

NBO 2008 (Jan-Dec) - 910 references
Compiled by Emily Wixson; Updated by Ariel Neff 4/16/13

- Adalsteinsson, H.; Debusschere, B. J.; Long, K. R.; Najm, H. N.
Components for atomistic-to-continuum multiscale modeling of flow in micro- and nanofluidic systems
Scientific Programming, (16): 297-313 2008.
- Adcock, W.; Trout, N. A.
Diastereofacial selectivity in some 4-substituted (X) 2-adamantyl derivatives: electronic versus steric effects
Journal of Physical Organic Chemistry, (21): 68-72 2008.
- Agapito, F.; Nunes, P. A.; Costa Cabral, B. J.; Borges dos Santos, R. A.; Martinho Simoes, J. A.
Energetic differences between the five- and six-membered ring hydrocarbons: Strain energies in the parent and radical molecules
Journal of Organic Chemistry, (73): 6213-6223 2008.
- Aguilar-Castro, L.; Tlahuextl, M.; Mendoza-Huizar, L. H.; Tapia-Benavides, A. R.; Tlahuext, H.
Hydrogen bond studies in substituted N-(2-hydroxyphenyl)-2-[(4-methylbenzenesulfonyl)amino]acetamides
Arkivoc: 210-226 2008.
- Alajarin, M.; Cabrera, J.; Pastor, A.; Sanchez-Andrada, P.; Bautista, D.
Polar hetero-Diels-alder reactions of 4-alkenylthiazoles with 1,2,4-triazoline-3,5-diones: An experimental and computational study
Journal of Organic Chemistry, (73): 963-973 2008.
- Albertin, G.; Antoniutti, S.; Baldan, D.; Castro, J.; Garcia-Fontan, S.
Preparation of benzyl azide complexes of iridium(III)
Inorganic Chemistry, (47): 742-748 2008.
- Alcoba, D. R.; Ona, O.
Determination of energies and electronic densities of functional groups according to partitionings in the physical space
Journal of Physical Chemistry A, (112): 10023-10028 2008.
- Alia, J. D.; Vlasisavljevich, B.
Prediction of molecular properties including symmetry from quantum-based molecular structural formulas, VIF
Journal of Physical Chemistry A, (112): 9784-9795 2008.
- Alizadeh, M. H.; Eshtiagh-Hosseini, H.; Mirzaei, M.; Salimi, A. R.; Razavi, H.
Synthesis, X-ray crystallography characterization, vibrational spectroscopy, and DFT theoretical studies of a new organic-inorganic hybrid material
Structural Chemistry, (19): 155-164 2008.

- Alkorta, I.; Blanco, F.; Elguero, J.
Molecular complexes of pentazolo[1,2-a]pentazole, N-8
Journal of Physical Chemistry A, (112): 1817-1822 2008.
- Alkorta, I.; Blanco, F.; Elguero, J.
 π -systems as simultaneous hydride and hydrogen bond acceptors
Journal of Physical Chemistry A, (112): 6753-6759 2008.
- Alkorta, I.; Blanco, F.; Solimannejad, M.; Elguero, J.
Competition of Hydrogen Bonds and Halogen Bonds in Complexes of Hypohalous Acids with Nitrogenated Bases
Journal of Physical Chemistry A, (112): 10856-10863 2008.
- Alkorta, I.; Elguero, J.; Grabowski, S. J.
How to determine whether intramolecular H center dot center dot center dot H interactions can be classified as dihydrogen bonds
Journal of Physical Chemistry A, (112): 2721-2727 2008.
- Alkorta, I.; Elguero, J.; Solimannejad, M.
Dihydrogen bond cooperativity in (HCCBeH)(n) clusters
Journal of Chemical Physics, (129) 2008.
- Alkorta, M.; Blanco, F.; Solimannejad, M.; Elguero, J.
Competition of Hydrogen Bonds and Halogen Bonds in Complexes of Hypohalous Acids with Nitrogenated Bases
Journal of Physical Chemistry A, (112): 10856-10863 2008.
- Alkorta, M.; Elguero, J.; Grabowski, S. J.
How to determine whether intramolecular H center dot center dot center dot H interactions can be classified as dihydrogen bonds
Journal of Physical Chemistry A, (112): 2721-2727 2008.
- Altamura, M.; Dapporto, P.; Guidi, A.; Harmat, N. J. S.; Jierry, L.; Libralesso, E.; Paoli, P.; Rossi, P.
Investigation on the flexibility of chiral tricyclic derivatives
New Journal of Chemistry, (32): 1617-1627 2008.
- Anane, H.; El Houssame, S.; El Guerraze, A.; Guermoune, A.; Boutalib, A.; Jarid, A.; Nebot-Gil, I.; Tomas, F.
A G2(MP2) theoretical study of substituent effects on H3BNHnCl3-n (n=3-0) donor-acceptor complexes
Central European Journal of Chemistry, (6): 400-403 2008.
- Andruniow, T.; Jaworska, M.; Lodowski, P.; Zgierski, M. Z.; Dreos, R.; Randaccio, L.; Kozlowski, P. M.
Time-dependent density functional theory study of cobalt corrinoids: Electronically excited states of methylcobalamin
Journal of Chemical Physics, (129) 2008.
- Anizelli, P. R.; Vilcachagua, J. D.; Cunha Neto, A.; Tormena, C. F.

- Stereoelectronic interaction and their effects on conformational preference for 2-substituted methylenecyclohexane: An experimental and theoretical investigation*
Journal of Physical Chemistry A, (112): 8785-8789 2008.
- Antonczak, S.
Electronic description of four flavonoids revisited by DFT method
Journal of Molecular Structure-Theochem, (856): 38-45 2008.
- Aragoni, M. C.; Arca, M.; Devillanova, F. A.; Hursthouse, M. B.; Huth, S. L.; Isaia, F.; Lippolis, V.; Mancini, A.; Verani, G.
Reactions of Halogens/Interhalogens with polypyridyl substrates: The case of 2,4,6-tris(2-pyridyl)-1,3,5-triazine
European Journal of Inorganic Chemistry: 3921-3928 2008.
- Aragoni, M. C.; Arca, M.; Devillanova, F. A.; Isaia, F.; Lippolis, V.
Polyiodides and polytellurides: Analogies and differences
Phosphorus Sulfur and Silicon and the Related Elements, (183): 1036-1045 2008.
- Arciniegas, M.; Pena, J.; Manero, J. M.; Paniagua, J. C.; Gil, F. J.
Quantum parameters for guiding the design of Ti alloys with shape memory and/or low elastic modulus
Philosophical Magazine, (88): 2529-2548 2008.
- Aronica, C.; Chumakov, Y.; Jeanneau, E.; Luneau, D.; Neugebauer, P.; Barra, A. L.; Gillon, B.; Goujon, A.; Cousson, A.; Tercero, J.; Ruiz, E.
Structure, Magnetic Properties, Polarized Neutron Diffraction, and Theoretical Study of a Copper(II) Cubane
Chemistry-a European Journal, (14): 9540-9548 2008.
- Auer, B. M.; Skinner, J. L.
Vibrational sum-frequency spectroscopy of the liquid/vapor interface for dilute HOD in D2O
Journal of Chemical Physics, (129) 2008.
- Autschbach, J.; Zheng, S. H.
Analyzing Pt chemical shifts calculated from relativistic density functional theory using localized orbitals: The role of Pt 5d lone pairs
Magnetic Resonance in Chemistry, (46): S45-S55 2008.
- Autschbach, J.
Analyzing NMR shielding tensors calculated with two-component relativistic methods using spin-free localized molecular orbitals
Journal of Chemical Physics, (128) 2008.
- Ayotte, P.; Plessis, S.; Marchand, P.
Trapping proton transfer intermediates in the disordered hydrogen-bonded network of cryogenic hydrofluoric acid solutions
Physical Chemistry Chemical Physics, (10): 4785-4792 2008.

