

NBO 2009 (Jan-Dec) - 1024 references  
Compiled by Ariel Neff; Updated 4/16/13

- Abdelatif, M. L.; Belmiloud, Y.; Brahimi, M.  
*HF, DFT Studies and NBO Analysis of Phosphazenes and Its-Na<sup>+</sup> Complex*  
Asian Journal of Chemistry, (21): 5029-5047 2009.
- Abdurahman, A.; Renger, T.  
*Density Functional Studies of Iron-Porphyrin Cation with Small Ligands X (X: O, CO, NO, O-2, N-2, H2O, N2O, CO2)*  
Journal of Physical Chemistry A, (113): 9202-9206 2009.
- Abiram, A.; Kolandaivel, P.  
*INTERACTION OF THE TAUTOMERIC STATES OF HISTIDINE WITH Cu AND Zn METAL IONS - A THEORETICAL STUDY*  
Journal of Theoretical & Computational Chemistry, (8): 657-676 2009.
- Abrahao, O., Jr.; Panconato Teixeira, T. S.; Madurro, J. M.; da Hora Machado, A. E.; Brito-Madurro, A. G.  
*Quantum mechanical investigation of polymer formation from aminophenols*  
Journal of Molecular Structure-Theochem, (913): 28-37 2009.
- Adcock, W.  
*Transmission of polar substituent effects across the cubane ring system: F-19 substituent chemical shifts (SCS) of 4-substitute (X) cub-1-yl fluorides revisited*  
Journal of Physical Organic Chemistry, (22): 1065-1069 2009.
- Adcock, W.; Schamschurin, A.; Taylor, J. F.  
*Nature of transmission of polar substituent effects in gamma-disposed bicyclo[2.2.1]heptane (norbornane) and adamantane ring systems as monitored by F-19 NMR: A DFT-GIAO and - NBO Analysis*  
Arkivoc: 23-37 2009.
- Adhikari, D.; Pink, M.; Mindiola, D. J.  
*Mild Protocol for the Synthesis of Stable Nickel Complexes Having Primary and Secondary Silyl Ligands*  
Organometallics, (28): 2072-2077 2009.
- Aghabozorg, H.; Manteghi, F.; Ghadermazi, M.; Mirzaei, M.; Salimi, A. R.; Shokrollahi, A.; Derki, S.; Eshtiagh-Hosseini, H.  
*A novel supramolecular compound of cadmium(II): Synthesis, characterization, crystal structure, ab initio HF, DFT calculations and solution study*  
Journal of Molecular Structure, (919): 381-388 2009.
- Agrawal, M. K.; Adimurthy, S.; Ganguly, B.; Ghosh, P. K.  
*Comparative study of the vicinal functionalization of olefins with 2:1 bromide/bromate and iodide/iodate reagents*  
Tetrahedron, (65): 2791-2797 2009.

- Akilandeswari, L.; Jaccob, M.; Venuvanalingam, P.  
*Fluorine effect on pericyclic and pseudopericyclic processes: Evidences and ab initio theory*  
Journal of Chemical Sciences, (121): 859-866 2009.
- Alagona, G.; Ghio, C.  
*Plicatin B conformational landscape and affinity to copper (I and II) metal cations. A DFT study*  
Physical Chemistry Chemical Physics, (11): 776-790 2009.
- Alajarin, M.; Bonillo, B.; Sanchez-Andrada, P.; Vidal, A.; Bautista, D.  
*Unexpected Formation of 2,1-Benzisothiazol-3-ones from Oxathiolano Ketenimines: A Rare Tandem Process*  
Organic Letters, (11): 1365-1368 2009.
- Alajarin, M.; Marin-Luna, M.; Ortin, M. M.; Sanchez-Andrada, P.; Vidal, A.  
*Benzyllic Newman-Kwart rearrangement of O-azidobenzyl thiocarbamates triggered by phosphines: pseudopericyclic [1,3] shifts via uncoupled concerted mechanisms*  
Tetrahedron, (65): 2579-2590 2009.
- Alcaide, B.; Almendros, P.; del Campo, T. M.; Soriano, E.; Marco-Contelles, J. L.  
*Metal-Catalyzed Cyclization of beta- and gamma-Allenols Derived from D-Glyceraldehyde-Synthesis of Enantiopure Dihydropyrans and Tetrahydroooxepines: An Experimental and Theoretical Study*  
Chemistry-a European Journal, (15): 9127-9138 2009.
- Alcaide, B.; Almendros, P.; del Campo, T. M.; Soriano, E.; Marco-Contelles, J. L.  
*Regioselectivity Control in the Metal-Catalyzed Functionalization of gamma-Allenols, Part 2: Theoretical Study*  
Chemistry-a European Journal, (15): 1909-1928 2009.
- Alcantara-Garcia, J.; Jancik, V.; Barroso, J.; Hidalgo-Bonilla, S.; Cea-Olivares, R.; Toscano, R. A.; Moya-Cabrera, M.  
*Coordination Diversity of Aluminum Centers Molded by Triazole Based Chalcogen Ligands*  
Inorganic Chemistry, (48): 5874-5883 2009.
- Alkorta, I.; Blanco, F.; Elguero, J.  
*A computational study of the cooperativity in clusters of interhalogen derivatives*  
Structural Chemistry, (20): 63-71 2009.
- Alkorta, I.; Blanco, F.; Elguero, J.  
*Theoretical studies of azapentalenes. Part 4: Theoretical study of the properties of 3a,6a-diazapentalene*  
Tetrahedron, (65): 5760-5766 2009.
- Alkorta, I.; Blanco, F.; Elguero, J.; Dobado, J. A.; Ferrer, S. M.; Vidal, I.  
*Carbon center dot center dot center dot Carbon Weak Interactions*  
Journal of Physical Chemistry A, (113): 8387-8393 2009.

Alkorta, I.; Blanco, F.; Elguero, J.; Estarellas, C.; Frontera, A.; Quinonero, D.; Deya, P. M.  
*Simultaneous Interaction of Tetrafluoroethene with Anions and Hydrogen-Bond Donors: A Cooperativity Study*  
Journal of Chemical Theory and Computation, (5): 1186-1194 2009.

Alkorta, I.; Del Bene, J. E.; Elguero, J.; Mo, O.; Yanez, M.  
*A theoretical study of diborenes HLB=BLH for L=CO, NH<sub>3</sub>, OH<sub>2</sub>, PH<sub>3</sub>, SH<sub>2</sub>, ClH: structures, energies, and spin-spin coupling constants*  
Theoretical Chemistry Accounts, (124): 187-195 2009.

Alonso, E.; Fornies, J.; Fortuno, C.; Lledos, A.; Martin, A.; Nova, A.  
*Behavior of P-Pt and P-Pd Bonds in Phosphido Complexes toward Electrophilic Fragments*  
Inorganic Chemistry, (48): 7679-7690 2009.

Al-Sehemi, A. G.; El-Gogary, T. M.  
*Geometry and thermodynamic stabilities of rhodanine tautomers and rotamers: Quantum chemical study*  
Journal of Molecular Structure-Theochem, (907): 66-73 2009.

Altman, M.; Zenkina, O. V.; Ichiki, T.; Iron, M. A.; Evmenenko, G.; Dutta, P.; van der Boom, M. E.  
*Positive Constructs: Charges Localized on Surface-Confining Organometallic Oligomers*  
Chemistry of Materials, (21): 4676-4684 2009.

Alvarez, M. A.; Garcia, M. E.; Garcia-Vivo, D.; Martinez, M. E.; Ruiz, M. A.  
*Reactions of the Unsaturated Complex [Mo-2(eta(5)-C<sub>5</sub>H<sub>5</sub>)(2)(mu-PEt<sub>2</sub>)(2)(CO)(2)] with [Au(PR<sub>3</sub>)](+) Cations: Kinetic Preference of the Mo-P Bonds as the Site of Attack of the Gold(I) Electrophile*  
Inorganic Chemistry, (48): 9767-9778 2009.

Aparicio, S.; Alcalde, R.  
*The green solvent ethyl lactate: an experimental and theoretical characterization*  
Green Chemistry, (11): 65-78 2009.

Aparicio, S.; Alcalde, R.  
*Insights into the Ethyl Lactate plus Water Mixed Solvent*  
Journal of Physical Chemistry B, (113): 14257-14269 2009.

Aragoni, M. C.; Arca, M.; Crespo, M.; Devillanova, F. A.; Hursthause, M. B.; Huth, S. L.; Isaia, F.; Lippolis, V.; Verani, G.  
*Investigation on the reactivity of dithiophosphonato/dithiophosphato Ni-II complexes towards 2,4,6-tris-2-pyridyl-1,3,5-triazine: developments and new perspectives*  
Dalton Transactions: 2510-2520 2009.

Archipov, T.; Santra, S.; Ene, A. B.; Stoll, H.; Rauhut, G.; Roduner, E.  
*Adsorption of Benzene to Copper in CuHY Zeolite*  
Journal of Physical Chemistry C, (113): 4107-4116 2009.

Arliguie, T.; Belkhiri, L.; Bouaoud, S. E.; Thuery, P.; Villiers, C.; Boucekkine, A.; Ephritikhine, M.

*Lanthanide(III) and Actinide(III) Complexes [M(BH<sub>4</sub>)<sub>2</sub>(THF)<sub>5</sub>][BPh<sub>4</sub>] and [M(BH<sub>4</sub>)<sub>2</sub>(18-crown-6)][BPh<sub>4</sub>] (M = Nd, Ce, U): Synthesis, Crystal Structure, and Density Functional Theory Investigation of the Covalent Contribution to Metal-Borohydride Bonding*  
Inorganic Chemistry, (48): 221-230 2009.

Arquier, D.; Vendier, L.; Miqueu, K.; Sotiropoulos, J. M.; Bastin, S.; Igau, A.  
*Crucial Role of the Amidine Moiety in Methylenamino Phosphine-Type Ligands for the Synthesis of Tethered eta(6)-Arene-eta(1)-P Ruthenium(II) Complexes: Experimental and Theoretical Studies*  
Organometallics, (28): 4945-4957 2009.

Arroyo, Y.; Meana, A.; Sanz-Tejedor, M. A.; Alonso, I.; Ruano, J. L. G.  
*Stereoselective Addition of alpha-Methylsulfonyl Benzyl Carbanions to N-Sulfinylketimines: Asymmetric Synthesis of alpha,alpha-Dibranched beta-Sulfonyl Amines*  
Journal of Organic Chemistry, (74): 764-772 2009.

Asensio, X.; Gonzalez-Lafont, A.; Marquet, J.; Lluch, J. M.; Geoffroy, M.  
*The effect of electron-withdrawing groups in the fragmentation of the radical anions of benzyl phenyl ethers*  
Journal of Molecular Structure-Theochem, (913): 228-235 2009.

Auer, A. A.; Mansfeld, D.; Nolde, C.; Schneider, W.; Schurmann, M.; Mehring, M.  
*Bismuth-Arene pi-Interaction: A Combined Experimental and Theoretical Approach*  
Organometallics, (28): 5405-5411 2009.

Auer, B. M.; Skinner, J. L.  
*Water: Hydrogen bonding and vibrational spectroscopy, in the bulk liquid and at the liquid/vapor interface*  
Chemical Physics Letters, (470): 13-20 2009.

Aullon, G.; Alvarez, S.  
*Oxidation states, atomic charges and orbital populations in transition metal complexes*  
Theoretical Chemistry Accounts, (123): 67-73 2009.

Aullon, G.; Alvarez, S.; Cao, R.; Ortiz, M.; Diaz-Garcia, A. M.  
*Substitution of chloride by nitrosyl ligand in a scorpionate ruthenium(III) compound: A theoretical study*  
Inorganica Chimica Acta, (362): 4651-4658 2009.

Aversa, M. C.; Barattucci, A.; Bonaccorsi, P.; Contini, A.  
*Addition of sulfenic acids to monosubstituted acetylenes: a theoretical and experimental study*  
Journal of Physical Organic Chemistry, (22): 1048-1057 2009.

Azami, S. M.; Pooladi, R.; Sheikhi, M. H.  
*Local sigma-pi mixing in C-60 buckminsterfullerene*  
Journal of Molecular Structure-Theochem, (901): 153-156 2009.

Azizi, K.; Safarpour, M. A.; Keykhaee, M.; Mehdipour, A. R.

*DFT-based QSAR study of alkanols and alkanthiols using the conductor-like polarizable continuum model (CPCM)*

Journal of Molecular Modeling, (15): 1509-1515 2009.

Bagheri, S.; Roohi, H.

*Proton-Transfer Mechanism in 2-Thioxoimidazolidin-4-one: A Competition between Keto/Enol and Thione/Thiol Tautomerism Reactions*

Bulletin of the Chemical Society of Japan, (82): 446-452 2009.

Bailey, J. M.; Check, C. E.; Gilbert, T. A.

*Computational Studies of Pericyclic Reactions between Aminoalanes and Ethyne, Ethene, and Dienes. A Reactive Aminoalane That Should Prefer [2+2] and [4+2] Cyclizations to Dimerization*

Organometallics, (28): 787-794 2009.

Balanay, M. P.; Kim, S. M.; Lee, M. J.; Lee, S. H.; Kim, D. H.

*Conformational Analysis and Electronic Properties of 2-Cyano-3-(thiophen-2-yl)acrylic Acid in Sensitizers for Dye-sensitized Solar Cells: A Theoretical Study*

Bulletin of the Korean Chemical Society, (30): 2077-2082 2009.

Balcells, D.; Moles, P.; Blakemore, J. D.; Raynaud, C.; Brudvig, G. W.; Crabtree, R. H.; Eisenstein, O.

*Molecular recognition in Mn-catalyzed C-H oxidation. Reaction mechanism and origin of selectivity from a DFT perspective*

Dalton Transactions: 5989-6000 2009.

Bande, A.; Michl, J.

*Conformational Dependence of sigma-Electron Delocalization in Linear Chains: Permethylated Oligosilanes*

Chemistry-a European Journal, (15): 8504-8517 2009.

Bandoli, G.; Barreca, D.; Gasparotto, A.; Seraglia, R.; Tondello, E.; Devi, A.; Fischer, R. A.; Winter, M.; Fois, E.; Gambae, A.; Tabacchi, G.

*An integrated experimental and theoretical investigation on Cu(hfa)(2)center dot TMEDA: structure, bonding and reactivity*

Physical Chemistry Chemical Physics, (11): 5998-6007 2009.

Banerjee, S.; Sengupta, P. S.; Mukherjee, A. K.

*A detailed theoretical study of the interaction of thiourea with cis-diaqua(ethylenediamine) platinum(II)*

Journal of Molecular Structure-Theochem, (913): 97-106 2009.

Barquera-Lozada, J. E.; Cuevas, G.

*Biogenesis of Sesquiterpene Lactones Pseudoguaianolides from Germacranoïdides: Theoretical Study on the Reaction Mechanism of Terminal Biogenesis of 8-Epicofertin*

Journal of Organic Chemistry, (74): 874-883 2009.

Barrientos-Salcedo, C.; Rico-Rosillo, G.; Gimenez-Scherer, J. A.; Soriano-Correa, C.

*Computational study of the electronic structure characterization of a novel anti-inflammatory tripeptide derived from monocyte locomotion inhibitory factor (MLIF)-pentapeptide*

European Journal of Medicinal Chemistry, (44): 3114-3119 2009.

Bauer, S.; Tschirschwitz, S.; Lonnecke, P.; Frank, R.; Kirchner, B.; Clarke, M. L.; Hey-Hawkins, E.  
*Enantiomerically Pure Bis(phosphanyl)carborane(12) Compounds:* 2776-2788 2009.

Begum, F. A.; Farah, A. A.; Hunter, H. N.; Lever, A. B. P.

*Synthesis and Characterization of Ruthenium bis-Bipyridine Mono- and Disulfinate Complexes*  
Inorganic Chemistry, (48): 2018-2027 2009.

Belpassi, L.; Tarantelli, F.; Pirani, F.; Candori, P.; Cappelletti, D.

*Experimental and theoretical evidence of charge transfer in weakly bound complexes of water*  
Physical Chemistry Chemical Physics, (11): 9970-9975 2009.

Ben Fredj, A.; Ben Lakhdar, Z.; Ruiz-Lopez, M. F.

*Six-coordination in Chlorophylls: The fundamental role of dispersion energy*  
Chemical Physics Letters, (472): 243-247 2009.

Benchouk, W.; Mekelleche, S. M.; Aurell, M. J.; Domingo, L. R.

*Understanding the regio- and chemoselective polar [3+2] cycloaddition of the Padwa carbonyl ylides with alpha-methylene ketones. A DFT study*  
Tetrahedron, (65): 4644-4651 2009.

Benisvy, L.; Wanke, R.; Kuznetsov, M. L.; Guedes da Silva, M. F. C.; Pombeiro, A. J. L.

*Towards the functionalization of the methine carbon of a sterically hindered tris(pyrazolyl)methane: is a radical pathway envisageable? Synthesis and structure of tetrakis(3,5-dimethylpyrazolyl)methane*  
Tetrahedron, (65): 9218-9223 2009.

Benitez, D.; Shapiro, N. D.; Tkatchouk, E.; Wang, Y. M.; Goddard, W. A.; Toste, F. D.

*A bonding model for gold(I) carbene complexes*  
Nature Chemistry, (1): 482-486 2009.

Benitez, D.; Tkatchouk, E.; Gonzalez, A. Z.; Goddard, W. A., III; Toste, F. D.

*On the Impact of Steric and Electronic Properties of Ligands on Gold(I)-Catalyzed Cycloaddition Reactions*  
Organic Letters, (11): 4798-4801 2009.

Bentabed-Ababsa, G.; Derdour, A.; Roisnel, T.; Saez, J. A.; Perez, P.; Chamorro, E.; Domingo, L. R.; Mongin, F.

*A Combined Experimental and Theoretical Study of the Polar [3+2] Cycloaddition of Electrophilically Activated Carbonyl Ylides with Aldehydes and Imines*  
Journal of Organic Chemistry, (74): 2120-2133 2009.

Bera, P. P.; Francisco, J. S.; Lee, T. J.

*Identifying the Molecular Origin of Global Warming*  
Journal of Physical Chemistry A, (113): 12694-12699 2009.

Berestovitskaya, V. M.; Makarenko, S. V.; Bushmarinov, I. S.; Lyssenko, K. A.; Smirnov, A. S.; Stukan, E. V.

*1-Aryl-2-nitro-3-trichloromethylaziridines: synthesis and structure*  
Russian Chemical Bulletin, (58): 1023-1033 2009.

Berionni, G.; Pegot, B.; Marrot, J.; Goumont, R.  
*Supramolecular association of 1,2,5-chalcogenadiazoles: an unexpected self-assembled dissymmetric [Se center dot center dot center dot N](2) four-membered ring*  
Crystengcomm, (11): 986-988 2009.

Bernal-Uruchurtu, M. I.; Kerenskaya, G.; Janda, K. C.  
*Structure, spectroscopy and dynamics of halogen molecules interacting with water*  
International Reviews in Physical Chemistry, (28): 223-265 2009.

Bernsdorf, A.; Brand, H.; Hellmann, R.; Kockerling, M.; Schulz, A.; Villinger, A.; Voss, K.  
*Synthesis, Structure, and Bonding of Weakly Coordinating Anions Based on CN Adducts*  
Journal of the American Chemical Society, (131): 8958-8970 2009.

Bhabak, K. P.; Mugesh, G.  
*Amide-Based Glutathione Peroxidase Mimics: Effect of Secondary and Tertiary Amide Substituents on Antioxidant Activity*  
Chemistry-an Asian Journal, (4): 974-983 2009.

Bil, A.; Latajka, Z.; Morrison, C. A.  
*C-70 Oxides and Ozonides and the Mechanism of Ozonolysis on the Fullerene Surface. A Theoretical Study*  
Journal of Physical Chemistry A, (113): 9891-9898 2009.

Billes, F.; Podea, P. V.; Mohammed-Ziegler, I.; Tosa, M.; Mikosch, H.; Irimie, D.-F.  
*Formyl- and acetylindols: Vibrational spectroscopy of an expectably pharmacologically active compound family*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (74): 1031-1045 2009.

Biswal, H. S.; Shirhatti, P. R.; Wategaonkar, S.  
*O-H center dot center dot center O versus O-H center dot center dot center S Hydrogen Bonding I: Experimental and Computational Studies on the p-Cresol center dot H<sub>2</sub>O and p-Cresol center dot H<sub>2</sub>S Complexes*  
Journal of Physical Chemistry A, (113): 5633-5643 2009.

Biswal, H. S.; Wategaonkar, S.  
*Nature of the N-H center dot center dot center S Hydrogen Bond*  
Journal of Physical Chemistry A, (113): 12763-12773 2009.

Biswal, H. S.; Wategaonkar, S.  
*Sulfur, Not Too Far Behind O, N, and C: SH center dot center dot center pi Hydrogen Bond*  
Journal of Physical Chemistry A, (113): 12774-12782 2009.

Blanco, F.; Alkorta, I.; Elguero, J.  
*Barriers about Double Carbon-Nitrogen Bond in Imine Derivatives (Aldimines, Oximes, Hydrazones, Azines)*

Croatica Chemica Acta, (82): 173-183 2009.

Blanco, F.; Alkorta, I.; Elguero, J.

*N-sigma versus pi configuration in mono- and bis-pyrrole and imidazole derivatives of alkaline earth metals*

Journal of Physical Organic Chemistry, (22): 747-755 2009.

Blanco, F.; Alkorta, I.; Elguero, J.

*Theoretical studies of azapentalenes. Part 5: Bimanes*

Tetrahedron, (65): 6244-6250 2009.

Blanco, F.; Alkorta, I.; Solimannejad, M.; Elguero, J.

*Theoretical Study of the 1:1 Complexes between Carbon Monoxide and Hypohalous Acids*

Journal of Physical Chemistry A, (113): 3237-3244 2009.

Bleiholder, C.; Rominger, F.; Gleiter, R.

*alpha-Metallocenylmethylium Ions and Their Isoelectronic Congeners: A Comparison Based on DFT Calculations*

Organometallics, (28): 1014-1017 2009.

Bock, C. W.; Larkin, J. D.; Hirsch, S. S.; Wright, J. B.

*Nucleophilic destruction of organophosphate toxins: A computational investigation*

Journal of Molecular Structure-Theochem, (915): 11-19 2009.

Bogdanov, S. E.; Faustov, V. I.; Shavrin, K. N.; Gvozdev, V. D.; Promyslov, V. M.; Egorov, M. P.; Nefedov, O. M.

*A Highly Delocalized Triplet Carbene, 5-Methylhexa-1,2,4-triene-1,3-diy: Matrix IR Identification, Structure, and Reactions*

Journal of the American Chemical Society, (131): 14688-14698 2009.

Bokach, N. A.; Kuznetsov, M. L.; Haukka, M.; Ovcharenko, V. I.; Tretyakov, E. V.; Kukushkin, V. Y.

*Platinum(II)-Complexed Tetrahydroimidazo[1,2-*b*][1,2,4]oxadiazoles Derived from Metal-Mediated 1,3-Dipolar Cycloaddition. Novel Type of Heterocycles, Which Do Not Exist without the Metal Center*

Organometallics, (28): 1406-1413 2009.

Bokarev, S. I.; Dolgov, E. K.; Bataev, V. A.; Godunov, I. A.

*Molecular Parameters of Tetraatomic Carbonyls X<sub>2</sub>CO and XYCO (X, Y = H, F, Cl) in the Ground and Lowest Excited Electronic States, Part 1: A Test of Ab Initio Methods*

International Journal of Quantum Chemistry, (109): 569-585 2009.

Bolano, T.; Collado, A.; Esteruelas, M. A.; Onate, E.

*Selectivity of Allenylidene versus Butadienyl Protonation in an Osmium-Bisphosphine System*

Organometallics, (28): 2107-2111 2009.

Bonnet, S.; van Lenthe, J. H.; Siegler, M. A.; Spek, A. L.; van Koten, G.; Gebbink, R.

*Bimetallic eta(6),eta(1) NCN-Pincer Ruthenium Palladium Complexes with eta(6)-RuCp*

*Coordination: Synthesis, X-ray Structures, and Catalytic Properties*

Organometallics, (28): 2325-2333 2009.

Bontemps, S.; Bouhadir, G.; Apperley, D. C.; Dyer, P. W.; Miqueu, K.; Bourissou, D.  
*Bridging M-Cl Bonds with Ambiphilic Phosphine-Borane Ligands*  
Chemistry-an Asian Journal, (4): 428-435 2009.

Bopp, J. C.; Alexandrova, A. N.; Elliott, B. M.; Herden, T.; Johnson, M. A.  
*Vibrational predissociation spectra of the O-n(-), n=3-10, 12 clusters: Even-odd alternation in the core ion*  
International Journal of Mass Spectrometry, (283): 94-99 2009.

Bortoluzzi, M.; Paolucci, G.; Annibale, G.; Pitteri, B.  
*A new pi-acidity scale for several N-donor heterocycles as ligands in neutral gold(III) complexes*  
Polyhedron, (28): 1079-1084 2009.

Braida, B.; Prana, V.; Hiberty, P. C.  
*The Physical Origin of Saytzeff's Rule*  
Angewandte Chemie-International Edition, (48): 5724-5728 2009.

Brand, H.; Martens, J.; Mayer, P.; Schulz, A.; Seibald, M.; Soller, T.  
*Salts and Ionic Liquids of Resonance Stabilized Amides*  
Chemistry-an Asian Journal, (4): 1588-1603 2009.

Branda, M. M.; Rodriguez, A. H.; Belelli, P. G.; Castellani, N. J.  
*Ethanol adsorption on MgO surface with and without defects from a theoretical point of view*  
Surface Science, (603): 1093-1098 2009.

Brandan, S. A.  
*Theoretical study of the structure and vibrational spectra of chromyl perchlorate, CrO<sub>2</sub>(ClO<sub>4</sub>)<sub>2</sub>*  
Journal of Molecular Structure-Theochem, (908): 19-25 2009.

Brandan, S. A.; Socolsky, C.; Ben Altabef, A.  
*DFT Calculations of the Molecular Force Field of Vanadyl Nitrate, VO(NO<sub>3</sub>)<sub>3</sub>*  
Zeitschrift fur Anorganische und Allgemeine Chemie, (635): 582-592 2009.

Brauer, B.; Grobosch, M.; Knupfer, M.; Weigend, F.; Vaynzof, Y.; Kahn, A.; Ruffer, T.; Salvan, G.  
*How Photoelectron Spectroscopy and Quantum Chemical Studies Can Help Understanding the Magnetic Properties of Molecules: An Example from the Class of Cu(II)-Bis(oxamato) Complexes*  
Journal of Physical Chemistry B, (113): 10051-10054 2009.

Braunschweig, H.; Brenner, P.; Dewhurst, R. D.; Kaupp, M.; Mueller, R.; Oestreicher, S.  
*A Trimetallic Gold Boride Complex with a Fluxional Gold-Boron Bond*  
Angewandte Chemie-International Edition, (48): 9735-9738 2009.

Braunschweig, H.; Christ, B.; Colling-Hendelkens, M.; Forster, M.; Gotz, K.; Kaupp, M.; Radacki, K.; Seeler, F.  
*Synthesis, Structure, and Bonding of Novel Homodinuclear Cobalt and Nickel Borylene Complexes*  
Chemistry-a European Journal, (15): 7150-7155 2009.

- Braunschweig, H.; Herbst, T.; Rais, D.; Ghosh, S.; Kupfer, T.; Radacki, K.; Crawford, A. G.; Ward, R. M.; Marder, T. B.; Fernandez, I.; Frenking, G.  
*Borylene-Based Direct Functionalization of Organic Substrates: Synthesis, Characterization, and Photophysical Properties of Novel pi-Conjugated Borirenes*  
Journal of the American Chemical Society, (131): 8989-8999 2009.
- Breda, S.; Reva, I.; Fausto, R.  
*UV-induced unimolecular photochemistry of 2(5H)-furanone and 2(5H)-thiophenone isolated in low temperature inert matrices*  
Vibrational Spectroscopy, (50): 57-67 2009.
- Bricks, J.; Ryabitskii, A.; Kachkovskii, A.  
*Studies of 2-Azaazulenium Derivatives: The Natures of Electron Transitions in the 2-Azaazulenium Cation and in Monomethine Cyanine Dyes Bearing 2-Azaazulenium Moieties as Terminal Groups*  
European Journal of Organic Chemistry: 3439-3449 2009.
- Browne, D. L.; Vivat, J. F.; Plant, A.; Gomez-Bengoa, E.; Harrity, J. P. A.  
*Investigation of the Scope and Regiochemistry of Alkynylboronate Cycloadditions with Sydrones*  
Journal of the American Chemical Society, (131): 7762-7769 2009.
- Bruschi, M.; Limacher, P. A.; Hutter, J.; Luthi, H. P.  
*A Scheme for the Evaluation of Electron Delocalization and Conjugation Efficiency in Linearly pi-Conjugated Systems*  
Journal of Chemical Theory and Computation, (5): 506-514 2009.
- Brusco, Y.; Berroteran, N.; Lorono, M.; Cordova, T.; Chuchani, G.  
*Theoretical calculations for neighboring group participation in gas-phase elimination kinetics of 2-hydroxyphenethyl chloride and 2-methoxyphenethyl chloride*  
Journal of Physical Organic Chemistry, (22): 1022-1029 2009.
- Bultinck, P.; Cooper, D. L.; Van Neck, D.  
*Comparison of the Hirshfeld-I and iterated stockholder atoms in molecules schemes*  
Physical Chemistry Chemical Physics, (11): 3424-3429 2009.
- Bunge, S. D.; Ocana, J. A.; Cleland, T. L.; Steele, J. L.  
*Synthetic, Structural, and Theoretical Investigation of Guanidinate Complexes Containing Planar Cu-6 Cores*  
Inorganic Chemistry, (48): 4619-4621 2009.
- Burck, S.; Gotz, K.; Kaupp, M.; Nieger, M.; Weber, J.; auf der Gunne, J. S.; Gudat, D.  
*Diphosphines with Strongly Polarized P-P Bonds: Hybrids between Covalent Molecules and Donor-Acceptor Adducts with Flexible Molecular Structures*  
Journal of the American Chemical Society, (131): 10763-10774 2009.
- Burk, P.; Tammiku-Taul, J.; Tamp, S.; Sikk, L.; Sillar, K.; Mayeux, C.; Gal, J. F.; Maria, P. C.

*Computational Study of Cesium Cation Interactions with Neutral and Anionic Compounds Related to Soil Organic Matter*  
Journal of Physical Chemistry A, (113): 10734-10744 2009.

Cabeza, J. A.; del Rio, I.; Goite, M. C.; Perez-Carreno, E.; Pruneda, V.  
*Cationic Heterocycles as Ligands: Synthesis and Reactivity with Anionic Nucleophiles of Cationic Triruthenium Clusters Containing C-Metalated N-Methylquinoxalinium or N-Methylpyrazinium Ligands*  
Chemistry-a European Journal, (15): 7339-7349 2009.

Cabeza, J. A.; Fernandez-Colinas, J. M.; Perez-Carreno, E.  
*DFT Mechanistic Study of the Transformation of Cyclohexa-1,3-diene into a Bridging Allyl Ligand upon Reaction with a Triruthenium Hydrido Carbonyl Cluster*  
Organometallics, (28): 4217-4220 2009.

Cai, X.; Sheng, N.; Zhang, Y. X.; Qi, D. D.; Jiang, J. Z.  
*Structure and spectroscopic properties of phthalocyaninato zinc(II) complexes fused with different number of 15-crown-5 moieties*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (72): 627-635 2009.

Cao, D.-l.; Ren, F.-d.; Liu, S.-n.; Chen, S.-s.  
*A MP2(full) and CCSD(T) theoretical investigation on unusual cation-pi interaction between OCB BCO and H<sup>+</sup>, Li<sup>+</sup>, Na<sup>+</sup>, Be<sup>2+</sup> or Mg<sup>2+</sup>*  
Journal of Molecular Structure-Theochem, (913): 221-227 2009.

Cao, Y. C.; Li, Y.  
*Dearsenication of Liquid Hydrocarbons and Interaction between Arsenic Compounds and Cuprous Probes*  
Acta Physico-Chimica Sinica, (25): 1495-1503 2009.

Capriati, V.; Florio, S.; Perna, F. M.; Salomone, A.; Abbotto, A.; Amedjkouh, M.; Lill, S. O. N.  
*On the Dichotomic Reactivity of Lithiated Styrene Oxide: A Computational and Multinuclear Magnetic Resonance Investigation*  
Chemistry-a European Journal, (15): 7958-7979 2009.

Caputo, C. A.; Jennings, M. C.; Tuononen, H. M.; Jones, N. D.  
*Phospha-Fischer Carbenes: Synthesis, Structure, Bonding, and Reactions of Pd(0)- and Pt(0)-Phosphonium Complexes*  
Organometallics, (28): 990-1000 2009.

Carnevale, V.; Raugei, S.  
*Structural aspects of the solvation shell of lysine and acetylated lysine: A Car-Parrinello and classical molecular dynamics investigation*  
Journal of Chemical Physics, (131) 2009.

Caronna, T.; Fontana, F.; Longhi, G.; Mele, A.; Sora, I. N.; Vigano, L.  
*2,13-Diaza[5]helicene: synthesis, theoretical calculations and spectroscopic properties*  
Arkivoc: 145-155 2009.

- Carvalho, J. F. S.; Silva, M. M. C.; Moreira, J. N.; Simoes, S.; Melo, M.  
*Efficient Chemoenzymatic Synthesis, Cytotoxic Evaluation, and SAR of Epoxysterols*  
Journal of Medicinal Chemistry, (52): 4007-4019 2009.
- Casanovas, J.; Canales, M.; Ferreira, C. A.; Aleman, C.  
*A First Principle Analysis of the Structure of Oligoanilines Doped with Alkylsulfonic Acids*  
Journal of Physical Chemistry A, (113): 8795-8800 2009.
- Casey, C. P.; Boller, T. M.; Samec, J. S. M.; Reinert-Nash, J. R.  
*Quantitative Determination of the Regioselectivity of Nucleophilic Addition to eta(3)-Propargyl Rhenium Complexes and Direct Observation of an Equilibrium between eta(3)-Propargyl Rhenium Complexes and Rhenacyclobutenes*  
Organometallics, (28): 123-131 2009.
- Castro, L.; Dommergue, A.; Ferrari, C.; Maron, L.  
*A DFT study of the reactions of O-3 with Hg degrees or Br*  
Atmospheric Environment, (43): 5708-5711 2009.
- Castro, R. A. E.; Canotilho, J.; Nunes, S. C. C.; Eusebio, M. E. S.; Redinha, J. S.  
*A study of the structure of the pindolol based on infrared spectroscopy and natural bond orbital theory*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (72): 819-826 2009.
- Celebi-Olcum, N.; Sanyal, A.; Aviyente, V.  
*Understanding the Stereoselection Induced by Chiral Anthracene Templates in Diels-Alder Cycloaddition: A DFT Study*  
Journal of Organic Chemistry, (74): 2328-2336 2009.
- Ceron-Carrasco, J. P.; Bastida, A.; Zuniga, J.; Requena, A.; Miguel, B.  
*Density Functional Theory Study of the Stability and Vibrational Spectra of the beta-Carotene Isomers*  
Journal of Physical Chemistry A, (113): 9899-9907 2009.
- Ceron-Carrasco, J. P.; Requena, A.; Michaux, C.; Perpete, E. A.; Jacquemin, D.  
*Effects of Hydration on the Proton Transfer Mechanism in the Adenine-Thymine Base Pair*  
Journal of Physical Chemistry A, (113): 7892-7898 2009.
- Cerpa, E.; Krapp, A.; Flores-Moreno, R.; Donald, K. J.; Merino, G.  
*Influence of Endohedral Confinement on the Electronic Interaction between He atoms: A He-2@C20H20 Case Study*  
Chemistry-a European Journal, (15): 1985-1990 2009.
- Chan, B.; Del Bene, J. E.; Radom, L.  
*What factors determine whether a proton-bound homodimer has a symmetric or an asymmetric hydrogen bond?*  
Molecular Physics, (107): 1095-1105 2009.

