BN)(n) (=) (3) (-) (5) NANOCLUSTERS
Surface Review and Letters, (22) 2015.

Zahedi-Tabrizi, M.; Gerivani, B.; Tayyari, S. F.
Hydrogen bond strength and vibrational assignment of the enol form of 3-(ortho-methoxyphenylthio) and 3-(para-methoxyphenylthio) pentane-2,4-dione
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (136): 731-742 2015.

Zahl, M. G.; Fossheim, R.; Borve, K. J.; Saethre, L. J.; Thomas, T. D.
Electronic Properties of Chlorine, Methyl, and Chloromethyl as Substituents to the Ethylene Group-Viewed from the Core of Carbon
Journal of Physical Chemistry A, (119): 9481-9493 2015.

Zaitsev, K. V.; Lermontova, E. K.; Churakov, A. V.; Tafeenko, V. A.; Tarasevich, B. N.; Poleshchuk, O. K.; Kharcheva, A. V.; Magdesieva, T. V.; Nikitin, O. M.; Zaitseva, G. S.; Karlov, S. S.
Compounds of Group 14 Elements with an Element-Element (E = Si, Ge, Sn) Bond: Effect of the Nature of the Element Atom
Organometallics, (34): 2765-2774 2015.

Zamorano, A.; Rendon, N.; Lopez-Serrano, J.; Valpuesta, J. E. V.; Alvarez, E.; Carmona, E.
Dihydrogen Catalysis of the Reversible Formation and Cleavage of C-H and N-H Bonds of Aminopyridinate Ligands Bound to (eta(5)-C5Me5)Ir-III
Chemistry-a European Journal, (21): 2576-2587 2015.

Zanuttini, D.; Gervais, B.
Ground and Excited States Of OH-(H2O)(n) Clusters
Journal of Physical Chemistry A, (119): 8188-8201 2015.

Zapata-Torres, G.; Fierro, A.; Barriga-Gonzalez, G.; Salgado, J. C.; Celis-Barros, C.
Revealing Monoamine Oxidase B Catalytic Mechanisms by Means of the Quantum Chemical Cluster Approach
Journal of Chemical Information and Modeling, (55): 1349-1360 2015.

Zarycz, M. N. C.; Provasi, P. F.
Investigation of the resonance-assisted hydrogen bond in model beta-diketones through localized molecular orbital analysis of the spin-spin coupling constants related to the O-H center dot center dot center dot O hydrogen bond
Magnetic Resonance in Chemistry, (53): 120-129 2015.

Zarycz, M. N. C.; Provasi, P. F.; Sauer, S. P. A.
On the truncation of the number of excited states in density functional theory sum-over-states calculations of indirect spin spin coupling constants
Journal of Chemical Physics, (143) 2015.

Zeng, J. P.; Dai, Y.; Shi, W. Y.; Shao, J. L.; Sun, G. X.
Molecular dynamics simulation on the interaction between polymer inhibitors and anhydrite surface
Surface and Interface Analysis, (47): 896-902 2015.

Zeng, T.; Hoffmann, R.; Nesper, R.; Ashcroft, N. W.; Strobel, T. A.; Proserpio, D. M.
Li-Filled, B-Substituted Carbon Clathrates
Journal of the American Chemical Society, (137): 12639-12652 2015.

Zeng, T.; Lancaster, K. M.; Ananth, N.; Hoffmann, R.
Anomalous orbital admixture in ammine complexes
Journal of Organometallic Chemistry, (792): 6-12 2015.

Zeng, X. L.; Wang, Y.

Mechanism and Regioselectivity of Addition Reactions of CH3OH to Germasilenes
Acta Physico-Chimica Sinica, (31): 1699-1707 2015.

Zeng, Y.; Yu, Y.; Feng, H.; King, R. B.; Schaefer, H. F.
Nickelacyclopentadienylchromium Tricarbonyl Unit as a Bulky Pseudohalogen in Cyclopentadienylchromium Complexes Leading to Low-Energy High-Spin Structures
Inorganic Chemistry, (54): 5309-5315 2015.