- Azam, K. A.; Bennett, D. W.
Double carbon-hydrogen activation of 2-vinylpyridine: Synthesis of tri- and pentanuclear clusters containing the μ -NC₅H₄CH=C ligand
Organometallics, (27): 5163-5166 2008.
- Azizoglu, A.; Balci, M.; Miesusset, J. L.; Brinker, U. H.
Substituent Effects on the Ring-Opening Mechanism of Lithium Bromocyclopropylidenoids to Allenes
Journal of Organic Chemistry, (73): 8182-8188 2008.
- Bach, R. D.; Dmitrenko, O.; Thorpe, C.
Mechanism of thiolate-disulfide interchange reactions in biochemistry
Journal of Organic Chemistry, (73): 12-21 2008.
- Bachmann, C.; Frapper, G.
Cl/F-exchange reaction in COCl₂/SbF₅ system: A theoretical investigation
Chemical Physics Letters, (457): 292-297 2008.
- Balcells, D.; Nova, A.; Clot, E.; Gnanamgari, D.; Crabtree, R. H.; Eisenstein, O.
Mechanism of homogeneous iridium-catalyzed alkylation of amines with alcohols from a DFT study
Organometallics, (27): 2529-2535 2008.
- Balcells, D.; Raynaud, C.; Crabtree, R. H.; Eisenstein, O.
A Rational Basis for the Axial Ligand Effect in C-H Oxidation by [MnO(porphyrin)(X)](+) (X = H₂O, OH-, O₂-) from a DFT Study
Inorganic Chemistry, (47): 10090-10099 2008.
- Balta, B.; Ozturk, C.; Aviyente, V.; Vincent, M. A.; Hillier, I. H.
Claisen rearrangement of aliphatic allyl vinyl ethers in the presence of copper(II) bisoxazoline
Journal of Organic Chemistry, (73): 4800-4809 2008.
- Baric, D.; Maksic, Z. B.
The Baeyer strain is strongly affected by the nucleus-electron attraction - a comment on the Letter of G. Hohlneicher and L. Packschies [Tetrahedron Lett. 2007, 48, 6429-6433]
Tetrahedron Letters, (49): 1428-1431 2008.
- Barnett, C. B.; Naidoo, K. J.
Stereoelectronic and Solvation Effects Determine Hydroxymethyl Conformational Preferences in Monosaccharides
Journal of Physical Chemistry B, (112): 15450-15459 2008.
- Barone, C. R.; Cini, R.; Clot, E.; Eisenstein, O.; Maresca, L.; Natile, G.; Tamasi, G.
A NMR, X-ray, and DFT combined study on the regio-chemistry of nucleophilic addition to platinum(II) coordinated terminal olefins
Journal of Organometallic Chemistry, (693): 2819-2827 2008.
- Barros, N.; Eisenstein, O.; Maron, L.; Tilley, T. D.

- DFT investigation of the catalytic hydromethylation of olefins by scandocenes. 2. Influence of the ansa ligand on propene and isobutene hydromethylation*
Organometallics, (27): 2252-2257 2008.
- Baumann, W.; Schulz, A.; Villinger, A.
A Blue Homoleptic Bismuth-Nitrogen Cation
Angewandte Chemie-International Edition, (47): 9530-9532 2008.
- Beckmann, J.; Finke, P.; Heitz, S.; Hesse, M.
Aryltellurenyl cation [R⁺Te(CR²)]⁺ stabilized by an N-heterocyclic carbene
European Journal of Inorganic Chemistry: 1921-1925 2008.
- Bei, Y.-L.; Zhu, C.-F.
Dynamical and thermodynamic studies on the isomerization reaction of cis-halogeno silylene to halogeno silyl(silylene)
Acta Chimica Sinica, (66): 810-816 2008.
- Bei, Y.-L.; Zhu, C.-F.; Liu, Q.-Y.; Qi, G.-B.
Addition reaction of pentacoordinated silicon compounds by R₃SiX with NR₃'
Acta Physico-Chimica Sinica, (24): 217-222 2008.
- Ben Said, R.; Tangour, B.; Barthelat, J.-C.
Quantum chemical investigations of intramolecular isomerization in RuH₂(CO)(2)(PMe₃)(2)
Journal of Molecular Structure-Theochem, (857): 115-122 2008.
- Bende, A.; Bogar, F.; Ladik, J.
The role of water and K⁺ ion in the charge transfer between PO₄⁻ groups of DNA and the lysine(+) and arginine(+) side chains of histone proteins
Chemical Physics Letters, (463): 211-213 2008.
- Bentabed-Ababsa, G.; Derdour, A.; Roisnel, T.; Saez, J. A.; Domingo, L. R.; Mongin, F.
Polar [3+2] cycloaddition of ketones with electrophilically activated carbonyl ylides. Synthesis of spirocyclic dioxolane indolinones
Organic & Biomolecular Chemistry, (6): 3144-3157 2008.
- Berkaine, N.; Reinhardt, P.; Alikhani, M. E.
Metal (Ti, Zr, Hf) insertion in the C-H bond of methane: Manifestation of an agostic interaction
Chemical Physics, (343): 241-249 2008.
- Bertin, D.; Gigmes, D.; Marque, S. R. A.; Siri, D.; Tordo, P.; Trappo, G.
Effect of the carboxylate salt on the C-ON bond homolysis of SG1-based alkoxyamines
Chemphyschem, (9): 272-281 2008.
- Besseau, F.; Graton, J.; Berthelot, M.
A Theoretical Evaluation of the pK(HB) and Delta H-HB(circle minus) Hydrogen-Bond Scales of Nitrogen Bases
Chemistry-a European Journal, (14): 10656-10669 2008.