- Chaturvedi, J.; Bhattacharya, S.; Nethaji, M.  
*Synthesis of a one-dimensional coordination polymer containing pendant hydrosulfide groups*  
Dalton Transactions: 8018-8024 2009.
- Chaudret, R.; Trinquier, G.; Poteau, R.; Maron, L.  
*Theoretical proposal for an organometallic route to cis-peptides*  
New Journal of Chemistry, (33): 1833-1836 2009.
- Chen, A. Q.; Pu, X. M.; He, S. H.; Guo, Y. Z.; Wen, Z. N.; Li, M. L.; Wong, N. B.; Tian, A. M.  
*Solvent effects on isolated formamide and its monohydrated complex: observations from PCM study*  
New Journal of Chemistry, (33): 1709-1719 2009.
- Chen, B.-G.; Ho, C.-H.; Lee, C.-J.; Shieh, M.  
*Copper Halide-incorporated Tellurium-Iron Carbonyl Complexes: Transformation, Electrochemical Properties, and Theoretical Calculations*  
Inorganic Chemistry, (48): 10757-10768 2009.
- Chen, C. S.; Yu, Y. P.; Lin, B. C.; Gervay-Hague, J.; Fang, J. M.; Hsu, C. P.; Wu, S. H.  
*The Observation of the C-H center dot center dot center dot O-sp<sub>3</sub> Hydrogen Bond in Trisialic Acid Lactone and Its Implications for Cooperative Lactonization*  
European Journal of Organic Chemistry: 3351-3356 2009.
- Chen, H. S.; Meng, F. S.; Li, X. F.; Zhang, S. L.  
*Theoretical study of the adsorption of water molecule on (TiO<sub>2</sub>)<sub>n</sub> (n=3-6) clusters*  
Acta Physica Sinica, (58): 887-892 2009.
- Chen, J. C.; Chen, L. M.; Liao, S. Y.; Zheng, K. C.; Ji, L. N.  
*A DFT study on the hydrolysis mechanism of the potential antitumor Ru(III) complex TzNAMI*  
Journal of Molecular Structure-Theochem, (901): 137-144 2009.
- Chen, J. C.; Chen, L. M.; Liao, S. Y.; Zheng, K. C.; Ji, L. N.  
*A theoretical study on the hydrolysis process of two Kepler-type antitumor complexes [TzH][trans-RuCl<sub>4</sub>(Tz)(2)] and [2-NH(2)TzH][trans-RuCl<sub>4</sub>(2-NH(2)Tz)(2)]*  
Physical Chemistry Chemical Physics, (11): 3401-3410 2009.
- Chen, L.; Woon, D. E.; Dunning, T. H., Jr.  
*Bonding in ClF<sub>n</sub> (n=1-7) Molecules: Further Insight into the Electronic Structure of Hypervalent Molecules and Recounted Pair Bonds*  
Journal of Physical Chemistry A, (113): 12645-12654 2009.
- Chen, R.; Zhu, H.; Xie, D.; Yan, G.  
*Theoretical prediction of the noble gas complexes HeAuF and NeAuF*  
Science in China Series B-Chemistry, (52): 1987-1990 2009.
- Chen, X.; Qiao, Q. A.; Jin, Y. Q.; Jing, J.; Liu, Q. W.; Sun, L. X.; Wang, M. S.; Yang, C. L.  
*Theoretical study of the scavenging mechanism to 1,4-dicarbonyls by pyridoxamine: The water-assisted reaction*

Journal of Molecular Structure-Theochem, (911): 70-74 2009.

Chen, X.; Qiao, Q.-A.; Jin, Y.-Q.; Jing, J.; Cai, Z.-T.; Feng, D.-C.

*DFT Study on the Catalytic Mechanism of Aspartoacylase and Hydrolysis Pathway of the Inhibitor*  
Chemical Journal of Chinese Universities-Chinese, (30): 68-72 2009.

Chen, X.; Qiao, Q. G.; Cai, Z. T.; Jin, Y. Q.; Jing, J.; Sun, X. M.; Sun, L. X.; Cai, H. L.; Feng, D. C.

*Investigation on the Scavenging Mechanism of 1,4-Dicarbonyls by Pyridoxamine: A Density Functional Theory Study*  
Chinese Journal of Chemistry, (27): 1452-1458 2009.

Chen, X.; Xing, D.; Zhang, L.; Cukier, R. I.; Bu, Y.

*Effect of Metal Ions on Radical Type and Proton-Coupled Electron Transfer Channel: sigma-Radical vs pi-Radical and sigma-Channel vs pi-Channel in the Imide Units*  
Journal of Computational Chemistry, (30): 2694-2705 2009.

Chen, X. J.; Wu, F.; Yan, M.; Li, H. B.; Tian, S. X.; Shan, X.; Wang, K. D.; Li, Z. J.; Xu, K. Z.

*Hyperconjugative effect on the electronic wavefunctions of ethanol*  
Chemical Physics Letters, (472): 19-22 2009.

Chen, Z.; Song, J.; Shaik, S.; Hiberty, P. C.; Wu, W.

*Valence Bond Perturbation Theory. A Valence Bond Method That Incorporates Perturbation Theory*  
Journal of Physical Chemistry A, (113): 11560-11569 2009.

Chen, Z. H.; Song, J. S.; Shaik, S.; Hiberty, P. C.; Wu, W.

*Valence Bond Perturbation Theory. A Valence Bond Method That Incorporates Perturbation Theory*  
Journal of Physical Chemistry A, (113): 11560-11569 2009.

Chen, Z. Q.; Zhang, C. H.; Xue, Y.

*Theoretical Studies on the Thermodynamics and Kinetics of the N-Glycosidic Bond Cleavage in Deoxythymidine Glycol*  
Journal of Physical Chemistry B, (113): 10409-10420 2009.

Chenesseau, S.; Ferre, N.; Marque, S. R. A.; Siri, D.

*Imidazoline-N-oxyl: A DFT Study of Its Protonation Reaction*  
Chemphyschem, (10): 2419-2428 2009.

Cheng, J. B.; Wang, Y. L.; Li, Q. Z.; Liu, Z. B.; Li, W. Z.; Gong, B. A.

*Gigantic Blue Shift of the H-Ar Stretch Vibration in pi Hydrogen-Bonded C2H2 center dot center dot center dot HArCCF Complex*  
Journal of Physical Chemistry A, (113): 5235-5239 2009.

Cheng, Q.; Evangelista, F. A.; Simmonett, A. C.; Yamaguchi, Y.; Schaefer, H. F., III

*Water Dimer Radical Cation: Structures, Vibrational Frequencies, and Energetics*  
Journal of Physical Chemistry A, (113): 13779-13789 2009.

- Cheng, W.; Jiang, H. H.; Zhang, D. J.; Zhang, C. Q.  
*A DFT study of the reactions of the Cu<sup>+</sup> ion with methylamine and dimethylamine*  
Journal of Molecular Structure-Theochem, (895): 77-81 2009.
- Cherkaoui, M.; Boutalib, A.  
*AB INITIO CHEMICAL INVESTIGATION OF THE ARSENIC-ALANES COMPLEXES (CH<sub>3</sub>)<sub>(n)</sub>H<sub>3-n</sub>AlAsY<sub>3</sub>(Y = H, F, Cl, and Br; n=0-3)*  
Annales De Chimie-Science Des Materiaux, (34): 203-209 2009.
- Cheshmedzhieva, D.; Ilieva, S.; Hadjieva, B.; Galabov, B.  
*The mechanism of alkaline hydrolysis of amides: a comparative computational and experimental study of the hydrolysis of N-methylacetamide, N-methylbenzamide, and acetanilide*  
Journal of Physical Organic Chemistry, (22): 619-631 2009.
- Cheshmedzhieva, D.; Ilieva, S.; Hadjieva, B.; Trayanova, T.; Galabov, B.  
*Reactivity of acetanilides in the alkaline hydrolysis reaction: theory vs. experiment*  
Molecular Physics, (107): 1187-1192 2009.
- Chiang, Y. K.; Kuo, C. C.; Wu, Y. S.; Chen, C. T.; Coumar, M. S.; Wu, J. S.; Hsieh, H. P.; Chang, C. Y.; Jseng, H. Y.; Wu, M. H.; Leou, J. S.; Song, J. S.; Chang, J. Y.; Lyu, P. C.; Chao, Y. S.; Wu, S. Y.  
*Generation of Ligand-Based Pharmacophore Model and Virtual Screening for Identification of Novel Tubulin Inhibitors with Potent Anticancer Activity*  
Journal of Medicinal Chemistry, (52): 4221-4233 2009.
- Cho, H. G.  
*Agostic Structure of Titanium Methylidene Hydride (CH<sub>2</sub>=TiH<sub>2</sub>): A Theoretical Investigation for the Elusive Intramolecular Interaction*  
Bulletin of the Korean Chemical Society, (30): 1631-1633 2009.
- Cho, H. G.; Andrews, L.  
*Matrix Infrared Spectra of Dihydrido Cyclic and Trihydrido Ethynyl Products from Reactions of Th and U Atoms with Ethylene Molecules*  
Journal of Physical Chemistry A, (113): 5073-5081 2009.
- Cho, H. G.; Andrews, L.; Vlaisavljevich, B.; Gagliardi, L.  
*Infrared Spectra of Small Insertion and Methylidene Complexes in Reactions of Laser-Ablated Nickel Atoms with Halomethanes*  
Organometallics, (28): 5623-5632 2009.
- Cho, H. G.; Cheong, B. S.  
*Agostic Interaction of the Smallest Zirconium Methylidene Hydride: Reproduction of the Distorted Structure Experimentally Observed in Matrix Infrared Spectra*  
Bulletin of the Korean Chemical Society, (30): 479-481 2009.
- Cholewinski, G.; Chojnacki, J.; Pikies, J.; Rachon, J.  
*Synthesis and structural investigation of N-acyl selenophosphoramides*  
Organic & Biomolecular Chemistry, (7): 4095-4100 2009.

- Choudhary, A.; Gandla, D.; Krow, G. R.; Raines, R. T.  
*Nature of Amide Carbonyl-Carbonyl Interactions in Proteins*  
Journal of the American Chemical Society, (131): 7244-+ 2009.
- Chrostowska, A.; Lemierre, V.; Dargelos, A.; Baylere, P.; Leigh, W. J.; Rima, G.; Weber, L.; Schimmel, M.  
*Gas-phase synthesis and characterization of heteroleptic divalent germanium compounds by FVT/UV-PES*  
Journal of Organometallic Chemistry, (694): 43-51 2009.
- Ciclosi, M.; Lloret, J.; Estevan, F.; Sanau, M.; Perez-Prieto, J.  
*Intramolecular apical Metal-H-C-sp<sub>3</sub> interaction in molybdenum and silver complexes*  
Dalton Transactions: 5077-5082 2009.
- Cid, M. B.; Alfonso, F.; Alonso, I.; Martin-Lomas, M.  
*On the origin of the regioselectivity in glycosylation reactions of 1,2-diols*  
Organic & Biomolecular Chemistry, (7): 1471-1481 2009.
- Coelho, J. V.; Freitas, M. P.; Tormena, C. F.; Rittner, R.  
*On the (4)J(HH) long-range coupling in 2-bromocyclohexanone: conformational insights*  
Magnetic Resonance in Chemistry, (47): 348-351 2009.
- Coi, A.; Bianucci, A. M.; Calderone, V.; Testai, L.; Digaocomo, M.; Rapposelli, S.; Balsamo, A.  
*Predictive models, based on classification algorithms, for compounds potentially active as mitochondrial ATP-sensitive potassium channel openers*  
Bioorganic & Medicinal Chemistry, (17): 5565-5571 2009.
- Colaneri, M. J.; Vitali, J.; Peisach, J.  
*Aspects of Structure and Bonding in Copper-Amino Acid Complexes Revealed by Single-Crystal EPR/ENDOR Spectroscopy and Density Functional Calculations*  
Journal of Physical Chemistry A, (113): 5700-5709 2009.
- Coles, M. P.; Aragon-Saez, P. J.; Oakley, S. H.; Hitchcock, P. B.; Davidson, M. G.; Maksic, Z. B.; Vianello, R.; Leito, I.; Kaljurand, I.; Apperley, D. C.  
*Superbasicity of a Bis-guanidino Compound with a Flexible Linker: A Theoretical and Experimental Study*  
Journal of the American Chemical Society, (131): 16858-16868 2009.
- Comelli, N. C.; Massa, N. E.; Castro, E. A.; Blanch, L. B.; Jubert, A. H.  
*Experimental and theoretical study of the structure and vibrational spectra of valpromide, C<sub>7</sub>H<sub>15</sub>CONH<sub>2</sub>*  
Journal of Raman Spectroscopy, (40): 6-17 2009.
- Comelli, N. C.; Massa, N. E.; Castro, E. A.; Jubert, A. H.  
*Spectroscopy properties of the amide group in valpromide and some derivatives with antiepileptic activity*  
Journal of Raman Spectroscopy, (40): 1797-1809 2009.
- Constantino, E.; Rimola, A.; Sodupe, M.; Rodriguez-Santiago, L.

*Coordination of (Glycyl)(n)glycine (n=1-3) to Co<sup>+</sup> and Co<sup>2+</sup>*  
Journal of Physical Chemistry A, (113): 8883-8892 2009.

Contreras, J. G.; Hurtado, S. M.  
*The Effect of C2 and C5 Substitutions on the Nitrogen Lone Pair Inversion in 1,3-Oxazines*  
Journal of the Chilean Chemical Society, (54): 99-104 2009.

Contreras, R. H.; Llorente, T.; Pagola, G. I.; Bustamante, M. G.; Pasqualini, E. E.; Melo, J. I.; Tormena, C. F.  
*Qualitative Study of Substituent Effects on NMR N-15 and O-17 Chemical Shifts*  
Journal of Physical Chemistry A, (113): 9874-9880 2009.

Contreras, R. H.; Provasi, P. F.; dos Santos, F. P.; Tormena, C. F.  
*Stereochemical dependence of NMR geminal spin-spin coupling constants*  
Magnetic Resonance in Chemistry, (47): 113-120 2009.

Corani, A.; Domanskaya, A.; Khriachtchev, L.; Rasanen, M.; Lignell, A.  
*Matrix-Isolation and Ab Initio Study of the HKrCl center dot center dot center dot HCl Complex*  
Journal of Physical Chemistry A, (113): 10687-10692 2009.

Cormier, K. W.; Lewis, M.  
*Lithium and sodium cation binding of cyclopentadienyl anions: Electronic effects of cyclopentadienyl substitution*  
Polyhedron, (28): 3120-3128 2009.

Corn, B.; Malinovskaya, S. A.  
*An Ab Initio Analysis of Charge Redistribution upon Isomerization of Retinal in Rhodopsin and Bacteriorhodopsin*  
International Journal of Quantum Chemistry, (109): 3131-3141 2009.

Correa, J. V.; Jaque, P.; Olah, J.; Toro-Labbe, A.; Geerlings, P.  
*Nucleophilicity and electrophilicity of silylenes from a molecular electrostatic potential and dual descriptor perspectives*  
Chemical Physics Letters, (470): 180-186 2009.

Costa, R. D.; Viruela, P. M.; Bolink, H. J.; Orti, E.  
*Lowest triplet excited states of a novel heteroleptic iridium(III) complex and their role in the emission colour*  
Journal of Molecular Structure-Theochem, (912): 21-26 2009.

Coucouvanis, D.; Paital, A. R.; Zhang, Q. W.; Lehnert, N.; Ahlrichs, R.; Fink, K.; Fenske, D.; Powell, A. K.; Lan, Y. H.  
*Synthesis, Electronic Structure, and Structural Characterization of the New, "Non-Innocent" 4,5-Dithio-Catecholate Ligand, Its Metal Complexes, and Their Oxidized 4,5-Dithio-o-quinone Derivatives*  
Inorganic Chemistry, (48): 8830-8844 2009.

Craciun, S.; Donald, K. J.

*Radical Bonding: Structure and Stability of Bis(Phenalenyl) Complexes of Divalent Metals from across the Periodic Table*  
Inorganic Chemistry, (48): 5810-5819 2009.

Cui, J.; Zhang, Y.; Zhao, F. J.; Yang, J.; Shen, G. Y.; Xu, Y.  
*HB(N-5)(3)M (M = Li, Na, K, and Rb): A new kind of pentazolides as HEDMs*  
Progress in Natural Science, (19): 41-45 2009.

Cui, Y. H.; Tian, W. Q.; Feng, J. K.; Li, W. Q.; Liu, Z. Z.  
*Aromaticity of Ni bis-dithiolenes complexes*  
Journal of Molecular Structure-Theochem, (897): 61-65 2009.

Da Silva, J. C. S.; De Almeida, W. B.; Rocha, W. R.  
*Theoretical investigation of the structure and nature of the interaction in metal-alkane sigma-complexes of the type [M(CO)(5)(C<sub>2</sub>H<sub>6</sub>)] (M = Cr, Mo, and W)*  
Chemical Physics, (365): 85-93 2009.

da Silva, M.; Santos, A.; Gomes, J. R. B.; Roux, M. V.; Temprado, M.; Jimenez, P.; Notario, R.  
*Thermochemistry of Bithiophenes and Thienyl Radicals. A Calorimetric and Computational Study*  
Journal of Physical Chemistry A, (113): 11042-11050 2009.

Dai, Q.; Lei, X.; Yang, J.; Cheng, Q.; Gao, C.; Li, H.  
*Crystal Structure of Baicalin*  
Acta Chimica Sinica, (67): 2363-2367 2009.

Dans, P. D.; Coitino, E. L.  
*Density Functional Theory Characterization and Descriptive Analysis of Cisplatin and Related Compounds*  
Journal of Chemical Information and Modeling, (49): 1407-1419 2009.

Das, A. R.; Medda, A.; Singha, R.; Guchhait, N.  
*A highly active catalyst supported molecular sieves-NaHCO<sub>3</sub> mixture for the selective and advantageous N-monoalkylation of amines*  
Journal of the Indian Chemical Society, (86): 841-848 2009.

Dash, C.; Shaikh, M. M.; Ghosh, P.  
*Fluoride-Free Hiyama and Copper- and Amine-Free Sonogashira Coupling in Air in a Mixed Aqueous Medium by a Series of PEPPSI-Themed Precatalysts*  
European Journal of Inorganic Chemistry: 1608-1618 2009.

de Almeida, K. J.; Duarte, H. A.  
*Gas-Phase Methane Activation by the Ac<sup>+</sup>-Pu<sup>+</sup> Ions: Theoretical Insights into the Role of 5f Electrons/Orbitals in Early Actinide Chemistry*  
Organometallics, (28): 3203-3211 2009.

De Dobbeleer, C.; Pospisil, J.; De Vleeschouwer, F.; De Proft, F.; Marko, I. E.  
*Unexpected nucleophilic behaviour of free-radicals generated from alpha-iodoketones*  
Chemical Communications: 2142-2144 2009.

- de Sousa, A. S.; Reisinger, S. A.; Fernandes, M. A.; Perry, C. B.; Varadwaj, P. R.; Marques, H. M.  
*The structure of N,N'-bis(2-hydroxyethyl)ethane-1,2-diamine and its complexes with Zn(II) and Cd(II)*  
Dalton Transactions: 10208-10218 2009.
- De Vleeschouwer, F.; Toro-Labbe, A.; Gutierrez-Oliva, S.; Van Speybroeck, V.; Waroquier, M.; Geerlings, P.; De Proft, F.  
*Reversibility from DFT-Based Reactivity Indices: Intramolecular Side Reactions in the Polymerization of Poly(vinyl chloride)*  
Journal of Physical Chemistry A, (113): 7899-7908 2009.
- Deakyne, C. A.; Thomas, H. M.; Liebman, J. F.  
*The structure and energetics of triplet [B, C, F, H-2]*  
Journal of Fluorine Chemistry, (130): 836-845 2009.
- Decken, A.; Knapp, C.; Nikiforov, G. B.; Passmore, J.; Rautiainen, J. M.; Wang, X. P.; Zeng, X. Q.  
*Silver(I) Complexes of the Weakly Coordinating Solvents SO<sub>2</sub> and CH<sub>2</sub>Cl<sub>2</sub>: Crystal Structures, Bonding, and Energetics of Ag(OSO)Al{OC(CF<sub>3</sub>)(3)}(4), Ag(OSO)(2/2)SbF<sub>6</sub>, and Ag(CH<sub>2</sub>Cl<sub>2</sub>)(2)SbF<sub>6</sub>*  
Chemistry-a European Journal, (15): 6504-6517 2009.
- Defonsi Lestard, M. E.; Eugenia Tuttolomondo, M.; Wann, D. A.; Robertson, H. E.; Rankin, D. W. H.; Ben Altabef, A.  
*A conformational and vibrational study of CF<sub>3</sub>COSCH<sub>2</sub>CH<sub>3</sub>*  
Journal of Chemical Physics, (131) 2009.
- Defonsi Lestard, M. E.; Tuttolomondo, M. E.; Varetti, E. L.; Wann, D. A.; Robertson, H. E.; Rankin, D. W. H.; Ben Altabef, A.  
*Gas-phase structure and new vibrational study of methyl trifluoroacetate (CF<sub>3</sub>C(O)OCH<sub>3</sub>)*  
Journal of Raman Spectroscopy, (40): 2053-2062 2009.
- Degirmenci, I.; Aviyente, V.; Van Speybroeck, V.; Waroquier, M.  
*DFT Study on the Propagation Kinetics of Free-Radical Polymerization of alpha-Substituted Acrylates*  
Macromolecules, (42): 3033-3041 2009.
- Del Bene, J. E.; Mo, O.; Yanez, M.  
*Substituent Effects on B-N Bonding and Coupling Constants in Five-membered Rings N<sub>3</sub>B<sub>2</sub>H<sub>4</sub>X and N<sub>2</sub>B<sub>3</sub>H<sub>4</sub>X, for X = H, F, and Li*  
Croatica Chemica Acta, (82): 149-155 2009.
- Del Bene, J. E.; Yanez, M.; Alkorta, I.; Elguero, J.  
*An Ab Initio Study of the Structures and Selected Properties of 1,2-Dihydro-1,2-azaborine and Related Molecules*  
Journal of Chemical Theory and Computation, (5): 2239-2247 2009.
- del Rosal, I.; Jolibois, F.; Maron, L.; Philippot, K.; Chaudret, B.; Poteau, R.

*Ligand effect on the NMR, vibrational and structural properties of tetra- and hexanuclear ruthenium hydrido clusters: a theoretical investigation*  
Dalton Transactions: 2142-2156 2009.

Delferro, M.; Tegoni, M.; Verdolino, V.; Cauzzi, D.; Graiff, C.; Tiripicchio, A.  
*Oxidative Addition of Iodomethane to Charge-Tuned Rhodium(I) Complexes*  
Organometallics, (28): 2062-2071 2009.

Delfino, R. T.; Figueroa-Villar, J. D.  
*Nucleophilic Reactivation of Sarin-Inhibited Acetylcholinesterase: A Molecular Modeling Study*  
Journal of Physical Chemistry B, (113): 8402-8411 2009.

Dhaouadi, Z.; Nsangou, M.; Garrab, N.; Anouar, E. H.; Marakchi, K.; Lahmar, S.  
*DFT study of the reaction of quercetin with center dot O-2(-) and center dot OH radicals*  
Journal of Molecular Structure-Theochem, (904): 35-42 2009.

Dhumal, N. R.; Kim, H. J.; Kiefer, J.  
*Molecular Interactions in 1-Ethyl-3-methylimidazolium Acetate Ion Pair: A Density Functional Study*  
Journal of Physical Chemistry A, (113): 10397-10404 2009.

Di Santo, E.; Michelini, M. D.; Russo, N.  
*Methane C-H Bond Activation by Gas-Phase Th+ and U+: Reaction Mechanisms and Bonding Analysis*  
Organometallics, (28): 3716-3726 2009.

Diao, K. S.; Wang, H. J.  
*The nitrogen position effect on the selectivity of diazacrown ethers to metal ion*  
Journal of Molecular Structure-Theochem, (910): 163-168 2009.

Diao, K. S.; Wang, H. J.; Qiu, Z. M.  
*A DFT Study on the Selective Extraction of Metallic Ions by 12-Crown-4*  
Journal of Solution Chemistry, (38): 713-724 2009.

Diao, K.-S.; Wang, F.; Wang, H.-j.  
*Ab initio theoretical study of the interactions between CFCs and CO2*  
Journal of Molecular Structure-Theochem, (913): 195-199 2009.

Dias, H. V. R.; Flores, J. A.; Wu, J.; Kroll, P.  
*Monomeric Copper(I), Silver(I), and Gold(I) Alkyne Complexes and the Coinage Metal Family Group Trends*  
Journal of the American Chemical Society, (131): 11249-11255 2009.

Dias, L. C.; Pinheiro, S. M.; de Oliveira, V. M.; Ferreira, M. A. B.; Tormena, C. F.; Aguilar, A. M.; Zukerman-Schpector, J.; Tiekkink, E. R. T.  
*Addition of kinetic boron enolates generated from beta-alkoxy methyl ketones to aldehydes. Density functional theory calculations on the transition structures*  
Tetrahedron, (65): 8714-8721 2009.

Dimitrova, M.; Galabov, B.

*Predicting the Acidities of Substituted Phenols Using Electrostatic Potential at Nuclei*  
Croatica Chemica Acta, (82): 21-25 2009.

Dinelli, L. R.; Von Poelhsitz, G.; Castellano, E. E.; Ellena, J.; Galembek, S. E.; Batista, A. A.

*On an Electrode Modified by a Supramolecular Ruthenium Mixed Valence (Ru-II/Ru-III) Diphosphine-Porphyrin Assembly*  
Inorganic Chemistry, (48): 4692-4700 2009.

Ding, J.-N.; Yuan, N.-Y.; Li, F.; Ding, G.-Q.; Chen, Z.-G.; Chen, X.-S.; Lu, W.

*Geometry and stability of Cu<sub>n</sub>N (*n*=1-6) and Cu<sub>3n</sub>N<sub>n</sub> (*n*=1-5) clusters*  
Journal of Chemical Physics, (131) 2009.

Ding, Y. Q.; He, M. X.; Niu, Y. Z.; Wang, D. X.; Cui, Y.; Feng, S. Y.

*Electronic Structures of Bis- and Monothiophene Complexes with Fe, Co, Ni: A Density Functional Theory Study*  
Journal of Physical Chemistry A, (113): 10291-10298 2009.

Dipojono, H. K.; Saputro, A. G.; Belkada, R.; Nakanishi, H.; Kasai, H.; David, M.; Dy, E. S.

*Adsorption of O-2 on Cobalt-(n)Pyrrole Molecules from First-Principles Calculations*  
Journal of the Physical Society of Japan, (78) 2009.

Djukic, J. P.; Parkhomenko, K.; Hijazi, A.; Chemmi, A.; Allouche, L.; Brelot, L.; Pfeffer, M.; Ricard, L.; Le Goff, X. F.

*mu-Chlorido, mu-hydroxo-bridged dicarbonyl ruthenacycles: synthesis, structure and catalytic properties in hydrogen atom transfer*  
Dalton Transactions: 2695-2711 2009.

Djukic, J.-P.; Boulho, C.; Sredojevic, D.; Scheeren, C.; Zaric, S.; Ricard, L.; Pfeffer, M.

*The Stereospecific Ligand Exchange at a Pseudo-Benzylid T-4 Iridium Centre in Planar-Chiral Cycloiridium (eta(6)-Arene)tricarbonylchromium Complexes*  
Chemistry-a European Journal, (15): 10830-10842 2009.

Dobrzynska, D.; Lis, T.; Wozniak, J.; Jezierska, J.; Duczmal, M.; Wojciechowska, A.; Wysokinski, R.

*Crystal structure, spectroscopic, magnetic and theoretical studies of [bis(hippurato)bis(benzimidazole)copper(II)] propanol 1/4hydrate*  
Polyhedron, (28): 3150-3154 2009.

Dogaru, D.; Motiu, S.; Gogonea, V.

*Inactivation of [Fe-Fe]-Hydrogenase by O-2. Thermodynamics and Frontier Molecular Orbitals Analyses*  
International Journal of Quantum Chemistry, (109): 876-889 2009.

Domagala, M.; Grabowski, S. J.

*X-H center dot center dot center dot pi and X-H center dot center dot center dot N hydrogen bonds - Acetylene and hydrogen cyanide as proton acceptors*  
Chemical Physics, (363): 42-48 2009.

- Domagala, S.; Korybut-Daszkiewicz, B.; Straver, L.; Wozniak, K.  
*Determination of Experimental Charge Density in Model Nickel Macrocycle: [3,11-Bis(methoxycarbonyl)-1,5,9,13-tetraazacyclohexadeca-1,3,9,11-tetra enato-(2-)kappa N-4]nickel(II)*  
Inorganic Chemistry, (48): 4010-4020 2009.
- Domagal-Goldman, S. D.; Paul, K. W.; Sparks, D. L.; Kubicki, J. D.  
*Quantum chemical study of the Fe(III)-desferrioxamine B siderophore complex-Electronic structure, vibrational frequencies, and equilibrium Fe-isotope fractionation*  
Geochimica et Cosmochimica Acta, (73): 1-12 2009.
- Domingo, L. R.; Arno, M.; Saez, J. A.  
*DFT Study of the Molecular Mechanism of Lewis Acid Induced [4+3] Cycloadditions of 2-Alkylacroleins with Cyclopentadiene*  
Journal of Organic Chemistry, (74): 5934-5940 2009.
- Domingo, L. R.; Aurell, M. J.; Arno, M.  
*Understanding the mechanism of the N-heterocyclic carbene-catalyzed ring-expansion of 4-formyl-beta-lactams to succinimide derivatives*  
Tetrahedron, (65): 3432-3440 2009.
- Domingo, L. R.; Chamorro, E.; Perez, P.  
*An Analysis of the Regioselectivity of 1,3-Dipolar Cycloaddition Reactions of Benzonitrile N-Oxides Based on Global and Local Electrophilicity and Nucleophilicity Indices*  
European Journal of Organic Chemistry: 3036-3044 2009.
- Domingo, L. R.; Perez-Ruiz, R.; Arguello, J. E.; Miranda, M. A.  
*DFT Study on the Molecular Mechanism of the [4+2] Cycloaddition between Thiobenzophenone and Arylalkenes via Radical Cations*  
Journal of Physical Chemistry A, (113): 5718-5722 2009.
- Domingo, L. R.; Picher, M. T.; Saez, J. A.  
*Toward an Understanding of the Unexpected Regioselective Hetero-Diels-Alder Reactions of Asymmetric Tetrazines with Electron-Rich Ethylenes: A DFT Study*  
Journal of Organic Chemistry, (74): 2726-2735 2009.
- Domingo, L. R.; Saez, J. A.  
*Understanding the mechanism of polar Diels-Alder reactions*  
Organic & Biomolecular Chemistry, (7): 3576-3583 2009.
- Donald, K. J.; Hargittai, M.; Hoffmann, R.  
*Group 12 Dihalides: Structural Predilections from Gases to Solids*  
Chemistry-a European Journal, (15): 158-177 2009.
- Du, J. G.; Sun, X. Y.; Jiang, G.  
*A DFT study on small M-doped titanium (M = V, Fe, Ni) clusters: structures, chemical bonds and magnetic properties*

European Physical Journal D, (55): 111-120 2009.

Du, S. Y.; Francisco, J. S.

*OH center dot N-2 and SH center dot N-2 radical-molecule van der Waals complex*  
Journal of Chemical Physics, (131) 2009.

Du, S. Y.; Francisco, J. S.

*Spectroscopic properties and stability of the SH center dot H<sub>2</sub>O open shell complex*  
Journal of Chemical Physics, (130) 2009.

Du, S. Y.; Francisco, J. S.; Kais, S.

*Study of electronic structure and dynamics of interacting free radicals influenced by water*  
Journal of Chemical Physics, (130) 2009.

Dul, M. C.; Ottenwaelder, X.; Pardo, E.; Lescouezec, R.; Journaux, Y.; Chamoreau, L. M.; Ruiz-Garcia, R.; Cano, J.; Julve, M.; Lloret, F.

*Ferromagnetic Coupling by Spin Polarization in a Trinuclear Copper(II) Metallacyclophane with a Triangular Cage-Like Structure*  
Inorganic Chemistry, (48): 5244-5249 2009.

DuPre, D. B.

*Multiple Bonding in the Chromium Dimer Supported by Two Diazadiene Ligands*  
Journal of Physical Chemistry A, (113): 1559-1563 2009.

Dureen, M. A.; Welch, G. C.; Gilbert, T. M.; Stephan, D. W.

*Heterolytic Cleavage of Disulfides by Frustrated Lewis Pairs*  
Inorganic Chemistry, (48): 9910-9917 2009.

Ebrahimi, A.; Habibi, M.; Hesabi, N.

*Development of Eclipsed and Staggered Forms in Some Hydrogen Bonded Complexes*  
International Journal of Quantum Chemistry, (109): 629-638 2009.

Ebrahimi, A.; Habibi, M.; Masoodi, H. R.

*The role of H center dot center dot center dot pi interaction on some calculated NMR data*  
Chemical Physics Letters, (478): 120-126 2009.

Ebrahimi, A.; Habibi, M.; Masoodi, H. R.; Gholipour, A. R.

*Relationship between calculated NMR data and intermolecular hydrogen bond properties in X-pyridine center dot center dot center dot HF*  
Chemical Physics, (355): 67-72 2009.

Ebrahimi, A.; Habibi, M.; Neyband, R. S.; Gholipour, A. R.

*Cooperativity of pi-stacking and hydrogen bonding interactions and substituent effects on X-phenyl parallel to pyr center dot center dot center dot H-F complexes*  
Physical Chemistry Chemical Physics, (11): 11424-11431 2009.

Ebrahimi, A.; Habibi, S. M.; Neyband, R. S.

*Substituent Effect on Intramolecular Hydrogen Bonding in 2-Hydroxybenzaldehyde*

International Journal of Quantum Chemistry, (109): 1274-1282 2009.

Ebrahimi, A.; Khorassani, S. M. H.; Delarami, H.

*Estimation of individual binding energies in some dimers involving multiple hydrogen bonds using topological properties of electron charge density*  
Chemical Physics, (365): 18-23 2009.

Eckert-Maksic, M.; Lischka, H.; Maksic, Z. B.; Vazdar, M.

*The Isomerization Barrier in Cyanocyclobutadienes: An ab Initio Multireference Average Quadratic Coupled Cluster Study*  
Journal of Physical Chemistry A, (113): 8351-8358 2009.

Edge, R.; Less, R. J.; McInnes, E. J. L.; Muther, K.; Naseri, V.; Rawson, J. M.; Wright, D. S.

*Formation of a new class of 7 pi radicals via sterically induced P-P bond cleavage of the dimers [(CH)(2)(NR)(2)P](2)*  
Chemical Communications: 1691-1693 2009.

Eger, W. A.; Jahn, B. O.; Anders, E.

*The zinc complex catalyzed hydration of alkyl isothiocyanates*  
Journal of Molecular Modeling, (15): 433-446 2009.

Eitner, K.; Koch, U.

*From Fragment Screening to Potent Binders: Strategies for Fragment-to-Lead Evolution*  
Mini-Reviews in Medicinal Chemistry, (9): 956-961 2009.

Eklof, A. M.; Ottosson, H.

*Effects of substituents and counterions on the structures of silenolates: a computational investigation*  
Tetrahedron, (65): 5521-5526 2009.

Eloi, A.; Rose-Munch, F.; Rose, E.; Chavarot-Kerlidou, M.; Gerard, H.

*A Simple Route to Keto-Substituted (eta(5)-Cyclohexadienyl)Mn(CO)(3) Complexes Using Organomanganese Transmetalation: Structural and Theoretical Characterizations*  
Organometallics, (28): 925-928 2009.

Erdelyiova, A.; Gyoryova, K.; Gyepes, R.; Halas, L.; Kovarova, J.

*Synthesis, spectral, thermal and structural study of bis(2-bromobenzoato-O,O')-bis(methyl-3-pyridylcarbamate-N)-zinc(II)*  
Polyhedron, (28): 131-137 2009.

Esquivel, R. O.; Flores-Gallegos, N.; Carrera, E. M.; Dehesa, J. S.; Angulo, J. C.; Antolin, J.; Soriano-Correa, C.

*Theoretic-information entropies analysis of nanostructures: ab initio study of PAMAM precursors and dendrimers G0 to G3*  
Molecular Simulation, (35): 498-511 2009.

Esrafili, M. D.; Beheshtian, J.; Hadipour, N. L.

*N-15 CHEMICAL SHIFT CALCULATIONS AND NATURAL BONDING ORBITAL ANALYSES OF  
(BENZAMIDE)(n=1-6) CLUSTERS*

Journal of Theoretical & Computational Chemistry, (8): 973-982 2009.

Esseffar, M.; El Messaoudi, M.; Azzouzi, S.; Jalal, R.; Saez, J. A.; Domingo, L. R.; Latorre, J.; Liu-Gonzalez, M.

*Formation of pyrazol-1,3,4-thiadiazoles through 1,3-dipolar cycloadditions of 3-thioxo-[1,2,4]-triazepin-5-one with nitrilimines: an experimental and computational study*  
Journal of Physical Organic Chemistry, (22): 31-41 2009.

Etienne, M.; McGrady, J. E.; Maseras, F.

*Agostic interactions in alkyl derivatives of sterically hindered tris(pyrazolyl)borate complexes of niobium*  
Coordination Chemistry Reviews, (253): 635-646 2009.

Evans, W. J.; Fang, M.; Zucchi, G.; Furche, F.; Ziller, J. W.; Hoekstra, R. M.; Zink, J. I.

*Isolation of Dysprosium and Yttrium Complexes of a Three-Electron Reduction Product in the Activation of Dinitrogen, the (N-2)(3-) Radical*  
Journal of the American Chemical Society, (131): 11195-11202 2009.

Evans, W. J.; Walensky, J. R.; Furche, F.; DiPasquale, A. G.; Rheingold, A. L.

*Trigonal-Planar versus Pyramidal Geometries in the Tris(ring) Heteroleptic Divalent Lanthanide Complexes (C5Me5)Ln(mu-eta(6):eta(1)-Ph)(2)BPh2: Crystallographic and Density Functional Theory Analysis*  
Organometallics, (28): 6073-6078 2009.

Fakhraee, S.; Azami, S. M.

*Orbital representation of kinetic energy pressure*  
Journal of Chemical Physics, (130) 2009.

Fallas, J. A.; Gonzalez, L.; Corral, I.

*Density functional theory rationalization of the substituent effects in trifluoromethyl-pyridinol derivatives*  
Tetrahedron, (65): 232-239 2009.

Fan, H.; Eliason, J. K.; Moliva A, C. D.; Olson, J. L.; Flancher, S. M.; Gealy, M. W.; Ulness, D. J.

*Halogen Bonding in Iodo-perfluoroalkane/Pyridine Mixtures*  
Journal of Physical Chemistry A, (113): 14052-14059 2009.

Fang, H.; Zhang, X. G.

*Density functional study on rare gas-noble metal closed-shell interaction in XeMX (M = Au, Ag, Cu; X = F, Cl, Br) systems*  
Theoretical Chemistry Accounts, (123): 443-453 2009.