Zenn, R. K.; Abad, E.; Kastner, J.
Influence of the Environment on the Oxidative Deamination of p-Substituted Benzylamines in Monoamine Oxidase
Journal of Physical Chemistry B, (119): 3678-3686 2015.

Zeonjuk, L. L.; Petkov, P. S.; Heine, T.; Roschenthaler, G. V.; Eicher, J.; Vankova, N.
Are intramolecular frustrated Lewis pairs also intramolecular catalysts? A theoretical study on H-2 activation
Physical Chemistry Chemical Physics, (17): 10687-10698 2015.

Zeyrek, C. T.; Alpaslan, G.; Alyar, H.; Yildiz, M.; Dilek, N.; Unver, H.
Synthesis, molecular structure, spectroscopic and theoretical studies on E-2-ethoxy-4- (4-ethoxyphenylimino)methyl phenol
Journal of Molecular Structure, (1088): 14-27 2015.

Zeyrek, C. T.; Kocak, S. B.; Unver, H.; Pektas, S.; Basterzi, N. S.; Celik, O.
Molecular structure and density functional modelling studies of 2- (E)-2-(4-hydroxyphenyl)ethyliminomethyl phenol
Journal of Molecular Structure, (1100): 570-581 2015.

Zeyrek, C. T.; Unver, H.; Arpaci, O. T.; Polat, K.; Iskeleli, N. O.; Yildiz, M.
Experimental and theoretical characterization of the 2-(4-bromobenzyl)-5-ethylsulphonyl-1,3-benzoxazole
Journal of Molecular Structure, (1081): 22-37 2015.

Zhang, C.; Santiago, C. B.; Crawford, J. M.; Sigman, M. S.
Enantioselective Dehydrogenative Heck Arylations of Trisubstituted Alkenes with Indoles to Construct Quaternary Stereocenters
Journal of the American Chemical Society, (137): 15668-15671 2015.

Zhang, C.; Santiago, C. B.; Kou, L.; Sigman, M. S.
Alkenyl Carbonyl Derivatives in Enantioselective Redox Relay Heck Reactions: Accessing alpha,beta-Unsaturated Systems
Journal of the American Chemical Society, (137): 7290-7293 2015.

Zhang, C. J.; Zhao, H.; Li, J. X.
Poly-membered macrometallacyclic complexes of silver and gold with functionalized N-Heterocyclic carbene and functionalized 2-borabicyclo 1.1.0 but-1(3)-ene ligands: A DFT study
Computational and Theoretical Chemistry, (1054): 22-28 2015.

Zhang, D. D.; Chen, X. K.; Liu, H. L.; Huang, X. R.
An theoretical investigation of reaction site of 2,4,6-trifluorobenzophenone, 2,4,6-trifluorophenylsulfone with hydroquinone
High Performance Polymers, (27): 868-876 2015.

Zhang, G. Q.; Wang, H.; Yue, H. J.; Li, H.; Zhang, S. N.; Fu, L.
Ligand effects due to resonance character in LAuCCH- (L=F, Cl, Br, I, CCH) complexes: an NBO/NRT analysis
Journal of Molecular Modeling, (21) 2015.

Zhang, G. Q.; Yue, H. J.; Weinhold, F.; Wang, H.; Li, H.; Chen, D. Z.
Resonance Character of Copper/Silver/Gold Bonding in Small MoleculeMX (X=F, Cl, Br, CH3, CF3) Complexes
Chemphyschem, (16): 2424-2431 2015.

Zhang, H.; Zheng, G. L.; Lv, G.; Geng, Y. Z.; Ji, Q.

Covalent intermolecular interaction of the nitric oxide dimer (NO)(2)
Chinese Physics B, (24) 2015.

Zhang, H. H.
A DFT study on direct hydrogenation of amide catalyzed by a PNN Ru(II) pincer complex
Computational and Theoretical Chemistry, (1066): 1-6 2015.