- Betts, H. M.; Barnard, P. J.; Bayly, S. R.; Dilworth, J. R.; Gee, A. D.; Holland, J. P.
Controlled Axial Coordination: Solid-Phase Synthesis and Purification of Metallo-Radiopharmaceuticals
Angewandte Chemie-International Edition, (47): 8416-8419 2008.
- Bhabak, K. P.; Mugesh, G.
A Simple and Efficient Strategy To Enhance the Antioxidant Activities of Amino-Substituted Glutathione Peroxidase Mimics
Chemistry-a European Journal, (14): 8640-8651 2008.
- Bigmore, H. R.; Meyer, J.; Krummenacher, I.; Ruegger, H.; Clot, E.; Mountford, P.; Breher, F.
Syntheses, reactivity and DFT studies of group 2 and group 12 metal complexes of tris(pyrazolyl)methanides featuring "Free" pyramidal carbanions
Chemistry-a European Journal, (14): 5918-5934 2008.
- Billes, F.; Varady, B.
A DFT study on the vibrational spectroscopy of protoporphyrin IX
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (70): 729-734 2008.
- Biswal, H. S.; Chakraborty, S.; Wategaonkar, S.
Experimental evidence of O-H-S hydrogen bonding in supersonic jet
Journal of Chemical Physics, (129) 2008.
- Blanco, F.; Alkorta, I.; Elguero, J.
The structure of alkali metal derivatives of azoles: N-sigma versus pi structures
Journal of Physical Chemistry A, (112): 7682-7688 2008.
- Blanco, F.; Alkorta, I.; Elguero, J.; Cruz, V.; Abarca, B.; Ballesteros, R.
[1,2,3]Triazolo[1,5-a]pyridines. A theoretical (DFT) study of the ring-chain isomerization
Tetrahedron, (64): 11150-11158 2008.
- Blanco, F.; Donovan, D. H. O.; Alkorta, I.; Elguero, J.
Substitution effects on neutral and protonated pyridine derivatives along the periodic table
Structural Chemistry, (19): 339-352 2008.
- Bodkin, J. A.; Bacskay, G. B.; McLeod, M. D.
The Sharpless asymmetric aminohydroxylation reaction: optimising ligand/substrate control of regioselectivity for the synthesis of 3-and 4-aminosugars
Organic & Biomolecular Chemistry, (6): 2544-2553 2008.
- Bogdan, D.
Electronic structure and driving forces in alpha-cyclodextrin : butylparaben inclusion complexes
Physics Letters A, (372): 4257-4262 2008.
- Bohlin, J.; Unge, M.; Stafstrom, S.
TDAE chemisorbed on gold
Journal of Physics-Condensed Matter, (20) 2008.

Bontemps, S.; Sircoglou, M.; Bouhadir, G.; Puschmann, H.; Howard, J. A. K.; Dyer, P. W.; Miqueu, K.; Bourissou, D.

Ambiphilic diphosphine-borane ligands: Metal → borane interactions within isoelectronic complexes of rhodium, platinum and palladium
Chemistry-a European Journal, (14): 731-740 2008.

Boo, B. H.; Kim, S.-J.; Lee, M. H.; Nishi, N.

Molecular structures and energies of low-lying $LixSix$ ($x=1-4$) clusters: Comparison with $LixCx$ ($x=1, 2, 4$) clusters
Chemical Physics Letters, (453): 150-159 2008.

Boshaala, A. M. A.; Simpson, S. J.

Synthesis and Characterization of the Trihalophosphine Compounds of Ruthenium $[RuX_2(\eta(6)\text{-cymene})(PY_3)]$ ($X = Cl, Br, Y = F, Cl, Br$) and the Related $PF_2(NMe_2)$ and $P(NMe_2)_3$ Compounds; Multinuclear NMR Spectroscopy and the X-ray Single Crystal Structures of $[RuBr_2(\eta(6)\text{-cymene})(PF_3)]$, $[RuBr_2(\eta(6)\text{-cymene})(PF_2\{NMe_2\})]$, and $[RuI_2(\eta(6)\text{-cymene})(P\{NMe_2\}_3)]$
Inorganic Chemistry, (47): 9279-9292 2008.

Boulet, B.; Joubert, L.; Cote, G.; Bouvier-Capely, C.; Cossonnet, C.; Adamo, C.

Theoretical study of the uranyl complexation by hydroxamic and carboxylic acid groups
Inorganic Chemistry, (47): 7983-7991 2008.

Boyarskaya, I. A.; Akopyan, S. K.

Quantum-Chemical Calculation of Spectral Characteristics and Structure of Complexes $[Mg(DMF)(i)(CH_3CN)(6-i)](2+)$ and IR Spectra of the Tricomponent Solutions $Mg(ClO_4)_2$ -DMF- CH_3CN
Russian Journal of General Chemistry, (78): 2317-2329 2008.

Braeuer, B.; Weigend, F.; Fittipaldi, M.; Gatteschi, D.; Reijerse, E. J.; Guerri, A.; Ciattini, S.; Salvan, G.; Rueffer, T.

Electron paramagnetic resonance and density-functional theory studies of Cu(II)-bis(oxamato) complexes
Inorganic Chemistry, (47): 6633-6644 2008.

Branca, M.; Alezra, V.; Kouklovsky, C.; Archirel, P.

Accurate conformation analysis in solution: NMR and DFT/PCM study of the S -3-(1-naphthoyl)-4-isopropyl-2,2-dimethyloxazolidin-5-one in $CDCl_3$
Tetrahedron, (64): 1743-1752 2008.

Brancato, G.; Rega, N.; Barone, V.

Accurate density functional calculations of near-edge X-ray and optical absorption spectra of liquid water using nonperiodic boundary conditions: The role of self-interaction and long-range effects
Physical Review Letters, (100) 2008.

Brand, D. J.; Steenkamp, J. A.; Omata, K.; Kabuto, K.; Fujiwara, T.; Takeuchi, Y.