Fang, H.; Zhang, X. G.; Wang, S. G.

*Density functional study of aurophilic interaction in X(AuPH3)(2)(+) (2) (X = F, Cl, Br, I)*  
Physical Chemistry Chemical Physics, (11): 5796-5804 2009.

- Farbos, B.; Tassaing, T.  
*Substituent effect on the interaction of aromatic primary amines and diamines with supercritical CO<sub>2</sub> from infrared spectroscopy and quantum calculations*  
Physical Chemistry Chemical Physics, (11): 5052-5061 2009.
- Fard, Z. H.; Muller, C.; Harmening, T.; Pottgen, R.; Dehnen, S.  
*Thiostannate Tin-Tin Bond Formation in Solution: In Situ Generation of the Mixed-Valent, Functionalized Complex [{(RSnIV)(2)(μ-S)(2)}(3)(Sn<sub>2</sub>S<sub>6</sub>)-S-III]*  
Angewandte Chemie-International Edition, (48): 4441-4444 2009.
- Farmanzadeh, D.; Amirazami, A.  
*Electric Field Dependence of (4,0) Zigzag Model Single-Walled Carbon Nanotube*  
Acta Physico-Chimica Sinica, (25): 2343-2349 2009.
- Farmanzadeh, D.; Ghazanfary, S.  
*First principle electric field response of single-walled boron nitride nanotube: a case study of zigzag (4,0) model*  
Structural Chemistry, (20): 709-717 2009.
- Fayet, G.; Rotureau, P.; Joubert, L.; Adamo, C.  
*On the prediction of thermal stability of nitroaromatic compounds using quantum chemical calculations*  
Journal of Hazardous materials, (171): 845-850 2009.
- Feng, X. T.; Yu, J. G.; Lei, M.; Fang, W. H.; Liu, S. B.  
*Toward Understanding Metal-Binding Specificity of Porphyrin: A Conceptual Density Functional Theory Study*  
Journal of Physical Chemistry B, (113): 13381-13389 2009.
- Ferbinteanu, M.; Cimpoesu, F.; Kajiwara, T.; Yamashita, M.  
*Magnetic anisotropy and molecular assembling in d complex cation-f complex anion type coordination compounds*  
Solid State Sciences, (11): 760-765 2009.
- Ferguson, G. A.; Rivillon, S.; Chabal, Y.; Raghavachari, K.  
*The Structure and Vibrational Spectrum of the Si(111)-H/Cl Surface*  
Journal of Physical Chemistry C, (113): 21713-21720 2009.
- Fernanda Zalazar, M.; Duarte, D. J. R.; Peruchena, N. M.  
*Adsorption of Alkenes on Acidic Zeolites. Theoretical Study Based on the Electron Charge Density*  
Journal of Physical Chemistry A, (113): 13797-13807 2009.
- Fernandez, I.; Dyker, C. A.; DeHope, A.; Donnadieu, B.; Frenking, G.; Bertrand, G.  
*Exocyclic Delocalization at the Expense of Aromaticity in 3,5-bis(pi-Donor) Substituted Pyrazolium Ions and Corresponding Cyclic Bent Allenes*  
Journal of the American Chemical Society, (131): 11875-11881 2009.
- Ferreira, A. M.; Krishnamurthy, M.; II, B. M. M.; Finkelstein, D.; Bashford, D.

*Quantitative structure-activity relationship (QSAR) for a series of novel cannabinoid derivatives using descriptors derived from semi-empirical quantum-chemical calculations*  
Bioorganic & Medicinal Chemistry, (17): 2598-2606 2009.

Ferreiros-Martinez, R.; Esteban-Gomez, D.; de Blas, A.; Platas-Iglesias, C.; Rodriguez-Blas, T.  
*Eight-Coordinate Zn(II), Cd(II), and Pb(II) Complexes Based on a 1,7-Diaza-12-crown-4 Platform Endowed with a Remarkable Selectivity over Ca(II)*  
Inorganic Chemistry, (48): 11821-11831 2009.

Ferreiros-Martinez, R.; Esteban-Gomez, D.; Platas-Iglesias, C.; de Blas, A.; Rodriguez-Blas, T.  
*Selective Chelation of Cd(II) and Pb(II) versus Ca(II) and Zn(II) by Using Octadentate Ligands Containing Pyridinecarboxylate and Pyridyl Pendants*  
Inorganic Chemistry, (48): 10976-10987 2009.

Ferullo, R. M.; Fuente, S. A.; Belelli, P. G.; Castellani, N. J.  
*CO interaction with Au atoms adsorbed on terrace, edge and corner sites of the MgO(100) surface. Electronic structure and vibrational analysis from DFT*  
Surface Science, (603): 1262-1269 2009.

Fey, N.; Orpen, A. G.; Harvey, J. N.  
*Building ligand knowledge bases for organometallic chemistry: Computational description of phosphorus(III)-donor ligands and the metal-phosphorus bond*  
Coordination Chemistry Reviews, (253): 704-722 2009.

Fievez, T.; Weckhuysen, B. M.; Geerlings, P.; De Proft, F.  
*Chemical Reactivity Indices as a Tool for Understanding the Support-Effect in Supported Metal Oxide Catalysts*  
Journal of Physical Chemistry C, (113): 19905-19912 2009.

Fifen, J. J.; Nsangou, M.; Dhaouadi, Z.; Motapon, O.; Lahmar, S.  
*Single or double hydrogen atom transfer in the reaction of metal - Associated phenolic acids with (OH)-O-center dot radical: DFT study*  
Journal of Molecular Structure-Theochem, (901): 49-55 2009.

Filippou, A. C.; Chernov, O.; Schnakenburg, G.  
*SiBr<sub>2</sub>(Idipp): A Stable N-Heterocyclic Carbene Adduct of Dibromosilylene*  
Angewandte Chemie-International Edition, (48): 5687-5690 2009.

Filippov, O. A.; Tsupreva, V. N.; Golubinskaya, L. M.; Krylova, A. I.; Bregadze, V. I.; Lledos, A.; Epstein, L. M.; Shubina, E. S.  
*Proton-Transfer and H-2-Elimination Reactions of Trimethylamine Alane: Role of Dihydrogen Bonding and Lewis Acid-Base Interactions*  
Inorganic Chemistry, (48): 3667-3678 2009.

FitzGibbons, J.; Op, S.; Hobson, A.; Schaffter, L.  
*Novel Approach to Optimization of a High-Throughput Semipreparative LC/MS System*  
Journal of Combinatorial Chemistry, (11): 592-597 2009.

- Florez, E.; Fuentealba, P.  
*A Theoretical Study of Alkali Metal Atomic Clusters: From Li-n to Cs-n (n=2-8)*  
International Journal of Quantum Chemistry, (109): 1080-1093 2009.
- Flugge, S.; Anoop, A.; Goddard, R.; Thiel, W.; Furstner, A.  
*Structure and Bonding in Neutral and Cationic 14-Electron Gold Alkyne pi Complexes*  
Chemistry-a European Journal, (15): 8558-8565 2009.
- Foo, C.; Lau, K.-C.; Yang, Y.-F.; So, C.-W.  
*Synthesis and characterization of a germanium bismethanediide complex*  
Chemical Communications: 6816-6818 2009.
- Fraga, A. R. L.; Collins, A.; Forte, G.; Rescifina, A.; Punzo, F.  
*Structures and properties in different media of N,N-(diethylcarbamothioyl)furan-2-carboxamide: A ionophore for sensor membranes*  
Journal of Molecular Structure, (929): 174-181 2009.
- Francisco, E.; Pendas, A. M.; Blanco, M. A.  
*A connection between domain-averaged Fermi hole orbitals and electron number distribution functions in real space*  
Journal of Chemical Physics, (131) 2009.
- Freeman, P. K.  
*Resonance Energies of Vinylcarbenes*  
Journal of Organic Chemistry, (74): 830-833 2009.
- Frenking, G.; Tonner, R.  
*Divalent carbon(0) compounds*  
Pure and Applied Chemistry, (81): 597-614 2009.
- Fu, Y.; Li, M.; Shen, W.  
*Theoretical investigation on the geometries and electronic properties of thiophene ring-containing compounds: monomer, oligomer and polymer*  
Molecular Simulation, (35): 1279-1287 2009.
- Fuente, S. A.; Belelli, P. G.; Branda, M. M.; Ferullo, R. M.; Castellani, N. J.  
*Formation of Ag-2, Au-2 and AgAu particles on MgO(100): DFT study on the role of support-induced charge transfer in metal-metal interactions*  
Applied Surface Science, (255): 7380-7384 2009.
- Fujita, T.; Fukuzawa, K.; Mochizuki, Y.; Nakano, T.; Tanaka, S.  
*Accuracy of fragmentation in ab initio calculations of hydrated sodium cation*  
Chemical Physics Letters, (478): 295-300 2009.
- Fumino, K.; Wulf, A.; Ludwig, R.  
*The potential role of hydrogen bonding in aprotic and protic ionic liquids*  
Physical Chemistry Chemical Physics, (11): 8790-8794 2009.

Gajewski, M.; Klobukowski, M.  
*DFT studies of complexes between ethylenediamine tetraacetate and alkali and alkaline earth cations*  
Canadian Journal of Chemistry-Revue Canadienne De Chimie, (87): 1492-1498 2009.

Galamba, N.; Costa Cabral, B. J.  
*Born-Oppenheimer Molecular Dynamics of the Hydration of Na<sup>+</sup> in a Water Cluster*  
Journal of Physical Chemistry B, (113): 16151-16158 2009.

Galvez, O.; Gomez, P. C.; Pacios, L. F.  
*Characterization of Two Types of Intermolecular Interactions on Halogen Monoxide Monohydrates*  
Journal of Computational Chemistry, (30): 2538-2549 2009.

Gamoke, B.; Neff, D.; Simons, J.  
*Nature of PO Bonds in Phosphates*  
Journal of Physical Chemistry A, (113): 5677-5684 2009.

Gamoke, B.; Neff, D.; Simons, J.  
*Nature of PO Bonds in Phosphates*  
Journal of Physical Chemistry A, (113): 5677-5684 2009.

Gancheff, J. S.; Albuquerque, R. Q.; Guerrero-Martinez, A.; Pape, T.; De Cola, L.; Hahn, F. E.  
*A Dinuclear Double-Stranded Oxido Complex of Re-V with a Bis(benzene-o-dithiolato) Ligand*  
European Journal of Inorganic Chemistry: 4043-4051 2009.

Gao, B.; Wyttenbach, T.; Bowers, M. T.  
*Hydration of Protonated Aromatic Amino Acids: Phenylalanine, Tryptophan, and Tyrosine*  
Journal of the American Chemical Society, (131): 4695-4701 2009.

Gao, G. H.; Xu, X.; Kang, H. S.  
*A Theoretical Study on Fullerene-Dizincocene Hybrids*  
Journal of Computational Chemistry, (30): 978-982 2009.

Gao, J. G.; Wang, F.; Meng, Q. X.; Li, M.  
*Density functional computations of Rh(I)-catalysed hydroacylation and hydrogenation of ethene using formic acid*  
Molecular Simulation, (35): 419-427 2009.

Gao, J. Y.; Zeng, Y.; Zhang, C. H.; Xue, Y.  
*Theoretical Studies on the Water-Assisted Hydrolysis of N,N-Dimethyl-N'-(2',3'-dideoxy-3'-thiacytidine) Formamidine with Three Water Molecules*  
Journal of Physical Chemistry A, (113): 325-331 2009.

Gao, S. L.; Wu, W.; Mo, Y. R.  
*The B-H center dot center dot center dot H-P Dihydrogen Bonding in Ion Pair Complexes (CF<sub>3</sub>)<sub>2</sub>BH-HPH<sub>3</sub>-n(Me)(n)(+) (n=0-3) and Its Implication in H-2 Elimination and Activation Reactions*

Journal of Physical Chemistry A, (113): 8108-8117 2009.

Gao, Y. L.; Sun, S. G.; Han, K. L.

*Electronic structures and spectroscopic properties of rhenium (I) tricarbonyl photosensitizer:*

*[Re(4,4'-*(COEt*)(2)-2,2'-bpy)(CO)(3)py]PF<sub>6</sub>*

Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (71): 2016-2022 2009.

Gapurenko, O. A.; Minyaev, R. M.; Minkin, V. I.

*Theoretical design of new sandwich compounds of boron, carbon, nitrogen, and oxygen*

Russian Journal of General Chemistry, (79): 728-739 2009.

Garcia, B.; Ibeas, S.; Ruiz, R.; Leal, J. M.; Biver, T.; Boggioni, A.; Secco, F.; Venturini, M.

*Solvent Effects on the Thermodynamics and Kinetics of Coralyne Self-Aggregation*

Journal of Physical Chemistry B, (113): 188-196 2009.

Garcia, M. E.; Garcia-Vivo, D.; Melon, S.; Ruiz, M. A.; Graiff, C.; Tiripicchio, A.

*Low-Temperature N-O Bond Cleavage in Nitrosyl Ligands Induced by the Unsaturated*

*Dimolybdenum Anion [Mo-2(eta(5)-C<sub>5</sub>H<sub>5</sub>)(2)(mu-PPh<sub>2</sub>)(mu-CO)(2)](-)*

Inorganic Chemistry, (48): 9282-9293 2009.

Garon, C. N.; Gorelsky, S. I.; Sigouin, O.; Woo, T. K.; Fontaine, F. G.

*Structural Study of Acidic Metallocavatands and Characterization of their Interactions with Lewis Bases*

Inorganic Chemistry, (48): 1699-1710 2009.

Gathy, T.; Peeters, D.; Leyssens, T.

*Mechanism of ketone hydrosilylation by Cu(I) catalysts: A theoretical study*

Journal of Organometallic Chemistry, (694): 3943-3950 2009.

Gauze, G. F.; Basso, E. A.; Contreras, R. H.; Tormena, C. F.

*Effect of Sulfur Oxidation on the Transmission Mechanism of (4)J(HH) NMR Coupling Constants in 1,3-Dithiane*

Journal of Physical Chemistry A, (113): 2647-2651 2009.

Gawinecki, R.; Stanovnik, B.; Valkonen, A.; Kolehmainen, E.; Osmialowski, B.; Dobosz, R.; Zakrzewska, A.

*Effect of vinylene and 1,4-phenylene spacers on efficiency of the ground-state intramolecular charge-transfer in enlarged 4-dimethylamino-1-methylpyridinium cations*

Structural Chemistry, (20): 655-662 2009.

Ge, G. X.; Yang, Z. Q.; Cao, H. B.

*Density functional study of the interaction of CO with nickel clusters*

Acta Physica Sinica, (58): 6128-6133 2009.

Geethalakshmi, K. R.; Waller, M. P.; Thiel, W.; Buhl, M.

*V-51 NMR Chemical Shifts Calculated from QM/MM Models of Peroxo Forms of Vanadium Haloperoxidases*

Journal of Physical Chemistry B, (113): 4456-4465 2009.

Gheorghiu, M. D.; Racoveanu, A.  
*Electronic and molecular structure of aminimides (1-acyl-2,2,2-trimethyl-diazan-2-iun-1-ide). 2. Substituted aminimides (R-CON-N+Me3)*  
Journal of Molecular Structure-Theochem, (908): 84-91 2009.

Ghiasi, R.  
*Theoretical insights into the properties of the borazine center dot center dot center X-complexes (X- = H, F, Cl, CN, NC or NCO)*  
Journal of the Serbian Chemical Society, (74): 1105-1111 2009.

Ghosh, S.; Hogarth, G.; Kabir, S. E.; Miah, A. L.; Salassa, L.; Sultana, S.; Garino, C.  
*Synthesis and Molecular Structure of [Fe-4(CO)(10)(mu(4)-O)(kappa(K)2-dppn)] (dppn=1,8-bis(diphenylphosphino)naphthalene): A Missing Piece in the [M-4(CO)(12)(mu(4)-E)](n-) (M = Fe, Ru; E = C, N, O; n=2, 1, 0) Puzzle*  
Organometallics, (28): 7047-7052 2009.

Ghosh, S.; Kabir, S. E.; Pervin, S.; Raha, A. K.; Hossain, G. M. G.; Haworth, D. T.; Lindeman, S. V.; Bennett, D. W.; Siddiquee, T. A.; Salassa, L.; Roesky, H. W.  
*Tetranuclear group 7/8 mixed-metal and open trinuclear group 7 metal carbonyl clusters bearing bridging 2-mercapto-1-methylimidazole ligands*  
Dalton Transactions: 3510-3518 2009.

Gil, A.; Branchadell, V.; Bertran, J.; Oliva, A.  
*An Analysis of the Different Behavior of DNA and RNA through the Study of the Mutual Relationship between Stacking and Hydrogen Bonding*  
Journal of Physical Chemistry B, (113): 4907-4914 2009.

Gil, A.; Sodupe, M.; Bertran, J.  
*Influence of Ionization on the Conformational Preferences of Peptide Models. Ramachandran Surfaces of N-Formyl-glycine Amide and N-Formyl-alanine Amide Radical Cations*  
Journal of Computational Chemistry, (30): 1771-1784 2009.

Giordana, A.; Ghigo, G.; Tonachini, G.; Ascenzi, D.; Tosi, P.; Guella, G.  
*The reaction of N2O with phenylium ions C-6(H, D)(5)(+): An integrated experimental and theoretical mechanistic study*  
Journal of Chemical Physics, (131) 2009.

Gloaguen, Y.; Alcaraz, G.; Pecharman, A. F.; Clot, E.; Vendier, L.; Sabo-Etienne, S.  
*Phosphinoborane and Sulfidoborohydride as Chelating Ligands in Polyhydride Ruthenium Complexes: Agostic sigma-Borane versus Dihydroborate Coordination*  
Angewandte Chemie-International Edition, (48): 2964-2968 2009.

Gobel, M.; Tchitchanov, B. H.; Murray, J. S.; Politzer, P.; Klapotka, T. M.  
*Chlorotrinitromethane and its exceptionally short carbon-chlorine bond*  
Nature Chemistry, (1): 229-235 2009.

Goedecke, C.; Hillebrecht, P.; Uhlemann, T.; Haunschmid, R.; Frenking, G.

*The Dewar-Chatt-Duncanson model reversed - Bonding analysis of group-10 complexes [(PMe<sub>3</sub>)(2)M-EX<sub>3</sub>] (M = Ni, Pd, Pt; E = B, Al, Ga, In, Tl; X = H, F, Cl, Br, I)*  
Canadian Journal of Chemistry-Revue Canadienne De Chimie, (87): 1470-1479 2009.

Goldfuss, B.  
*C-H Functionalizations by Means of Direct Borane-Hydrocarbon Dehydrogenations and Dehydrocarbonations*  
Chemistry-a European Journal, (15): 12856-12861 2009.

Golubeva, E. N.; Zhidomirov, G. M.; Kokorin, A. I.  
*On the stability of copper(II) organic compounds with the sigma bond Cu-C: A quantum-chemical study*  
Doklady Chemistry, (426): 143-145 2009.

Gomez, E.; Marco-Contelles, J.; Soriano, E.; Jimeno, M. L.  
*N-Arylmethyl-7-azabicyclo[2.2.1]heptane derivatives: synthesis and reaction mechanisms*  
Tetrahedron, (65): 9224-9232 2009.

Gomez-Bengoa, E.  
*DFT Studies on Double Hydrogen Bond Catalysis of Reactions of Distinct Polarity*  
European Journal of Organic Chemistry: 1207-1213 2009.

Gomez-Jeria, J. S.  
*An Empirical Way to Correct Some Drawbacks of Mulliken Population Analysis*  
Journal of the Chilean Chemical Society, (54): 482-485 2009.

Gong, L. F.; Wu, X. M.; Qi, C. S.; Li, W.; Xiong, J. M.; Guo, W. L.  
*Structures and stabilities of P5Mg<sub>n</sub>P5 (n=1-3) compounds containing P5 ligands. Theoretical investigation*  
Molecular Physics, (107): 197-204 2009.

Gong, L. F.; Xiong, J. M.; Wu, X. M.; Qi, C. S.; Li, W.; Guo, W. L.  
*Density Functional Study of Structures and Electron Affinities of BrO<sub>4</sub>F/BrO<sub>4</sub>F*  
International Journal of Molecular Sciences, (10): 3128-3148 2009.

Gonzalez, B.; Lorenzo-Luis, P.; Romerosa, A.; Serrano-Ruiz, M.; Gili, P.  
*Theoretical aspects on water soluble [RuClCp(PPh<sub>3</sub>)(2)], [RuClCp(PTA)(PPh<sub>3</sub>)], [RuClCp(PTA)(2)], [RuClCp(mPTA)(PPh<sub>3</sub>)](+)* and [RuClCp(mPTA)(2)](2+) (PTA=1,3,5-triaza-7-phosphaadamantane; mPTA = N-methyl-1,3,5-triaza-7-phosphaadamantane)  
Journal of Molecular Structure-Theochem, (894): 59-63 2009.

Gotz, K.; Kaupp, M.; Braunschweig, H.; Stalke, D.  
*Comparative Analysis of Electron-Density and Electron-Localization Function for Dinuclear Manganese Complexes with Bridging Boron-and Carbon-Centered Ligands*  
Chemistry-a European Journal, (15): 623-632 2009.

Gourlaouen, C.; Ujaque, G.; Lledos, A.; Medio-Simon, M.; Asensio, G.; Maseras, F.

*Why Is the Suzuki-Miyaura Cross-Coupling of sp(3) Carbons in alpha-Bromo Sulfoxide Systems Fast and Stereoselective? A DFT Study on the Mechanism*  
Journal of Organic Chemistry, (74): 4049-4054 2009.

Grabowski, S. J.  
*Covalent Character of Hydrogen Bonds Enhanced by pi-Electron Delocalization*  
Croatica Chemica Acta, (82): 185-192 2009.

Grabowski, S. J.; Leszczynski, J.  
*The enhancement of X-H center dot center dot center dot pi hydrogen bond by cooperativity effects - Ab initio and QTAIM calculations*  
Chemical Physics, (355): 169-176 2009.

Grant, D. J.; Dixon, D. A.; Camaiioni, D.; Potter, R. G.; Christe, K. O.  
*Lewis Acidities and Hydride, Fluoride, and V Affinities of the BH<sub>3</sub>-X-n(n) Compounds for (X = F, Cl, Br, I, NH<sub>2</sub>, OH, and SH) from Coupled Cluster Theory*  
Inorganic Chemistry, (48): 8811-8821 2009.

Gray, T. G.  
*Divergent Electronic Structures of Isoelectronic Metalloclusters: Tungsten(II) Halides and Rhenium(III) Chalcogenide Halides*  
Chemistry-a European Journal, (15): 2581-2593 2009.

Gregus, Z.; Roos, G.; Geerlings, P.; Nemeti, B.  
*Mechanism of Thiol-Supported Arsenate Reduction Mediated by Phosphorolytic-Arsenolytic Enzymes*  
Toxicological Sciences, (110): 282-292 2009.

Groen, C. P.; Varga, Z.; Kolonits, M.; Peterson, K. A.; Hargittai, M.  
*Does the 4f Electron Configuration Affect Molecular Geometries? A Joint Computational, Vibrational Spectroscopic, and Electron Diffraction Study of Dysprosium Tribromide*  
Inorganic Chemistry, (48): 4143-4153 2009.

Groves, M. N.; Chan, A. S. W.; Malardier-Jugroot, C.; Jugroot, M.  
*Improving platinum catalyst binding energy to graphene through nitrogen doping*  
Chemical Physics Letters, (481): 214-219 2009.

Grubbs, G. S.; Bailey, W. C.; Cooke, S. A.  
*Changes at the iodine nucleus in 1-iodopropane when one hydrogen at the carbon-3 position is replaced by fluorine*  
Chemical Physics Letters, (477): 37-40 2009.

Gruber, S.; Zaitsev, A. B.; Worle, M.; Pregosin, P. S.; Veiros, L. F.  
*Rapid, Selective Ru-Sulfonate-Catalyzed Allylation of Indoles Using Alcohols as Substrates*  
Organometallics, (28): 3437-3448 2009.

Grubisic, S.; Gruden-Pavlovic, M.; Radanovic, D. D.; Peric, M.; Niketic, S. R.

*Molecular mechanics description of the stabilized effects in (ethylenediamine-N,N'-diacetato)chromate(III) dinuclear complex bridged by pyrazole-3,5-dicarboxylate: DFT calculations of magnetic properties*  
Journal of Molecular Structure, (919): 54-58 2009.

Gu, J. D.; Xie, Y. M.; Schaefer, H. F.  
*Electron attachment to oligonucleotide dimers in water: Microsolvation-assisted base-stacking forms*  
Chemical Physics Letters, (473): 213-219 2009.

Guerrero, A.; Herrero, R.; Davalos, J. Z.; Koppel, I.; Abboud, J. L. M.; Chana, A.; Koppel, I. A.  
*Hydrogen-Bonding Interactions of (CF<sub>3</sub>)<sub>3</sub>CH and (CF<sub>3</sub>)<sub>3</sub>C- in the Gas Phase. An Experimental (FT-ICR) and Computational Study*  
Journal of Physical Chemistry A, (113): 6422-6429 2009.

Guino-o, M. A.; Alexander, J. S.; McKee, M. L.; Hope, H.; Englich, U. B.; Ruhlandt-Senge, K.  
*When VSEPR Fails: Experimental and Theoretical Investigations of the Behavior of Alkaline-Earth-Metal Acetyliides*  
Chemistry-a European Journal, (15): 11842-11852 2009.

Gumbart, J.; Wiener, M. C.; Tajkhorshid, E.  
*Coupling of Calcium and Substrate Binding through Loop Alignment in the Outer-Membrane Transporter BtuB*  
Journal of Molecular Biology, (393): 1129-1142 2009.

Guo, C. H.; Wu, H. S.; Zhang, X. M.; Song, J. Y.; Zhang, X.  
*A Comprehensive Theoretical Study on the Coupling Reaction Mechanism of Propylene Oxide with Carbon Dioxide Catalyzed by Copper(I) Cyanomethyl*  
Journal of Physical Chemistry A, (113): 6710-6723 2009.

Guo, C.-H.; Zhang, X.-M.; Jia, J.-F.; Wu, H.-S.  
*Theoretical study on the mechanism of nickel(0)-mediated coupling between carbon dioxide and epoxymethane*  
Journal of Molecular Structure-Theochem, (916): 125-134 2009.

Guo, H. M.; Zhang, J.; Zhao, P. S.; Jian, F. F.  
*Synthesis, Crystal Structure, Characterization and Ab Initio Calculations on a Dicyclic Pyrazoline Derivative*  
Polish Journal of chemistry, (83): 263-274 2009.

Habibi-Khorassani, S. M.; Ebrahimi, A.; Maghsoodlou, M. T.; Saravani, H.; Zakarianezhad, M.; Ghahramaninezhad, M.; Kazemian, M. A.; Nassiri, M.; Khajehali, Z.  
*Theoretical Study, an Efficient Synthesis Route to, and Kinetic Investigation of, Stable Phosphorus Ylides Derived from Benzamide*  
Progress in Reaction Kinetics and Mechanism, (34): 261-288 2009.

Haghjadi, M.; Amiri, R.; Price, L. S.  
*DFT studies on structures and stability of some keto-fructose analogues*

Journal of Molecular Structure-Theochem, (904): 57-63 2009.

Hamann, D. R.; Vanderbilt, D.

*Maximally localized Wannier functions for GW quasiparticles*  
Physical Review B, (79) 2009.

Hammerum, S.

*Alkyl Radicals as Hydrogen Bond Acceptors: Computational Evidence*  
Journal of the American Chemical Society, (131): 8627-8635 2009.

Hammerum, S.

*Alkyl Radicals as Hydrogen Bond Acceptors: Computational Evidence*  
Journal of the American Chemical Society, (131): 8627-8635 2009.

Hamza, A.; Stirling, A.; Rokob, T. A.; Papai, I.

*Mechanism of Hydrogen Activation by Frustrated Lewis Pairs: A Molecular Orbital Approach*  
International Journal of Quantum Chemistry, (109): 2416-2425 2009.

Han, Y.; Kim, H.; Lee, M. H.; Kim, Y.; Lee, J.; Lee, Y. S.; Do, Y.

*Aminosilylene-bridged ansa-zirconocenes for branched polyethylenes with bimodal molecular weight distributions*  
Journal of Organometallic Chemistry, (694): 4216-4222 2009.

Han, Y. X.; Geng, Z. Y.; Wang, Y. C.; Liang, J. X.; Yan, P. J.

*Theoretical Study of Reaction Mechanism of Silylene with Isothiocyanic Acid*  
Acta Chimica Sinica, (67): 773-780 2009.

Hanninen, M. M.; Peuronen, A.; Tuononen, H. M.

*Do Extremely Bent Allenes Exist?*  
Chemistry-a European Journal, (15): 7287-7291 2009.

Hanusek, J.; Belohlavova, H.

*Acid-catalyzed decomposition of stable 1-(2,1-benzisothiazol-3-yl)-3-phenyltriazenes*  
Dyes and Pigments, (80): 136-140 2009.

Hao, C. T.; Turecek, F.

*Host-Guest Hydrogen Atom Transfer Induced by Electron Capture*  
Journal of the American Society for Mass Spectrometry, (20): 639-651 2009.

Hayashi, S.; Nakanishi, W.; Furuta, A.; Drabowicz, J.; Sasamori, T.; Tokitoh, N.

*How does non-covalent Se center dot center dot center dot Se = O interaction stabilize selenoxides at naphthalene 1,8-positions: structural and theoretical investigations*  
New Journal of Chemistry, (33): 196-206 2009.

Hayashi, S.; Yamane, K.; Nakanishi, W.

*H/D Isotope Effect on Se-77 NMR Chemical Shifts in 8-Methyl-1-(arylselanyl)naphthalenes and Related Selenides: Nonbonded C-H-Se Through-Space Versus Through-Bond Mechanisms*  
Phosphorus Sulfur and Silicon and the Related Elements, (184): 1481-1495 2009.

- Hayes, C. J.; Hadad, C. M.  
*Combustion Pathways of the Alkylated Heteroaromatics: Bond Dissociation Enthalpies and Alkyl Group Fragmentations*  
Journal of Physical Chemistry A, (113): 12370-12379 2009.
- Hayes, C. J.; Simpkins, N. S.; Kirk, D. T.; Mitchell, L.; Baudoux, J.; Blake, A. J.; Wilson, C.  
*Bridgehead Lithiation-Substitution of Bridged Ketones, Lactones, Lactams, and Imides: Experimental Observations and Computational Insights*  
Journal of the American Chemical Society, (131): 8196-8210 2009.
- Haynes, M. K.; Strouse, J. J.; Waller, A.; Leitao, A.; Curpan, R. F.; Bologa, C.; Oprea, T. I.; Prossnitz, E. R.; Edwards, B. S.; Sklar, L. A.; Thompson, T. A.  
*Detection of Intracellular Granularity Induction in Prostate Cancer Cell Lines by Small Molecules Using the HyperCyt (R) High-Throughput Flow Cytometry System*  
Journal of Biomolecular Screening, (14): 596-609 2009.
- He, Q.; Yang, J.; Meng, X.-j.  
*Hydrogen Bonding Character Between the Glycine and BF<sub>4</sub>*  
Chinese Journal of Chemical Physics, (22): 517-522 2009.
- He, X.; Wang, B.; Merz, K. M.  
*Protein NMR Chemical Shift Calculations Based on the Automated Fragmentation QM/MM Approach*  
Journal of Physical Chemistry B, (113): 10380-10388 2009.
- Hedegard, E. D.; Bendix, J.; Sauer, S. P. A.  
*Partial charges as reactivity descriptors for nitrido complexes*  
Journal of Molecular Structure-Theochem, (913): 1-7 2009.
- Helios, K.; Wysokinski, R.; Zierkiewicz, W.; Proniewicz, L. M.; Michalska, D.  
*Unusual Noncovalent Interaction Between the Chelated Cu(II) Ion and the pi Bond in the Vitamin B-13 Complex, cis-Diammine(orotato)copper(II): Theoretical and Vibrational Spectroscopy Studies*  
Journal of Physical Chemistry B, (113): 8158-8169 2009.
- Helten, H.; Fankel, S.; Feier-lova, O.; Nieger, M.; Ferao, A. E.; Streubel, R.  
*Strong Evidence for an Unprecedented Borderline Case of Dissociation and Cycloaddition in Open-Shell 1,3-Dipole Chemistry: Transient Nitrilium Phosphane-Ylide Complex Radical Cations*  
European Journal of Inorganic Chemistry: 3226-3237 2009.
- Herize, A.; Mora, J. R.; Lezama, J.; Marquez, E.; Cordova, T.; Chuchani, G.  
*Experimental and theoretical study of the mechanism for the kinetic of elimination of methyl carbazate in the gas phase*  
Journal of Physical Organic Chemistry, (22): 170-176 2009.
- Hewitt, N.; Rauk, A.

*Mechanism of Hydrogen Peroxide Production by Copper-Bound Amyloid Beta Peptide: A Theoretical Study*  
Journal of Physical Chemistry B, (113): 1202-1209 2009.

Hiremath, C. S.; Sundius, T.  
*Vibrational spectra, ab initio/DFT electronic structure calculations, and normal coordinate analysis of 2-bromo-5-fluorobenzaldehyde*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (74): 1260-1267 2009.

Hirokawa, S.; Imasaka, T.; Imasaka, T.  
*The S-1 <- S-0 0-0 transition energies of polychlorinated dibenzofurans (PCDFs) revisited: CIS(D) and MP2 calculations with correction for correlation energies*  
Journal of Molecular Structure-Theochem, (915): 79-85 2009.

Hoeltzl, T.; Ngan, V. T.; Nguyen, M. T.; Vespremi, T.  
*Resonance structures of N-heterocyclic carbenes*  
Chemical Physics Letters, (481): 54-57 2009.

Hollo, B.; Tomic, Z. D.; Pogany, P.; Kovacs, A.; Leovac, V. M.; Szecsenyi, K. M.  
*Transition metal complexes with pyrazole-based ligands. Part 28. Synthesis, structural, DFT and thermal studies of cadmium(II) halides and zinc(II) chloride complexes with 3,5-dimethylpyrazole-1-carboxamidine*  
Polyhedron, (29): 3881-3889 2009.

Holt, A.; Karlstrom, G.; Roos, B. O.  
*The Charge Capacitance of the Chemical Bond: Application to Bonds Containing Metals*  
International Journal of Quantum Chemistry, (109): 618-628 2009.

Holt, B. T. O.; Vance, M. A.; Mirica, L. M.; Heppner, D. E.; Stack, T. D. P.; Solomon, E. I.  
*Reaction Coordinate of a Functional Model of Tyrosinase: Spectroscopic and Computational Characterization*  
Journal of the American Chemical Society, (131): 6421-6438 2009.

Holtztl, T.; Veldeman, N.; Vespremi, T.; Lievens, P.; Nguyen, M. T.  
*Cu<sub>6</sub>Sc<sup>+</sup> and Cu<sub>5</sub>Sc: Stable, high symmetry and aromatic scandium-doped coinage metal clusters*  
Chemical Physics Letters, (469): 304-307 2009.

Hooshyar, H.; Rahemi, H.; Hossein, M.; Shad, A.; Khezri, B.  
*Density functional and Moller-Plesset studies of cyclobutanonea <-HF and a <-HCl complexes*  
Journal of Molecular Modeling, (15): 525-536 2009.

Hooshyar, H.; Zare, K.; Modirshahla, N.; Khanahmadzadeh, S.  
*The effect of ring size on vibrational spectroscopy and hydrogen bonding properties for the complexes between small ring carbonyl compounds with HF and HCl: Theoretical analysis*  
Journal of Molecular Modeling, (15): 247-256 2009.

Hou, R. B.; Li, W. W.; Yi, X. H.

*Molecular Geometries and Electronic Structures of Adducts between 2'-Deoxycytidine-5'-monophosphate Acid and Hydroxyl Radical*  
Acta Physico-Chimica Sinica, (25): 291-298 2009.

Hu, G. S.; Han, D. F.; Jia, G. Q.; Chen, T.; Feng, Z. C.; Li, C.  
*Coadsorption of trimethyl phosphine and thiocyanate on colloidal silver: a SERS study combined with theoretical calculations*  
Journal of Raman Spectroscopy, (40): 387-393 2009.

Hu, T. P.; Ren, F. D.; Ren, J.  
*Theoretical investigation on geometries and aromaticity of mixed boron-, nitrogen- and furanoxo-containing five-membered rings B<sub>2</sub>N<sub>2</sub>O<sub>p</sub>H<sub>p</sub> (p=0-2)*  
Journal of Molecular Structure-Theochem, (909): 13-18 2009.

Hu, W.  
*Electronic Structure and Conductivity of Polypyrrolo[3,4-c]pyrrole*  
Acta Chimica Sinica, (67): 2402-2406 2009.

Hu, Z. Q.; Ye, X. Z.; Shi, S. M.; Mao, W. L.; Meng, X. G.  
*Syntheses, Crystal Structures, Luminescent Property and Theoretical Study of the Complexes [M(AAABA)(2)(py)(2)(H<sub>2</sub>O)(2), M=Zn, Mn]*  
Chinese Journal of Inorganic Chemistry, (25): 1389-1395 2009.

Huang, H.; Hurubeanu, N. R.; Bourgeois, C. J.; Cheah, S. M.; Yuan, J.; Rheingold, A. L.; Hughes, R. P.  
*Octahedral perfluoroalkyl complexes of Ir(III) formed by oxidative addition of perfluoroalkyl iodides to Ir(acac)(CO)(2)*  
Canadian Journal of Chemistry-Revue Canadienne De Chimie, (87): 151-160 2009.