Zhang, H. H.; Zhao, X.; Chen, D. Z.
A Computational Investigation of the Hydrogenation of Imines Catalyzed by Rhodium Thiolate Complexes
International Journal of Quantum Chemistry, (115): 1-5 2015.

Zhang, J. J.; Fu, X. D.; Lin, Z. Y.; Xie, Z. W.
Supercarborane Radical Anions with 2n+3 Electron Counts: A Combined Experimental and Theoretical Study
Inorganic Chemistry, (54): 1965-1973 2015.

Zhang, J. J.; Lin, Z. Y.; Xie, Z. W.
DFT Studies on Structures, Stabilities, and Electron Affinities of closo-Supercarboranes C2Bn-2Hn (n=13-20)
Organometallics, (34): 5576-5588 2015.

Zhang, J. Y.; Gong, X. D.
Computer simulations and analysis of structural and energetic features of crystalline cage energetic compound: 2, 4, 6, 8, 12-pentanitro-10-(3, 5, 6-trinitro (2-pyridyl))-2, 4, 6, 8, 12-hexaazatetracyclo 5.5.0.0(3,11).0(5,9) dodecane
Journal of Physical Organic Chemistry, (28): 577-585 2015.

Zhang, L.; Wang, J. M.; Wang, Q. R.; Zhang, D. W.; Li, Z. T.; Li, Z. M.
Theoretical investigation on SnCl4-catalyzed tandem dimerization/oxy-2-azonia-Cope rearrangements between beta,gamma-unsaturated ketones and imines
Theoretical Chemistry Accounts, (134) 2015.

Zhang, L. D.; Chen, Q. X.; Zhang, P.
A theoretical kinetics study of the reactions of methylbutanoate with hydrogen and hydroxyl radicals
Proceedings of the Combustion Institute, (35): 481-489 2015.

Zhang, M.; Gao, K. Q.; Sheng, L.
Predicted Organic Noble-Gas Hydrides Derived from Acrylic Acid
Journal of Physical Chemistry A, (119): 2393-2400 2015.

Zhang, M. X.; Zhang, M. J.; Li, W. Z.; Li, Q. Z.; Cheng, J. B.
Structure of H2GeFMgF and its insertion reactions with RH (R = F, OH, NH2)
Journal of Theoretical & Computational Chemistry, (14) 2015.

Zhang, N.; Luo, M. B.; Chi, C. X.; Wang, G. J.; Cui, J. M.; Zhou, M. F.
Infrared Photodissociation Spectroscopy of Mass-Selected Heteronuclear Iron-Copper Carbonyl Cluster Anions in the Gas Phase
Journal of Physical Chemistry A, (119): 4142-4150 2015.

Zhang, S.; Katz, A.; Gates, B. C.; Dixon, D. A.
Structures, relative energies, and ligand dissociation energies of iridium carbonyl phosphine clusters
Computational and Theoretical Chemistry, (1069): 18-35 2015.

Zhang, S. L.; Huang, L.; Sun, L. J.
The mechanism, electronic and ligand effects for reductive elimination from arylPd(II) trifluoromethyl complexes: a systematic DFT study
Dalton Transactions, (44): 4613-4622 2015.

Zhang, S. X.; Ganguly, A.; Goyal, P.; Bingaman, J. L.; Bevilacqua, P. C.; Hammes-Schiffer, S.
Role of the Active Site Guanine in the glmS Ribozyme Self-Cleavage Mechanism: Quantum Mechanical/Molecular Mechanical Free Energy Simulations

Journal of the American Chemical Society, (137): 784-798 2015.

Zhang, S. Z.; Chen, Z. Q.; Lu, Y. X.; Xu, Z. J.; Wu, W. H.; Zhu, W. L.; Peng, C. J.; Liu, H. L.
Halogen bonding interactions in ion pairs versus conventional charge-assisted and neutral halogen bonds: a theoretical study based on imidazolium species
Rsc Advances, (5): 74284-74294 2015.