The origin of an unusually large F -19 chemical shift difference between the diastereomeric α -cyano- α -fluoro- p -tolylacetic acid (CFTA) esters of 3',4',5,7-tetra- O -methylepicatechin

- Chirality, (20): 351-356 2008.
- Brand, H.; Liebman, J. F.
Cyano-, nitro- and nitrosomethane derivatives: Structures and gas-phase acidities
European Journal of Organic Chemistry: 4665-4675 2008.
- Brand, H.; Mayer, P.; Schulz, A.; Soller, T.; Villinger, A.
Synthesis and structure of monomeric, trimeric, and mixed phenylcyanamides
Chemistry-an Asian Journal, (3): 1050-1058 2008.
- Bras, N. F.; Moura-Tamames, S. A.; Fernandes, P. A.; Ramos, M. J.
Mechanistic Studies on the Formation of Glycosidase-Substrate and Glycosidase-Inhibitor Covalent Intermediates
Journal of Computational Chemistry, (29): 2565-2574 2008.
- Breckenridge, W. H.; Ayles, V. L.; Wright, T. G.
Evidence for emergent chemical bonding in Au⁺-Rg complexes (Rg = Ne, Ar, Kr, and Xe)
Journal of Physical Chemistry A, (112): 4209-4214 2008.
- Breda, S.; Reva, I.
Molecular structure and vibrational spectra of 2(5H)-furanone and 2(5H)-thiophenone isolated in low temperature inert matrix
Journal of Molecular Structure, (887): 75-86 2008.
- Bryantsev, V. S.; de Jong, W. A.; Cossel, K. C.; Diallo, M. S.; Goddard, W. A., III; Groenewold, G. S.; Chien, W.; Van Stipdonk, M. J.
Two-electron three-centered bond in side-on (eta(2)) uranyl(V) superoxo complexes
Journal of Physical Chemistry A, (112): 5777-5780 2008.
- Bryantsev, V. S.; Diallo, M. S.; van Duin, A. C. T.; Goddard, W. A., III
Hydration of copper(II): New insights from density functional theory and the COSMO solvation model
Journal of Physical Chemistry A, (112): 9104-9112 2008.
- Bucher, G.; Koehler, F.
Tetrahydroadamantane-1,3,5,7-di- and tetracations and their helium and hydride inclusion complexes: Spherical aromaticity and evidence for a bonding interaction between carbon and helium
Journal of Physical Chemistry A, (112): 9906-9910 2008.
- Budzisz, E.; Lorenz, I. P.; Mayer, P.; Paneth, P.; Szatkowski, L.; Krajewska, U.; Rozalski, M.; Miernicka, M.
Synthesis, crystal structure, theoretical calculation and cytotoxic effect of new Pt(II), Pd(II) and Cu(II) complexes with pyridine-pyrazoles derivatives
New Journal of Chemistry, (32): 2238-2244 2008.
- Burgett, R. A.; Bao, X.; Villamena, F. A.
Superoxide radical anion adduct of 5,5-dimethyl-1-pyrroline N-oxide (DMPO). 3. Effect of mildly acidic pH on the thermodynamics and kinetics of adduct formation

- Journal of Physical Chemistry A, (112): 2447-2455 2008.
- Bushmarinov, I. S.; Antipin, M. Y.; Akhmetova, V. R.; Nadyrgulova, G. R.; Lyssenko, K. A.
Stereoelectronic effects in N-C-S and N-N-C systems: Experimental and ab initio AIM study
Journal of Physical Chemistry A, (112): 5017-5023 2008.
- Cabeza, J. A.; Perez-Carreno, E.
Double C-H bond activation of an NHCN-methyl group on triruthenium and triosmium carbonyl clusters: A DFT mechanistic study
Organometallics, (27): 4697-4702 2008.
- Canotilho, J.; Castro, R. A. E.; Rosado, M. T. S.; Silva, M. R.; Beja, A. M.; Paixao, J. A.; Redinha, J. S.
The structure of betaxolol from single crystal X-ray diffraction and natural bond orbital analysis
Journal of Molecular Structure, (891): 437-442 2008.
- Cantat, T.; Mezailles, N.; Auffrant, A.; Le Floch, P.
Bis-phosphorus stabilised carbene complexes
Dalton Transactions: 1957-1972 2008.
- Cao, D.-l.; Ren, F.-d.; Feng, X.-q.; Wang, J.-l.; Li, Y.-x.; Hu, Z.-y.; Chen, S.-s.
Unusual intermolecular T-shaped X-H...pi interactions between CH₃CN/CH₃N₂C and H₂O, NH₃ or C₂H₂: A B3LYP and MP2 theoretical study
Journal of Molecular Structure-Theochem, (849): 76-83 2008.
- Cappelli, C.; Mennucci, B.
Modeling the solvation of peptides. The case of (s)-N-acetylproline amide in liquid water
Journal of Physical Chemistry B, (112): 3441-3450 2008.
- Carabineiro, S. A.; Bellabarba, R. M.
Synthesis, structure and magnetic behavior of five-coordinate bis(iminopyrrolyl) complexes of cobalt(II) containing PMe₃ and THF ligands
Inorganic Chemistry, (47): 8896-8911 2008.
- Caramori, G. F.; Frenking, G.
Analysis of the metal-ligand bonds in [Mo(X)(NH₂)(3)] (X = P, N, PO, and NO), [Mo(CO)(5)(NO)](+), and [Mo(CO)(5)(PO)](+)
Theoretical Chemistry Accounts, (120): 351-361 2008.
- Caramori, G. F.; Galembeck, S. E.
A Computational Study of Tetrafluoro-[2.2]Cyclophanes
Journal of Physical Chemistry A, (112): 11784-11800 2008.
- Cardozo, K. H. M.; Vessecchi, R.; Carvalho, V. M.; Pinto, E.; Gates, P. J.; Colepiccolo, P.; Galembeck, S. E.; Lopes, N. P.
A theoretical and mass spectrometry study of the fragmentation of mycosporine-like amino acids
International Journal of Mass Spectrometry, (273): 11-19 2008.
- Carissan, Y.; Hagebaum-Reignier, D.; Goudard, N.; Humbel, S.

- Huckel-Lewis Projection Method: A "Weights Watcher" for Mesomeric Structures*
Journal of Physical Chemistry A, (112): 13256-13262 2008.
- Carra, C.; Scaiano, J. C.
Nucleohomolytic substitution at boron: A computational approach
European Journal of Organic Chemistry: 4454-4459 2008.
- Castano, J. A. G.; Fantoni, A.; Romano, R. M.
Matrix-isolation FTIR study of carbon dioxide: Reinvestigation of the CO₂ dimer and CO₂ center dot center dot center dot N-2 complex
Journal of Molecular Structure, (881): 68-75 2008.
- Cavallotti, C.; Metrangolo, P.
Binding energies and F-19 nuclear magnetic deshielding in paramagnetic halogen-bonded complexes of TEMPO with haloperfluorocarbons
Journal of Physical Chemistry A, (112): 9911-9918 2008.
- Chaitanya, G. K.; Thomas, A.; Sinu, C. R.; Francis, B.; Subhashchandran, K. P.; Ramakrishna, K.; Bhanuprakash, K.
Insight Into the electron delocalization in phenylacetylenes and phenylvinylenes: An NBO analysis
Indian Journal of Chemistry Section a-Inorganic Bio-Inorganic Physical Theoretical & Analytical Chemistry, (47): 1171-1180 2008.
- Chandra, A. K.; Parveen, S.; Das, S.; Zeegers-Huyskens, T.
Blue shifts of the C-H stretching vibrations in hydrogen-bonded and protonated trimethylamine. Effect of hyperconjugation on bond properties
Journal of Computational Chemistry, (29): 1490-1496 2008.
- Chang, C.-R.; Xu, K.-Z.; Song, J.-R.; Yan, B.; Ma, H.-X.; Gao, H.-X.; Zhao, F.-Q.
Preparation, crystal structure and theoretical calculation of 1-amino-1-hydrazino-2,2-dinitroethene
Acta Chimica Sinica, (66): 1399-1404 2008.
- Chattaraj, P. K.; Roy, D. R.; Duley, S.
Bonding and aromaticity in an all-metal sandwich-like compound, Be-8(2-)
Chemical Physics Letters, (460): 382-385 2008.
- Chen, D.-L.; Tian, W. Q.; Feng, J.-K.; Sun, C.-C.
Theoretical investigation of C-56 fullerene isomers and related compounds
Journal of Chemical Physics, (128) 2008.
- Chen, H.; Ikeda-Saito, M.; Shaik, S.
Nature of the Fe-O-2 Bonding in Oxy-Myoglobin: Effect of the Protein
Journal of the American Chemical Society, (130): 14778-14790 2008.
- Chen, J.-M.
Spectroscopic and theoretical studies on axial coordination of bis(pyrrol-2-ylmethyleneamine)phenyl complexes

Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (71): 191-198 2008.

Cheng, H.-Y.; Chang, J.-T.

Study on chromium-containing aluminophosphate CrAPO-5 via density functional theory
Journal of the Chinese Chemical Society, (55): 29-38 2008.

Cheng, M.; Pu, X.; Wong, N.-B.; Lia, M.; Tian, A.

Substituent effects on the hydrogen-bonded complex of aniline-H₂O: a computational study
New Journal of Chemistry, (32): 1060-1070 2008.

Cheng, X. H.; Jin, M. X.; Hu, Z.; Hu, F. F.; Ding, D. J.

*Adsorption Behavior of CH₂ and CH₃ on Metal Clusters Cu-*n* (n=1-6)*
Chinese Journal of Chemical Physics, (21): 445-450 2008.

Cheng-Hua, Z.; Ying, X.; Yong, G.; Guo-Sen, Y.

Theoretical Study on the Hydrolysis of N, N-Bis (p-fluorobenzyl) - N'-(2',3'-dideoxy-3'-thiacytidinyl) Formamidine
Chemical Journal of Chinese Universities-Chinese, (29): 2354-2359 2008.

Chis, V.; Pirnau, A.; Vasilescu, M.; Varga, R. A.; Oniga, O.

X-ray, H-1 NMR and DFT study on 5-para-X-benzylidene-thiazolidine derivatives with x = Br, F
Journal of Molecular Structure-Theochem, (851): 63-74 2008.

Cho, H. G.; Andrews, L.

Infrared Spectra of Metallacyclopropane, Insertion, and Dihydrido Complex Products in Reactions of Laser-Ablated Group 6 Metal Atoms with Ethylene Molecules
Journal of Physical Chemistry A, (112): 12071-12080 2008.

Cho, H. G.; Andrews, L.

Preparation and Characterization of Simple Dihalomethylidene Platinum Dihalide Complexes in Reactions of Laser-Ablated Pt Atoms with Tetrahalomethanes
Journal of the American Chemical Society, (130): 15836-15841 2008.

Cho, H.-G.; Andrews, L.

Infrared spectra of insertion, methylidene, and methylidyne complexes in reactions of laser-ablated ruthenium atoms with halomethanes and methane
European Journal of Inorganic Chemistry: 2537-2549 2008.

Cho, H.-G.; Andrews, L.

Infrared spectra of methylidyne complexes formed in reactions of Re atoms with methane, methyl halides, methylene halides, and ethane: Methylidyne C-H stretching absorptions, bond lengths, and s character
Inorganic Chemistry, (47): 1653-1662 2008.

Chojnacki, J.

DFT and NBO theoretical study of protonation of tri-tert-butoxysilanethiol and its anion
Polyhedron, (27): 969-976 2008.

- Chojnacki, J.
Relationship between electronic structure and geometry of silanethiols and their derivatives: Elucidation of copper group silanethiolates
Journal of Molecular Structure-Theochem, (862): 112-117 2008.
- Choomwattana, S.; Maihom, T.; Khongpracha, P.; Probst, M.; Limtrakul, J.
Structures and mechanisms of the carbonyl-ene reaction between MOF-11 encapsulated formaldehyde and propylene: An ONIOM study
Journal of Physical Chemistry C, (112): 10855-10861 2008.
- Chung, T. W.; Turecek, F.
Electronic properties of charge-tagged peptides upon electron capture
European Journal of Mass Spectrometry, (14): 367-378 2008.
- Chung, T. W.; Turecek, F.
Selecting fixed-charge groups for electron-based peptide dissociations - A computational study of pyridinium tags
International Journal of Mass Spectrometry, (276): 127-135 2008.
- Chval, Z.; Sip, M.
The trans effect in square-planar platinum(II) complexes - A density functional study
Journal of Computational Chemistry, (29): 2370-2381 2008.
- Clark, A. E.
Density functional and basis set dependence of hydrated Ln(III) properties
Journal of Chemical Theory and Computation, (4): 708-718 2008.
- Clark, J.; English, A. M.; Hansen, J. C.; Francisco, J. S.
Computational study on the existence of organic peroxy radical-water complexes (RO₂ center dot H₂O)
Journal of Physical Chemistry A, (112): 1587-1595 2008.
- Clark, T.; Murray, J. S.; Lane, P.; Politzer, P.
Why are dimethyl sulfoxide and dimethyl sulfone such good solvents?
Journal of Molecular Modeling, (14): 689-697 2008.
- Coelho, J. V.; de Freitas, M. P.; Ramalho, T. C.
The role of carbonyl and thiocarbonyl groups in the conformational isomerism of haloacetones and halothioacetones
Structural Chemistry, (19): 671-677 2008.
- Constantino, E.; Tortajada, J.; Sodupe, M.; Rodriguez-Santiago, L.
Coordination Properties of Lysine Interacting with Co(I) and Co(II). A Theoretical and Mass Spectrometry Study
Journal of Physical Chemistry A, (112): 12385-12392 2008.
- Contreras, J. G.; Gerli, L. A.
Conformational preference in 4,6-dimethyl-1,3-thioxane