Huang, H.; Rheingold, A. L.; Hughes, R. P.  
*Serendipitous Discovery of a Simple Compound with an Unsupported Ir-Ir Bond*  
Organometallics, (28): 1575-1578 2009.

Huang, H.; Zhang, T.; Zhang, J.; Wang, L.  
*A screened hybrid density functional study on energetic complexes: Alkaline-earth metal carbohydrazide perchlorates*  
Journal of Molecular Structure-Theochem, (915): 43-46 2009.

Huang, X. X.; Xu, X.  
*Ir-Hg Interactions and the Nature of Redox Reactions in Ir(CO)Cl-a(Ph(2)Ppy)(2)HgClb(HgCl<sub>2</sub>)(c) (a, b=1, 2; c=0, 1)*  
Acta Physico-Chimica Sinica, (25): 1362-1366 2009.

Huber, S. M.; Ertem, M. Z.; Aquilante, F.; Gagliardi, L.; Tolman, W. B.; Cramer, C. L.  
*Generating Cu-II-Oxyl/Cu-III-Oxo Species from Cu-I-alpha-Ketocarboxylate Complexes and O-2: In Silico Studies on Ligand Effects and C-H-Activation Reactivity*  
Chemistry-a European Journal, (15): 4886-4895 2009.

Hue, M. T. N.; Pham, N. D.; Zeegers-Huyskens, T.

*Theoretical study of the interaction between monohalogenated ethylenes and water*  
Journal of Molecular Structure-Theochem, (897): 48-54 2009.

Hughes, M. J.; Mercier, H. P. A.; Schrobilgen, G. J.

*Synthesis and X-ray Crystal Structure of (OsO<sub>3</sub>F<sub>2</sub>)<sub>(2)</sub>center dot 2XeOF(4) and the Raman Spectra of (OsO<sub>3</sub>F<sub>2</sub>)<sub>(infinity)</sub>, (OsO<sub>3</sub>F<sub>2</sub>)<sub>(2)</sub>, and (OsO<sub>3</sub>F<sub>2</sub>)<sub>(2)</sub>center dot 2XeOF(4)*  
Inorganic Chemistry, (48): 4478-4490 2009.

Hurtado, M.; Mo, O.; Yanez, M.; Guillemin, J.-C.

*Acidity Enhancement of the Cyclopentadiene Ring by PH<sub>2</sub> and AsH<sub>2</sub> Substitution*  
Croatica Chemica Acta, (82): 1-6 2009.

Hurtado, M.; Yanez, M.; Guillemin, J. C.

*Enhanced acidity of cyclopenta-2,4-dienylborane and its Al and Ga analogues. The role of aromatization*  
Physical Chemistry Chemical Physics, (11): 8759-8766 2009.

Hyla-Kryspin, I.; Grimme, S.; Djukic, J. P.

*The Cr-Mn Interaction in syn-Facial [Tricarbonyl(benzyl)chromium]manganese tricarbonyl Complexes: A Non-Covalent Metal-Metal Bond*  
Organometallics, (28): 1001-1013 2009.

Hyla-Kryspin, I.; Mueck-Lichtenfeld, C.; Grimme, S.

*DFT Studies on Molecular and Electronic Structures of Cationic Carbene Complexes [L-2(eta(5)-C<sub>5</sub>H<sub>5</sub>)Fe=CR<sub>2</sub>](+)* (L = CO, PH<sub>3</sub>, dhpe, PPh<sub>3</sub>; R = H, F, CH<sub>3</sub>)  
Croatica Chemica Acta, (82): 115-127 2009.

Ignatyev, I. S.; Montejo, M.; Gonzalez, J. J. L.

*Role of structures with penta- and hexacoordinate silicon in the nucleophile-catalyzed hydrolysis of tetramethoxysilane*  
Physical Chemistry Chemical Physics, (11): 841-847 2009.

Ikeda, A.; Nakao, Y.; Sato, H.; Sakaki, S.

*Generalization of the New Resonance Theory: Second Quantization Operator, Localization Scheme, and Basis Set*  
Journal of Chemical Theory and Computation, (5): 1741-1748 2009.

Indrakanti, V. P.; Schobert, H. H.; Kubicki, J. D.

*Quantum Mechanical Modeling of CO<sub>2</sub> Interactions with Irradiated Stoichiometric and Oxygen-Deficient Anatase TiO<sub>2</sub> Surfaces: Implications for the Photocatalytic Reduction of CO<sub>2</sub>*  
Energy & Fuels, (23): 5247-5256 2009.

Injan, N.; Megyes, T.; Radnai, T.; Bakó, I.; Balint, S.; Limtrakul, J.; Spangberg, D.; Probst, M.

*Potential energy surface and molecular dynamics simulation of gold(I) in liquid nitromethane*  
Journal of Molecular Liquids, (147): 64-70 2009.

Irani, M.; Haqgu, M.; Talebi, A.; Gholami, M. R.

*A joint experimental and theoretical study of kinetic and mechanism of rearrangement of allyl p-tolyl ether*

Journal of Molecular Structure-Theochem, (893): 73-76 2009.

Iron, M. A.; Ben-Ari, E.; Cohen, R.; Milstein, D.

*Metal-ligand cooperation in the trans addition of dihydrogen to a pincer Ir(I) complex: a DFT study*

Dalton Transactions: 9433-9439 2009.

Irshaidat, T.

*A DFT study on the mono lithium and sodium salts of N-(2-hydroxyphenyl)salicylaldimine*

Tetrahedron Letters, (50): 825-830 2009.

Isaia, F.; Aragoni, M. C.; Arca, M.; Demartin, F.; Devillanova, F. A.; Ennas, G.; Garau, A.; Lippolis, V.; Mancini, A.; Verani, G.

*Molecular Iodine Stabilization in an Extended N center dot center dot center dot I-I center dot center dot center dot N Assembly*

European Journal of Inorganic Chemistry: 3667-3672 2009.

Ito, K.; Hara, Y.; Mori, S.; Kusama, H.; Iwasawa, N.

*Theoretical Study of the Cycloaddition Reaction of a Tungsten-Containing Carbonyl Ylide*

Chemistry-a European Journal, (15): 12408-12416 2009.

Itoh, K.; Kishimoto, S.

*Novel formation of phenylcyclopropanes from the reaction of beta-cyanostyrenes and related compounds with 2-methoxyfuran: experimental and theoretical studies*

New Journal of Chemistry, (33): 1127-1138 2009.

Ivashkevich, O. A.; Matulis, V. E.; Elkind, P. D.; Gaponik, P. N.; Sukhanov, G. T.; Sukhanova, A. G.

*Standard enthalpies of formation in the gas phase and relative stability of tautomers of C-nitro-*

*1,2,4-triazole and isomers of N-alkyl-C-nitro-1,2,4-triazole: quantum-chemical studies*

Chemistry of Heterocyclic Compounds, (45): 70-79 2009.

Izod, K.; Wills, C.; Clegg, W.; Harrington, R. W.

*Acyclic Dialkylstannylene and -Plumbylene Compounds That Are Monomeric in the Solid State*

Organometallics, (28): 5661-5668 2009.

Izod, K.; Wills, C.; Clegg, W.; Harrington, R. W.

*Seven-Membered Cyclic Dialkylstannylene and -Plumbylene Compounds Stabilized by Agostic-type B-H center dot center dot center dot E Interactions [E = Sn, Pb]*

Organometallics, (28): 2211-2217 2009.

Jacobsen, H.

*Chemical Bonding in View of Electron Charge Density and Kinetic Energy Density Descriptors*

Journal of Computational Chemistry, (30): 1093-1102 2009.

Jacobsen, H.

*Hypovalency-a kinetic-energy density description of a 4c-2e bond*

Dalton Transactions: 4252-4258 2009.

Jacobsen, H.

*Hypovalency-a kinetic-energy density description of a 4c-2e bond*

Dalton Transactions: 4252-4258 2009.

Jaeger, H. M.; Schaefer, H. F.

*Characterizing Radiation-Induced Oxidation of DNA by Way of the Monohydrated Guanine-Cytosine Radical Cation*

Journal of Physical Chemistry B, (113): 8142-8148 2009.

Jalbout, A. F.; Naseri, M. A.; Fazli, M.; Raissi, H.; Rezaei, M.; Nowroozi, A.; De Leon, A.

*Molecular Structure and Vibrational Assignment of alpha-Chloro Acetylacetone: A Density Functional Theory Study*

International Journal of Quantum Chemistry, (109): 1481-1496 2009.

James, C.; Ravikumar, C.; Jayakumar, V. S.; Joe, I. H.

*Vibrational spectra and potential energy distributions for 1-benzyl-1H-imidazole by normal coordinate analysis*

Journal of Raman Spectroscopy, (40): 537-545 2009.

James, W. H.; Baquero, E. E.; Shubert, V. A.; Choi, S. H.; Gellman, S. H.; Zwier, T. S.

*Single-Conformation and Diastereomer Specific Ultraviolet and Infrared Spectroscopy of Model Synthetic Foldamers: alpha/beta-Peptides*

Journal of the American Chemical Society, (131): 6574-6590 2009.

James, W. H.; Baquero, E. E.; Shubert, V. A.; Choi, S. H.; Gellman, S. H.; Zwier, T. S.

*Single-Conformation and Diastereomer Specific Ultraviolet and Infrared Spectroscopy of Model Synthetic Foldamers: alpha/beta-Peptides*

Journal of the American Chemical Society, (131): 6574-6590 2009.

Jaramillo, P.; Perez, P.; Fuentealba, P.

*On the Nucleophilicity of Boryllithium Compounds. A Theoretical Study*

Journal of Physical Chemistry A, (113): 6812-6817 2009.

Jeanvoine, Y.; Spezia, R.

*Mn<sup>2+</sup>, Fe<sup>2+</sup>, Co<sup>2+</sup>, Ni<sup>2+</sup>, Cu<sup>2+</sup>, and Zn<sup>2+</sup>-Binding Chalcogen-Chalcogen Bridges: A Compared MP2 and B3LYP Study*

Journal of Physical Chemistry A, (113): 7878-7887 2009.

Jena, N. R.; Mishra, P. C.; Suhai, S.

*Protection Against Radiation-Induced DNA Damage by Amino Acids: A DFT Study*

Journal of Physical Chemistry B, (113): 5633-5644 2009.

Ji, H.; Li, L.; Xu, X. L.; Ham, S. Y.; Hammad, L. A.; Birney, D. M.

*Multiphoton Infrared Initiated Thermal Reactions of Esters: Pseudopericyclic Eight-Centered cis-Elimination*

Journal of the American Chemical Society, (131): 528-537 2009.

Jia, Z. F.; Feng, S. Y.; Song, E. F.; Sun, W. Y.; Cong, L. X.  
*Theoretical Study on the Mechanism for the Thermal Rearrangement Reactions of 2-Silyleethyl Acetate H<sub>3</sub>SiCH<sub>2</sub>CH<sub>2</sub>OOCCH<sub>3</sub>*  
International Journal of Quantum Chemistry, (109): 342-348 2009.

Jiang, N.; Ma, J.  
*Theoretical study of proton encircling modes in proton sponges with tetraamido/diamino quaternized macrocycles: the role of pi-conjugated and aliphatic bridges*  
Physical Chemistry Chemical Physics, (11): 5100-5109 2009.

Jiang, Z. Y.; Hou, Y. Q.; Lee, K. H.; Chu, S. Y.  
*Density Functional Study of Structural and Electronic Properties of Maximum-Spin n+1Aun-1Ag Clusters*  
International Journal of Quantum Chemistry, (109): 1348-1356 2009.

Jiao, D. S.; Wang, H. Y.; Zhang, Y. L.; Tang, Y.  
*A DFT study of thymine and its tautomers*  
Canadian Journal of Chemistry-Revue Canadienne De Chimie, (87): 406-415 2009.

Jimenez, A.; Clapes, P.; Crehuet, R.  
*Protein Flexibility and Metal Coordination Changes in DHAP-Dependent Aldolases*  
Chemistry-a European Journal, (15): 1422-1428 2009.

Jimenez-Halla, J. O. C.; Matito, E.; Blancafort, L.; Robles, J.; Sola, M.  
*Tuning Aromaticity in Trigonal Alkaline Earth Metal Clusters and Their Alkali Metal Salts*  
Journal of Computational Chemistry, (30): 2764-2776 2009.

Joe, I. H.; Kostova, I.; Ravikumar, C.; Amalanathan, M.; Pinzaru, S. C.  
*Theoretical and vibrational spectral investigation of sodium salt of acenocoumarol*  
Journal of Raman Spectroscopy, (40): 1033-1038 2009.

John, A.; Shaikh, M. M.; Ghosh, P.  
*Palladium complexes of abnormal N-heterocyclic carbenes as precatalysts for the much preferred Cu-free and amine-free Sonogashira coupling in air in a mixed-aqueous medium*  
Dalton Transactions: 10581-10591 2009.

Joshi, Y. V.; Ghosh, P.; Venkataraman, P. S.; Delgass, W. N.; Thomson, K. T.  
*Electronic Descriptors for the Adsorption Energies of Sulfur-Containing Molecules on Co/MoS<sub>2</sub>, Using DFT Calculations*  
Journal of Physical Chemistry C, (113): 9698-9709 2009.

Ju, X. H.; Wang, Z. Y.  
*Theoretical Study of 2,4,6-Tris(3',5'-Diamino-2',4',6'-Trinitrophenylamino)-1,3,5-Triazine*  
Journal of Energetic Materials, (27): 51-62 2009.

Kageura, Y.; Sakota, K.; Sekiya, H.

*Charge Transfer Interaction of Intermolecular Hydrogen Bonds in 7-Azaindole(MeOH)(n) (n=1, 2) with IR-Dip Spectroscopy and Natural Bond Orbital Analysis*  
Journal of Physical Chemistry A, (113): 6880-6885 2009.

Kageura, Y.; Sakota, K.; Sekiya, H.

*Charge Transfer Interaction of Intermolecular Hydrogen Bonds in 7-Azaindole(MeOH)(n) (n=1, 2) with IR-Dip Spectroscopy and Natural Bond Orbital Analysis*  
Journal of Physical Chemistry A, (113): 6880-6885 2009.

Kaneno, D.; Tomoda, S.

*The Danishefsky pyranone puzzle: an explanation based on the exterior frontier orbital extension model*  
Tetrahedron Letters, (50): 329-332 2009.

Kang, G. J.; Chen, Z. X.; Li, Z.

*Theoretical studies of the interactions of ethylene and formaldehyde with gold clusters*  
Journal of Chemical Physics, (131) 2009.

Karafiloglou, P.

*An efficient generalized polyelectron population analysis in orbital spaces: The hole-expansion methodology*  
Journal of Chemical Physics, (130) 2009.

Karlsen, E. M.; Spanget-Larsen, J.

*FTIR investigation of the reaction between pyridine and iodine in a polyethylene host. Formation of N-iodopyridinium polyiodide*  
Chemical Physics Letters, (473): 227-232 2009.

Karnezis, A.; O'Hair, R. A. J.; White, J. M.

*Carbon-Germanium Hyperconjugation: Solid-State and Gas-Phase Investigations of (Trialkylgermyl)methyl-Substituted Pyridinium Ions*  
Organometallics, (28): 6480-6488 2009.

Karton, A.; Gruzman, D.; Martin, J. M. L.

*Benchmark Thermochemistry of the C<sub>n</sub>H<sub>2n+2</sub> Alkane Isomers (n=2-8) and Performance of DFT and Composite Ab Initio Methods for Dispersion-Driven Isomeric Equilibria*  
Journal of Physical Chemistry A, (113): 8434-8447 2009.

Kassaee, M. Z.; Soleimani-Amiri, S.

*Racemizations of diazacycloheptatetraenes through singlet diazacycloheptatrienylidenes at theoretical levels*  
Journal of Molecular Structure-Theochem, (913): 185-194 2009.

Kassaee, M. Z.; Soleimani-Amiri, S.; Buazar, F.; Rad, H. A.

*Novel disilyleno- and digermylenocarbenes and Si=Si containing cyclopropenylidenes at theoretical levels*  
Journal of Molecular Structure-Theochem, (893): 48-55 2009.

Kato, M.; Takayanagi, T.; Fujihara, T.; Nagasawa, A.  
*Linkage isomerism of pentaammine(dimethylsulfoxide)ruthenium(II/III) complexes: A theoretical study*  
Inorganica Chimica Acta, (362): 1199-1203 2009.

Katsumoto, Y.; Tanaka, T.; Ozaki, Y.; Hosoi, S.  
*Effects of dipole interaction and solvation on the C=O stretching band of N,N-dimethylacetamide in nonpolar solutions: Infrared, isotropic and anisotropic Raman measurements*  
Vibrational Spectroscopy, (51): 119-124 2009.

Kaur, D.; Kaur, R. P.; Kohli, R.  
*Correlation between proton affinity and conjugation effects in carbamic acid and its higher chalcogenide analogs*  
Journal of Molecular Structure-Theochem, (913): 90-96 2009.

Kaur, D.; Kohli, R.; Kaur, R. P.  
*The role of isomerism and medium effects on stability of anions of formo- and thioformohydroxamic acid*  
Journal of Molecular Structure-Theochem, (911): 30-39 2009.

Kesharwani, M. K.; Ganguly, B.  
*Solvent Effects on the Stereoselectivity of Reaction of Methyl Acrylate, Methyl Methacrylate and Methyl trans-Crotonate with Cyclopentadiene: A Computational Study*  
Croatica Chemica Acta, (82): 291-298 2009.

Ketkov, S. Y.; Isachenkov, N. A.; Braunschweig, H.; Kupfer, T.  
*Electronic structures of mixed sandwich ansa-complexes of chromium as studied by gas-phase absorption spectroscopy and quantum chemistry*  
Russian Chemical Bulletin, (58): 682-690 2009.

Khaliullin, R. Z.; Bell, A. T.; Head-Gordon, M.  
*Electron Donation in the Water-Water Hydrogen Bond*  
Chemistry-a European Journal, (15): 851-855 2009.

Khan, M. A. S.; Kesharwani, M. K.; Bandyopadhyay, T.; Ganguly, B.  
*Solvolytic of chemical warfare agent VX is more efficient with hydroxylamine anion: A computational study*  
Journal of Molecular Graphics and Modelling, (28): 177-182 2009.

Khartabil, H. K.; Martins-Costa, M. T. C.; Gros, P. C.; Fort, Y.; Ruiz-Lopez, M. F.  
*Structure of Mixed Alkyllithium/Lithium Alkoxide Aggregates in Etheral Solvents. Insights from Combined QM/MM Molecular Dynamics Simulations*  
Journal of Physical Chemistry B, (113): 6459-6467 2009.

Kilbas, B.; Azizoglu, A.; Balci, M.  
*Endo- and Exo-Configured Cyclopropylidenes Incorporated into the Norbornadiene Skeleton: Generation, Rearrangement to Allenes, and the Effect of Remote Substituents on Carbene Stability*

Journal of Organic Chemistry, (74): 7075-7083 2009.

Kim, H.; Jung, J.; Han, Y. K.

*Molecular Orbital Interpretation of Magic Clusters with Non-Magic Numbers*  
Chemphyschem, (10): 341-343 2009.

Kim, H. W.; Rhee, Y. M.

*Dispersion-Oriented Soft Interaction in a Frustrated Lewis Fair and the Entropic Encouragement Effect in its Formation*  
Chemistry-a European Journal, (15): 13348-13355 2009.

Kim, J.; Kim, T. K.; Ihee, H.

*Theoretical Study on the Reaction of Ti+ with Acetone and the Role of Intersystem Crossing*  
Journal of Physical Chemistry A, (113): 11382-11389 2009.

Kimmel, A. V.; Ramo, D. M.; Sushko, P. V.; Shluger, A. L.; Kuklja, M. M.

*Modeling proton transfer and polarons in a molecular crystal diamino-dinitroethylene*  
Physical Review B, (80) 2009.

Kiyota, Y.; Hasegawa, J. Y.; Fujimoto, K.; Swerts, B.; Nakatsuji, H.

*A Multicore QM/MM Approach for the Geometry Optimization of Chromophore Aggregate in Protein*  
Journal of Computational Chemistry, (30): 1351-1359 2009.

Kochina, T. A.; Vrazhnov, D. V.

*Silylium cations and their analogs: Radiochemical approach (A review)*  
Glass Physics and Chemistry, (35): 443-454 2009.

Kolakowski, R. V.; Manpadi, M.; Zhang, Y.; Emge, T. J.; Williams, L. J.

*Allene Synthesis via C-C Fragmentation: Method and Mechanistic Insight*  
Journal of the American Chemical Society, (131): 12910-+ 2009.

Kolakowski, R. V.; Manpadi, M.; Zhang, Y.; Emge, T. J.; Williams, L. J.

*Allene Synthesis via C-C Fragmentation: Method and Mechanistic Insight*  
Journal of the American Chemical Society, (131): 12910-+ 2009.

Koleva, G.; Galabov, B.; Wu, J. I.; Schaefer, H. F., III; Schleyer, P. v. R.

*Electrophile Affinity: A Reactivity Measure for Aromatic Substitution*  
Journal of the American Chemical Society, (131): 14722-14727 2009.

Kolocouris, A.

*C-H-ax center dot center dot center dot Y-ax Contacts in Cyclohexane Derivatives Revisited-Identification of Improper Hydrogen-Bonded Contacts*  
Journal of Organic Chemistry, (74): 1842-1849 2009.

Kona, F.; Tao, P.; Martin, P.; Xu, X. J.; Gatti, D. L.

*Electronic Structure of the Metal Center in the Cd2+, Zn2+, and Cu2+ Substituted Forms of KDO8P Synthase: Implications for Catalysis*

Biochemistry, (48): 3610-3630 2009.

Konrad, F.; Fillol, J. L.; Wadeohl, H.; Gade, L. H.

*Bis(oxazolinylmethyl)pyrrole Derivatives and Their Coordination as Chiral "Pincer" Ligands to Rhodium*

Inorganic Chemistry, (48): 8523-8535 2009.

Koshevoy, I. O.; Smirnova, E. S.; Domenech, A.; Karttunen, A. J.; Haukka, M.; Tunik, S. P.; Pakkanen, T. A.  
*Synthesis, electrochemical and theoretical studies of the Au(I)-Cu(I) heterometallic clusters bearing ferrocenyl groups*  
Dalton Transactions: 8392-8398 2009.

Krahulic, K. E.; Tuononen, H. M.; Parvez, M.; Roesler, R.

*Isolation of Free Phenylide-like Carbanions with N-Heterocyclic Carbene Frameworks*  
Journal of the American Chemical Society, (131): 5858-5865 2009.

Kraka, E.; Cremer, D.

*Characterization of CF Bonds with Multiple-Bond Character: Bond Lengths, Stretching Force Constants, and Bond Dissociation Energies*  
Chemphyschem, (10): 686-698 2009.

Kraus, F.; Baer, S. A.

*UF<sub>6</sub> and UF<sub>4</sub> in Liquid Ammonia: [UF<sub>7</sub>(NH<sub>3</sub>)]<sup>(3-)</sup> and [UF<sub>4</sub>(NH<sub>3</sub>)<sup>(4-)</sup>]*  
Chemistry-a European Journal, (15): 8269-8274 2009.

Kruszynski, R.

*Intermolecular Interactions in o-Tolidinium Dichloride Dihydrate: X-ray Structural and Quantum Mechanical Study*  
Polish Journal of chemistry, (83): 615-623 2009.

Kruszynski, R.

*Weak intermolecular interactions in isomorphous 5-(2-chloroethoxy)-2,3-dihydro-1,4-benzodioxine and 5-(2-bromoethoxy)-2,3-dihydro-1,4-benzodioxine: bonding or nonbonding interactions*  
Acta Crystallographica Section C-Crystal Structure Communications, (65): O396-O399 2009.

Kruszynski, R.; Trzesowska-Kruszynska, A.

*2,3-Dihydro-1,3-benzothiazol-2-iminium monohydrogen sulfate and 2-imino-2,3-dihydro-1,3-benzothiazole-6-sulfonate: a combined structural and theoretical study*  
Acta Crystallographica Section C-Crystal Structure Communications, (65): O624-O629 2009.

Krygowski, T. M.; Zachara-Horeglad, J. E.

*Resonance-assisted hydrogen bonding in terms of substituent effect*  
Tetrahedron, (65): 2010-2014 2009.

Krygowski, T. M.; Zachara-Horeglad, J. E.

*Resonance-assisted hydrogen bonding in terms of substituent effect*  
Tetrahedron, (65): 2010-2014 2009.

- Kubicki, J. D.; Halada, G. P.; Jha, P.; Phillips, B. L.  
*Quantum mechanical calculation of aqueous uranium complexes: carbonate, phosphate, organic and biomolecular species*  
Chemistry Central Journal, (3) 2009.
- Kun, Y.; Liu, Y. Z.; Lu, L. L.  
*Theoretical study of N(C)-H<sub>a</sub> <-H-B multi-dihydrogen bonds*  
Chinese Science Bulletin, (54): 1182-1189 2009.
- Kurian, R.; Filatov, M.  
*Calibration of Sn-119 isomer shift using ab initio wave function methods*  
Journal of Chemical Physics, (130) 2009.
- Kusama, H.; Sugihara, H.; Sayama, K.  
*Nitrogen-Containing Heterocycles' Interaction with Ru Dye in Dye-Sensitized Solar Cells*  
Journal of Physical Chemistry C, (113): 20764-20771 2009.
- Kutt, A.; Koppel, I.; Koppel, I. A.; Leito, I.  
*Boratabenzene Anions C5B(CN)(6)(-) and C5B(CF<sub>3</sub>)(6)(-) and the Superacidic Properties of their Conjugate Acids*  
Chemphyschem, (10): 499-502 2009.
- Kuwabara, J.; Mori, H.; Teratani, T.; Akita, M.; Kanbara, T.  
*Regioregulated Syntheses of Poly(aminopyridine)s by Pd-catalyzed Amination Reactions*  
Macromolecular Rapid Communications, (30): 997-1001 2009.
- Kuz'mina, L. G.; Kucherepa, N. S.; Pestov, S. M.; Kochetov, A. N.; Rukk, N. S.; Syrbu, S. A.  
*Molecular and Crystal Structure of 4-Alkoxybenzoic Acids: Design of the Mesogenic Phase*  
Crystallography Reports, (54): 862-879 2009.
- Kuznetsov, M. L.; Bokach, N. A.; Kukushkin, V. Y.; Dement'ev, A. I.  
*Theoretical Study of Ammonia Nucleophilic Addition to Nitriles in Platinum Complexes*  
Russian Journal of General Chemistry, (79): 232-241 2009.
- Kuznetsov, M. L.; Pessoa, J. C.  
*Epoxidation of olefins catalysed by vanadium-salan complexes: a theoretical mechanistic study*  
Dalton Transactions: 5460-5468 2009.
- Kuzora, R.; Schulz, A.; Villinger, A.; Wustrack, R.  
*Hypersilylated cyclodiphosphadiazanes and cyclodiphosphadiazonium salts*  
Dalton Transactions: 9304-9311 2009.
- Kyvala, M.  
*Calculation of Transition Matrix Elements by Nonsingular Orbital Transformations*  
International Journal of Quantum Chemistry, (109): 1200-1227 2009.
- Lage, M. L.; Mancheno, M. J.; Martinez-Alvarez, R.; Gomez-Gallego, M.; Fernandez, I.; Sierra, M. A.

*Behavior of Group 6 Fischer Aminocarbene Complexes in a Supercharged Medium: A Single Electron Transfer-H Atom Transfer Process*  
Organometallics, (28): 2762-2772 2009.

Lammermann, A.; Szatmari, I.; Fulop, F.; Kleinpeter, E.  
*Inter- or Intramolecular N center dot center dot center dot H-O or N-H center dot center dot center dot O Hydrogen Bonding in 1,3-Amino-alpha/beta-naphthols: An Experimental NMR and Computational Study*  
Journal of Physical Chemistry A, (113): 6197-6205 2009.

Lamsabhi, A. M.; Mo, O.; Gutierrez-Oliva, S.; Perez, P.; Toro-Labbe, A.; Yanez, M.  
*The Mechanism of Double Proton Transfer in Dimers of Uracil and 2-Thiouracil-The Reaction Force Perspective*  
Journal of Computational Chemistry, (30): 389-398 2009.

Langer, V.; Mach, P.; Smrcok, L.; Milata, V.  
*(E)-Methyl 2-[(2-fluorophenyl)aminomethylene]-3-oxobutanoate: X-ray and density functional theory (DFT) study*  
Acta Crystallographica Section C-Crystal Structure Communications, (65): O183-O185 2009.

Larkin, J. D.; Markham, G. D.; Milkevitch, M.; Brooks, B. R.; Bock, C. W.  
*Computational Investigation of the Oxidative Deboronation of Boroglycine, H<sub>2</sub>N-CH<sub>2</sub>-B(OH)(2), Using H<sub>2</sub>O and H<sub>2</sub>O<sub>2</sub>*  
Journal of Physical Chemistry A, (113): 11028-11034 2009.

Latelli, N.; May, A.; Ouddai, N.; Mokhtari, M.  
*Quantitative Characterization of Reactivity Descriptors of Nitrobenzofuroxan*  
Journal of Computational and Theoretical Nanoscience, (6): 599-604 2009.

Latosinska, J. N.; Latosinska, M.; Seliger, J.; Zagar, V.; Kazimierczuk, Z.  
*Electron density distribution in cladribine (2-chloro-2'-deoxyadenosine) - A drug against leukemia and multiple sclerosis - Studied by multinuclear NQR spectroscopy and DFT calculations*  
Chemical Physics Letters, (476): 293-302 2009.

Latosinska, J. N.; Seliger, J.; Zagar, V.; Burchardt, D. V.  
*Hydrogen Bonding and Stacking pi-pi Interactions in Solid 6-Thioguanine and 6-Mercaptopurine (Antileukemia and Antineoplastic Drugs) Studied by NMR-NQR Double Resonance Spectroscopy and Density Functional Theory*  
Journal of Physical Chemistry A, (113): 8781-8790 2009.

Laungani, A. C.; Keller, M.; Slattery, J. M.; Krossing, I.; Breit, B.  
*Cooperative Effect of a Classical and a Weak Hydrogen Bond for the Metal-Induced Construction of a Self-Assembled beta-Turn Mimic*  
Chemistry-a European Journal, (15): 10405-10422 2009.

Laurence, C.; Brameld, K. A.; Graton, J.; Le Questel, J. Y.; Renault, E.  
*The pK(BHX) Database: Toward a Better Understanding of Hydrogen-Bond Basicity for Medicinal Chemists*

Journal of Medicinal Chemistry, (52): 4073-4086 2009.

Le, T. D.; Arquier, D.; Miqueu, K.; Sotiropoulos, J. M.; Coppel, Y.; Bastin, S.; Igau, A.

*Unprecedented rearrangement during the formation of P-P homoatomic N-phosphino formamidine complexes*

Journal of Organometallic Chemistry, (694): 229-236 2009.

Ledesma, A. E.; Zinczuk, J.; Ben Altabef, A.; Gonzalez, J. J. L.; Brandan, S. A.

*Synthesis and vibrational analysis of N-(2'-Furyl)-Imidazole*

Journal of Raman Spectroscopy, (40): 1004-1010 2009.

Ledesma, A. E.; Zinczuk, J.; Gonzalez, J. J. L.; Ben Altabef, A.; Brandan, S. A.

*Structural and vibrational study of 4-(2'-furyl)-1-methylimidazole*

Journal of Molecular Structure, (924-26): 322-331 2009.

Lehmann, M.; Schulz, A.; Villinger, A.

*Bisilylated Halonium Ions: [Me<sub>3</sub>Si-X-SiMe<sub>3</sub>][B(C<sub>6</sub>F<sub>5</sub>)<sub>4</sub>] (X = F, Cl, Br, I)*

Angewandte Chemie-International Edition, (48): 7444-7447 2009.

Lehmann, S. B. C.; Spickermann, C.; Kirchner, B.

*Quantum Cluster Equilibrium Theory Applied in Hydrogen Bond Number Studies of Water. 1.*

*Assessment of the Quantum Cluster Equilibrium Model for Liquid Water*

Journal of Chemical Theory and Computation, (5): 1640-1649 2009.

Lein, M.

*Characterization of agostic interactions in theory and computation*

Coordination Chemistry Reviews, (253): 625-634 2009.

Lesar, A.; Milosev, I.

*Density functional study of the corrosion inhibition properties of 1,2,4-triazole and its amino derivatives*

Chemical Physics Letters, (483): 198-203 2009.

Less, R. J.; Naseri, V.; Wright, D. S.

*The Carbanionic Phosphoylide Dianion PhP(CH<sub>2</sub>)<sub>3</sub> (2-), Isoelectronic with Phosphonate Dianions*

*RP(O)<sub>3</sub> (2-)*

Organometallics, (28): 3594-3596 2009.

Lestard, M. E. D.; Tuttolomondo, M. E.; Varetti, E. L.; Wann, D. A.; Robertson, H. E.; Rankin, D. W. H.; Ben Altabef, A.

*Experimental and theoretical studies of the vibrations and structure of 2,2,2-trifluoroethyl trifluoroacetate, CF<sub>3</sub>CO<sub>2</sub>CH<sub>2</sub>CF<sub>3</sub>*

Journal of Molecular Structure, (917): 183-192 2009.

Lever, A. B. P.

*Density functional theory analyses of bis(bipyridine)ruthenium noninnocent quinonoid and thiolosulfinate complexes containing ligands formally in the semiquinone oxidation state*

Canadian Journal of Chemistry-Revue Canadienne De Chimie, (87): 1451-1459 2009.

- Leverentz, H. R.; Truhlar, D. G.  
*Electrostatically Embedded Many-Body Approximation for Systems of Water, Ammonia, and Sulfuric Acid and the Dependence of Its Performance on Embedding Charges*  
Journal of Chemical Theory and Computation, (5): 1573-1584 2009.
- Lezama, J.; Marquez, E.; Mora, J. R.; Cordova, T.; Chuchani, G.  
*Theoretical calculations on the mechanisms of the gas phase elimination kinetics of chlorocyclohexane, 3-chlorocyclohexene and 4-chlorocyclohexene*  
Journal of Molecular Structure-Theochem, (916): 17-22 2009.
- Li, F. F.; Gao, X.; Zheng, M.  
*Why [6,6]- and 1,2-Benzal-3-N-4-O-Cyclic Phenylimidate C-60 Undergo Electrochemically Induced Retro-Addition Reactions while 1,4-Dibenzyl-2,3-Cyclic Phenylimidate C-60 Does Not? C-H center dot center dot center dot X (X = N, O) Intramolecular Interactions in Organofullerenes*  
Journal of Organic Chemistry, (74): 82-87 2009.
- Li, H.; Zhang, L.; Han, L.; Cukier, R. I.; Bu, Y.  
*Theoretical prediction of size-expansion effect on the C8-site activity in the modified guanine-cytosine analogs*  
Journal of Physical Organic Chemistry, (22): 1114-1119 2009.
- Li, H. B.; Bin Bai, Y.; Tian, S. X.; Yang, J. L.  
*ELECTRON TOPOLOGICAL AND ENERGETIC STUDY OF THE INTERMOLECULAR HALOGEN BONDING INTERACTIONS IN COMPLEXES H<sub>2</sub>O center dot center dot center dot M (M = F-2, ClF, AND CF4)*  
Journal of Theoretical & Computational Chemistry, (8): 615-629 2009.
- Li, H. B.; Bin Bai, Y.; Tian, S. X.; Yang, J. L.  
*ELECTRON TOPOLOGICAL AND ENERGETIC STUDY OF THE INTERMOLECULAR HALOGEN BONDING INTERACTIONS IN COMPLEXES H<sub>2</sub>O center dot center dot center dot M (M = F-2, ClF, AND CF4)*  
Journal of Theoretical & Computational Chemistry, (8): 615-629 2009.
- Li, J.; Chen, X. Y.; Qiu, Y. X.; Wang, S. G.  
*Spin-Flip Reaction of Re + CH<sub>4</sub>-A Relativistic Density Functional Theory Investigation*  
Journal of Physical Chemistry A, (113): 8471-8477 2009.
- Li, J.; Qiu, Y. X.; Wang, S. G.  
*Metal-Phosphorus Bonding in Complexes W@Au<sub>12</sub>PX<sub>3</sub> (X = H, F, Cl, Br, I, Me, OMe) and [M@Au-12](PH<sub>3</sub>)-P-q (M-q = Hf<sub>2</sub>-, Ta-, W, Re+, Os<sub>2</sub>+, Ir<sub>3</sub>+, pt(4+), Au<sub>5</sub>+): Relativistic DFT Investigations*  
Journal of Physical Chemistry A, (113): 1646-1652 2009.
- Li, L. C.; Hu, F.; Cai, W. F.; Tian, A. M.; Wong, N. B.  
*Density functional theory study on hydrogen bonding interaction of luteolin-(H<sub>2</sub>O)(n)*  
Journal of Molecular Structure-Theochem, (911): 98-104 2009.
- Li, L. D.; Gomes, C. S. B.; Gomes, P. T.; Veiros, L. F.; Kim, S. Y.

*An unexpected one-pot synthesis of 7-isopropyl-3,3-dimethyl-10<sup>1</sup>H-spiro(indoline-2,9'-phenanthren)-10'-one*  
Arkivoc: 95-111 2009.

Li, P.

*DFT Predictions on Structures and Stabilities of Eleven-vertex nido- and closo-Heteroboranes*  
Chemical Research in Chinese Universities, (25): 247-256 2009.

Li, Q. G.; Xue, Y.