Zhang, X. H.; Xu, Z. G.; Gong, L. Z.; Xu, X.; Shen, G. X.; Chen, H. B.; Liu, H. Y.
Stability of trans-Dioxo Manganese(V) Corrole Complex
Acta Physico-Chimica Sinica, (31): 1069-1076 2015.

Zhang, X. L.; Gong, X. D.
DFT, QTAIM, and NBO investigations of the ability of the Fe or Ni doped CNT to absorb and sense CO and NO
Journal of Molecular Modeling, (21) 2015.

Zhang, X. L.; Gong, X. D.
Theoretical investigation of rare gas adsorption on and inside B-doped carbon nanotubes by DFT, QTAIM and NBO
Rsc Advances, (5): 65604-65612 2015.

Zhang, X. X.; Robinson, P. J.; Gantefor, G.; Alexandrova, A.; Bowen, K. H.
Photoelectron spectroscopic and theoretical study of the HPd(eta(2)-H-2) -cluster anion
Journal of Chemical Physics, (143) 2015.

Zhang, X. Y.; Li, X. Y.; Zeng, Y. L.; Zheng, S. J.; Meng, L. P.
Enhancing sigma/pi-type copper(I) center dot center dot center dot thiophene interactions by metal doping (metal = Li, Na, K, Ca, Sc)
Dalton Transactions, (44): 1283-1291 2015.

Zhang, Y. F.; Huang, R. Y.; Wang, J. W.; Kong, X. J.
Composition-dependent association behavior in the mixture of isopropanol and trichloromethane: a volumetric, vibration spectroscopic and quantum chemical study
Rsc Advances, (5): 63719-63725 2015.

Zhang, Z.; Pu, L.; Li, Q. S.; King, R. B.
Pathways to the Polymerization of Boron Monoxide Dimer To Give Low-Density Porous Materials Containing Six-Membered Boroxine Rings
Inorganic Chemistry, (54): 2910-2915 2015.

Zhao, G. M.; Liu, H. L.; Huang, X. R.; Yang, X.; Xie, Y. P.
DFT Study on the Homogeneous Palladium-Catalyzed N-Alkylation of Amines with Alcohols
Acs Catalysis, (5): 5728-5740 2015.

Zhao, H.; Zhang, C. J.
Theoretical study of group 6 metallacyclic complexes with planar tetracoordinate carbon
Computational and Theoretical Chemistry, (1055): 42-50 2015.

Zhao, H. X.; Li, L. Y.; Wang, J. Y.; Wang, R. H.
Spherical core-shell magnetic particles constructed by main-chain palladium N-heterocyclic carbenes
Nanoscale, (7): 3532-3538 2015.

Zhao, J. F.; Li, P.
The investigation of ESPT for 2,8-diphenyl-3,7-dihydroxy-4H, 6H-pyrano 3,2-g -chromene-4,6-dione: single or double?
Rsc Advances, (5): 73619-73625 2015.

Zhao, L. L.; Jones, C.; Frenking, G.
Reaction Mechanism of the Symmetry-Forbidden 2+2 Addition of Ethylene and Acetylene to Amido-Substituted Digermynes and Distannynes Ph2N-EE-NPh2, (E=Ge, Sn): A Theoretical Study
Chemistry-a European Journal, (21): 12405-12413 2015.

Zhao, L. M.; Ding, Q. Y.; Xu, W. B.; Sang, P. P.; He, X. L.; Shi, Z. M.; Chi, Y. H.; Lu, X. Q.; Guo, W. Y.
The ligand effect on the selective C-H versus C-C bond activation of propane by NiBr+: a theoretical study
Theoretical Chemistry Accounts, (134) 2015.

Zhao, S.; Tian, X. Z.; Liu, J. L.; Ren, Y. L.; Ren, Y. L.; Wang, J. J.
Density Functional Study of Molecular Hydrogen Adsorption on Small Gold-Copper Binary Clusters
Journal of Cluster Science, (26): 491-503 2015.

Zhao, S.; Tian, X. Z.; Liu, J. N.; Ren, Y. L.; Wang, J. J.
Interaction of H-2 with gold-palladium binary clusters: Molecular and dissociative adsorption
Computational and Theoretical Chemistry, (1055): 1-7 2015.