- Journal of the Chilean Chemical Society, (53): 1389-1392 2008.
- Contreras, R. H.; Suardiaz, R.; Perez, C.; Crespo-Otero, R.; Fabian, J. S.; de la Vega, J. M. G.
Karplus equation for (3)J(HH) spin-spin couplings with unusual (3)J(180 degrees) < (3)J(0 degrees) relationship
Journal of Chemical Theory and Computation, (4): 1494-1500 2008.
- Contreras-Torres, F. F.; Basiuk, V. A.; Basiuk, E. V.
Regioselectivity in azahydro[60]fullerene derivatives: Application of general-purpose reactivity indicators
Journal of Physical Chemistry A, (112): 8154-8163 2008.
- Coro, J.; Alvarez-Puebla, R.; Montero, A. L.; Suarez, M.; Martin, N.; Perez-Pineiro, R.
A computational approach to the synthesis of 1,3,5-thiadiazinane-2-thiones in aqueous medium: theoretical evidence for water-promoted heterocyclization
Journal of Molecular Modeling, (14): 641-647 2008.
- Corsaro, A.; Chiacchio, M. A.; Pistara, V.; Rescifina, A.; Vittorino, E.
Cyclopropanation of 5-methylene galactopyranosides by dihalo-, ethoxycarbonyl-, and unsubstituted carbenes
Tetrahedron, (64): 8652-8658 2008.
- Crabtree, K. N.; Hostetler, K. J.; Munsch, T. E.; Neuhaus, P.; Lahti, P. A.; Sander, W.; Poole, J. S.
Comparative study of the photochemistry of the azidopyridine 1-oxides
Journal of Organic Chemistry, (73): 3441-3451 2008.
- Crawford, N. R. M.; Schrodt, C.; Rothenberger, A.; Shi, W.; Ahlrichs, R.
DFT modeling of silver disorder and mobility in the semiconductor cluster [Ag₂₈S₂₆(P(O)PhOMe)(12)(PPh₃)(12)]
Chemistry-a European Journal, (14): 319-324 2008.
- Cremer, D.; Kraka, E.; Filatov, M.
Bonding in Mercury Molecules Described by the Normalized Elimination of the Small Component and Coupled Cluster Theory
Chemphyschem, (9): 2510-2521 2008.
- Crespo-Otero, R.; Sanchez-Garcia, E.; Suardiaz, R.; Montero, L. A.; Sander, W.
Interactions between simple radicals and water
Chemical Physics, (353): 193-201 2008.
- Crisponi, G.; Nurchi, V. M.; Pivetta, T.; Galezowska, J.; Gumienna-Kontecka, E.; Bailly, T.; Burgada, R.; Kozlowski, H.
Towards a new attenuating compound: A potentiometric, spectrophotometric and NMR equilibrium study on Fe(III), Al(III) and a new tetradentate mixed bisphosphonate-hydroxypyridinonate ligand
Journal of Inorganic Biochemistry, (102): 1486-1494 2008.
- Cui, G.; Ke, X.; Liu, H.; Zhao, J.; Song, S.; Shen, P. K.

- First-principles considerations on spontaneous replacement of copper by tin in the presence of thiourea*
Journal of Physical Chemistry C, (112): 13546-13553 2008.
- Cui, G.; Liu, H.; Wu, G.; Zhao, J.; Song, S.; Shen, P. K.
Electrochemical impedance spectroscopy and first-principle investigations on the oxidation mechanism of hypophosphite anion in the electroless deposition system of nickel
Journal of Physical Chemistry C, (112): 4601-4607 2008.
- Cui, Y.; Zhang, T. L.; Zhang, J. G.; Yang, L.; Zhang, J.; Hu, X. C.
Preparation, molecular structure, and thermal analyses of a novel coordination compound [Cd(AZT)(4)(H₂O)(2)](PA)(2) center dot 4H(2)O (AZT = 3-azido-1,2,4-triazole, PA = picrate)
Structural Chemistry, (19): 269-278 2008.
- Cui, Y. H.; Tian, W. Q.; Feng, J. K.; Chen, D. L.
Structures, Stabilities, Electronic, and Optical Properties of C-64 Fullerene Isomers, Anions (C-64(2-) and C-64(4-)), Metallofullerene Sc-2@C-64, and Sc2C2@C-64
Journal of Computational Chemistry, (29): 2623-2630 2008.
- Cuypers, R.; Burghoff, B.; Marcelis, A. T. M.; Sudholter, E. J. R.; de Haan, A. B.; Zuilhof, H.
Complexation of Phenols and Thiophenol by Phosphine Oxides and Phosphates. Extraction, Isothermal Titration Calorimetry, and ab Initio Calculations
Journal of Physical Chemistry A, (112): 11714-11723 2008.
- Czarnik-Matusiewicz, B.; Pilorz, S.; Bienko, D.; Michalska, D.
Molecular and electronic structures, infrared spectra, and vibrational assignment for ap and sc conformers of hexafluoro-iso-propanol
Vibrational Spectroscopy, (47): 44-52 2008.
- Dai, Y.; Blaisten-Barojas, E.
Energetics, structure, and charge distribution of reduced and oxidized n-pyrrole oligomers: A density functional approach
Journal of Chemical Physics, (129) 2008.
- Dai, Y.; Zhang, X.; Zhang, X.; Wang, H.; Lu, Z.
DFT and GA studies on the QSAR of 2-aryl-5-nitro-1H-indole derivatives as NorA efflux pump inhibitors
Journal of Molecular Modeling, (14): 807-812 2008.
- Daniel, K. A.; Kopff, L. A.; Patterson, E. V.
Computational studies on the solvolysis of the chemical warfare agent VX
Journal of Physical Organic Chemistry, (21): 321-328 2008.
- Danilov, A. I.; Nazmutdinov, R. R.; Zinkicheva, T. T.; Molodkina, E. B.; Rudnev, A. V.; Polukarov, Y. M.; Feliu, J. M.
Mechanism of copper underpotential deposition at Pt(hkl)-electrodes: Quantum-chemical modelling
Russian Journal of Electrochemistry, (44): 697-708 2008.