*Effects of Substituent and Leaving Group on the Gas-Phase S(N)2 Reactions of Phenoxides with Halomethanes: A DFT Investigation*  
Journal of Physical Chemistry A, (113): 10359-10366 2009.

Li, Q. Z.; Cheng, J. B.; Li, W. Z.; Gong, B. A.; Sun, J. Z.

*Comparative Study on the Nonadditivity of Methyl Group in Lithium Bonding and Hydrogen Bonding*  
International Journal of Quantum Chemistry, (109): 1127-1134 2009.

Li, Q. Z.; Liu, Z. B.; Li, W. Z.; Cheng, J. B.; Gong, B. A.; Sun, J. Z.

*Theoretical study on the pi hydrogen-bonded complex between HArF and ethylene*  
Journal of Molecular Structure-Theochem, (897): 69-72 2009.

Li, Q. Z.; Wang, Y. F.; Li, W. Z.; Cheng, J. B.; Gong, B. A.; Sun, J. Z.

*Prediction and characterization of the HMgH center dot center dot center dot LiX (X = H, OH, F, CCH, CN, and NC) complexes: a lithium-hydride lithium bond*  
Physical Chemistry Chemical Physics, (11): 2402-2407 2009.

Li, Q. Z.; Zhu, H. J.; An, X. L.; Gong, B. A.; Cheng, J. B.

*Nonadditivity of Methyl Group in Single-Electron Hydrogen Bond of Methyl Radical-Water Complex*  
International Journal of Quantum Chemistry, (109): 605-611 2009.

Li, R.; Feng, D. C.; Feng, S. Y.

*Computational study on decarboxylation mechanism of beta-lactamases inhibitors: Clavulanate vs. sulbactam*  
Chemical Physics Letters, (472): 248-253 2009.

Li, X.; Cao, X.; Jiang, J. H.; Zhao, Y. F.

*Structure and stability of AgXenZ (n=1-3, Z = -1, 0,+1) clusters. Theoretical insights*  
European Physical Journal D, (55): 87-91 2009.

Li, X.; Zhou, C.; Cao, X.; Zhao, Y.

*Theoretical investigation of stabilities and interactions of AuNenZ (n=1-3, Z = -1, 0,+1) clusters*  
Molecular Physics, (107): 2531-2536 2009.

Li, X. H.; Tang, Z. X.; Zhang, X. Z.

*Natural bond orbital (NBO) population analysis of para-substituted S-Nitroso-thiophenols*  
Journal of Molecular Structure-Theochem, (900): 50-54 2009.

- Li, X.-H.; Chen, Q.-D.; Zhang, X.-Z.  
*Natural bond orbital population analysis of para-substituted O-nitrosyl carboxylate compounds*  
Structural Chemistry, (20): 1043-1048 2009.
- Li, X.-H.; Zhang, R.-Z.; Zhang, X.-Z.  
*Natural bond orbital analysis of some para-substituted N-nitrosoacetanilide biological molecules*  
Structural Chemistry, (20): 1049-1054 2009.
- Li, X. M.; Tian, W. Q.; Huang, X. R.; Sun, C. C.; Jiang, L.  
*Theoretical explorations on the armchair BN nanotube with defects*  
Journal of Nanoparticle Research, (11): 395-403 2009.
- Li, X. Y.; Cao, X.; Zhao, Y. F.  
*Ab initio study of MArn+ (M = Cu, Ag, and Au, n=1-3)*  
Journal of Physics B-Atomic Molecular and Optical Physics, (42) 2009.
- Li, X. Y.; Xue, C.; Zhao, Y. F.  
*Structure and stability of AuXe (n) (Z) (n=1-3, Z = -1, 0, +1) clusters*  
Theoretical Chemistry Accounts, (123): 469-475 2009.
- Li, Y.; Ai, H. Q.; Qi, Z. N.; He, W.; Mang, L.  
*Stability Analysis of the Neutral Noble Gas Molecules FN<sub>g</sub>X and Their Anions FN<sub>g</sub>X(-) (Ng = He, Ar, Kr; X = O, S)*  
International Journal of Quantum Chemistry, (109): 782-789 2009.
- Li, Y.; Liu, Y. J.; Wu, D.; Li, Z. R.  
*Evolution of the structures and stabilities of boron-doped lithium cluster cations: ab initio and DFT studies*  
Physical Chemistry Chemical Physics, (11): 5703-5710 2009.
- Li, Z.; Ma, H.; Yan, B.; Guan, Y.; Song, J.  
*Synthesis, Crystal Structure, Theoretical Calculation and Thermal Behavior of DNAZ center dot NTO*  
Chinese Journal of Chemistry, (27): 2284-2290 2009.
- Li, Z. F.; Shi, X. N.; Liu, Y. Z.; Tang, H. A.; Zhang, J. Y.  
*Non-additivity of Methyl Group in the Single-electron Lithium Bond of H3C center dot center dot Li-H Complex*  
Chinese Journal of Chemical Physics, (22): 303-309 2009.
- Li, Z. H.; Liu, J. L.; Qiao, M. H.; Fan, K. N.  
*A theoretical study on the metal cation-pi complexes of Zn<sup>2+</sup> and Cd<sup>2+</sup> with benzene and cyclohexene*  
Molecular Physics, (107): 1271-1282 2009.
- Li, Z. J.; Li, Z. R.; Wang, F. F.; Ma, F.; Chen, M. M.; Huang, X. R.

*The charge transfer anion-radical alkali-metal salts M(+)TCNQ(-) (M = Li, Na, K): The structures and static hyperpolarizabilities*  
Chemical Physics Letters, (468): 319-324 2009.

Liang, B. L.; Zhang, Y. X.; Wang, Y. F.; Xu, W.; Li, X. Y.  
*Structures and properties of 1,7-disubstituted perylene tetracarboxylic diimides: The substitutional effect study based on density functional theory calculations*  
Journal of Molecular Structure, (917): 133-141 2009.

Liang, B. Y.; Wang, X. F.; Andrews, L.  
*Infrared Spectra and Density Functional Theory Calculations of Group 10 Transition Metal Sulfide Molecules and Complexes*  
Journal of Physical Chemistry A, (113): 3336-3343 2009.

Liang, J. X.; Geng, Z. Y.; Wang, Y. C.  
*Theoretical Study on Reaction of Furan Anion with N<sub>2</sub>O in Gas Phase*  
Chinese Journal of Chemistry, (27): 1261-1268 2009.

Lips, F.; Dehnen, S.  
*[Zn<sub>6</sub>Sn<sub>3</sub>Bi<sub>8</sub>](4-): Expanding the Intermetalloid Zintl Anion Concept to Ternary Systems*  
Angewandte Chemie-International Edition, (48): 6435-6438 2009.

Lips, F.; Schellenberg, I.; Poettgen, R.; Dehnen, S.  
*The Subtle Influence of Binary versus Homoatomic Zintl Ions: The Phenyl-Ligated Trimetallic Cage [Sn<sub>2</sub>Sb<sub>5</sub>(ZnPh)(2)](3-)*  
Chemistry-a European Journal, (15): 12968-12973 2009.

Liu, C.; Chung, S.-Y.; Lee, S.; Weiss, S.; Neuhauser, D.  
*Adsorbate-induced absorption redshift in an organic-inorganic cluster conjugate: Electronic effects of surfactants and organic adsorbates on the lowest excited states of a methanethiol-CdSe conjugate*  
Journal of Chemical Physics, (131) 2009.

Liu, C. G.; Guan, W.; Yan, L. K.; Song, P.; Su, Z. M.  
*Theoretical studies on nitrido ruthenium (VI) porphyrin and high valent ruthenium nitrido derivatives of Keggin typical polyoxometalate ([PW<sub>11</sub>O<sub>39</sub>{(RuN)-N-VI}](4-)): electronic structures and bonding features*  
Dalton Transactions: 6208-6213 2009.

Liu, C. G.; Su, Z. M.; Guan, W.; Yan, L. K.  
*Quantum Chemical Studies on High-Valent Metal Nitrido Derivatives of Keggin-Type Polyoxometalates ([PW<sub>11</sub>O<sub>39</sub>{(MN)-N-VI}](4-) (M = Ru, Os, Re)): M-VI-N Bonding and Electronic Structures*  
Inorganic Chemistry, (48): 541-548 2009.

Liu, F. L.  
*Heterofullerene molecules C<sub>58</sub>X (X = S, Se, Te): A DFT study*  
Chemical Physics Letters, (471): 116-121 2009.

- Liu, J. H.; Cao, S. X.; Jia, B.; Wei, D. H.; Liao, X. C.; Lu, J. S.; Zhao, Y. F.  
*A theoretical and mass spectrometry study of the novel mechanism of N-glycosidic bond cleavage in nucleoside*  
International Journal of Mass Spectrometry, (282): 1-5 2009.
- Liu, L. P.; Hammond, G. B.  
*Reactions of Cationic Gold(I) with Allenoates: Synthesis of Stable Organogold(I) Complexes and Mechanistic Investigations on Gold-Catalyzed Cyclizations*  
Chemistry-an Asian Journal, (4): 1230-1236 2009.
- Liu, Y.-Z.; Shi, X.-N.; Li, Z.-F.; Tang, H.-A.; Yuan, K.; Zhang, J.-Y.  
*Structures and Electron Density Topological Properties of the CH<sub>3</sub>SH center dot center dot center dot HOO Hydrogen Bond Complexes*  
Chemical Journal of Chinese Universities-Chinese, (30): 2049-2054 2009.
- Liu, Z.; Goddard, J. D.  
*Predictions of the Fluorine NMR Chemical Shifts of Perfluorinated Carboxylic Acids, C<sub>n</sub>F<sub>2n+1</sub>COOH (n=6-8)*  
Journal of Physical Chemistry A, (113): 13921-13931 2009.
- Lloret, J.; Estevan, F.; Lahuerta, P.; Hirva, P.; Perez-Prieto, J.; Sanau, M.  
*Dirhodium(II) Compounds with Bridging Thienylphosphines: Studies on Reversible P,C/P,S Coordination*  
Chemistry-a European Journal, (15): 7706-7716 2009.
- Lobayan, R. M.; Jubert, A. H.; Vitale, M. G.; Pomilio, A. B.  
*Conformational and electronic (AIM/NBO) study of unsubstituted A-type dimeric proanthocyanidin*  
Journal of Molecular Modeling, (15): 537-550 2009.
- Long, G. J.; Tanase, S.; Remacle, F.; Periyasamy, G.; Grandjean, F.  
*Combined Mossbauer Spectral and Density Functional Theory Determination of the Magnetic Easy-Axis in Two High-Spin Iron(II) 2-Pyrazinecarboxylate Complexes*  
Inorganic Chemistry, (48): 8173-8179 2009.
- Long, H.; King, P. W.; Ghirardi, M. L.; Kim, K.  
*Hydrogenase/Ferredoxin Charge-Transfer Complexes: Effect of Hydrogenase Mutations on the Complex Association*  
Journal of Physical Chemistry A, (113): 4060-4067 2009.
- Lopes Jesus, A. J.; Redinha, J. S.  
*On the structure of erythritol and L-threitol in the solid state: An infrared spectroscopic study*  
Journal of Molecular Structure, (938): 156-164 2009.
- Lopez-Alberca, M. P.; Mancheno, M. J.; Fernandez, I.; Gomez-Gallego, M.; Sierra, M. A.; Torres, R.  
*Synthesis and Properties of Mononuclear Group 10 Alkoxy-Biscarbene Complexes*  
Chemistry-a European Journal, (15): 3595-3603 2009.

- Lopez-Tarifa, P.; Martin, F.; Yanez, M.; Alcami, M.  
*Theoretical Study of Doubly Charged [X(H<sub>2</sub>O)] and [X(NH<sub>3</sub>)] (X = Si, Ge, Sn, Pb) Molecular Ions*  
Croatica Chemica Acta, (82): 129-137 2009.
- Lu, Q. X.; Li, X. C.; Wang, Y.; Chen, G. J.  
*Catalytic activities of dismutation reactions of Cu(bpy)Br-2 compound and its derivatives as SOD mimics: A theoretical study*  
Journal of Molecular Modeling, (15): 1397-1405 2009.
- Lu, Z. H.; Jiang, L.; Xu, Q.  
*Infrared spectra and density functional theory calculations of the tantalum and niobium carbonyl dinitrogen complexes*  
Journal of Chemical Physics, (131) 2009.
- Lucas, X.; Estarellas, C.; Escudero, D.; Frontera, A.; Quinonero, D.; Deya, P. M.  
*Very Long-Range Effects: Cooperativity between Anion-pi and Hydrogen-Bonding Interactions*  
Chemphyschem, (10): 2256-2264 2009.
- Ludwig, R.; Paschek, D.  
*Applying the Inductive Effect for Synthesizing Low-Melting and Low-Viscosity Imidazolium-Based Ionic Liquids*  
Chemphyschem, (10): 516-519 2009.
- Lue, L.-L.; Yang, S.; Yuan, K.; Wang, X.-F.; Wang, Y.-C.  
*Theoretical Study on the Excited-state Intramolecular Hydrogen Abstraction Reactions of Butanal*  
Chinese Journal of Structural Chemistry, (28): 1226-1235 2009.
- Lukowski, M.; Jacobs, K.; Hsueh, P.; Lindsay, H. A.; Milletti, M. C.  
*Thermodynamic and kinetic factors in the aza-Cope rearrangement of a series of iminium cations*  
Tetrahedron, (65): 10311-10316 2009.
- Luo, G. G.; Wu, R. B.; Sun, D.; Chen, J. H.; Zhang, N.; Huang, R. B.; Lin, L. R.; Zheng, L. S.  
*Microwave-assisted synthesis, crystal structures and DFT calculations of two novel silver(I) dimers [Ag-2(mu-X)(2)(mu-dppm)(PPh<sub>3</sub>)(2)] (X = Br, I) with butterfly-shaped dinuclear cores*  
Journal of Molecular Structure, (930): 9-14 2009.
- Luo, S. X.; Zhang, S. T.; Zhang, X. Y.; Zhu, H. W.; Hu, J. W.; Wei, G.  
*Density Functional Theory Study on the Photocatalytic Degradation of Mercapto-Azobenzene Carboxylic Acids with Different Substituents Catalyzed by TiO<sub>2</sub>*  
Chinese Journal of Catalysis, (30): 654-658 2009.
- Lv, G.; Wei, F.; Jiang, H.; Zhou, Y.; Wang, X.  
*DFT study on the intermolecular interactions between Au-n (n=2-4) and thymine*  
Journal of Molecular Structure-Theochem, (915): 98-104 2009.
- Lv, L. L.; Liu, X. W.; Yuan, K.; Wang, X. F.; Wang, Y. C.

*Theoretical study of the mechanism for C-H bond activation in spin-forbidden reaction between Ti+ and C<sub>2</sub>H<sub>4</sub>*  
Science in China Series B-Chemistry, (52): 295-303 2009.

Lv, L.-L.; Wang, Y.-C.; Geng, Z.-Y.; Si, Y.-B.; Wang, Q.; Liu, H.-W.  
*Activation of C<sub>2</sub>H<sub>6</sub> by Gas-Phase Ta+: Potential Energy Surfaces, Spin-Orbit Coupling, Spin-Inversion Probabilities, and Reaction Mechanisms*  
Organometallics, (28): 6160-6170 2009.

Lyalin, A.; Taketsugu, T.  
*Cooperative Adsorption of O<sub>2</sub> and C<sub>2</sub>H<sub>4</sub> on Small Gold Clusters*  
Journal of Physical Chemistry C, (113): 12930-12934 2009.

Lyngdoh, R. H. D.; Schaefer, H. F.  
*Elementary Lesions in DNA Subunits: Electron, Hydrogen Atom, Proton, and Hydride Transfers*  
Accounts of Chemical Research, (42): 563-572 2009.

Ma, F.; Li, R.-Y.; Li, Z.-R.; Chen, M.-M.; Xu, H.-L.; Li, Z.-J.; Wu, D.; Li, Z.-S.  
*Out-of-plane sigma-aromaticity and enhanced pi-aromaticity in superatom compounds Li<sub>3</sub>+N<sub>42</sub>-M<sub>3</sub><sup>+</sup> (M = Li, Na and K)*  
Journal of Molecular Structure-Theochem, (913): 80-84 2009.

Ma, F.; Li, Z. R.; Xu, H. L.; Li, Z. J.; Wu, D.; Li, Z. S.; Gu, F. L.  
*Proton Transfer in the Complex H<sub>3</sub>N center dot center dot center dot HCl Catalyzed by Encapsulation into a C-60 Cage*  
Chemphyschem, (10): 1112-1116 2009.

Ma, J.; Zhang, X. L.; Zhao, N.; Xiao, F. K.; Wei, W.; Sun, Y. H.  
*Mechanism of TBD-catalyzed hydrolysis of acetonitrile*  
Journal of Molecular Structure-Theochem, (911): 40-45 2009.

Ma, X. Y.; Wang, J. P.  
*Differentiating Subtle Variation of Weak Intramolecular Hydrogen Bond in Vicinal Diols by Linear Infrared Spectroscopy*  
Journal of Physical Chemistry A, (113): 6070-6076 2009.

Ma, Y. P.; He, S. G.; Ding, X. L.; Wang, Z. C.; Xue, W.; Shi, Q.  
*Theoretical study of intermolecular interactions in meso-tetraphenylporphyrin diacid dimer (H<sub>4</sub>TPPCl<sub>2</sub>)<sub>2</sub>*  
Physical Chemistry Chemical Physics, (11): 2543-2552 2009.

Macchi, P.  
*Resonance Structures and Electron Density Analysis*  
Angewandte Chemie-International Edition, (48): 5793-5795 2009.

Madi, F.; Khatmi, D.; Dhaoui, N.; Bouzitouna, A.; Abdaoui, M.; Boucekkine, A.  
*Molecular model of CENS piperidine beta-CD inclusion complex: DFT study*  
Comptes Rendus Chimie, (12): 1305-1312 2009.

- Mahindroo, N.; Connelly, M. C.; Punchihewa, C.; Kimura, H.; Smeltzer, M. P.; Wu, S.; Fujii, N.  
*Structure-Activity Relationships and Cancer-Cell Selective Toxicity of Novel Inhibitors of Glioma-Associated Oncogene Homologue 1 (Gli1) Mediated Transcription*  
Journal of Medicinal Chemistry, (52): 4277-4287 2009.
- Malaspina, T.; Costa, L. T.; Fileti, E. E.  
*Ab Initio Analysis of Monomers and Dimers of Trialkylphosphine Oxides: Structural and Thermodynamic Stability*  
International Journal of Quantum Chemistry, (109): 250-258 2009.
- Malecki, J. G.; Kruszynski, R.; Mazurak, Z.  
*Synthesis, spectroscopic and structural characterizations of two new complexes of ruthenium with 2-(hydroxymethyl)benzimidazole and 1,10-phenanthroline ligands*  
Polyhedron, (28): 3891-3898 2009.
- Malenkov, G.  
*Liquid water and ices: understanding the structure and physical properties*  
Journal of Physics-Condensed Matter, (21) 2009.
- Mang, C.-Y.; Zi, J.-Q.; Zhao, X.; Wu, K.-C.  
*The Lowest Triplet Excited States of Ph<sub>3</sub>PAuX and Ph<sub>3</sub>AsAuX (X=Cl, Br)*  
Acta Physico-Chimica Sinica, (25): 2113-2117 2009.
- Markovic, S.; Petrovic, Z. D.; Petrovic, V.  
*DFT study on the preactivation reaction of a palladium catalyst precursor in phosphine-free Heck reactions*  
Monatshefte fur Chemie, (140): 171-175 2009.
- Markovic, S.; Stankovic, S.; Radenkovic, S.; Gutman, I.  
*Thermal isomerization in cyclopenta[fg]aceanthrylene*  
Monatshefte fur Chemie, (140): 153-156 2009.
- Markovic, Z. S.; Manojlovic, N. T.  
*DFT study on the reactivity of OH groups in emodin: structural and electronic features of emodin radicals*  
Monatshefte fur Chemie, (140): 1311-1318 2009.
- Maron, L.; Bourissou, D.  
*2,6-Bis(imidazol-2-ylidene)pyridine Complexes of Lanthanoids: A Theoretical Study of the Bonding Situation and Selective Complexation*  
Organometallics, (28): 3686-3690 2009.
- Maron, L.; Eisenstein, O.; Andersen, R. A.  
*The Bond between CO and Cp' U-3 in Cp' U-3(CO) Involves Back-bonding from the Cp' U-3 Ligand-Based Orbitals of pi-Symmetry, where Cp' Represents a Substituted Cyclopentadienyl Ligand*  
Organometallics, (28): 3629-3635 2009.

Marquez, E.; Mora, J. R.; Cordova, T.; Chuchani, G.  
*DFT Calculations of Triethyl and Trimethyl Orthoacetate Elimination Kinetics in the Gas Phase*  
Journal of Physical Chemistry A, (113): 2600-2606 2009.

Martin, C. B.; Walker, D.; Soniat, M.  
*Density functional theory study of possible mechanisms of folic acid photodecomposition*  
Journal of Photochemistry and Photobiology a-Chemistry, (208): 1-6 2009.

Martins-Costa, M.; Anglada, J. M.; Ruiz-Lopez, M. F.  
*Hyperconjugation in adjacent OO bonds: Remarkable odd/even effects*  
Chemical Physics Letters, (481): 180-182 2009.

Marton, A.; Parvulescu, L.; Draghici, C.; Varga, R. A.; Gheorghiu, M. D.  
*Reaction of Moore's ketene (tert-butylcyanoketene) with 1,3-cyclopentadiene and 1,3-cyclohexadiene. Is periselectivity controlled by the dynamic of trajectories at the bifurcation point?*  
Tetrahedron, (65): 7504-7509 2009.

Masoodi, H. R.; Ebrahimi, A.; Habibi, M.  
*The effect of carbon hybridization and halogen-acceptor type on some calculated NMR data in C-X center dot center dot center dot H-F hydrogen bonds*  
Chemical Physics Letters, (483): 43-48 2009.

Mata, I.; Molins, E.; Alkorta, I.; Espinosa, E.  
*Effect of an external electric field on the dissociation energy and the electron density properties: The case of the hydrogen bonded dimer HF center dot HF*  
Journal of Chemical Physics, (130) 2009.

Matos, M. A. R.; Sousa, C. C. S.; Morais, V. M. F.  
*Experimental and computational thermochemistry of the isomers: Chromanone, 3-isochromanone, and dihydrocoumarin*  
Journal of Chemical Thermodynamics, (41): 308-314 2009.

Matsumoto, K.; Hagiwara, R.  
*A New Series of Ionic Liquids Based on the Difluorophosphate Anion*  
Inorganic Chemistry, (48): 7350-7358 2009.

Matulis, V. E.; Halauko, Y. S.; Ivashkevich, O. A.; Gaponik, P. N.  
*CH acidity of five-membered nitrogen-containing heterocycles: DFT investigation*  
Journal of Molecular Structure-Theochem, (909): 19-24 2009.

Mayhall, N. J.; Rothgeb, D. W.; Hossain, E.; Jarrold, C. C.; Raghavachari, K.  
*Water reactivity with tungsten oxides: H-2 production and kinetic traps*  
Journal of Chemical Physics, (131) 2009.

Mayhall, N. J.; Rothgeb, D. W.; Hossain, E.; Raghavachari, K.; Jarrold, C. C.

*Electronic structures of MoWO<sub>y</sub>- and MoWO<sub>y</sub> determined by anion photoelectron spectroscopy and DFT calculations*  
Journal of Chemical Physics, (130) 2009.

McDowell, S. A. C.  
*Displacement of the proton in hydrogen-bonded complexes of hydrogen fluoride by beryllium and magnesium ions*  
Journal of Chemical Physics, (130) 2009.

McDowell, S. A. C.; Golovko, V. B.  
*A computational study of a novel seven-membered cyclic diyne and its cobalt-carbonyl complex*  
Journal of Molecular Structure-Theochem, (909): 111-115 2009.

McGrady, G. S.; Sirsch, P.; Chatterton, N. P.; Ostermann, A.; Gatti, C.; Altmannshofer, S.; Herz, V.; Eickerling, G.; Scherer, W.

*Nature of the Bonding in Metal-Silane sigma-Complexes*  
Inorganic Chemistry, (48): 1588-1598 2009.

Mebs, S.; Henn, J.; Dittrich, B.; Paulmann, C.; Luger, P.  
*Electron Densities of Three B-12 Vitamins*  
Journal of Physical Chemistry A, (113): 8366-8378 2009.

Medved, M.; Budzak, S.; Jacquemin, D.; Perpete, E. A.  
*Enhancement of the second-order NLO responses of boron-nitrogen oligomers by copolymerization with polyyne*  
Journal of Molecular Structure-Theochem, (901): 194-201 2009.

Mei, Y.; Zhang, J. Z. H.  
*Numerical Stabilities in Fitting Atomic Charges to Electric Field and Electrostatic Potential*  
Journal of Theoretical & Computational Chemistry, (8): 925-942 2009.

Meier, D. C.; Raman, B.; Semancik, S.  
*Detecting Chemical Hazards with Temperature-Programmed Microsensors: Overcoming Complex Analytical Problems with Multidimensional Databases*  
Annual Review of Analytical Chemistry, (2): 463-484 2009.

Melero, C.; Guijarro, A.; Yus, M.  
*Structural characterization and bonding properties of lithium naphthalene radical anion, [Li<sup>+</sup>(TMEDA)(2)][C<sub>10</sub>H<sub>8</sub> center dot-], and lithium naphthalene dianion [(Li<sup>+</sup>)TMEDA](2)C<sub>10</sub>H<sub>8</sub>-2]*  
Dalton Transactions: 1286-1289 2009.

Mendez, P. S.; Cachau, R. E.; Seoane, G.; Ventura, O. N.  
*Regioselective epoxide ring-opening using boron trifluoride diethyl etherate: DFT study of an alternative mechanism to explain the formation of syn-fluorohydrins*  
Journal of Molecular Structure-Theochem, (904): 21-27 2009.

Menezes, F. M. C.; Kuznetsov, M. L.; Pombeiro, A. J. L.

*Isocyanide Complexes with Platinum and Palladium and Their Reactivity toward Cycloadditions with Nitrones to Form Aminooxycarbenes: A Theoretical Study*  
Organometallics, (28): 6593-6602 2009.

Menjon, B.; Martinez-Salvador, S.; Gomez-Saso, M. A.; Fornies, J.; Falvello, L. R.; Martin, A.; Tsipis, A.  
*Oxidative Addition of Halogens to Homoleptic Perfluoromethyl or Perfluorophenyl Derivatives of Platinum(II): A Comparative Study*  
Chemistry-a European Journal, (15): 6371-6382 2009.

Mera, R.; Mendizabal, F.  
*Theoretical study of the d(10)-s(2) interaction between Au(I) and Tl(I) in the [AuCl(PH<sub>3</sub>)(2)]Tl<sup>+</sup> hypothetical complex*  
Chemical Physics Letters, (479): 156-159 2009.

Mercy, M.; Maron, L.  
*Can 1,3-butadiene be catalytically hydrophosphinated in the presence of Cp<sub>2</sub>EuH? A DFT investigation*  
Dalton Transactions: 3014-3025 2009.

Merouani, H.; Ouddai, N.; Mokhtari, M.; Latelli, N.  
*Density Functional Theory Study of the Reactivity of Nitrobenzofurazan with a Series of 4-X-Substituted Phenols*  
Journal of Computational and Theoretical Nanoscience, (6): 1658-1662 2009.

Miller, S. R.; Schultz, N. E.; Truhlar, D. G.; Leopold, D. G.  
*A study of the ground and excited states of Al-3 and Al-3(-). II. Computational analysis of the 488 nm anion photoelectron spectrum and a reconsideration of the Al-3 bond dissociation energy*  
Journal of Chemical Physics, (130) 2009.

Minasian, S. G.; Krinsky, J. L.; Rinehart, J. D.; Coping, R.; Tyliszczak, T.; Janousch, M.; Shuh, D. K.; Arnold, J.  
*A Comparison of 4f vs 5f Metal-Metal Bonds in (CpSiMe<sub>3</sub>)(3)M-ECp<sup>\*</sup> (M = Nd, U; E = Al, Ga; Cp<sup>\*</sup> = C<sub>5</sub>Me<sub>5</sub>): Synthesis, Thermodynamics, Magnetism, and Electronic Structure*  
Journal of the American Chemical Society, (131): 13767-13783 2009.

Mitani, M.; Yoshioka, Y.  
*A B3LYP study on counterpoise-corrected geometry optimizations for hydrated complexes of [K(H<sub>2</sub>O)(n)]<sup>(+)</sup> and [Na(H<sub>2</sub>O)(n)]<sup>(+)</sup>*  
Journal of Molecular Structure-Theochem, (915): 160-169 2009.

Mitin, A. V.; Kubicki, J. D.  
*Quantum Mechanical Investigations of Heme Structure and Vibrational Spectra: Effects of Conformation, Oxidation State, and Electric Field*  
Langmuir, (25): 548-554 2009.

Mitoraj, M. P.; Michalak, A.; Ziegler, T.  
*A Combined Charge and Energy Decomposition Scheme for Bond Analysis*  
Journal of Chemical Theory and Computation, (5): 962-975 2009.

Mizuno, K.; Masuda, Y.; Yamamura, T.; Kitamura, J.; Ogata, H.; Bako, I.; Tamai, Y.; Yagasaki, T.  
*Roles of the Ether Oxygen in Hydration of Tetrahydrofuran Studied by IR, NMR, and DFT Calculation Methods*  
Journal of Physical Chemistry B, (113): 906-915 2009.

Mladek, A.; Sharma, P.; Mitra, A.; Bhattacharyya, D.; Sponer, J.; Sponer, J. E.  
*Trans Hoogsteen/Sugar Edge Base Pairing in RNA. Structures, Energies, and Stabilities from Quantum Chemical Calculations*  
Journal of Physical Chemistry B, (113): 1743-1755 2009.

Mladenovic, M.; Elhiyani, M.; Lewerenz, M.  
*Electric and magnetic properties of the four most stable CHNO isomers from ab initio CCSD(T) studies*  
Journal of Chemical Physics, (131) 2009.

Mocci, F.  
*Torsion angle relationship of the O-17 NMR chemical shift in alpha,beta-unsaturated carbonyl compounds*  
Magnetic Resonance in Chemistry, (47): 862-867 2009.

Moens, J.; Jaque, P.; De Proft, F.; Geerlings, P.  
*A New View on the Spectrochemical and Nephelauxetic Series on the Basis of Spin-Polarized Conceptual DFT*  
Chemphyschem, (10): 847-854 2009.

Mohajeri, A.; Pakiari, A. H.; Bagheri, N.  
*Theoretical studies on the nature of bonding in sigma-hole complexes*  
Chemical Physics Letters, (467): 393-397 2009.

Monakhov, K. Y.; Linti, G.  
*Theoretical Study of Structure, Bonding, and Electronic Behavior of Low-Valent Bismuth Cyclopentadienyl and Pentamethylcyclopentadienyl Half-Sandwich Compounds*  
Inorganic Chemistry, (48): 6986-6996 2009.

Monbaliu, J. C.; Marchand-Brynaert, J.; Peeters, D.  
*Is anthracene cofactor or spectator for the thermolysis of anthracenyl acylnitroso cycloadducts in the presence of a diene?*  
Tetrahedron Letters, (50): 2555-2558 2009.

Mora, J. R.; Lezama, J.; Albornoz, J. M.; Hernandez, A.; Cordova, T.; Chuchani, G.  
*Theoretical calculations of the kinetics and mechanisms of the gas phase elimination of primary, secondary, and tertiary 2-hydroxyalkylbenzenes*  
Journal of Physical Organic Chemistry, (22): 1198-1207 2009.

Mora, J. R.; Tosta, M.; Cordova, T.; Chuchani, G.  
*Ab initio and DFT calculations on the gas phase elimination kinetics of 2,2-diethoxy-ethylamine and 2,2-diethoxy-N,N-diethyl-ethylamine*

Journal of Physical Organic Chemistry, (22): 367-377 2009.

Moreno, A.; Pregosin, P. S.; Fuentes, B.; Veiros, L. F.; Albinati, A.; Rizzato, S.

*Ion Pairing and Allyl Dynamics in a Series of [Pd(eta(3)-allyl)(N,N-chelate)][anion] Salts. On the Influence of the BPh<sub>4</sub>- Anion*

Organometallics, (28): 6489-6506 2009.

Morera-Boado, C.; Alonso-Becerra, E.; Gonzalez-Jonte, R.; Montero-Cabrera, L. A.; Garcia-De-La-Vega, J. M.

*A theoretical approach to the solvation of brassinosteroids*

Journal of Molecular Graphics and Modelling, (27): 600-610 2009.

Morzyk-Ociepa, B.

*Vibrational spectroscopic studies of indolecarboxylic acids and their metal complexes Part VIII. 5-Methoxyindole-2-carboxylic acid and its Zn(II) complex*

Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (72): 236-243 2009.

Muck, L. A.; Timoshkin, A. Y.; von Hopffgarten, M.; Frenking, G.

*Donor Acceptor Complexes of Noble Gases*

Journal of the American Chemical Society, (131): 3942-3949 2009.

Mukhopadhyay, A.; Mukherjee, M.; Pandey, P.; Samanta, A. K.; Bandyopadhyay, B.; Chakraborty, T.

*Blue Shifting C-H center dot center dot center dot O Hydrogen Bonded Complexes between Chloroform and Small Cyclic Ketones: Ring-Size Effects on Stability and Spectral Shifts*

Journal of Physical Chemistry A, (113): 3078-3087 2009.

Mukhopadhyay, C.; Datta, A.; Butcher, R. J.; Paul, B. K.; Guchhait, N.; Singha, R.

*Water mediated expeditious and highly selective synthesis of 2-aryl-1-arylmethyl-1H-benzimidazoles by Dowex 50W: fluorescence properties of some representative compounds*

Arkivoc: 1-22 2009.

Munha, R. F.; Veiros, L. F.; Duarte, M. T.; Fryzuk, M. D.; Martins, A. M.

*Synthesis and structural studies of amido, hydrazido and imido zirconium(IV) complexes incorporating a diamido/diamine cyclam-based ligand*

Dalton Transactions: 7494-7508 2009.

Munro, O. Q.; Camp, G. L.; Carlton, L.

*Structural, Rh-103 NMR and DFT Studies of a Bis(phosphane)Rh-III-Porphyrin Derivative*

European Journal of Inorganic Chemistry: 2512-2523 2009.

Murray, J. S.; Lane, P.; Politzer, P.

*Expansion of the sigma-hole concept*

Journal of Molecular Modeling, (15): 723-729 2009.

Murugavel, R.; Prabusankar, G.; Sharma, A.; Sunoj, R. B.; Butcher, R. J.

*Conformational and Isomeric Preferences of Six-Membered Inorganic Heterocycles*

*[EtNP(E)(OR)](3) (E = Lone Pair, O, S, or Se): A Synthetic, Spectroscopic, Structural, and Computational Study*

Inorganic Chemistry, (48): 2048-2059 2009.

Musio, R.; Sciacovelli, O.

*Conformational studies on 2-substituted ethanesulfonates in aqueous solution by H-1 NMR spectroscopy and DFT calculations*

Journal of Molecular Structure, (934): 57-65 2009.

Muthukumar, M.; Balasubramanian, V.

*Theoretical Studies on Structure of Acetylacetones of Zn(II), Cd(II) and Hg(II)*

Asian Journal of Chemistry, (21): 716-724 2009.

Muya, J. T.; Nguyen, M. T.; Ceulemans, A.

*Quantum chemistry study of symmetric methyne substitution patterns in the boron buckyball*

Chemical Physics Letters, (483): 101-106 2009.

Nakamura, S.; Liu, C. Y.; Muranaka, A.; Uchiyama, M.

*Theoretical Study on the Halogen-Zinc Exchange Reaction by Using Organozincate Compounds*

Chemistry-a European Journal, (15): 5686-5694 2009.

Nakazawa, T.; Igarashi, T.; Tsuru, T.; Kaji, Y.

*Ab initio calculations of Fe-Ni clusters*

Computational Materials Science, (46): 367-375 2009.

Nechaev, M. S.; Aksamentova, T. N.; Voronkov, M. G.; Chipanina, N. N.; Trofimova, O. M.; Bolgova, Y. I.; Turchaninov, V. K.

*Nature of intramolecular O -> Si bond in N-(trifluorosilylmethy)succinimide and N-(trifluorosilylmethy)phthalimide*

Russian Journal of General Chemistry, (79): 1086-1089 2009.

Nelyubina, Y. V.; Antipin, M. Y.; Lyssenko, K. A.

*Interactions between nitrate ions and their effect on charge redistribution in pentaerythrityltetraammonium tetranitrate crystal*

Russian Chemical Bulletin, (58): 751-757 2009.

Nemeth, B.; Khater, B.; Vespremi, T.; Guillemin, J. C.

*Synthesis, photoelectron spectroscopy and quantum chemical study of kinetically unstabilized phosphines complexed by borane*

Dalton Transactions: 3526-3535 2009.

Neto, A. C.; Ducati, L. C.; Rittner, R.; Tormena, C. F.; Contreras, R. H.; Frenking, G.

*Heavy Halogen Atom Effect on C-13 NMR Chemical Shifts in Monohalo Derivatives of*

*Cyclohexane and Pyran. Experimental and Theoretical Study*

Journal of Chemical Theory and Computation, (5): 2222-2228 2009.

Niu, S. Q.; Ichijo, T.

*Probing Ligand Effects on the Redox Energies of [4Fe-4S] Clusters Using Broken-Symmetry Density Functional Theory*

Journal of Physical Chemistry A, (113): 5671-5676 2009.