Zhao, W. Y.; Yu, J.; Ren, S. J.; Wei, X. G.; Qiu, F. Z.; Li, P. H.; Li, H.; Zhou, Y. P.; Yin, C. Z.; Chen, A. P.; Li, H.; Zhang, L.; Zhu, J.; Ren, Y.; Lau, K. C.
Probing the Reactivity of Microhydrated alpha-Nucleophile in the Anionic Gas-Phase S(N)2 Reaction
Journal of Computational Chemistry, (36): 844-852 2015.

Zhao, X.; Sun, C. Z.; Lu, Y. T.; Xing, Z.; Sun, N.; Chen, D. Z.
A DFT study on the difference of C-H bond activation by Pd(II) and Pd(IV) complex
Computational and Theoretical Chemistry, (1056): 41-46 2015.

Zhao, Y. L.; Zhou, Q.; Lian, Y. F.; Yu, H. T.
Molecular structures of Pr@C-72 and Pr@C-72(C6H3Cl2): a combined experimental-theoretical investigation
Rsc Advances, (5): 97568-97578 2015.

Zhao, Y. Y.; Zhang, Y. C.; Liu, X.; Fan, K. X.; Zheng, X. M.
Formation, characterization, structure and bonding analysis of the metal-carbon bond OM-(eta(6)-C6H6) (M = Sc, Ti) complexes in solid matrix: Infrared spectroscopic and theoretical study
Journal of Organometallic Chemistry, (777): 25-30 2015.

Zheng, B. X.; Die, D.; Zhu, B.; Zhao, Z. Q.
Probing the structural, electronic and magnetic properties of small Au4M (M= Sc-Zn) clusters
Molecular Physics, (113): 3395-3402 2015.

Zheng, X. W.; Wang, L.; Han, S. M.; Cui, X. Y.; Du, C. Y.; Liu, T.
Theoretical Studies of Weak Interactions of Formamide with Methanol and Its Derivates
Russian Journal of Physical Chemistry A, (89): 1419-1428 2015.

Zheng, Y. Z.; Deng, G.; Zhou, Y.; Sun, H. Y.; Yu, Z. W.
Comparative Study of Halogen- and Hydrogen-Bond Interactions between Benzene Derivatives and Dimethyl Sulfoxide
Chemphyschem, (16): 2594-2601 2015.

Zhong, A. G.; Chen, D.; Li, R. R.
Revisiting the beryllium bonding interactions from energetic and wavefunction perspectives
Chemical Physics Letters, (633): 265-272 2015.

Zhou, D. G.; Zhou, P. P.; Jing, H. W.
Mechanisms of water-promoted aryl azide conversion into N-alkylated aniline: Two competitive pathways
Computational and Theoretical Chemistry, (1070): 76-81 2015.

Zhou, F. F.; Liu, R. R.; Li, P.; Zhang, H. Y.
On the properties of S center dot center dot center dot O and S center dot center dot center dot pi noncovalent interactions: the analysis of geometry, interaction energy and electron density
New Journal of Chemistry, (39): 1611-1618 2015.

Zhou, L.; Li, Y.; Lin, F. R.; Tian, D. Y.; Lei, Q. F.; Fang, W. J.; Xie, H. J.

Reaction Mechanism for the Alkoxylation of a Silyl Ligand in the Silyl(silylene)ruthenium Complex: A Density Functional Theory Study
Chinese Journal of Organic Chemistry, (35): 698-704 2015.

Zhou, P. P.; Zhang, R. Q.
Physisorption of benzene derivatives on graphene: critical roles of steric and stereoelectronic effects of the substituent
Physical Chemistry Chemical Physics, (17): 12185-12193 2015.

Zhou, Q. H.; Li, Y. X.
The Real Role of N-Heterocyclic Carbene in Reductive Functionalization of CO2: An Alternative Understanding from Density Functional Theory Study
Journal of the American Chemical Society, (137): 10182-10189 2015.