- Das, D.; Roy, G.; Mugesh, G.
Antithyroid Drug Carbimazole and Its Analogues: Synthesis and Inhibition of Peroxidase-Catalyzed Iodination of L-Tyrosine
Journal of Medicinal Chemistry, (51): 7313-7317 2008.
- Davari, M. D.; Taghizadeh, A.; Bahrami, H.; Zahedi, M.; Shaabani, A.
THEORETICAL STUDY ON THE KINETICS AND MECHANISM OF THE REACTION OF CYCLOHEXYL ISOCYANIDE AND 1,1,1,5,5,5-HEXAFLUOROPENTANE-2,4-DIONE USING DFT METHOD
Journal of Theoretical & Computational Chemistry, (7): 1227-1250 2008.
- De, S.; Drew, M. G. B.; Rzepa, H. S.; Datta, D.
Linking number analysis of a self-assembled lemniscular Mobius-metallamacrocycle
New Journal of Chemistry, (32): 1831-1834 2008.
- De Vleeschouwer, F.; Van Speybroeck, V.; Waroquier, M.; Geerlings, P.; De Proft, F.
An Intrinsic Radical Stability Scale from the Perspective of Bond Dissociation Enthalpies: A Companion to Radical Electrophilicities
Journal of Organic Chemistry, (73): 9109-9120 2008.
- Deepa, P.; Kolandaivel, P.; Senthilkumar, K.
Interactions of anticancer drugs with usual and mismatch base pairs - Density functional theory studies
Biophysical Chemistry, (136): 50-58 2008.
- Del Bene, J. E.; Alkorta, I.; Elguero, J.
Spin-spin coupling across intramolecular N-H...N hydrogen bonds in models for proton sponges: an ab initio investigation
Magnetic Resonance in Chemistry, (46): 457-463 2008.
- del Rosal, I.; Maron, L.; Poteau, R.; Jolibois, F.
DFT calculations of H-1 and C-13 NMR chemical shifts in transition metal hydrides
Dalton Transactions: 3959-3970 2008.
- Dem'yanov, P.; Polestshuk, P.; Gschwind, R.
Hydrogen-bonding interactions in monomeric dimethylcuprates. A theoretical study
Journal of Molecular Structure-Theochem, (861): 85-96 2008.
- Deng, C.; Li, Q.-G.; Ren, Y.; Wong, N.-B.; Chu, S.-Y.; Zhu, H.-J.
A comprehensive theoretical study on the hydrolysis of carbonyl sulfide in the neutral water
Journal of Computational Chemistry, (29): 466-480 2008.
- Dennehy, M.; Ferullo, R. M.; Quinzani, O. V.; Mandolesi, S. D.; Castellani, N.; Jennings, M.
Unusual coordination in a silver thionate complex. Synthesis, structural characterization and theoretical calculations of dinuclear and polynuclear silver(I) thiosaccharinates with pyridine and 1,10-phenanthroline
Polyhedron, (27): 2243-2250 2008.

- Di Salvo, F.; Estrin, D. A.; Leitus, G.; Doctorovich, F.
Synthesis, structure, and reactivity of aliphatic primary nitrosamines stabilized by coordination to [IrCl5](2-)
Organometallics, (27): 1985-1995 2008.
- Dikarev, E. V.; Li, B.; Rogachev, A. Y.; Zhang, H.; Petrukhina, M. A.
Metal-site-controlled arene coordination in a heterobimetallic Bi-Rh complex with pyrene
Organometallics, (27): 3728-3735 2008.
- Dimitrova, Y.
Structure and vibrational spectrum of the hydrogen-bonded system between 4-tert-butylphenol and N-bases: Ab initio and DFT studies
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (69): 517-523 2008.
- Dinescu, A.; Clark, A. E.
Thermodynamic and Structural Features of Aqueous Ce(III)
Journal of Physical Chemistry A, (112): 11198-11206 2008.
- Ding, N.; Zhang, S.; Chen, X.
How does the Fe+-mediated demethanation of CH3OCH3 occur? A density functional theoretical study
Chemical Physics Letters, (458): 33-38 2008.
- Domingo, L. R.; Chamorro, E.; Perez, P.
An understanding of the electrophilic/nucleophilic behavior of electro-deficient 2,3-disubstituted 1,3-butadienes in polar Diels-Alder reactions. A density functional theory study
Journal of Physical Chemistry A, (112): 4046-4053 2008.
- Domingo, L. R.; Chamorro, E.; Perez, P.
Understanding the reactivity of captodative ethylenes in polar cycloaddition reactions. A theoretical study
Journal of Organic Chemistry, (73): 4615-4624 2008.
- Domingo, L. R.; Saez, J. A.; Zaragoza, R. J.; Arno, M.
Understanding the Participation of Quadricyclane as Nucleophile in Polar [2 sigma+2 sigma+2 pi] Cycloadditions toward Electrophilic pi Molecules
Journal of Organic Chemistry, (73): 8791-8799 2008.
- Donghi, D.; D'Alfonso, G.; Mauro, M.; Panigati, M.; Mercandelli, P.; Sironi, A.; Mussini, P.; D'Alfonso, L.
A new class of luminescent tricarbonyl rhenium(I) complexes containing bridging 1,2-diazine ligands: Electrochemical, photophysical, and computational characterization
Inorganic Chemistry, (47): 4243-4255 2008.
- Dorn, V. B.; Badajoz, M. A.; Lockhart, M. T.; Chopra, A. B.; Pierini, A. B.
Synthesis of cyclohexadienylstannanes - Novel example of vinylic S(RN)1 mechanism: A theoretical and experimental study
Journal of Organometallic Chemistry, (693): 2458-2462 2008.

- dos Santos, F. P.; Tormena, C. F.; Contreras, R. H.; Rittner, R.; Magalhaes, A.
The effect of carbonyl group in the asymmetry Of (3,4)J(CH) coupling constants in norbornanones
Magnetic Resonance in Chemistry, (46): 107-109 2008.
- Dostal, L.; Jambor, R.; Ruzicka, A.; Lycka, A.; Brus, J.; de Proft, F.
Synthesis and Structure of Organoantimony(III) Compounds Containing Antimony-Selenium and -Tellurium Terminal Bonds
Organometallics, (27): 6059-6062 2008.
- Du, J.; Sun, X.; Wang, H.
The confirmation of accurate combination of functional and basis set for transition-metal dimers: Fe-2, Co-2, Ni-2, Ru-2, Rh-2, Pd-2, Os-2, Ir-2, and Pt-2
International Journal of Quantum Chemistry, (108): 1505-1517 2008.
- Du, S.; Francisco, J. S.
Interaction between OH radical and the water interface
Journal of Physical Chemistry A, (112): 4826-4835 2008.
- Duefert, A.; Werz, D. B.
Theoretical investigations of substituent effects in dimethyldioxirane epoxidation reactions
Journal of Organic Chemistry, (73): 5514-5519 2008.
- Durand, G.; Choteau, F.; Pucci, B.; Villamena, F. A.
Reactivity of Superoxide Radical Anion and Hydroperoxyl Radical with alpha-Phenyl-N-tert-butylNitrone (PBN) Derivatives
Journal of Physical Chemistry A, (112): 12498-12509 2008.
- Dureen, M. A.; Lough, A.
B-H Activation by frustrated Lewis pairs: borenium or boryl phosphonium cation?
Chemical Communications: 4303-4305 2008.
- Ebrahimi, A.; Habibi, M.; Sayyad, O.
Anion-pi interactions: CP-corrected vs. standard optimisation, AIM and NBO analyses
Molecular Simulation, (34): 689-697 2008.
- Ebrahimi, A.; Habibi, M.; Sayyadi, O.
Interaction between some anions and deficient olefinic and aromatic centers
Journal of Molecular Structure-Theochem, (859): 46-50 2008.
- Ebrahimi, A.; Habibi, S. M.; Sanati, A.; Mohammadi, M.
A comparison of C-C rotational barrier in [2]staffane, [2]tetrahedrane and ethane
Chemical Physics Letters, (466): 32-36 2008.
- Echegaray, E.; Toro-Labbe, A.
Reaction Electronic Flux: A New Concept To Get Insights into Reaction Mechanisms. Study of Model Symmetric Nucleophilic Substitutions
Journal of Physical Chemistry A, (112): 11801-11807 2008.