Noguera, M.; Rios-Font, R.; Rodriguez-Santiago, L.; Solans-Monfort, X.; Oliva, A.; Bertran, J.; Sodupe, M.  
*Influence of pi-stacking on the N7 and O6 proton affinity of guanine*  
Theoretical Chemistry Accounts, (123): 105-111 2009.

Noor, A.; Glatz, G.; Muller, R.; Kaupp, M.; Demeshko, S.; Kempe, R.  
*Carboalumination of a chromium-chromium quintuple bond*  
Nature Chemistry, (1): 322-325 2009.

Noor, A.; Glatz, G.; Muller, R.; Kaupp, M.; Demeshko, S.; Kempe, R.  
*Metal-Metal Distances at the Limit: Cr-Cr 1.73 angstrom - the Importance of the Ligand and its Fine Tuning*  
Zeitschrift fur Anorganische und Allgemeine Chemie, (635): 1149-1152 2009.

Nori-Shargh, D.; Yahyaei, H.  
*Stereoelectronic interaction effects (associated with the anomeric effects) on the conformational properties of 2-methylaminotetrahydropyran, 2-methylaminotetrahydrothiopyran, 2-methylaminotetrahydroselenopyran and their analogous containing P and As atoms: An Ab initio study and NBO analysis*  
Journal of Molecular Structure-Theochem, (913): 8-15 2009.

Noro, S.; Tanaka, D.; Sakamoto, H.; Shimomura, S.; Kitagawa, S.; Takeda, S.; Uemura, K.; Kita, H.; Akutagawa, T.; Nakamura, T.  
*Selective Gas Adsorption in One-Dimensional, Flexible Cu-II Coordination Polymers with Polar Units*  
Chemistry of Materials, (21): 3346-3355 2009.

Novak, I.; Kovac, B.  
*Polyoxometalates and vanadium alkoxides: Electronic structure and properties*  
Chemical Physics Letters, (474): 33-35 2009.

Nowroozi, A.; Jalbout, A. F.; Roohi, H.; Khalilinia, E.; Sadeghi, M.; De Leon, A.; Raissi, H.  
*Hydrogen Bonding in Acetylacetalddehyde: Theoretical Insights from the Theory of Atoms in Molecules*  
International Journal of Quantum Chemistry, (109): 1505-1514 2009.

Noyman, M.; Zilberg, S.; Haas, Y.  
*Stability of Polynitrogen Compounds: The Importance of Separating the sigma and pi Electron Systems*  
Journal of Physical Chemistry A, (113): 7376-7382 2009.

Ochi, N.; Nakao, Y.; Sato, H.; Matano, Y.; Imahori, H.; Sakaki, S.  
*New Palladium(II) Complex of P,S-Containing Hybrid Calixphyrin. Theoretical Study of Electronic Structure and Reactivity for Oxidative Addition*  
Journal of the American Chemical Society, (131): 10955-10963 2009.

Ochi, N.; Nakao, Y.; Sato, H.; Sakaki, S.

*Theoretical prediction of O-H, Si-H, and Si-C Sigma-bond activation reactions by titanium(IV)-imido complex*

Canadian Journal of Chemistry-Revue Canadienne De Chimie, (87): 1415-1424 2009.

O'Donovan, D. H.; Rozas, I.; Blanco, F.; Alkorta, I.; Elguero, J.

*Chiral Recognition in Bicyclic Guanidines*

Collection of Czechoslovak Chemical Communications, (74): 299-312 2009.

Oehlke, A.; Auer, A. A.; Schreiter, K.; Hofmann, K.; Riedel, F.; Spange, S.

*Electrophilic Substituent Constant sigma(+) of Electron Donor Substituents, in Nonpolar Media*

Journal of Organic Chemistry, (74): 3316-3322 2009.

Ogini, F. O.; Elder, P. J. W.; Britten, J. F.; Vargas-Baca, I.

*An investigation of (C5H5)Fe(C5H4-C(OBF3)-CH3)(1,2)*

Canadian Journal of Chemistry-Revue Canadienne De Chimie, (87): 1055-1062 2009.

Ogorodnikova, N. A.

*On invariance of the Mulliken substituent-induced charge changes in quantum-chemical calculations of different levels*

Journal of Molecular Structure-Theochem, (894): 41-49 2009.

Olah, G. A.; Prakash, G. K. S.; Rasul, G.

*Calculational Study of Fluoroammonium and Related Cations and Dications*

Chemistry-a European Journal, (15): 8443-8448 2009.

Olesen, S. G.; Hammerum, S.

*Redshift or adduct stabilization-a computational study of hydrogen bonding in adducts of protonated carboxylic acids*

European Journal of Mass Spectrometry, (15): 239-248 2009.

Oliveira, B. G.; Araujo, R.; Carvalho, A. B.; Ramos, M. N.

*The molecular properties of heterocyclic and homocyclic hydrogen-bonded complexes evaluated by DFT calculations and AIM densities*

Journal of Molecular Modeling, (15): 123-131 2009.

Orrego, J. F.; Zapata, F.; Truong, T. N.; Mondragon, F.

*Heterogeneous CO<sub>2</sub> Evolution from Oxidation of Aromatic Carbon-Based Materials*

Journal of Physical Chemistry A, (113): 8415-8420 2009.

Orzechowski, L.; Jansen, G.; Lutz, M.; Harder, S.

*Calcium carbene complexes with boranophosphorano side-arms: CaC[P(Ph)(2)BH3](2)*

Dalton Transactions: 2958-2964 2009.

Ostermeier, M.; Limberg, C.; Herwig, C.; Ziemer, B.

*Stabilizing the Boat Conformation of Piperazines Coordinated to Iron(II): iso-Butyl Substituents Lead to Robust Oxidation Catalysts via Hyperconjugation*

Zeitschrift fur Anorganische und Allgemeine Chemie, (635): 1823-1830 2009.

Oulie, P.; Nebra, N.; Saffon, N.; Maron, L.; Martin-Vaca, B.; Bourissou, D.  
*2-Indenylidene Pincer Complexes of Zirconium and Palladium*  
Journal of the American Chemical Society, (131): 3493-3498 2009.

Ouyang, Y. F.; Wang, J. C.; Liu, F. L.; Liu, Y. X.; Du, Y.; He, Y. H.; Feng, Y. P.  
*Density functional study of 3d-transition metal aluminides*  
Journal of Molecular Structure-Theochem, (905): 106-112 2009.

Ozen, C.; Konuklar, F. A. S.; Tuzun, N. S.  
*Mechanistic Study on [3+2] Cycloaddition and Cyclopropanation Reactions of 1,3-Dioxepine Derivatives in the Presence of Copper(I) Catalyst*  
Organometallics, (28): 4964-4973 2009.

Oziminski, W. P.  
*Computational note on steric interactions within COOH moiety from the Natural Steric Analysis point of view*  
Journal of Molecular Structure-Theochem, (902): 114-115 2009.

Oziminski, W. P.; Dobrowolski, J. C.  
*sigma- and pi-electron contributions to the substituent effect: natural population analysis*  
Journal of Physical Organic Chemistry, (22): 769-778 2009.

Padilla-Campos, L.  
*Theoretical investigation of the adsorption of carbon monoxide on small bimetallic LimCun ( $m, n \leq 4$ ) clusters*  
Journal of Molecular Structure-Theochem, (895): 34-43 2009.

Padilla-Campos, L.  
*Theoretical Investigation of the Adsorption of Oxygen on Small Bimetallic LimCun( $m, n \leq 4$ ) Clusters*  
International Journal of Quantum Chemistry, (109): 1357-1367 2009.

Padmaja, L.; Amalanathan, M.; Ravikumar, C.; Joe, I. H.  
*NBO analysis and vibrational spectra of 2,6-bis(*p*-methyl benzylidene cyclohexanone) using density functional theory*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (74): 349-356 2009.

Padmaja, L.; Ravikumar, C.; Sajan, D.; Joe, I. H.; Jayakumar, V. S.; Pettit, G. R.; Nielsen, O. F.  
*Density functional study on the structural conformations and intramolecular charge transfer from the vibrational spectra of the anticancer drug combretastatin-A2*  
Journal of Raman Spectroscopy, (40): 419-428 2009.

Pakiari, A. H.; Azami, S. M.  
*A localized picture of back bonding in CH<sub>3</sub>-nX<sub>n</sub> (X = F, Cl and Br; n=1, 2 or 3) radical and cation systems*  
Journal of Molecular Structure-Theochem, (901): 96-102 2009.

Palacios, M. A.; Rodriguez-Dieguez, A.; Sironi, A.; Herrera, J. M.; Mota, A. J.; Cano, J.; Colacio, E.

*Enhanced ferromagnetic interaction in metallacyclic complexes incorporating m-phenylenediamido bridges*  
Dalton Transactions: 8538-8547 2009.

Palacios, M. A.; Rodriguez-Dieguez, A.; Sironi, A.; Herrera, J. M.; Mota, A. J.; Moreno, V.; Cano, J.; Colacio, E.

*Double and triple stranded mesocates containing the bis(bidentate) bridging ligand 1,3-bis(pyridine-2-carboxamide)benzene. Structure, properties and DNA interaction*  
New Journal of Chemistry, (33): 1901-1908 2009.

Palafox, M. A.; Iza, N.; de la Fuente, M.; Navarro, R.

*Simulation of the First Hydration Shell of Nucleosides D4T and Thymidine: Structures Obtained Using MP2 and DFT Methods*  
Journal of Physical Chemistry B, (113): 2458-2476 2009.

Pandey, K. K.; Lledos, A.

*Linear M E-Me Versus Bent M-E-Me: Bonding Analysis in Heavier Metal-ylidyne Complexes [(Cp)(CO)(2)M EMe] and Metallo-ylidenes [(Cp)(CO)(3)M-E-Me] (M = Cr, Mo, W; E = Si, Ge, Sn, Pb)*  
Inorganic Chemistry, (48): 2748-2759 2009.

Pandey, K. K.; Lledos, A.; Maseras, F.

*The Nature of M-B Versus M = B Bonds in Cationic Terminal Borylene Complexes: Structure and Energy Analysis in the Borylene Complexes [(eta(5)-C5H5)(CO)(2)M{B(eta(5)-C5Me5)}](+), [(eta(5)-C5H5)(CO)(2)M(BMes)](+), and [(eta(5)-C5H5)(CO)(2)M(BNMe2)](+) (M = Fe, Ru, Os)*  
Organometallics, (28): 6442-6449 2009.

Parameswaran, P.; Frenking, G.

*Transition-Metal Complexes [(PMe3)(2)Cl2M(E)] and [(PMe3)(2)(CO)(2)M(E)] with Naked Group 14 Atoms (E = C-Sn) as Ligands; Part 1: Parent Compounds*  
Chemistry-a European Journal, (15): 8807-8816 2009.

Parameswaran, P.; Frenking, G.

*Transition-Metal Complexes [(PMe3)(2)Cl2M(E)] and [(PMe3)(2)(CO)(2)M(E)] with Naked Group 14 Atoms (E = C-Sn) as Ligands; Part 2: Complexation with W(CO)(5)*  
Chemistry-a European Journal, (15): 8817-8824 2009.

Parks, J. M.; Guo, H.; Momany, C.; Liang, L. Y.; Miller, S. M.; Summers, A. O.; Smith, J. C.

*Mechanism of Hg-C Protonolysis in the Organomercurial Lyase MerB*  
Journal of the American Chemical Society, (131): 13278-13285 2009.

Parveen, S.; Chandra, A. K.

*Theoretical Studies on Kinetics and Reactivity of the Gas-Phase Addition and H-Abstraction Reactions of Pyridine with Atomic Chlorine*  
Journal of Physical Chemistry A, (113): 177-183 2009.

Parveen, S.; Chandra, A. K.; Zeegers-Huyskens, T.

*Theoretical Investigation of the Interaction between Fluorinated Dimethyl Ethers ( $n(F)=1-5$ ) and Water: Role of the Acidity and Basicity on the Competition between OH center dot center dot O and CH center dot center dot center dot O Hydrogen Bonds*  
Journal of Physical Chemistry A, (113): 6182-6191 2009.

Parvulescu, L.; Marton, A.; Mihai, M.; Draghici, C.; Varga, R. A.; Gheorghiu, M. D.  
*6,6-Dimethyl- and 6,6-Diphenylfulvene as Cycloaddends in Reaction with Moore's Ketene*  
Revue Roumaine de Chimie, (54): 895-+ 2009.

Pasdar, H.; Ghiasi, R.  
*Effect of substitution on the structures, properties, and aromaticity of 1-H-boratabenzene anion*  
Main Group Chemistry, (8): 143-150 2009.

Pasinszki, T.; Bazso, G.; Krebsz, M.; Tarczay, G.  
*A matrix isolation and computational study of the [C, N, F, S] isomers*  
Physical Chemistry Chemical Physics, (11): 9458-9467 2009.

Patil, M. P.; Sunoj, R. B.  
*On the Relative Preference of Enamine/Iminium Pathways in an Organocatalytic Michael Addition Reaction*  
Chemistry-an Asian Journal, (4): 714-724 2009.

Payaka, A.; Tongraar, A.; Rode, B. M.  
*Combined QM/MM MD Study of HCOO--Water Hydrogen Bonds in Aqueous Solution*  
Journal of Physical Chemistry A, (113): 3291-3298 2009.

Pendas, A. M.; Blanco, M. A.; Francisco, E.  
*Steric Repulsions, Rotation Barriers, and Stereoelectronic Effects: A Real Space Perspective*  
Journal of Computational Chemistry, (30): 98-109 2009.

Peng, S.; Li, X. J.  
*DFT study of structural, electronic, and spectroscopic properties of D-6d endohedral fullerenes: X@C<sub>24</sub>H<sub>12</sub> (X = Li<sup>+</sup>, Na<sup>+</sup>, K<sup>+</sup>)*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (73): 67-71 2009.

Peng, S.; Li, X. J.; Zhang, D. X.; Zhang, Y.  
*A computational study of the endohedral fullerene GeH<sub>4</sub>@C-60*  
Structural Chemistry, (20): 789-794 2009.

Perrin, L.; Maron, L.; Eisenstein, O.; Tilley, T. D.  
*Bond Activations of PhSiH<sub>3</sub> by CP<sub>2</sub>SmH: A Mechanistic Investigation by the DFT Method*  
Organometallics, (28): 3767-3775 2009.

Perrin, L.; Sarazin, Y.; Kirillov, E.; Carpentier, J. F.; Maron, L.  
*On the Initiation Mechanism of Syndiospecific Styrene Polymerization Catalyzed by Single-Component ansa-Lanthanidocenes*  
Chemistry-a European Journal, (15): 3773-3783 2009.

Pet, M. A.; Cain, M. F.; Hughes, R. P.; Glueck, D. S.; Golen, J. A.; Rheingold, A. L.  
*Synthesis and structure of ferrocenylmethylphosphines, their borane adducts, and some related derivatives*  
Journal of Organometallic Chemistry, (694): 2279-2289 2009.

Petz, W.; Oexler, F.; Neumueller, B.; Tonner, R.; Frenking, G.  
*Carbodiphosphorane C(PPh<sub>3</sub>)<sub>2</sub> as a Single and Twofold Lewis Base with Boranes: Synthesis, Crystal Structures and Theoretical Studies on [H<sub>3</sub>B{C(PPh<sub>3</sub>)<sub>2</sub>}]] and [{(mu-H)H<sub>4</sub>B<sub>2</sub>}C(PPh<sub>3</sub>)<sub>2</sub>}](+)*  
European Journal of Inorganic Chemistry: 4507-4517 2009.

Pfletschinger, A.; Dolg, M.  
*Haptotropic migration of M(CO)<sub>3</sub> (M = Cr, Mo, W) on substituted phenanthrene*  
Journal of Organometallic Chemistry, (694): 3338-3342 2009.

Pichierri, F.; Kumar, V.  
*Geometries and electronic structures of phosphorous-doped silicon fullerenes: A DFT study*  
Journal of Molecular Structure-Theochem, (900): 71-76 2009.

Plumley, J. A.; Evanseck, J. D.  
*Periodic Trends and Index of Boron Lewis Acidity*  
Journal of Physical Chemistry A, (113): 5985-5992 2009.

Ponec, R.; Feixas, F.  
*Domain Averaged Fermi Hole Analysis for Open-Shell Systems*  
Journal of Physical Chemistry A, (113): 5773-5779 2009.

Poole, J. S.  
*A computational study of the chemistry of substituted 3-nitrenopyridine 1-oxides*  
Journal of Molecular Structure-Theochem, (894): 93-102 2009.

Popelier, P. L. A.; Bremond, E. A. G.  
*Geometrically Faithful Homeomorphisms Between the Electron Density and the Bare Nuclear Potential*  
International Journal of Quantum Chemistry, (109): 2542-2553 2009.

Popp, B. V.; Stahl, S. S.  
*Mechanism of Pd(OAc)<sub>2</sub>/Pyridine Catalyst Reoxidation by O<sub>2</sub>: Influence of Labile Monodentate Ligands and Identification of a Biomimetic Mechanism for O<sub>2</sub> Activation*  
Chemistry-a European Journal, (15): 2915-2922 2009.

Praveena, G.; Kolandaivel, P.  
*Structural Properties and Anion Binding Affinity of cyclo (1R,3S)-gamma-Acc-Gly (3) Hexapeptide*  
Journal of Biomolecular Structure and Dynamics, (27): 37-47 2009.

Prestianni, A.; Martorana, A.; Labat, F.; Ciofini, I.; Adamo, C.  
*A DFT investigation of CO oxidation over neutral and cationic gold clusters*  
Journal of Molecular Structure-Theochem, (903): 34-40 2009.

- Pu, Z. F.; Li, Q. S.; Xie, Y. M.; Schaefer, H. F.  
*Hypervalent molecules, sulfuranes, and persulfuranes: review and studies related to the recent synthesis of the first persulfurane with all substituents carbon-linked*  
Theoretical Chemistry Accounts, (124): 151-159 2009.
- Puchta, R.; Pasgreta, E.; van Eldik, R.  
*Ligand Exchange Processes on the Smallest Solvated Alkali and Alkaline Earth Metal Cations: An Experimental and Theoretical Approach*  
Advances in Inorganic Chemistry, Vol 61: Metal Ion Controlled Reactivity, (61): 523-571 2009.
- Puga, A. V.; Teixidor, F.; Sillanpaa, R.; Kivekas, R.; Arca, M.; Barbera, G.; Vinas, C.  
*From Mono- to Poly-Substituted Frameworks: A Way of Tuning the Acidic Character of C-c-H in o-Carbon Derivatives*  
Chemistry-a European Journal, (15): 9755-9763 2009.
- Qi, Y. H.; Feng, D. C.; Li, R.; Feng, S. Y.  
*Theoretical study on the substitution and insertion reactions of silylenoid H<sub>2</sub>SiLiF with CH<sub>3</sub>XH<sub>n</sub>-1 (X = F, Cl, Br, O, N; n=1, 1, 1, 2, 3)*  
Journal of Organometallic Chemistry, (694): 771-779 2009.
- Qian, Z. S.; Feng, H.; Yang, W. J.; Jin, X. Y.; Bi, S. P.  
*Density functional study of the water exchange reaction of the polyoxocation GeO<sub>4</sub>Al<sub>12</sub>(OH)(24)(H<sub>2</sub>O)(12)(8+) (K-GeAl12) in aqueous solution*  
Dalton Transactions: 8013-8017 2009.
- Raber, M. L.; Castillo, A.; Greer, A.; Townsend, C. A.  
*A Conserved Lysine in beta-Lactam Synthetase Assists Ring Cyclization: Implications for Clavam and Carbapenem Biosynthesis*  
Chembiochem, (10): 2904-2912 2009.
- Raiissi, H.; Jalbout, A. F.; Farsi, H.; Abbasi, B.; De Leon, A.; Moghiminia, S.  
*Intramolecular Hydrogen Bonding in 3-Imino-propenylamine: Theoretical Investigations*  
International Journal of Quantum Chemistry, (109): 1609-1616 2009.
- Rajapandian, V.; Hakkim, V.; Subramanian, V.  
*ONIOM Calculation on Azurin: Effect of Metal Ion Substitutions*  
Journal of Physical Chemistry A, (113): 8615-8625 2009.
- Rajeev, R.; Sunoj, R. B.  
*On the Origin of Reversible Hydrogen Activation by Phosphine-Boranes*  
Chemistry-a European Journal, (15): 12846-12855 2009.
- Ramalho, T. C.; Oliveira, L. C. A.; Carvalho, K. T. G.; Souza, E. F.; da Cunha, E. F. F.; Nazzaro, M.  
*The molecular basis for the behaviour of niobia species in oxidation reaction probed by theoretical calculations and experimental techniques*  
Molecular Physics, (107): 171-179 2009.

- Ramalho, T. C.; Pereira, D. H.  
*Understanding the substituent effect on the acidity of alcohols and para-substituted phenols*  
Molecular Simulation, (35): 1269-1278 2009.
- Ramirez-Anguita, J. M.; Gonzalez-Lafont, A.; Lluch, J. M.  
*Formation Pathways of DMSO<sub>2</sub> in the Addition Channel of the OH-Initiated DMS Oxidation: A Theoretical Study*  
Journal of Computational Chemistry, (30): 1477-1489 2009.
- Ramirez-Solis, A.; Kirtman, B.; Bernal-Jaquez, R.; Zicovich-Wilson, C. M.  
*Periodic density functional theory studies of Li-doped polythiophene: Dependence of electronic and structural properties on dopant concentration*  
Journal of Chemical Physics, (130) 2009.
- Ramos, D. R.; Castillo, R.; Canle, M.; Garcia, M. V.; Andres, J.; Santaballa, J. A.  
*A theoretical study on the mechanism of the base-promoted decomposition of N-chloro,N-methylethanolamine*  
Organic & Biomolecular Chemistry, (7): 1807-1814 2009.
- Rannulu, N. S.; Rodgers, M. T.  
*Noncovalent Interactions of Ni<sup>+</sup> with N-Donor Ligands (Pyridine, 4,4'-Dipyridyl, 2,2'-Dipyridyl, and 1,10-Phenanthroline): Collision-Induced Dissociation and Theoretical Studies*  
Journal of Physical Chemistry A, (113): 4534-4548 2009.
- Rapacioli, M.; Spiegelman, F.; Talbi, D.; Mineva, T.; Goursot, A.; Heine, T.; Seifert, G.  
*Correction for dispersion and Coulombic interactions in molecular clusters with density functional derived methods: Application to polycyclic aromatic hydrocarbon clusters*  
Journal of Chemical Physics, (130) 2009.
- Rappoport, D.; Furche, F.  
*Structure of endohedral fullerene Eu@C-74*  
Physical Chemistry Chemical Physics, (11): 6353-6358 2009.
- Ratajczyk, T.; Szymanski, S.  
*Are the silyl group hydrogens in peri-substituted-9-silyltryptecenes engaged in blue-shifting hydrogen bonds?*  
Physical Chemistry Chemical Physics, (11): 2335-2338 2009.
- Ray, A.; Rosair, G. M.; Rajeev, R.; Sunoj, R. B.; Rentschler, E.; Mitra, S.  
*Na-I/Cu-II heterometallic cages interconnected by unusual linear 2-coordinate OCN-Cu(I)-NCO links: synthesis, structural, magnetostructural correlation and computational studies*  
Dalton Transactions: 9510-9519 2009.
- Rayon, V. M.; Redondo, P.; Valdes, H.; Barrientos, C.; Largo, A.  
*Polyisocyanides of Titanium*  
Journal of Physical Chemistry A, (113): 1574-1577 2009.
- Re, S.; Jung, J.; Ten-no, S.; Sugita, Y.

*A two-dimensional energy surface of the phosphoryl transfer reaction catalyzed by phosphoserine phosphatase*  
Chemical Physics Letters, (480): 284-288 2009.

Rehbein, J.; Hiersemann, M.  
*Gosteli-Claisen Rearrangement: DFT Study of Substituent-Rate Effects*  
Journal of Organic Chemistry, (74): 4336-4342 2009.

Ren, F. D.; Cao, D. L.; Wang, W. L.; Ren, J.; Chen, S. S.  
*Can the BB multiple bonds be as the stronger hydrogen-bond proton acceptors than the CC multiple bonds: A comparative theoretical investigation on unusual intermolecular T-shaped X-H center dot center dot center dot pi interaction between HF and HB=BH ((3)Sigma(-)(g)), HB=BH ((1)Delta(g)), OCB BCO, H2C=CH2 or HC CH*  
Journal of Molecular Structure-Theochem, (896): 38-43 2009.

Ren, F. D.; Cao, D. L.; Wang, W. L.; Ren, J.; Hou, S. Q.; Chen, S. S.  
*A theoretical study on unusual intermolecular T-shaped X-H center dot center dot center dot pi interactions between the singlet state HB=BH and HF, HCl, HCN or H2C2*  
Journal of Molecular Modeling, (15): 515-523 2009.

Ren, Y.; Yamataka, H.  
*Does alpha-Effect Exist in E2 Reactions? A G2(+) Investigation*  
Journal of Computational Chemistry, (30): 358-365 2009.

Renner, S.; van Otterlo, W. A. L.; Seoane, M. D.; Mocklinghoff, S.; Hofmann, B.; Wetzel, S.; Schuffenhauer, A.; Ertl, P.; Oprea, T. I.; Steinhilber, D.; Brunsved, L.; Rauh, D.; Waldmann, H.  
*Bioactivity-guided mapping and navigation of chemical space*  
Nature Chemical Biology, (5): 585-592 2009.

Robertson, S. D.; Chivers, T.; Tuononen, H. M.  
*Experimental and Theoretical Investigations of the Contact Ion Pairs Formed by Reactions of the Anions (EPR2)(2)N (-) (R = Pr-i, Bu-t; E = S, Se) with the Cations (TePR2)(2)N (+) (R = Pr-i, Bu-t)*  
Inorganic Chemistry, (48): 6755-6762 2009.

Roering, A. J.; Maddox, A. F.; Elrod, L. T.; Chan, S. M.; Ghebreab, M. B.; Donovan, K. L.; Davidson, J. J.; Hughes, R. P.; Shalumova, T.; MacMillan, S. N.; Tanski, J. M.; Waterman, R.  
*General Preparation of (N3N)ZrX (N3N = N(CH<sub>2</sub>CH<sub>2</sub>NSiMe<sub>3</sub>)(3)(3-)) Complexes from a Hydride Surrogate*  
Organometallics, (28): 573-581 2009.

Rogachev, A. Y.; Petrukhina, M. A.  
*Insights Into Metal-pi Arene Interactions of the Highly Lewis Acidic Rh-2(4+) Core with a Broad Set of pi-Ligands: From Ethylene to Corannulene and C-60-Fullerene*  
Journal of Physical Chemistry A, (113): 5743-5753 2009.

Rojas, J. R.; Lorono, M.; Mora, J. R.; Dominguez, R. M.; Cordova, T.; Chuchani, G.  
*Theoretical Studies of the Gas-Phase Pyrolysis Kinetics of omega-Bromonitriles, ZCH(2)CH(2)Br [Z = NC, NCCH<sub>2</sub>, NCCH<sub>2</sub>CH<sub>2</sub>]*

International Journal of Chemical Kinetics, (41): 168-175 2009.

Romero, M. L.; Cordova, T.; Chuchani, G.

*Theoretical study of neighboring group participation of methyl omega-chloroesters elimination kinetics in the gas phase*

Journal of Physical Organic Chemistry, (22): 403-409 2009.

Roohi, H.; Baghery, S.

*Influence of hydration on the protomeric tautomerism in selenium analogue of methimazole: A computational chemistry study*

Journal of Molecular Structure-Theochem, (910): 41-49 2009.

Roos, G.; Foloppe, N.; Van Laer, K.; Wyns, L.; Nilsson, L.; Geerlings, P.; Messens, J.

*How Thioredoxin Dissociates Its Mixed Disulfide*

Plos Computational Biology, (5) 2009.

Rosado, M. T. S.; Jesus, A. J. L.; Reva, I. D.; Fausto, R.; Redinha, J. S.

*Conformational Cooling Dynamics in Matrix-Isolated 1,3-Butanediol*

Journal of Physical Chemistry A, (113): 7499-7507 2009.

Rossini, A. J.; Mills, R. W.; Briscoe, G. A.; Norton, E. L.; Geier, S. J.; Hung, I.; Zheng, S.; Autschbach, J.; Schurko, R. W.

*Solid-State Chlorine NMR of Group IV Transition Metal Organometallic Complexes*

Journal of the American Chemical Society, (131): 3317-3330 2009.

Rotinov, A.; Escalante, L.; Ramirez, B.; Pereira, D.; Cordova, T.; Chuchani, G.

*Gas Phase Elimination Kinetics of Methyl Mandelate: Experimental and DFT Studies*

Journal of Physical Chemistry A, (113): 12157-12162 2009.

Rotinov, A.; Ramirez, B.; Escalante, L.; Pereira, D.; Cordova, T.; Chuchani, G.

*Joint Experimental and Theoretical Studies of the Mechanism for the Gas Phase Elimination Kinetics of Methyl 2,2-Dimethyl-3-hydroxypropionate*

Journal of Physical Chemistry A, (113): 3491-3497 2009.

Roux, M. V.; Temprado, M.; Jimenez, P.; Foces-Foces, C.; Notario, R.; Parameswar, A. R.; Demchenko, A. V.; Chickos, J. S.; Deakyne, C. A.; Ludden, A. K.; Liebman, J. F.

*Experimental and Theoretical Study of the Structures and Enthalpies of Formation of the Synthetic Reagents 1,3-Thiazolidine-2-thione and 1,3-Oxazolidine-2-thione*

Journal of Physical Chemistry A, (113): 10772-10778 2009.

Roy, D.; Navarro-Vazquez, A.; Schleyer, P. V. R.

*Modeling Dinitrogen Activation by Lithium: A Mechanistic Investigation of the Cleavage of N-2 by Stepwise Insertion into Small Lithium Clusters*

Journal of the American Chemical Society, (131): 13045-13053 2009.

Ruiz, J.; Cutillas, N.; Dolores Villa, M.; Lopez, G.; Espinosa, A.; Bautista, D.

*N1-Coordination in palladium(II) and platinum(II) complexes with 9-methylhypoxanthine: crystal structures and theoretical calculations*

Dalton Transactions: 9637-9644 2009.

Ryde, U.; Schulzke, C.; Starke, K.

*Which functional groups of the molybdopterin ligand should be considered when modeling the active sites of the molybdenum and tungsten cofactors? A density functional theory study*  
Journal of Biological Inorganic Chemistry, (14): 1053-1064 2009.

Sabolovic, J.; Gomzi, V.

*Structure Prediction of Bis(amino acidato)copper(II) Complexes with a New Force Field for Molecular Modeling*  
Journal of Chemical Theory and Computation, (5): 1940-1954 2009.

Sadlej-Sosnowska, N.

*Quantum chemical considerations on degeneracy of the genetic code: Anticodon-codon wobble base pairing*  
Journal of Molecular Structure-Theochem, (913): 270-276 2009.

Safi, Z. S.; Alhendawi, H. M.

*Tautomerization and Substituent Effects on the Intramolecular Hydrogen Bonding in 4-Formyl-1-methylpyrazol-5-ol A Density Functional Theory*  
Asian Journal of Chemistry, (21): 4772-4784 2009.

Saha, S.; Roy, R. K.; Ayers, P. W.

*Are the Hirshfeld and Mulliken Population Analysis Schemes Consistent With Chemical Intuition?*  
International Journal of Quantum Chemistry, (109): 1790-1806 2009.

Sahnoun, R.; Fujimura, Y.; Kabuto, K.; Takeuchi, Y.; Noyori, R.

*Substituent effects on conformational preference in alpha-substituted alpha-fluorophenylacetic acid methyl ester model systems for chiral derivatizing agents*  
Journal of Physical Organic Chemistry, (22): 903-912 2009.

Sakata, K.; Miyake, Y.; Nishibayashi, Y.

*A DFT Study on the Reaction Pathways for Carbon-Carbon Bond-Forming Reactions between Propargylic Alcohols and Alkenes or Ketones Catalyzed by Thiolate-Bridged Diruthenium Complexes*  
Chemistry-an Asian Journal, (4): 81-88 2009.

Sakota, K.; Shimazaki, Y.; Sekiya, H.

*Formation of a dual hydrogen bond in the N-H center dot center dot center dot C=O moiety in the indole-(N-methylacetamide)(1) cluster revealed by IR-dip spectroscopy with natural bond orbital analysis*  
Journal of Chemical Physics, (130) 2009.

Salassa, L.; Phillips, H. I. A.; Sadler, P. J.

*Decomposition pathways for the photoactivated anticancer complex cis,trans,cis-[Pt(N-3)(2)(OH)(2)(NH3)(2)]: insights from DFT calculations*  
Physical Chemistry Chemical Physics, (11): 10311-10316 2009.

- Sanz, P.; Mo, O.; Yanez, M.; Elguerob, J.  
*The effects of C by N replacement on the hydrogen bonding of malonaldehyde: N-formylformimidic acid, N-(hydroxymethyl)formamide and related compounds*  
Physical Chemistry Chemical Physics, (11): 762-769 2009.
- Sarma, B. K.; Mugesh, G.  
*Theoretical Investigation on the Effect of Different Nitrogen Donors on Intramolecular Se center dot center dot center dot N Interactions*  
Chemphyschem, (10): 3013-3020 2009.
- Sasanuma, Y.  
*Conformational Characteristics, Configurational Properties, and Thermodynamic Characteristics of Poly(ethylene terephthalate) and Poly(ethylene-2,6-naphthalate)*  
Macromolecules, (42): 2854-2862 2009.
- Scemama, A.; Caffarel, M.; Ramirez-Solis, A.  
*Bond Breaking and Bond Making in Tetraoxygen: Analysis of the O-2(X-3 Sigma(-)(g)) + O-2(X-3 Sigma(-)(g)) reversible arrow O-4 Reaction Using the Electron Pair Localization Function*  
Journal of Physical Chemistry A, (113): 9014-9021 2009.
- Scheiner, S.; Seybold, P. G.  
*Quantum chemical analysis of the energetics of the anti and gauche conformers of ethanol*  
Structural Chemistry, (20): 43-48 2009.
- Schenk, S.; Reiher, M.  
*Ligands for Dinitrogen Fixation at Schrock-Type Catalysts*  
Inorganic Chemistry, (48): 1638-1648 2009.
- Schenk, S.; Reiher, M.  
*Ligands for Dinitrogen Fixation at Schrock-Type Catalysts*  
Inorganic Chemistry, (48): 1638-1648 2009.
- Schoeller, W. W.  
*Autocatalytic degradation of white phosphorus with silylenes*  
Physical Chemistry Chemical Physics, (11): 5273-5280 2009.
- Schreiner, P. R.; Reisenauer, H. P.; Romanski, J.; Mloston, G.  
*A Formal Carbon-Sulfur Triple Bond: H-CE S-O-H*  
Angewandte Chemie-International Edition, (48): 8133-8136 2009.
- Schulz, A.; Villinger, A.  
*Cyclic Arsenic-Nitrogen Cations*  
Inorganic Chemistry, (48): 7359-7367 2009.
- Schwobel, J.; Ebert, R. U.; Kuhne, R.; Schuurmann, G.  
*Modeling the H Bond Donor Strength of -OH, -NH, and -CH Sites by Local Molecular Parameters*  
Journal of Computational Chemistry, (30): 1454-1464 2009.

Seburg, R. A.; Patterson, E. V.; McMahon, R. J.  
*Structure of Triplet Propynylidene (HCCCH) as Probed by IR, UV/vis, and EPR Spectroscopy of Isotopomers*  
Journal of the American Chemical Society, (131): 9442-9455 2009.

See, R. F.  
*Which Method of Assigning Bond Orders in Lewis Structures Best Reflects Experimental Data? An Analysis of the Octet Rule and Formal Charge Systems for Period 2 and 3 Nonmetallic Compounds*  
Journal of Chemical Education, (86): 1241-1247 2009.

Selvaraj, K.; Kurian, R.  
*Dependence of Si-29 NMR chemical shielding properties of precursor silicate species, Q(0) on its local structure at the pre-nucleation stages of zeolite synthesis - A DFT based computational correlation*  
Microporous and Mesoporous Materials, (122): 105-113 2009.

Semenov, S. G.; Bedrina, M. E.  
*Highly Symmetrical Phthalocyanines and Perfluorophthalocyanines: The Quantum-Chemical Study*  
Russian Journal of General Chemistry, (79): 1741-1747 2009.

Sen, K.; Hackett, J. C.  
*Molecular Oxygen Activation and Proton Transfer Mechanisms in Lanosterol 14 alpha-Demethylase Catalysis*  
Journal of Physical Chemistry B, (113): 8170-8182 2009.

Serrano-Andres, L.; Avramopoulos, A.; Li, J.; Labeguerie, P.; Begue, D.; Kelloe, V.; Papadopoulos, M. G.  
*Linear and nonlinear optical properties of a series of Ni-dithiolene derivatives*  
Journal of Chemical Physics, (131) 2009.

Shainyan, B. A.; Lazareva, N. F.  
*P=O → Si Intramolecular Coordination in the Derivatives of 1,4-Phosphasilacyclohexane 1-Oxides*  
International Journal of Quantum Chemistry, (109): 301-307 2009.

Sharma, P.; Sharma, S.; Mitra, A.; Singh, H.  
*A Theoretical Study on Interaction of Small Gold Clusters Au-n (n=4, 6, 8) with xDNA Base Pairs*  
Journal of Biomolecular Structure and Dynamics, (27): 65-81 2009.

Sharma, S.; Baligar, R. S.; Singh, H. B.; Butcher, R. J.  
*Reaction of a Metallamacrocycle Leading to a Mercury(II)center dot center dot center dot Palladium(H)center dot center dot center dot Mercury(II) Interaction*  
Angewandte Chemie-International Edition, (48): 1987-1990 2009.