Zhou, S. D.; Schlangen, M.; Schwarz, H.
Mechanistic Aspects of the Gas-Phase Reactions of Halobenzenes with Bare Lanthanide Cations: A Combined Experimental/Theoretical Investigation
Chemistry-a European Journal, (21): 2123-2131 2015.

Zhu, C.; Rasanen, M.; Khriachtchev, L.
Fluorinated noble-gas cyanides FKrCN, FXeCN, and FXeNC
Journal of Chemical Physics, (143) 2015.

Zhu, C.; Rasanen, M.; Khriachtchev, L.
Matrix-isolation and ab initio study of HKrCCCl and HXeCCCl
Journal of Chemical Physics, (143) 2015.

Zhu, C.; Tsuge, M.; Rasanen, M.; Khriachtchev, L.
Experimental and theoretical study of the HXeI center dot center dot center dot HCl and HXeI center dot center dot center dot HCCH complexes
Journal of Chemical Physics, (142) 2015.

Zhu, H. Y.; Huang, B. L.; Li, J. F.; Jiang, Z. Y.; Wang, B.; Wang, Z. G.; Zhang, R. Q.
Tunable dipole induced hydrogen bonds between a hydrogen molecule and alkali halides
Physical Chemistry Chemical Physics, (17): 20361-20367 2015.

Zhu, W. Y.; Liu, Y. J.; Zhang, R.
A QM/MM study of the reaction mechanism of (R)-hydroxynitrile lyases from Arabidopsis thaliana (AtHNL)
Proteins-Structure Function and Bioinformatics, (83): 66-77 2015.

Zhu, Y. Q.; Su, H.; Tang, J. L.; Yang, Y. Q.
Mechanism of palladium(II)-catalyzed reaction between styrene and carbazole
Computational and Theoretical Chemistry, (1068): 47-51 2015.

Zhuo, H. Y.; Li, Q. Z.
Novel pnicogen bonding interactions with silylene as an electron donor: covalency, unusual substituent effects and new mechanisms
Physical Chemistry Chemical Physics, (17): 9153-9160 2015.

Zhuo, H. Y.; Li, Q. Z.; Li, W. Z.; Cheng, J. B.
The dual role of pnicogen as Lewis acid and base and the unexpected interplay between the pnicogen bond and coordination interaction in H3N center dot center dot center dot FH2X center dot center dot center dot MCN (X = P and As; M = Cu, Ag, and Au)
New Journal of Chemistry, (39): 2067-2074 2015.

Zierkiewicz, W.; Bienko, D. C.; Michalska, D.; Zeegers-Huyskens, T.
Theoretical Investigation of the Halogen Bonded Complexes Between Carbonyl Bases and Molecular Chlorine
Journal of Computational Chemistry, (36): 821-832 2015.

Zimmerman, P. M.; Molina, A. R.; Smereka, P.
Orbitals with intermediate localization and low coupling: Spanning the gap between canonical and localized orbitals
Journal of Chemical Physics, (143) 2015.

Zins, E. L.; Silvi, B.; Alikhani, M. E.
Activation of C-H and B-H bonds through agostic bonding: an ELF/QTAIM insight
Physical Chemistry Chemical Physics, (17): 9258-9281 2015.

Zobac, V.; Lewis, J. P.; Abad, E.; Mendieta-Moreno, J. I.; Hapala, P.; Jelinek, P.; Ortega, J.
Photo-induced reactions from efficient molecular dynamics with electronic transitions using the FIREBALL local-orbital density functional theory formalism
Journal of Physics-Condensed Matter, (27) 2015.

Zukerman-Schpector, J.; Madureira, L. S.; Poplaukhin, P.; Arman, H. D.; Miller, T.; Tiekink, E. R. T.
Conformational preferences for isomeric N,N '-bis(pyridin-n-ylmethyl)ethanedithiodiamides, n=2, 3 and 4: a combined crystallographic and DFT study
Zeitschrift Fur Kristallographie-Crystalline Materials, (230): 531-541 2015.