Shin, W. H.; Yang, S. H.; Choi, Y. J.; Jung, H. M.; Song, C. O.; Kang, J. K.  
*Charge polarization-dependent activity of catalyst nanoparticles on carbon nitride nanotubes for hydrogen generation*  
Journal of Materials Chemistry, (19): 4505-4509 2009.

- Shishkin, O. V.; Konovalova, I. S.; Gorb, L.; Leszczynski, J.  
*Novel type of mixed O-H center dot center dot center dot N/O-H center dot center dot center dot pi hydrogen bonds: monohydrate of pyridine*  
Structural Chemistry, (20): 37-41 2009.
- Shum, W. W.; Epstein, A. J.; Miller, J. S.  
*Spin-polarized electronic structure for the layered two-dimensional [Fe-II(TCNE)(NCMe)(2)][(FeCl4)-Cl-III] organic-based magnet*  
Physical Review B, (80) 2009.
- Siebert, W.; Kudinov, A. R.; Zanello, P.; Antipin, M. Y.; Scherban, V. V.; Romanov, A. S.; Muratov, D. V.; Starikova, Z. A.; Corsini, M.  
*Synthesis of mu-Diborolyl Triple-Decker Complexes by Electrophilic Stacking. Similar Bonding Properties of Anions [CpCo(1,3-C3B2H5)](-) and Cp- toward Transition Metals*  
Organometallics, (28): 2707-2715 2009.
- Silva, P. J.; Ramos, M. J.  
*Computational Studies on the Reactivity of Substituted 1,2-Dihydro-1,2-azaborines*  
Journal of Organic Chemistry, (74): 6120-6129 2009.
- Sinitsyn, N. A.  
*The stochastic pump effect and geometric phases in dissipative and stochastic systems*  
Journal of Physics a-Mathematical and Theoretical, (42) 2009.
- Siu, C. K.; Zhao, J. F.; Laskin, J.; Chu, I. K.; Hopkinson, A. C.; Siu, K. W. M.  
*Kinetics for Tautomerizations and Dissociations of Triglycine Radical Cations*  
Journal of the American Society for Mass Spectrometry, (20): 996-1005 2009.
- Sizova, O. V.; Skripnikov, L. V.; Sokolov, A. Y.; Sizov, V. V.  
*Atomic-Orbital-Symmetry Based sigma-, pi-, and delta-Decomposition Analysis of Bond Orders*  
International Journal of Quantum Chemistry, (109): 2581-2590 2009.
- Skinner, J. L.; Auer, B. M.; Lin, Y. S.  
*Vibrational Line Shapes, Spectral Diffusion, and Hydrogen Bonding in Liquid Water*  
Advances in Chemical Physics, Vol 142, (142): 59-103 2009.
- Snehalatha, M.; Joe, I. H.; Ravikumar, C.; Jayakumar, V. S.  
*Azure A chloride: computational and spectroscopic study*  
Journal of Raman Spectroscopy, (40): 176-182 2009.
- Snehalatha, M.; Ravikumar, C.; Joe, I. H.; Jayakumar, V. S.  
*Vibrational spectra and scaled quantum chemical studies of the structure of Martius yellow sodium salt monohydrate*  
Journal of Raman Spectroscopy, (40): 1121-1126 2009.
- Snehalatha, M.; Ravikumar, C.; Joe, I. H.; Sekar, N.; Jayakumar, V. S.  
*Spectroscopic analysis and DFT calculations of a food additive Carmoisine*

Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (72): 654-662 2009.

Soliman, M. E. S.; Pernia, J. J. R.; Greig, I. R.; Williams, I. H.

*Mechanism of glycoside hydrolysis: A comparative QM/MM molecular dynamics analysis for wild type and Y69F mutant retaining xylanases*

Organic & Biomolecular Chemistry, (7): 5236-5244 2009.

Solimannejad, M.; Alkorta, I.; Elguero, J.

*Stabilities and properties of ozone-nitrosyl hydride ( $O_3\text{-HNO}$ ) complexes: A computational study*

Chemical Physics Letters, (474): 253-257 2009.

Solimannejad, M.; Massahi, S.; Alkorta, I.

*A computational study of dimers and trimers of nitrosyl hydride: Blue shift of NH bonds that are involved in H-bond and orthogonal interactions*

Chemical Physics, (362): 1-7 2009.

Solimannejad, M.; Massahi, S.; Scheiner, S.

*Existence and characterization of  $\text{HOO}\text{-HOOOH}$  radical-molecule complexes: A computational study*

Journal of Molecular Structure-Theochem, (913): 50-53 2009.

Sommer, H.; Drebov, N.; Eichhoefer, A.; Ahlrichs, R.; Fenske, D.

*Syntheses, Structures and Theoretical Investigations of  $[\text{Li}(\text{thf})(4)](2)[\text{Ti}_2\text{Cu}_8\text{S}_4(\text{SPh})(10)]$  and  $[\text{Ti}_2\text{Ag}_6\text{S}_6\text{Cl}_2(\text{PPhiPr}(2))(6)]$*

European Journal of Inorganic Chemistry: 4329-4334 2009.

Song, P.; Yan, L. K.; Guan, W.; Feng, J. D.; Liu, C. G.; Su, Z. M.

*The comparative investigation on redox property and second-order nonlinear response of Keggin-type alpha-[ $\text{PM}_{12}\text{O}_{39}\text{NPh}$ ](3-) ( $M = \text{W}$  and  $\text{Mo}$ ) and  $\text{Mo}_6\text{NPh}$*

Chinese Science Bulletin, (54): 203-211 2009.

Soran, A.; Breunig, H. J.; Lippolis, V.; Arca, M.; Silvestru, C.

*Monoorganobismuth(III) dihalides containing the new pincer 2,6-{ $\text{MeN}(\text{CH}_2\text{CH}_2)(2)\text{NCH}_2(2)\text{C}_6\text{H}_3$ } ligand: solution NMR, vibrational and single-crystal X-ray studies*

Dalton Transactions: 77-84 2009.

Soriano, E.; Marco-Contelles, J.

*Mechanistic Analysis of Intramolecular Free Radical Reactions toward Synthesis of 7-Azabicyclo[2.2.1]heptane Derivatives*

Journal of Organic Chemistry, (74): 4061-4067 2009.

Soto-Delgado, J.; Domingo, L. R.; Araya-Maturana, R.; Contreras, R.

*Understanding the stereo- and regioselectivities of the polar Diels-Alder reactions between 2-acetyl-1,4-benzoquinone and methyl substituted 1,3-butadienes: a DFT study*

Journal of Physical Organic Chemistry, (22): 578-584 2009.

Soto-Delgado, J.; Domingo, L. R.; Contreras, R.

*Understanding the influence of Lewis acids in the regioselectivity of the Diels-Alder reactions of 2-methoxy-5-methyl-1,4-benzoquinone: A DFT study*  
Journal of Molecular Structure-Theochem, (902): 103-108 2009.

Srebro, M.; Michalak, A.  
*Theoretical Analysis of Bonding in N-Heterocyclic Carbene-Rhodium Complexes*  
Inorganic Chemistry, (48): 5361-5369 2009.

Srebro, M.; Mitoraj, M.  
*Role of Ancillary Ligands in a Description of Copper(I)-Bis(trimethylsilyl)acetylene bonding. A Theoretical Study*  
Organometallics, (28): 3650-3655 2009.

Srebro, M.; Mitoraj, M.; Michalak, A.  
*Binding of polar monomers in the complexes with organometallic ethylene polymerization catalysts - Natural orbitals for chemical valence and energy decomposition analysis*  
Canadian Journal of Chemistry-Revue Canadienne De Chimie, (87): 1039-1054 2009.

Srinivas, G. N.; Schwartz, M.  
 *$\mu$ - and  $\mu(4)$ -eta(2) coordination of  $A(2)H(2)$  ( $A = C, Si, Ge, Sn$  and  $Pb$ ) ligands with transition metals*  
Inorganica Chimica Acta, (362): 2172-2176 2009.

Stankovic, S.; Markovic, S.; Radenkovic, S.; Gutman, I.  
*Formation and isomerization of dicyclopenta[de,mn] anthracene. Electronic Structure Study*  
Journal of Molecular Modeling, (15): 953-958 2009.

Stare, J.; Henson, N. J.; Eckert, J.  
*Mechanistic Aspects of Propene Epoxidation by Hydrogen Peroxide. Catalytic Role of Water Molecules, External Electric Field, and Zeolite Framework of TS-1*  
Journal of Chemical Information and Modeling, (49): 833-846 2009.

Stefanic, I.; Ljubic, I.; Bonifacic, M.; Sabljic, A.; Asmus, K. D.; Armstrong, D. A.  
*A surprisingly complex aqueous chemistry of the simplest amino acid. A pulse radiolysis and theoretical study on H/D kinetic isotope effects in the reaction of glycine anions with hydroxyl radicals*  
Physical Chemistry Chemical Physics, (11): 2256-2267 2009.

Steglenko, D. V.; Kletsky, M. E.; Kurbatov, S. V.; Minkin, V. I.; Goumont, R.; Terrier, F.  
*A mechanism of addition of a new aromatic electrophile, nitrobenzofuran, to cyclopentadiene*  
Russian Chemical Bulletin, (58): 1602-1608 2009.

Steglenko, D. V.; Kletsky, M. E.; Kurbatov, S. V.; Tatarov, A. V.; Minkin, V. I.; Goumont, R.; Terrier, F.  
*A theoretical and experimental study of the polar Diels-Alder cycloaddition of cyclopentadiene with nitrobenzodifuran*  
Journal of Physical Organic Chemistry, (22): 298-307 2009.

Sternberg, U.; Klipfel, M.; Grage, S. L.; Witter, R.; Ulrich, A. S.

*Calculation of fluorine chemical shift tensors for the interpretation of oriented F-19-NMR spectra of gramicidin A in membranes*  
Physical Chemistry Chemical Physics, (11): 7048-7060 2009.

Steudel, R.; Steudel, Y.  
*Microsolvation of Thiosulfuric Acid and Its Tautomeric Anions [HSSO<sub>3</sub>](-) and [SSO<sub>2</sub>(OH)](-) Studied by B3LYP-PCM and G3X(MP2) Calculations*  
Journal of Physical Chemistry A, (113): 9920-9933 2009.

Steudel, R.; Steudel, Y.  
*Sulfur Dioxide and Water: Structures and Energies of the Hydrated Species SO<sub>2</sub> center dot nH(2)O, [HSO<sub>3</sub>](-)center dot nH(2)O, [SO<sub>3</sub>H](-)center dot nH(2)O, and H<sub>2</sub>SO<sub>3</sub> center dot nH(2)O (n=0-8)*  
European Journal of Inorganic Chemistry: 1393-1405 2009.

Sukumaran, S. M.; Potsaid, B.; Lee, M. Y.; Clark, D. S.; Dordick, J. S.  
*Development of a Fluorescence-Based, Ultra High-Throughput Screening Platform for Nanoliter-Scale Cytochrome P450 Microarrays*  
Journal of Biomolecular Screening, (14): 668-678 2009.

Sumpter, B. G.; Huang, J.; Meunier, V.; Romo-Herrera, J. M.; Cruz-Silva, E.; Terrones, H.; Terrones, M.  
*A Theoretical and Experimental Study On Manipulating the Structure and Properties of Carbon Nanotubes Using Substitutional Dopants*  
International Journal of Quantum Chemistry, (109): 97-118 2009.

Sun, H.; Zhang, D. J.; Liu, C. B.; Zhang, C. Q.  
*Geometrical and electronic structures of the dication and ion pair in the geminal dicationic ionic liquid 1,3-bis[3-methylimidazolium-yl]propane bromide*  
Journal of Molecular Structure-Theochem, (900): 37-43 2009.

Sun, W. J.; Yang, L. M.; Yu, L. Y.; Saeys, M.  
*Ab Initio Reaction Path Analysis for the Initial Hydrogen Abstraction from Organic Acids by Hydroxyl Radicals*  
Journal of Physical Chemistry A, (113): 7852-7860 2009.

Sun, X.-L.; Huang, C.-P.; Zhang, J.  
*Guest-Host Interactions of Tetraethylammonium Cations and Zeolite Framework for Distributions of Al in beta Zeolite: a Density Functional Theory Calculation*  
Chinese Journal of Inorganic Chemistry, (25): 2053-2061 2009.

Sun, Y.; Fournier, R.; Zhang, M.  
*Structural and electronic properties of 13-atom 4d transition-metal clusters*  
Physical Review A, (79) 2009.

Sun, Z.; Li, X.; Tian, M.; Zhao, G.; Li, J.; Ma, B.  
*Comparative study on metal-encapsulated TM@C-24 and TM@C<sub>24</sub>H<sub>12</sub> (TM = Ti, Zr and Hf)*  
Journal of Molecular Structure-Theochem, (913): 265-269 2009.

- Sung, C. Y.; Broadbelt, L. J.; Snurr, R. Q.  
*QM/MM Study of the Effect of Local Environment on Dissociative Adsorption in BaY Zeolites*  
Journal of Physical Chemistry C, (113): 15643-15651 2009.
- Sung, D. D.; Kim, T. J.; Lee, I.  
*Theoretical Studies of the Nucleophilic Substitution of Halides and Amine at a Sulfonyl Center*  
Journal of Physical Chemistry A, (113): 7073-7079 2009.
- Suponitsky, K. Y.; Lyssenko, K. A.; Antipin, M. Y.; Aleksandrova, N. S.; Sheremetev, A. B.; Novikova, T. S.  
*4,4'-Bis(nitramino)azofurazan and its salts. Study of molecular and crystal structure based on X-ray and quantum chemical data*  
Russian Chemical Bulletin, (58): 2129-2136 2009.
- Sutrisno, A.; Lo, A. Y. H.; Tang, J. A.; Dutton, J. L.; Farrar, G. J.; Ragogna, P. J.; Zheng, S.; Autschbach, J.; Schurko, R. W.  
*Experimental and theoretical investigations of selenium nuclear magnetic shielding tensors in Se-N heterocycles*  
Canadian Journal of Chemistry-Revue Canadienne De Chimie, (87): 1546-1564 2009.
- Swaminathan, J.; Ramalingam, M.; Sethuraman, V.; Sundaraganesan, N.; Sebastian, S.  
*Vibrational spectroscopic studies and DFT calculations of 4-aminoantipyrine*  
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (73): 593-600 2009.
- Swanson, J. M. J.; Simons, J.  
*Role of Charge Transfer in the Structure and Dynamics of the Hydrated Proton*  
Journal of Physical Chemistry B, (113): 5149-5161 2009.
- Swinnen, S.; Nguyen, V. S.; Sakai, S.; Nguyen, M. T.  
*Calculations suggest facile hydrogen release from water using boranes and alanes as catalysts*  
Chemical Physics Letters, (472): 175-180 2009.
- Szarek, P.; Urakami, K.; Zhou, C. G.; Cheng, H. S.; Tachibana, A.  
*On reversible bonding of hydrogen molecules on platinum clusters*  
Journal of Chemical Physics, (130) 2009.
- Tahan, A.; Mollaamin, F.; Monajjemi, M.  
*Thermochemistry and NBO Analysis of Peptide Bond: Investigation of Basis Sets and Binding Energy*  
Russian Journal of Physical Chemistry A, (83): 587-597 2009.
- Tanak, H.; Koysal, Y.; Unver, Y.; Yavuz, M.; Isik, S.; Sancak, K.  
*Experimental and DFT studies of ethyl N'-3-(1H-imidazol-1-yl) propylcarbamoyl benzohydrazone monohydrate*  
Structural Chemistry, (20): 409-416 2009.
- Tanaka, M.; Siehl, H. U.; Viefhaus, T.; Frey, W.; Kantlehner, W.  
*An ONIOM Study of a Guanidinium Salt Ionic Liquid. Experimental and Computational Characterization of N,N,N ''N ''N ''-Pentabutyl-N ''-benzylguanidinium Bromide*

Zeitschrift Fur Naturforschung Section B-a Journal of Chemical Sciences, (64): 765-772 2009.

Tang, S. W.; Sun, L. L.; Sun, H.; Feng, J. D.; Wang, R. S.; Chang, Y. F.; Hao, L. Z.

*Search for the most stable Ca@C-44 isomer: Structural stability and electronic property investigations*

Journal of Chemical Physics, (130) 2009.

Tanioku, A.; Hayashi, S.; Nakanishi, W.

*Analysis of One-Bond Se-Se Nuclear Couplings in Diselenides and 1,2-Diselenoles on the Basis of Molecular Orbital Theory: Torsional Angular Dependence, Electron Density Influence, and Origin in (1)J(Se, Se)*

Bioinorganic Chemistry and Applications, 2009.

Tanskanen, J. T.; Linnolahti, M.; Karttunen, A. J.; Pakkanen, T. A.

*Hydrogenated Monolayer Sheets of Group 13-15 Binary Compounds: Structural and Electronic Characteristics*

Journal of Physical Chemistry C, (113): 229-234 2009.

Tapia, O.

*Quantum Linear Superposition Theory for Chemical Processes: A Generalized Electronic Diabatic Approach*

Advances in Quantum Chemistry, Vol 56, (56): 31-93 2009.

Tapia, O.

*Quantum Linear Superposition Theory for Chemical Processes: A Generalized Electronic Diabatic Approach*

Advances in Quantum Chemistry, Vol 56, (56): 31-93 2009.

Taylor, M. S.; Ivanic, S. A.; Wood, G. P. F.; Easton, C. J.; Bacsikay, G. B.; Radom, L.

*Hydrogen Abstraction by Chlorine Atom from Small Organic Molecules Containing Amino Acid Functionalities: An Assessment of Theoretical Procedures*

Journal of Physical Chemistry A, (113): 11817-11832 2009.

Teixeira, F.; Rodriguez-Borges, J. E.; Melo, A.; Cordeiro, M.

*Stereoselectivity of the aza-Diels-Alder reaction between cyclopentadiene and protonated phenylethylimine derived from glyoxylates. A density functional theory study*

Chemical Physics Letters, (477): 60-64 2009.

Tezer, N.; Karakus, N.

*Theoretical study on the ground state intramolecular proton transfer (IPT) and solvation effect in two Schiff bases formed by 2-aminopyridine with 2-hydroxy-1-naphthaldehyde and 2-hydroxy salicylaldehyde*

Journal of Molecular Modeling, (15): 223-232 2009.

Thakur, A. J.; Das, S.; Phukan, A. K.

*Reply of amide type resonance in 6- (dimethylamino)methylene 1,3-dimethylaminouracil: A dynamic NMR and density functional theory study*

Journal of Molecular Structure, (929): 134-140 2009.

- Thom, A. J. W.; Sundstrom, E. J.; Head-Gordon, M.  
*LOBA: a localized orbital bonding analysis to calculate oxidation states, with application to a model water oxidation catalyst*  
Physical Chemistry Chemical Physics, (11): 11297-11304 2009.
- Tiana, D.; Francisco, E.; Blanco, M. A.; Pendas, A. M.  
*Using Pseudopotentials within the Interacting Quantum Atoms Approach*  
Journal of Physical Chemistry A, (113): 7963-7971 2009.
- Tiznado, W.; Ona, O. B.; Caputo, M. C.; Ferraro, M. B.; Fuentealba, P.  
*Theoretical Study of the Structure and Electronic Properties of Si<sub>3</sub>On- and Si<sub>6</sub>On- (n=1-6) Clusters. Fragmentation and Formation Patterns*  
Journal of Chemical Theory and Computation, (5): 2265-2273 2009.
- Tiznado, W.; Perez-Peralta, N.; Islas, R.; Toro-Labbe, A.; Ugalde, J. M.; Merino, G.  
*Designing 3-D Molecular Stars*  
Journal of the American Chemical Society, (131): 9426-9431 2009.
- Tong, J.; Li, Y.; Wu, D.; Li, Z.-R.; Huang, X.-R.  
*Low ionization potentials of binuclear superalkali B<sub>2</sub>Li11*  
Journal of Chemical Physics, (131) 2009.
- Tong, S. R.; Ge, M. F.; Wang, W. G.; Vedova, C. O. D.  
*Experimental and theoretical study of a novel compound: Fluorocarbonylsulfenyl acetate, FC(O)SOC(O)CH<sub>3</sub>*  
Journal of Molecular Structure, (919): 83-88 2009.
- Tran, N. L.; Bohrer, F. I.; Trogler, W. C.; Kummel, A. C.  
*A density functional theory study of the correlation between analyte basicity, ZnPc adsorption strength, and sensor response*  
Journal of Chemical Physics, (130) 2009.
- Trevisanutto, P. E.; Sushko, P. V.; Beck, K. M.; Joly, A. G.; Hess, W. P.; Shluger, A. L.  
*Excitation, Ionization, and Desorption: How Sub-Band Gap Photons Modify the Structure of Oxide Nanoparticles*  
Journal of Physical Chemistry C, (113): 1274-1279 2009.
- Trung, N. T.; Hue, T. T.; Nguyen, M. T.  
*Interaction of CHX<sub>3</sub> (X = F, Cl, Br) with HNO induces remarkable blue shifts of both C-H and N-H bonds*  
Physical Chemistry Chemical Physics, (11): 926-933 2009.
- Trung, N. T.; Hue, T. T.; Nguyen, M. T.  
*Interaction of CHX<sub>3</sub> (X = F, Cl, Br) with HNO induces remarkable blue shifts of both C-H and N-H bonds*  
Physical Chemistry Chemical Physics, (11): 926-933 2009.

- Trzesowska, A.  
*P-Dimethylaminobenzaldehyde semicarbazone: The bonding abilities of imine nitrogen atom*  
Journal of Molecular Structure, (917): 125-132 2009.
- Trzesowska-Kruszynska, A.; Kruszynski, R.  
*2,3-Dihydro-1,3-benzothiazol-2iminium hydrogen oxydiacetate: a combined structural and theoretical study*  
Acta Crystallographica Section C-Crystal Structure Communications, (65): O19-O23 2009.
- Tsai, Y.-C.; Chang, C.-C.  
*Recent Progress in the Chemistry of Quintuple Bonds*  
Chemistry Letters, (38): 1122-1129 2009.
- Tsivion, E.; Gerber, R. B.  
*Lifetimes of compounds made of noble-gas atoms with water*  
Chemical Physics Letters, (482): 30-33 2009.
- Tubert-Brohman, I.; Schmid, M.; Meuwly, M.  
*Molecular Mechanics Force Field for Octahedral Organometallic Compounds with Inclusion of the Trans Influence*  
Journal of Chemical Theory and Computation, (5): 530-539 2009.
- Tukov, A. A.; Normand, A. T.; Nечаев, M. S.  
*N-heterocyclic carbenes bearing two, one and no nitrogen atoms at the ylidene carbon: insight from theoretical calculations*  
Dalton Transactions: 7015-7028 2009.
- Tundo, P.; Arico, F.; Rosamilia, A. E.; Rigo, M.; Maranzana, A.; Tonachini, G.  
*Reaction of dialkyl carbonates with alcohols: Defining a scale of the best leaving and entering groups*  
Pure and Applied Chemistry, (81): 1971-1979 2009.
- Turecek, F.; Holm, A. I. S.; Panja, S.; Nielsen, S. B.; Hvelplund, P.  
*Transition metals as electron traps. II. Structures, energetics and electron transfer dissociations of ternary Co, Ni and Zn-peptide complexes in the gas phase*  
Journal of Mass Spectrometry, (44): 1518-1531 2009.
- Turecek, F.; Jones, J. W.; Holm, A. I. S.; Panja, S.; Nielsen, S. B.; Hvelplund, P.  
*Transition metals as electron traps. I. Structures, energetics, electron capture, and electron-transfer-induced dissociations of ternary copper-peptide complexes in the gas phase*  
Journal of Mass Spectrometry, (44): 707-724 2009.
- Turecek, F.; Panja, S.; Wyer, J. A.; Ehlerding, A.; Zettergren, H.; Nielsen, S. B.; Hvelplund, P.; Bythell, B.; Paizs, B.  
*Carboxyl-Catalyzed Prototropic Rearrangements in Histidine Peptide Radicals upon Electron Transfer: Effects of Peptide Sequence and Conformation*  
Journal of the American Chemical Society, (131): 16472-16487 2009.

Turecek, F.; Yao, C. X.; Fung, Y. M. E.; Hayakawa, S.; Hashimoto, M.; Matsubara, H.  
*Histidine-Containing Radicals in the Gas Phase*  
Journal of Physical Chemistry B, (113): 7347-7366 2009.

Tuttolomondo, M. E.; Navarro, A.; Pena, T.; Fernandez-Liencres, M. P.; Granadino-Roldan, J. M.; Parker, S. F.; Fernandez-Gomez, M.  
*New insight into the structure, internal rotation barrier and vibrational analysis of 2-fluorostyrene*  
Chemical Physics, (361): 94-105 2009.

Tuttolomondo, M. E.; Navarro, A.; Pena, T.; Varetti, E. L.; Parker, S. F.; Ben Altabef, A.  
*Conformational and Vibrational Analysis of Methyl Methanesulfonate, CH<sub>3</sub>SO<sub>2</sub>OCH<sub>3</sub>*  
Journal of Physical Chemistry A, (113): 8401-8408 2009.

Tye, J. W.; Hartwig, J. F.  
*Computational Studies of the Relative Rates for Migratory Insertions of Alkenes into Square-Planar, Methyl, -Amido, and -Hydroxo Complexes of Rhodium*  
Journal of the American Chemical Society, (131): 14703-14712 2009.

Ueno-Noto, K.; Marynick, D. S.  
*A comparative computational study of matrix-peptide interactions in MALDI mass spectrometry: the interaction of four tripeptides with the MALDI matrices 2,5-dihydroxybenzoic acid, alpha-cyano-4-hydroxy-cinnamic acid and 3,5-dihydroxybenzoic acid*  
Molecular Physics, (107): 777-788 2009.

Ugur, I.; De Vleeschouwer, F.; Tuzun, N.; Aviyente, V.; Geerlings, P.; Liu, S. B.; Ayers, P. W.; De Proft, F.  
*Cyclopolymerization Reactions of Diallyl Monomers: Exploring Electronic and Steric Effects Using DFT Reactivity Indices*  
Journal of Physical Chemistry A, (113): 8704-8711 2009.

Ulshofer, R.; Podlech, J.  
*Stereoelectronic Effects in Vinyl Sulfoxides*  
Journal of the American Chemical Society, (131): 16618-+ 2009.

Usharani, D.; Podnska, A.; Nixon, J. F.; Jemmis, E. D.  
*Electronic Structure and Bonding in Neutral and Dianionic Boradiphospholes: R'BC<sub>2</sub>P<sub>2</sub>R<sub>2</sub> (R=H, tBu, R'=H, Ph)*  
Chemistry-a European Journal, (15): 8429-8442 2009.

Uzunova, E. L.  
*Intersystem Crossings of the Triplet and Singlet States in Cobalt and Copper Mononitrosyls*  
Journal of Physical Chemistry A, (113): 11266-11272 2009.

Uzunova, E. L.; Mikosch, H.; Hafner, J.  
*Theoretical study of transition metal cation exchanged zeolites: Interaction with NO*  
Journal of Molecular Structure-Theochem, (912): 88-94 2009.

Van Damme, S.; Bultinck, P.; Fias, S.

*Electrostatic Potentials from Self-Consistent Hirshfeld Atomic Charges*  
Journal of Chemical Theory and Computation, (5): 334-340 2009.

Van Nhien, A. N.; Cordonnier, R.; Le Bas, M.-D.; Delacroix, S.; Soriano, E.; Marco-Contelles, J.; Postel, D.  
*Highly functionalized, enantiomerically pure furo[x,y-c]pyrans via alkylidene carbenes derived from sugar templates: synthesis and mechanism study via computational chemistry*  
Tetrahedron, (65): 9378-9394 2009.

Van Nhien, A. N.; Soriano, E.; Marco-Contelles, J.; Postel, D.  
*The synthesis of polyoxygenated, enantiomerically pure cyclopentane derivatives on route to neplanocin A stereoisomers via alkylidene carbene species prepared from sugar templates*  
Carbohydrate Research, (344): 1605-1611 2009.

Van Regemorter, T.; Larsson, K.  
*Effect of Substitutional N on Important Chemical Vapor Deposition Diamond Growth Steps*  
Journal of Physical Chemistry A, (113): 3274-3284 2009.

Varadwaj, P. R.; Cukrowski, I.; Marques, H. M.  
*DFT RX3LYP and RPBE/PBE studies on the structural, electronic, and vibrational properties of some amino-alcohol ligands*  
Journal of Molecular Structure-Theochem, (915): 20-32 2009.

Varadwaj, P. R.; Cukrowski, I.; Marques, H. M.  
*Low-spin complexes of Ni<sup>2+</sup> with six NH<sub>3</sub> and H<sub>2</sub>O ligands: A DFT-RX3LYP study*  
Journal of Molecular Structure-Theochem, (902): 21-32 2009.

Varga, V.; Cisarova, I.; Gyepes, R.; Horacek, M.; Kubista, J.; Mach, K.  
*Evaluation of the Oxygen pi-Donation in Permethyltitanocene Silanlates and Alcoholates*  
Organometallics, (28): 1748-1757 2009.

Vasconcellos, M.; Lima, C. G.  
*Chlorination of Anisole, Toluene and Nitrobenzene Using Trichloroisocyanuric Acid (Tica): Computational Issues on Reactivity and Regioselectivity*  
Quimica Nova, (32): 244-U265 2009.

Vasilevsky, S. F.; Baranov, D. S.; Mamtyuk, V. I.; Gatilov, Y. V.; Alabugin, I. V.  
*An Unexpected Rearrangement That Disassembles Alkyne Moiety Through Formal Nitrogen Atom Insertion between Two Acetylenic Carbons and Related Cascade Transformations: New Approach to Sampangine Derivatives and Polycyclic Aromatic Amides*  
Journal of Organic Chemistry, (74): 6143-6150 2009.

Vasilevsky, S. F.; Mikhailovskaya, T. y. F.; Mamtyuk, V. I.; Salnikov, G. E.; Bogdanchikov, G. A.; Manoharan, M.; Alabugin, I. V.  
*Tuning Selectivity of Anionic Cyclizations: Competition between 5-Exo and 6-Endo-Dig Closures of Hydrazides of o-Acetylenyl Benzoic Acids and Based-Catalyzed Fragmentation/Recyclization of the Initial 5-Exo-Dig Products*  
Journal of Organic Chemistry, (74): 8106-8117 2009.

- Velez, E.; Quijano, J.; Notario, R.; Pabon, E.; Murillo, J.; Leal, J.; Zapata, E.; Alarcon, G.  
*A computational study of stereospecificity in the thermal elimination reaction of menthyl benzoate in the gas phase*  
Journal of Physical Organic Chemistry, (22): 971-977 2009.
- Velkov, Z. A.; Velkov, Y. Z.; Galunska, B. T.; Paskalev, D. N.; Tadjer, A. V.  
*Melatonin: Quantum-chemical and biochemical investigation of antioxidant activity*  
European Journal of Medicinal Chemistry, (44): 2834-2839 2009.
- Venayagamoorthy, M.; Ford, T. A.  
*Ab initio Molecular Orbital Studies of the Vibrational Spectra of some van der Waals Complexes. Part 4. Complexes of Sulphur Dioxide with Carbon Dioxide, Carbonyl Sulphide, Carbon Disulphide and Nitrous Oxide*  
South African Journal of Chemistry-Suid-Afrikaanse Tydskrif Vir Chemie, (62): 149-U147 2009.
- Venter, G. A.; Dillen, J.  
*A computational study of the effect of an external electric field on the geometry of selected donor-acceptor complexes*  
Journal of Molecular Structure-Theochem, (915): 112-121 2009.
- Verstraelen, T.; Van Speybroeck, V.; Waroquier, M.  
*The electronegativity equalization method and the split charge equilibration applied to organic systems: Parametrization, validation, and comparison*  
Journal of Chemical Physics, (131) 2009.
- Vessecchi, R.; Carollo, C. A.; Lopes, J. N. C.; Crotti, A. E. M.; Lopes, N. P.; Galembeck, S. E.  
*Gas-phase dissociation of 1,4-naphthoquinone derivative anions by electrospray ionization tandem mass spectrometry*  
Journal of Mass Spectrometry, (44): 1224-1233 2009.
- Vijayakumar, T.; Joe, I. H.; Nair, C. P. R.; Jayakumar, V. S.  
*Vibrational spectral studies on charge transfer and ionic hydrogen-bonding interactions of nonlinear optical material L-arginine nitrate hemihydrate*  
Journal of Raman Spectroscopy, (40): 18-30 2009.
- Vijayakumar, T.; Joe, I. H.; Nair, C. P. R.; Jazbinsek, M.; Jayakumar, V. S.  
*Electron-phonon coupling and vibrational modes contributing to linear electro-optic effect of the efficient NLO chromophore 4-N,N-dimethylamino)-N-methyl-4'-toluene sulfonate (DAST) from their vibrational spectra*  
Journal of Raman Spectroscopy, (40): 52-63 2009.
- Villamena, F. A.  
*Superoxide Radical Anion Adduct of 5,5-Dimethyl-1-pyrroline N-Oxide. 5. Thermodynamics and Kinetics of Unimolecular Decomposition*  
Journal of Physical Chemistry A, (113): 6398-6403 2009.
- Viswanathan, R.; Etra, A. M.; Jiang, J.

*Effect of solvent environment on the CO band position in the infrared spectrum of trans-[Fe-II(CN)(4)(CO)(2)](2-)*  
Inorganica Chimica Acta, (362): 2728-2734 2009.

Vitkovskaya, N. M.; Kobychev, V. B.; Larionova, E. Y.; Zaitseva, I. L.; Trofimov, B. A.  
*Theoretical evaluation of some interactions in the system of acetylene-alkali metal hydroxide-DMSO*  
Journal of Structural Chemistry, (50): 18-26 2009.

Vogt-Geisse, S.; Toro-Labbe, A.  
*The mechanism of the interstellar isomerization reaction HOC+ > HCO+ catalyzed by H-2: New Insights from the reaction electronic flux*  
Journal of Chemical Physics, (130) 2009.

Volkov, A.; Koritsanszky, T.; Chodkiewicz, M.; King, H. F.  
*On the Basis-Set Dependence of Local and Integrated Electron Density Properties: Application of a New Computer Program for Quantum-Chemical Density Analysis*  
Journal of Computational Chemistry, (30): 1379-1391 2009.

Wagner, F. R.; Noor, A.; Kempe, R.  
*Ultrashort metal-metal distances and extreme bond orders*  
Nature Chemistry, (1): 529-536 2009.

Wahl, B.; Erbe, M.; Gerisch, A.; Kloo, L.; Ruck, M.  
*Nobel-Metal Centered Polycations [Au@Bi-10](5+) or [Pd@Bi-10](4+) Embedded in Halogenido-Bismuthate(III)-Stannate(II) Frameworks*  
Zeitschrift fur Anorganische und Allgemeine Chemie, (635): 743-752 2009.

Wallasch, M. W.; Vollmer, G. Y.; Kafiyatullina, A.; Wolmershauser, G.; Jones, P. G.; Mang, M.; Meyer, W.; Sitzmann, H.  
*High-spin Cyclopentadienyl Complexes, Part 7. Ambivalent Interpretation of the Bonding in Iron-Copper Complexes: Metalated Arene versus Carbocyclic Carbene*  
Zeitschrift Fur Naturforschung Section B-a Journal of Chemical Sciences, (64): 18-24 2009.

Wallin, G.; Nervall, M.; Carlsson, J.; Aqvist, J.  
*Charges for Large Scale Binding Free Energy Calculations with the Linear Interaction Energy Method*  
Journal of Chemical Theory and Computation, (5): 380-395 2009.

Wan, H.; Wang, X. L.; Guan, G. F.  
*Interaction Between Cation and Anion in Ion-pairs of [EPy] [BF4] and [EPy] [PF6] in Gas and Liquid Phases*  
Chemical Journal of Chinese Universities-Chinese, (30): 1615-1620 2009.

Wang, F.; Meng, Q. X.; Wang, J. M.; Li, M.  
*Density functional computations of alkynylation of nitrones catalyzed by chiral zinc(II)-complexes*  
Structural Chemistry, (20): 129-137 2009.

- Wang, G.-x.; Ma, X.-y.; Wang, J.-p.  
*Anharmonic Vibrational Signatures of DNA Bases and Watson-Crick Base Pairs*  
Chinese Journal of Chemical Physics, (22): 563-570 2009.
- Wang, H.-Q.; Kuang, X.-Y.; Li, H.-F.  
*Structural, Electronic, and Magnetic Properties of Gold Cluster Anions Doped with Zinc: AunZn- (2 <= n <= 10)*  
Journal of Physical Chemistry A, (113): 14022-14028 2009.
- Wang, H. Y.; Zhao, P. S.; Li, R. Q.; Zhou, S. M.  
*Synthesis, Crystal Structure and Quantum Chemical Study on 3-Phenylamino-4-Phenyl-1,2,4-Triazole-5-Thione*  
Molecules, (14): 608-620 2009.
- Wang, H. Y.; Zhao, P. S.; Shao, D. L.; Li, R. Q.; Song, J.; Jian, F. F.  
*Density Functional Calculations on a Double Hydrogen Bonded Dimer of 1-(2-Furylmethylene)-4-phenyl Thiosemicarbazide*  
Asian Journal of Chemistry, (21): 6135-6143 2009.
- Wang, K. D.; Shan, X.; Chen, X. J.  
*Electron propagator theory study of 2-aminoethanol conformers*  
Journal of Molecular Structure-Theochem, (909): 91-95 2009.
- Wang, L.; Liu, Y. C.; Xu, C. S.; Qiu, Y. Q.; Zhao, L.; Rong, X. M.  
*Effect of nitrogenized Si(111) substrates on the quality of ZnO films grown by pulsed laser deposition*  
Journal of Physics D-Applied Physics, (42) 2009.
- Wang, L. F.  
*Halogenation effects of pheniramines on the complexation with beta-cyclodextrin*  
Journal of Pharmaceutical and Biomedical Analysis, (50): 392-396 2009.
- Wang, M. Y.; Cheng, L.; Hong, B.; Wu, Z. J.  
*Reaction Mechanism of Palladium-Catalyzed Silastannation of Allenes by Density Functional Theory*  
Journal of Computational Chemistry, (30): 1521-1531 2009.
- Wang, S. G.; Schwarz, W. H. E.  
*Icon of Chemistry: The Periodic System of Chemical Elements in the New Century*  
Angewandte Chemie-International Edition, (48): 3404-3415 2009.
- Wang, S. P.; Yan, K. M.; Hsu, W. Y.; Huang, M. Y.; Wu, H. Y.  
*The pi-Bonding Trend in VIB M(CO)(6) Observed by NMR Spectroscopy - A Natural Bond Orbital View*  
Journal of the Chinese Chemical Society, (56): 1205-1215 2009.
- Wang, S.-P.; Yan, K.-M.; Hsu, W.-Y.; Huang, M.-Y.; Wu, H.-Y.

*The pi-Bonding Trend in VIB M(CO)(6) Observed by NMR Spectroscopy - A Natural Bond Orbital View*

Journal of the Chinese Chemical Society, (56): 1205-1215 2009.

Wang, W. Z.; Ji, B. M.; Zhang, Y.

*Chalcogen Bond: A Sister Noncovalent Bond to Halogen Bond*

Journal of Physical Chemistry A, (113): 8132-8135 2009.

Wang, X.; Andrews, L.

*Infrared spectra and density functional calculations of triplet pnictinidene N divided by ThF<sub>3</sub>, P divided by ThF<sub>3</sub> and As divided by ThF<sub>3</sub> molecules*

Dalton Transactions: 9260-9265 2009.

Wang, X.; Lyon, J. T.; Andrews, L.

*Formation and Calculations of the Simple Terminal Triplet Pnictinidene Molecules N divided by MF<sub>3</sub>, P divided by MF<sub>3</sub>, and As divided by MF<sub>3</sub> (M = Ti, Zr, Hf)*

Inorganic Chemistry, (48): 6297-6302 2009.

Wang, X. F.; Andrews, L.

*Infrared spectra, structure and bonding in the LiO<sub>2</sub>, LiO<sub>2</sub>Li, LiO and Li<sub>2</sub>O molecules in solid neon*

Molecular Physics, (107): 739-748 2009.

Wang, Y.

*Perfect Planar Tetracoordinate Carbon in Neutral Unsaturated Hydrocarbon Cages: A New Strategy Utilizing Three-Dimensional Electron Delocalization*

Journal of Computational Chemistry, (30): 2122-2126 2009.

Wang, Y.; Hong, L.; Tapriyal, D.; Kim, I. C.; Paik, I.-H.; Crosthwaite, J. M.; Hamilton, A. D.; Thies, M. C.; Beckman, E. J.; Enick, R. M.; Johnson, J. K.

*Design and Evaluation of Nonfluorous CO<sub>2</sub>-Soluble Oligomers and Polymers*

Journal of Physical Chemistry B, (113): 14971-14980 2009.

Wang, Y. C.; Li, H. Z.; Geng, Z. Y.; Zhang, Q. L.; Si, Y. B.; Wang, Q. Y.

*The DFT study on C-H activation of ethene by YNH<sup>+</sup> and YC<sub>2</sub>H<sub>3</sub>N<sup>+</sup> in gas phase*

Chemical Physics, (363): 1-6 2009.

Wang, Y. F.; Li, Z. R.; Wang, F. F.; Sun, C. C.

*The inter-ring sigma/(pi/pi) covalent interactions of cyclodimes of benzenes*

Physical Chemistry Chemical Physics, (11): 455-462 2009.

Wang, Y. F.; Yang, G.; Liu, C. B.

*Electron transfers in proteins: Investigations with a modified through-bond coupling model*

Physical Review E, (80) 2009.

Wang, Y. F.; Yu, Z. Y.; Wu, J.; Liu, C. B.

*Electron Delocalization and Charge Transfer in Polypeptide Chains*

Journal of Physical Chemistry A, (113): 10521-10526 2009.

Wang, Y. L.; Xing, S. Y.; Cao, L.; Wang, S. P.; Zhou, D. H.

*Theoretical Study of the Lewis Acidity of TS-1 Zeolite*

Chinese Journal of Catalysis, (30): 24-30 2009.

Wang, Z.-x.; Zheng, B.-s.; Zhang, J.-c.; Cao, W.-l.

*Theoretical Investigation on Intermolecular Interactions Between HCCF and HCCR(R=F, Cl, Br)*

Chemical Research in Chinese Universities, (25): 929-935 2009.

Wei, X. F.; Zhang, D. J.; Liu, C. B.

*Characterizing the properties of the cation and ion pair for the cyclic tetra methylguanidinium nitrate ionic liquid*

Journal of Molecular Structure-Theochem, (909): 1-5 2009.

Weinberg, J.; Cimpoesu, F.; Lerner, D. A.; Humelnicu, I.

*The association of dehydro-epiandrosterone and adenosine triphosphate acid: A DFT study of interactions between prototypic biologically active molecules*

Journal of Molecular Structure-Theochem, (912): 32-37 2009.

Weitershaus, K.; Fillol, J. L.; Wadeohl, H.; Gade, L. H.

*Reactions of Titanium Hydrazinediido Complexes with Unsaturated Organic Substrates*

Organometallics, (28): 4747-4757 2009.

Werkema, E. L.; Andersen, R. A.; Yahia, A.; Maron, L.; Eisenstein, O.

*Hydrogen for X-Group Exchange in CH<sub>3</sub>X (X = Cl, Br, I, OMe, and NMe<sub>2</sub>) by Monomeric [1,2,4-(Me<sub>3</sub>C)<sub>2</sub>]C<sub>5</sub>H<sub>2</sub>]CeH: Experimental and Computational Support for a Carbenoid Mechanism*

Organometallics, (28): 3173-3185 2009.

Werz, D. B.; Klatt, G.; Raskatov, J. A.; Koeppe, H.; Gleiter, R.

*CpCo-Mediated Reactions of Cyclopropenones: A DFT Study*

Organometallics, (28): 1675-1682 2009.

Wiberg, K. B.; Wang, Y. G.; Petersson, G. A.; Bailey, W. F.

*Intramolecular Nonbonded Attractive Interactions: 1-Substituted Propenes*

Journal of Chemical Theory and Computation, (5): 1033-1037 2009.

Wilke, J. J.; Lind, M. C.; Schaefer, H. F.; Csaszar, A. G.; Allen, W. D.

*Conformers of Gaseous Cysteine*

Journal of Chemical Theory and Computation, (5): 1511-1523 2009.

Wolczanski, P. T.

*Structure and reactivity studies of transition metals ligated by (BuSi<sub>3</sub>X)-Bu-t (X = O, NH, N, S, and CC)*

Chemical Communications: 740-757 2009.

Wolczanski, P. T.

*Structure and reactivity studies of transition metals ligated by (BuSi<sub>3</sub>X)-Bu-t (X = O, NH, N, S, and CC)*

Chemical Communications: 740-757 2009.

- Wong, B. M.  
*Noncovalent Interactions in Supramolecular Complexes: A Study on Corannulene and the Double Concave Buckycatcher*  
Journal of Computational Chemistry, (30): 51-56 2009.
- Wong, K. Y.; Richard, J. P.; Gao, J. L.  
*Theoretical Analysis of Kinetic Isotope Effects on Proton Transfer Reactions between Substituted alpha-Methoxystyrenes and Substituted Acetic Acids*  
Journal of the American Chemical Society, (131): 13963-13971 2009.
- Woon, D. E.; Dunning, T. H.  
*A comparison between polar covalent bonding and hypervalent recoupled pair bonding in diatomic chalcogen halide species {O,S,Se} x {F,Cl,Br}*  
Molecular Physics, (107): 991-998 2009.
- Woon, D. E.; Dunning, T. H.  
*Theory of Hypervalency: Recoupled Pair Bonding in SF<sub>n</sub> (n=1-6)*  
Journal of Physical Chemistry A, (113): 7915-7926 2009.
- Wu, J. Y.; Yan, H.; Jin, Y. X.; Chen, H.; Dai, G. L.; Zhong, A. G.; Pan, F. Y.  
*Study on the nature of interaction of thiophene with various hydrides*  
Journal of Molecular Structure-Theochem, (911): 132-136 2009.
- Wu, Q. Y.; Tang, Y. P.; Zhang, X. H.  
*Boron rings containing planar octacoordinate iron and cobalt*  
Science in China Series B-Chemistry, (52): 288-294 2009.
- Wu, W.; Ma, B.; Wu, J. I. C.; Schleyer, P. V.; Mo, Y. R.  
*Is Cyclopropane Really the sigma-Aromatic Paradigm?*  
Chemistry-a European Journal, (15): 9730-9736 2009.
- Wu, X. P.; Sun, X. M.; Wei, X. G.; Ren, Y.; Wong, N. B.; Li, W. K.  
*Exploring the Reactivity Trends in the E2 and S(N)2 Reactions of X- + CH<sub>3</sub>CH<sub>2</sub>Cl (X = F, Cl, Br, HO, HS, HSe, NH<sub>2</sub>PH<sub>2</sub>, AsH<sub>2</sub>, CH<sub>3</sub>, SiH<sub>3</sub>, and GeH<sub>3</sub>)*  
Journal of Chemical Theory and Computation, (5): 1597-1606 2009.
- Wu, Y.; Sa, R. J.; Li, Q. H.; Wei, Y. Q.; Wu, K. C.  
*Theoretical studies on the bonding of Cd<sup>2+</sup> to adenine and thymine: Tautomeric equilibrium and metalation in base pairing*  
Chemical Physics Letters, (467): 387-392 2009.
- Wu, Y.; Zhang, T.  
*Structural and Electronic Properties of Amino Acid Based Ionic Liquids: A Theoretical Study*  
Journal of Physical Chemistry A, (113): 12995-13003 2009.
- Wu, Y.; Zhang, T. T.; Li, J. R.

*A Theoretical Investigation of Interaction between 1-Ethyl-3-methyl-imidazolium Cation and Cysteine Anion*  
Acta Chimica Sinica, (67): 1851-1858 2009.

Wu, Y.; Zhang, T. T.; Yu, N.  
*Interaction between 1-Ethyl-3-Methyl-Imidazolium Cation and Asparagine Anion*  
Acta Physico-Chimica Sinica, (25): 1689-1696 2009.

Wu, Y. B.; Lu, H. G.; Li, S. D.; Wang, Z. X.  
*Simplest Neutral Singlet C2E4 (E = Al, Ga, In, and Tl) Global Minima with Double Planar Tetracoordinate Carbons: Equivalence of C-2 Moieties in C2E4 to Carbon Centers in CAI42- and CAI5+*  
Journal of Physical Chemistry A, (113): 3395-3402 2009.

Wu, Y. H.; Zhou, X.; Zhang, H. X.  
*Theoretical Studies on the Electron Structures and Spectroscopic Properties of Diimine Os(II) Complexes [Os(L)(2)(CN)(2)(phen)] (L=PH3, DMSO; phen=1,10-phenanthroline) and [Os(PH3)(2)(phen)Br-2]*  
Acta Chimica Sinica, (67): 197-202 2009.

Wu, Y. J.; Ren, F. D.; Li, B. C.  
*A B3LYP and MP2 theoretical investigation on unusual cation-pi interaction between the singlet state HB=BH ((1)Delta(g)) and H+, Li+, Na+, Be2+ or Mg2+*  
Journal of Molecular Structure-Theochem, (909): 79-85 2009.

Xia, F.-F.; Yi, H.-B.; Zeng, D.  
*Hydrates of Copper Dichloride in Aqueous Solution: A Density Functional Theory and Polarized Continuum Model Investigation*  
Journal of Physical Chemistry A, (113): 14029-14038 2009.

Xia, F. T.; Zhu, H.; Xue, Y.; Guo, Y.; Xie, D. Q.  
*Theoretical Study on Reaction Pathways for Methanolysis of 3-Methyl Cyclic Ethylene Phosphate*  
Acta Chimica Sinica, (67): 937-944 2009.

Xia, S.-W.; Ma, X.-N.; Yu, L.-M.; Pan, G.  
*DFT Study of the Electronic Structure in As(V), Zn(II)/TiO2 System*  
Chemical Journal of Chinese Universities-Chinese, (30): 83-88 2009.

Xiao, D. Q.; Skourtis, S. S.; Rubtsov, I. V.; Beratan, D. N.  
*Turning Charge Transfer On and Off in a Molecular Interferometer with Vibronic Pathways*  
Nano Letters, (9): 1818-1823 2009.

Xiao, W.; Xia, Q. Q.; Zhang, Y. F.; Ning, L. X.; Cui, Z. F.  
*Density Functional Study on Structures and Relative Stability of Gd(H2O)(n)(3+) (n=8,9)*  
Chinese Journal of Chemical Physics, (22): 395-400 2009.

Xie, M. X.; Xu, X.

*Theoretical Studies on the Fe-Hg Interactions and the P-31 NMR in [Fe(CO)(x)(Ph(2)Ppy)(y)(HgCl2)(z)] (x=3, 4; y=1, 2; z=0, 1, 2)*  
Chemical Journal of Chinese Universities-Chinese, (30): 1861-1864 2009.

Xie, X. H.; Shen, W.; He, R. X.; Zhang, J. S.; Li, M.  
*Theoretical Studies on the Reaction Mechanisms of C3H2 (cyclopropenylidene) and O((3)p) Radicals*  
Chinese Journal of Chemistry, (27): 49-55 2009.

Xing, L. D.; Wang, C. Y.; Xu, M. Q.; Li, W. S.; Cai, Z. P.  
*Theoretical study on reduction mechanism of 1,3-benzodioxol-2-one for the formation of solid electrolyte interface on anode of lithium ion battery*  
Journal of Power Sources, (189): 689-692 2009.

Xu, H. L.; Li, Z. R.; Wu, D.; Ma, F.; Li, Z. J.  
*Lithiation and Li-Doped Effects of [5]Cyclacene on the Static First Hyperpolarizability*  
Journal of Physical Chemistry C, (113): 4984-4986 2009.

Xu, S. H.; Cui, Y. P.; Wang, C. L.  
*New insight into the stability and property of linear carbon clusters*  
Journal of Molecular Structure-Theochem, (895): 30-33 2009.

Xu, W.; Zhang, Y.; Zhai, L.  
*Structures and aromaticity of the planar Al2P2 (n-) (n=1-4) clusters*  
Science in China Series B-Chemistry, (52): 2237-2242 2009.

Xu, W. G.; Zhang, R. C.; Chang, H. Y.  
*Structures and Aromaticity of Planar XY(2)Z (X = Li, K, Y = P, As and Z = C, Si, Ge) Clusters*  
Chinese Journal of Structural Chemistry, (28): 1067-1076 2009.

Xu, W. G.; Zhang, R. C.; Chang, H. Y.; Lu, S. X.; Zhang, Y. C.  
*Structures and Aromaticity of Three-membered BeXP (X = C, Si, Ge) and CYP (Y = O, S, Se) Rings*  
Chinese Journal of Structural Chemistry, (28): 427-433 2009.

Xu, W. G.; Zhang, Y. C.; Lu, S. X.; Zhang, R. C.  
*Geometries, stability and aromaticity of Al2P22-, [M(Al2P2)](-) (M = Li, Na, K, Cu) and N(Al2P2) (N = Be, Mg, Ca, Zn) clusters*  
Journal of Molecular Structure-Theochem, (900): 44-49 2009.

Xu, W. G.; Zhang, Y. C.; Lu, S. X.; Zhang, R. C.  
*Structures and aromaticity of X2Y (2) (-) (X = C, Si, Ge and Y = N, P, As) anions*  
Journal of Molecular Modeling, (15): 1329-1336 2009.

Xu, W. G.; Zhang, Y. C.; Xi, Q.  
*Structures and aromaticity of the C2N2- anion, M(C2N2) (M = Li, Na, K) and [N(C2N2)](+) (N = Be, Mg, Ca) clusters*  
Journal of Molecular Structure-Theochem, (909): 129-136 2009.

Xu, Z.; Jin, J.; Li, Z. F.; Qiu, H. Y.; Jiang, J. X.; Lai, G. Q.; Kira, M.  
*Remarkable Substituent Effects on the Activation Energy of Silylene Insertion into Silicon-Chlorine Bonds*  
Chemistry-a European Journal, (15): 8605-8612 2009.

Yahia, A.; Maron, L.  
*Is Thorium a d Transition Metal or an Actinide? An Answer from a DFT Study of the Reaction between Pyridine N-Oxide and Cp2M(CH<sub>3</sub>)<sub>2</sub> with M = Zr, Th, and U*  
Organometallics, (28): 672-679 2009.

Yamagata, M.; Konno, S.; Matsumoto, K.; Hagiwara, R.  
*Room-Temperature Fluorohydrogenate Ionic Liquids of Alkylpyridinium Cations and Allylated Quaternary Cyclic Ammonium Cations*  
Electrochemical and Solid State Letters, (12): F9-F12 2009.

Yan, D.; Lu, J.; Wei, M.; Ma, J.; Evans, D. G.; Duan, X.  
*A combined study based on experiment and molecular dynamics: perylene tetracarboxylate intercalated in a layered double hydroxide matrix*  
Physical Chemistry Chemical Physics, (11): 9200-9209 2009.

Yan, H.; Wei, M.; Ma, J.; Li, F.; Evans, D. G.; Duan, X.  
*Theoretical Study on the Structural Properties and Relative Stability of M(II)-Al Layered Double Hydroxides Based on a Cluster Model*  
Journal of Physical Chemistry A, (113): 6133-6141 2009.

Yan, S. H.; Lee, J. Y.  
*Excess Electrons in LiAlH<sub>4</sub> Clusters: Implication for Hydrogen Storage*  
Journal of Physical Chemistry C, (113): 1104-1108 2009.

Yan, X.; Jiang, N.; Ma, J.  
*Theoretical study of interactions between human adult hemoglobin and acetate ion by polarizable force field and fragmentation quantum chemistry methods*  
Science in China Series B-Chemistry, (52): 1925-1931 2009.

Yanez, M.; Sanz, P.; Mo, O.; Alkorta, I.; Elguero, J.  
*Beryllium Bonds, Do They Exist?*  
Journal of Chemical Theory and Computation, (5): 2763-2771 2009.

Yang, B. Z.; Zhou, X.; Liu, T.; Bai, F. Q.; Zhang, H. X.  
*Theoretical Studies on Structures and Spectroscopic Properties of Cyclometalated Gold(III) Complexes*  
Journal of Physical Chemistry A, (113): 9396-9403 2009.

Yang, G.; Zhou, L. J.; Zu, Y. G.; Fu, Y. J.; Zhu, R. X.; Liu, C. B.  
*Effects of side chains in gas-phase amino acids: Conformational analysis and relative stabilities*  
Journal of Molecular Structure-Theochem, (901): 81-87 2009.

Yang, H. Q.; Qin, S.; Hu, C. W.

*Theoretical Study on the Gas-Phase Reaction Mechanism Between Nickel Monoxide and Methane for Syngas Production*  
Journal of Computational Chemistry, (30): 847-863 2009.

Yang, L.-Z.; Li, Y.; Zhuang, X.-M.; Jiang, L.; Chen, J.-M.; Luck, R. L.; Lu, T.-B.  
*Mechanistic Studies of C-C Bond Cleavage of Nitriles by Dinuclear Metal Cryptates*  
Chemistry-a European Journal, (15): 12399-12407 2009.

Yang, W. Y.; Breiner, B.; Kovalenko, S. V.; Ben, C.; Singh, M.; LeGrand, S. N.; Sang, Q. X. A.; Strouse, G. F.; Copland, J. A.; Alabugin, I. V.  
*C-Lysine Conjugates: pH-Controlled Light-Activated Reagents for Efficient Double-Stranded DNA Cleavage with Implications for Cancer Therapy*  
Journal of the American Chemical Society, (131): 11458-11470 2009.

Yang, Y.  
*Theoretical Study of the S-H center dot center dot center dot O Blue-Shifted Hydrogen Bond*  
International Journal of Quantum Chemistry, (109): 266-274 2009.

Yang, Y.; Cui, Q.  
*The Hydrolysis Activity of Adenosine Triphosphate in Myosin: A Theoretical Analysis of Anomeric Effects and the Nature of the Transition State*  
Journal of Physical Chemistry A, (113): 12439-12446 2009.

Yang, Y.; Cui, Q.  
*The Hydrolysis Activity of Adenosine Triphosphate in Myosin: A Theoretical Analysis of Anomeric Effects and the Nature of the Transition State*  
Journal of Physical Chemistry A, (113): 12439-12446 2009.

Yang, Y.; Zhang, W. J.  
*Theoretical Study on Blue-shifted Hydrogen Bonds in CH<sub>3</sub>CHO Dimers*  
Acta Chimica Sinica, (67): 599-606 2009.

Yang, Z.; Xiong, S.-J.  
*Structural, electronic and magnetic properties of small yttrium trioxide clusters from density functional calculations*  
Journal of Physics B-Atomic Molecular and Optical Physics, (42) 2009.

Yaziji, V.; Coelho, A.; El Maatougui, A.; Brea, J.; Loza, M. I.; Garcia-Mera, X.; Sotelo, E.  
*Divergent Solution-Phase Synthesis of Diarylpyrimidine Libraries as Selective A(3) Adenosine Receptor Antagonists*  
Journal of Combinatorial Chemistry, (11): 519-522 2009.

Yeung, C. S.; Tian, W. Q.; Liu, L. V.; Wang, Y. A.  
*Chemistry of Single-Walled Carbon Nanotubes*  
Journal of Computational and Theoretical Nanoscience, (6): 1213-1235 2009.

Yin, J.; Wei, P.; Li, Q.; Liu, Z.; Li, W.; Cheng, J.; Gong, B.  
*Theoretical study of lithium bond between XMgH (X = H, F, CH<sub>3</sub>) and LiCY<sub>3</sub> (Y = H, F)*

Journal of Molecular Structure-Theochem, (916): 28-32 2009.

Yin, J. H.; Zhou, Z. Y.; Wang, L. Y.; Wu, X.

*Theoretical Research on Intermolecular Interaction between 2,2'-Dimethyl-4,4'-bithiazole and Chloroform*

Acta Chimica Sinica, (67): 923-928 2009.

Yoshikai, N.; Zhang, S. L.; Yamagata, K.; Tsuji, H.; Nakamura, E.

*Mechanistic Study of the Manganese-Catalyzed [2+2+2] Annulation of 1,3-Dicarbonyl Compounds and Terminal Alkynes*

Journal of the American Chemical Society, (131): 4099-4109 2009.

Yu, H. L.

*Structures and aromaticities of doped P4Mq (M = S, Se, q=0; M = Si, Ge, q=2-) species from theoretical study*

Journal of Molecular Structure-Theochem, (906): 25-30 2009.

Yu, H. L.; Sang, R. L.; Wu, Y. Y.

*Structure and Aromaticity of B6H5<sup>+</sup> Cation: A Novel Borhydride System Containing Planar Pentacoordinated Boron*

Journal of Physical Chemistry A, (113): 3382-3386 2009.

Yu, H. Z.; Fu, Y.; Guo, Q. X.; Lin, Z. Y.

*DFT Studies on Reactions of Transition Metal Complexes with O-2 Organometallics*, (28): 4443-4451 2009.

Yuan, K.; Liu, Y. Z.; Lue, L. L.; Zhu, Y. C.; Zhang, J.; Junyan, Y.

*pi Type Lithium Bond Interaction between Ethylene, Acetylene, or Benzene and Amido-lithium*

Chinese Journal of Chemistry, (27): 697-702 2009.

Yuan, K.; Liu, Y. Z.; Ma, W. C.; Tang, H. A.; Zhu, Y. C.; Zhang, J.

*Theoretical Study on Structures and Properties of N2O center dot center dot center dot HOCl Complexes*

Chinese Journal of Chemistry, (27): 900-906 2009.

Yuan, K.; Liu, Y. Z.; Zhu, Y. C.; Zhang, J.; Zhang, J. Y.

*Structures and Properties of Halogen Bond and Hydrogen Bond Formed between CH3SH and HOCl*

Acta Chimica Sinica, (67): 499-506 2009.

Yun, S. Y.; Catak, S.; Lee, W. K.; D'Hooghe, M.; De Kimpe, N.; Van Speybroeck, V.; Waroquier, M.; Kim, Y.; Ha, H. J.

*Nucleophile-dependent regioselective ring opening of 2-substituted N,N-dibenzylaziridinium ions: bromide versus hydride*

Chemical Communications: 2508-2510 2009.

Zade, S. S.; Zamoshchik, N.; Bendikov, M.

*Oligo- and Polyselenophenes: A Theoretical Study*

Chemistry-a European Journal, (15): 8613-8624 2009.

Zahedi, E.; Aghaie, M.; Zare, K.

*A density functional study of NBO, NICS and N-14 NQR parameters of 5-methylcytosine tautomers in the gas phase*

Journal of Molecular Structure-Theochem, (905): 101-105 2009.

Zahn, S.; Reckien, W.; Kirchner, B.; Staats, H.; Matthey, J.; Lutzen, A.

*Towards Allosteric Receptors: Adjustment of the Rotation Barrier of 2,2'-Bipyridine Derivatives*

Chemistry-a European Journal, (15): 2572-2580 2009.

Zaitsev, A. B.; Caldwell, H. F.; Pregosin, P. S.; Veiros, L. E.

*Fast Ruthenium-Catalysed Allylation of Thiols by Using Allyl Alcohols as Substrates*

Chemistry-a European Journal, (15): 6468-6477 2009.

Zanti, G.; Peeters, D.

*DFT Study of Small Palladium Clusters Pd-n and Their Interaction with a CO Ligand (n=1-9)*

European Journal of Inorganic Chemistry: 3904-3911 2009.

Zapata, F.; Caballero, A.; Espinosa, A.; Tarraga, A.; Molina, P.

*A Selective Redox and Chromogenic Probe for Hg(II) in Aqueous Environment Based on a Ferrocene-Azaquinoxaline Dyad*

Inorganic Chemistry, (48): 11566-11575 2009.

Zarate, X.; Daza, M. C.; Villaveces, J. L.

*Hydrogen bonds C-H center dot center dot center dot O in superoxide anion radical-1,4-Pentadiene complexes*

Journal of Molecular Structure-Theochem, (893): 77-83 2009.

Zeng, X. Q.; Beckers, H.; Willner, H.

*Difluoro-lambda(5)-Phosphinonitrile F2P N: Matrix Isolation and Photoisomerization into FP = NF*

Angewandte Chemie-International Edition, (48): 4828-4831 2009.

Zhang, C. R.; Wu, Y. Z.; Chen, Y. H.; Ding, Y. T.; Zhang, D. J.; Chen, H. S.

*Geometry, Electronic Structure, and Related Properties of Dye Sensitizer: 3,4-bis[1-(carboxymethyl)-3-indolyl]-1H-pyrrole-2,5-dione*

Chinese Journal of Chemical Physics, (22): 63-68 2009.

Zhang, C.-r.; Liu, Z.-j.; Chen, Y.-h.; Ma, J.; Chen, H.-s.; Zhang, M.-l.

*Density Functional Theory Study on Organic Dye Sensitizers Containing Bis-dimethylfluorenyl Amino Benzofuran*

Chinese Journal of Chemical Physics, (22): 489-496 2009.

Zhang, H.; Fu, X.; Chen, J.; Wang, E.; Liu, Y.; Li, Y.

*Generation of Allenic/Propargylic Zirconium Complexes and Subsequent Cross-Coupling Reactions: A Facile Synthesis of Multisubstituted Allenes*

Journal of Organic Chemistry, (74): 9351-9358 2009.

- Zhang, H.; Li, J.; Liu, F.-L.  
*DFT Study on a Heterofullerene C<sub>58</sub>Sn with Odd Number of Atoms*  
Chinese Journal of Structural Chemistry, (28): 1296-1303 2009.
- Zhang, J.; Cui, M. Z.; Feng, S. Y.; Sun, X. M.; Feng, D. C.  
*Catalytic and Thermal 1,2-Rearrangement of (alpha-Mercaptobenzyl)trimethylsilane*  
Journal of Physical Chemistry A, (113): 11007-11014 2009.
- Zhang, J. G.; Zheng, H. H.; Zhang, T. L.; Wu, M.  
*Theoretical Study for High-Energy-Density Compounds Derived from Cyclophosphazene. IV. DFT Studies on 1,1-Diamino-3,3,5,5,7,7-hexaaazidocyclotetraphosphazene and Its Isomers*  
International Journal of Molecular Sciences, (10): 3502-3516 2009.
- Zhang, J. S.; Shen, W.; Li, L. Q.; Li, M.  
*Gold(I)-Catalyzed Cycloaddition of 1-(1-Alkynyl)cyclopropyl Ketones with Nucleophiles To Yield Substituted Furans: A DFT Study*  
Organometallics, (28): 3129-3139 2009.
- Zhang, J. S.; Shen, W.; Liu, R. Q.; Yu, Y. Q.; Wu, H. L.; Li, M.  
*DFT Study on Ru-II-Catalyzed Cyclization of Terminal Alkynals to Cycloalkenes*  
International Journal of Quantum Chemistry, (109): 679-687 2009.
- Zhang, L.; Xiao, Q.; Ma, C.; Xie, X. Q.; Floreancig, P. E.  
*Construction of a Bicyclic beta-Benzoyloxy and beta-Hydroxy Amide Library through a Multicomponent Cyclization Reaction*  
Journal of Combinatorial Chemistry, (11): 640-644 2009.
- Zhang, Q.; Yue, S. P.; Lu, X.; Chen, Z. F.; Huang, R. B.; Zheng, L. S.; Schleyer, P. V.  
*Homoconjugation/Homoaromaticity in Main Group Inorganic Molecules*  
Journal of the American Chemical Society, (131): 9789-9799 2009.
- Zhang, X.; Geng, Z. Y.; Wang, Y. C.; Li, W. Q.; Wang, Z.; Liu, F. X.  
*A theoretical study nickel-catalyzed cyclopropanation reactions. Nickel(0) versus nickel(II)*  
Journal of Molecular Structure-Theochem, (893): 56-66 2009.
- Zhang, X.; Schwarz, H.  
*A DFT-Based Analysis of the Grossly Varying Reactivity Pattern in Room-Temperature Activation and Dehydrogenation of CH<sub>4</sub> by Main-Group Atomic M<sup>+</sup> (M = Ga, Ge, As, and Se)*  
Chemistry-a European Journal, (15): 11559-11565 2009.
- Zhang, X.; Zummack, W.; Schroeder, D.; Weinhold, F. A.; Schwarz, H.  
*Isotope-Sensitive Degenerate [1,3]-Hydrogen Migration versus Competitive Enol-Keto Tautomerization*  
Chemistry-a European Journal, (15): 11815-11819 2009.
- Zhang, X. H.; Li, S.; Li, Q. S.  
*Characterizations of novel binuclear alkaline-earth metallocenes: M-2(eta(5)-E-5)(2) (M = Be, Mg and Ca; E = P and As)*

Molecular Physics, (107): 855-861 2009.

Zhang, Y.; Peng, S.; Li, X. J.; Zhang, D. X.

*The structure, electronic property and infrared spectroscopy of the endohedral fullerene SnH<sub>4</sub>@C-60*

Journal of Molecular Structure-Theochem, (906): 41-45 2009.

Zhang, Y.; Wang, W.

*The bifurcate chalcogen bond: Some theoretical observations*

Journal of Molecular Structure-Theochem, (916): 135-138 2009.

Zhang, Z.; Chen, S. H.; Feng, Y. Y.; Ding, Y. Q.; Zhou, J. J.; Jia, H. L.

*Electrochemical and molecular simulation studies on the corrosion inhibition of L-glutamine monolayers on an iron surface*

Journal of the Serbian Chemical Society, (74): 407-415 2009.

Zhao, J.; Khalizov, A.; Zhang, R. Y.; McGraw, R.

*Hydrogen-Bonding Interaction in Molecular Complexes and Clusters of Aerosol Nucleation Precursors*

Journal of Physical Chemistry A, (113): 680-689 2009.

Zhao, J. F.; Ng, C. M. D.; Chu, I. K.; Siu, K. W. M.; Hopkinson, A. C.

*Methionine, alpha-methylmethionine and S-methylcysteine radical cations: generations and dissociations in the gas phase*

Physical Chemistry Chemical Physics, (11): 7629-7639 2009.

Zhao, L. M.; Liu, Z. C.; Guo, W. Y.; Zhang, L. Z.; Zhang, F. Y.; Zhu, H. Y.; Shan, H. H.

*Theoretical investigation of the gas-phase Mn<sup>+</sup>- and Co<sup>+</sup>-catalyzed oxidation of benzene by N2O*

Physical Chemistry Chemical Physics, (11): 4219-4229 2009.

Zhao, L. X.; Cao, T. T.; Feng, X. J.; Xiao, L.; Lei, Y. M.; Luo, Y. H.

*A theoretical study of neutral and anionic Au<sub>5</sub>Al clusters*

Journal of Molecular Structure-Theochem, (895): 92-95 2009.

Zhao, L. X.; Feng, X. J.; Cao, T. T.; Liang, X.; Luo, Y. H.

*Density functional study of Al-doped Au clusters*

Chinese Physics B, (18): 2709-2718 2009.

Zhao, P. S.; Shangguan, R. C.; Wang, H. Y.; Qing, Y. Q.; Jian, F. F.

*Synthesis, characterization, crystal structure and ab initio studies on 5-ethoxycarbonyl-6-methyl-4-phenyl-2-thioxo-1,2,3,4-tetrahydropyrimidine*

Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (72): 61-67 2009.

Zhao, S.; Ren, Y. L.; Wang, J. J.; Yin, W. P.

*A Density Functional Study of the Interaction of NCO with Small Copper Clusters*

Journal of Physical Chemistry A, (113): 1075-1085 2009.

Zhou, H. W.; Zhang, Z. Q.; Cheung, H. Y.

*Theoretical Study on the Reactive Sites and Intramolecular Interactions in Taxol and Its Four Analogues*  
International Journal of Quantum Chemistry, (109): 362-372 2009.

Zhou, P.; Zou, J.; Tian, F.; Shang, Z.  
*Fluorine Bonding - How Does It Work In Protein-Ligand Interactions?*  
Journal of Chemical Information and Modeling, (49): 2344-2355 2009.

Zhou, P. P.; Qiu, W. Y.  
*Red- and Blue-Shifted Hydrogen Bonds in the Cis-Trans Noncyclic Formic Acid Dimer*  
Chemphyschem, (10): 1847-1858 2009.

Zhou, P. P.; Qiu, W. Y.  
*Red-Shifted Hydrogen Bonds and Blue-Shifted van der Waals Contact in the Standard Watson-Crick Adenine-Thymine Base Pair*  
Journal of Physical Chemistry A, (113): 10306-10320 2009.

Zhou, Z. J.; Liu, H. L.; Yu, J. K.; Yu, G. T.; Huang, X. R.  
*Bonding and Correlation Analysis of Various Si<sub>2</sub>CO Isomers on the Potential Energy Surface*  
International Journal of Quantum Chemistry, (109): 907-919 2009.

Zhu, R. X.; Wang, R. X.; Zhang, D. J.; Liu, C. B.  
*A Density Functional Theory Study on the Ring-Opening Polymerization of D-Lactide Catalyzed by a Bifunctional-Thiourea Catalyst*  
Australian Journal of Chemistry, (62): 157-164 2009.

Zhu, Y. L.; Zhou, S. Y.; Kan, Y. H.; Su, Z. M.  
*Theoretical investigation of electronic structures and excitation energies of hexaphyrin and its group 11 transition metal (III) complexes*  
Journal of Organometallic Chemistry, (694): 3012-3018 2009.

Zhu, Y. Y.; Chen, Z. F.; Guo, Z. J.; Wang, Y.; Chen, G. J.  
*Systematic characterization on electronic structures and spectra for a series of complexes, M(IDB)Cl-2 (M = Mn, Fe, Co, Ni, Cu and Zn): a theoretical study*  
Journal of Molecular Modeling, (15): 469-479 2009.

Zierkiewicz, W.; Michalska, D.; Zeegers-Huyskens, T.  
*Theoretical study of the interaction of a proton with the O, F and Cl atoms of enflurane (CHFCI-CF<sub>2</sub>-O-CHF<sub>2</sub>)*  
Journal of Molecular Structure-Theochem, (911): 58-64 2009.

Zimmermann, T.; Burda, J. V.  
*Charge-scaled cavities in polarizable continuum model: Determination of acid dissociation constants for platinum-amino acid complexes*  
Journal of Chemical Physics, (131) 2009.

Zottola, M. A.

*A partial exploration of the potential energy surfaces of SCN and HSCN: Implications for the enzyme-mediated detoxification of cyanide*  
Journal of Molecular Graphics and Modelling, (28): 183-186 2009.

Zou, P.; Li, Q.; Xue, Y.; Yan, G.

*Effects of Substituent and Temperature on the Gas-phase Pyrolysis of 4-Arylideneimino-1,2,4-triazol-3(2H)-ones: a DFT Investigation*  
Acta Chimica Sinica, (67): 2427-2432 2009.