- Eisler, D. J.; Less, R. J.; Naseri, V.; Rawson, J. M.; Wright, D. S.
The 6 pi, phosphide-stabilised stannylene dianion [C6H4P2Sn](2-); the first member of a new class of Arduengo-type carbene analogues
Dalton Transactions: 2382-2384 2008.
- Eizaguirre, A.; Mo, O.; Yanez, M.; Guillemin, J. C.
alpha,beta-Unsaturated and Saturated Derivatives of Be, Mg, and Ca: Are They Carbon or Metal Acids in the Gas Phase?
Chemistry-a European Journal, (14): 10423-10429 2008.
- Eklof, A. M.; Gullashvili, T.
Relation between the pi-Contribution to Reversed Si=C Bond Polarization and the Reaction Profile for the Thermolytic Formation of Silenes
Organometallics, (27): 5203-5211 2008.
- El-Gogary, T. M.; El-Nahas, A. M.
Origin of reverse stability of diphosphouracil tautomers compared to their analogue uracil: DFT and ab initio study
Journal of Molecular Structure-Theochem, (851): 54-62 2008.
- Esfarili, M. D.; Behzadi, H.
Theoretical study of N-H center dot center dot center dot O hydrogen bonding properties and cooperativity effects in linear acetamide clusters
Theoretical Chemistry Accounts, (121): 135-146 2008.
- Esfarili, M. D.; Behzadi, H.; Hadipour, N. L.
N-14 and O-17 electric field gradient tensors in benzamide clusters: Theoretical evidence for cooperative and electronic delocalization effects in N-H center dot center dot center dot O hydrogen bonding
Chemical Physics, (348): 175-180 2008.
- Esseffar, M.; El Messaoudi, M.; Jalala, R.; Domingo, L. R.; Aurell, M. J.
A combined experimental and theoretical study of the alkylation of 3,5-dithioxo-[1,2,4]triazepines
Journal of Physical Organic Chemistry, (21): 457-463 2008.
- Fan, J. F.; Wu, L. F.; Tao, F. M.
Poor enantioselectivity of the direct aldol reaction catalyzed by (S,S)-proline dipeptide: A density functional study
International Journal of Quantum Chemistry, (108): 66-74 2008.
- Fang, G. Y.; Xu, L.; Hu, X. G.; Li, X. H.
DFT study of the interaction between 3-nitro-1,2,4-triazole-5-one and hydrogen fluoride
Journal of Hazardous materials, (160): 51-55 2008.
- Farmanzadeh, D.; Sabzyan, H.
Characterization of a candidate multi-pole molecular switch using computational techniques
Journal of Molecular Modeling, (14): 1023-1033 2008.

- Fayet, G.; Joubert, L.; Rotureau, P.; Adamo, C.
Theoretical study of the decomposition reactions in substituted nitrobenzenes
Journal of Physical Chemistry A, (112): 4054-4059 2008.
- Fernandez, I.; Mancheno, M. J.; Vicente, R.; Lopez, L. A.; Sierra, M. A.
Transmetalation Reactions from Fischer Carbene Complexes to Late Transition Metals: A DFT Study
Chemistry-a European Journal, (14): 11222-11230 2008.
- Fernandez, I.; Sierra, M. A.
Deeper insight into the mechanism of the reaction of photogenerated metallaketenes and imines
Journal of the American Chemical Society, (130): 13892-13899 2008.
- Fernandez, I.; Sierra, M. A.; Cossio, F. P.
DFT study on the Diels-Alder cycloaddition between alkenyl-M(0) (M = Cr, W) carbene complexes and neutral 1,3-dienes
Journal of Organic Chemistry, (73): 2083-2089 2008.
- Fernandez, I.; Sierra, M. A.; Jose Mancheno, M.; Gomez-Gallego, M.; Cossio, F. P.
The noncarbonylative photochemistry of group 6 Fischer carbene complexes
European Journal of Inorganic Chemistry: 2454-2462 2008.
- Fernandez, L.; Viruela-Martin, P.; Latorre, J.; Guillem, C.; Beltran, A.; Amoros, P.
Theoretical study of oligomeric alumatranes present in the chemistry of materials from micro to mesoporous molecular sieves and alumina composites
Journal of Molecular Structure-Theochem, (850): 94-104 2008.
- Ferreiros-Martinez, R.; Esteban-Gomez, D.
Zn(II), Cd(II) and Pb(II) complexation with pyridinecarboxylate containing ligands
Dalton Transactions: 5754-5765 2008.
- Ferreiros-Martinez, R.; Esteban-Gomez, D.; Platas-Iglesias, C.; de Blas, A.; Rodriguez-Blas, T.
Zn(II), Cd(II) and Pb(II) complexation with pyridinecarboxylate containing ligands
Dalton Transactions: 5754-5765 2008.
- Field, S. A.; Villamena, F. A.
Theoretical and Experimental Studies of Tyrosyl Hydroperoxide Formation in the Presence of H-Bond Donors
Chemical Research in Toxicology, (21): 1923-1932 2008.
- Filatov, A. S.; Petrukhina, M. A.
Gas phase synthesis and X-ray crystal structures of supramolecular networks with bromocorannulene: Similarities and differences with their corannulene analogs
Journal of Organometallic Chemistry, (693): 1590-1596 2008.
- Filatov, A. S.; Rogachev, A. Y.; Petrukhina, M. A.

- Lanthanum(III) chloroaluminate and chlorogallate complexes with toluene and hexamethylbenzene: The effect of arene methylation on the structure*
Journal of Molecular Structure, (890): 116-122 2008.
- Filipuzzi, S.; Maennel, E.; Pregosin, P. S.; Albinati, A.; Rizzato, S.; Veiros, L. F.
Multinuclear NMR, X-ray, and DFT studies on RhCl(diene)(phosphoramidite) complexes
Organometallics, (27): 4580-4588 2008.
- Filipuzzi, S.; Pregosin, P. S.; Calhorda, M. J.; Costa, P. J.
Weak $\eta(2)$ -olefin bonding in palladium and platinum allyl cationic complexes containing chiral monodentate ligands with α -phenyl methyl amine side chains
Organometallics, (27): 2949-2958 2008.
- Fleischer, H.; Schollmeyer, D.
Cooperative Effects in Aminothiols: Acid-Base Equilibria and the Molecular Structure of 2-(N, N-Dimethylaminomethyl)thiophenol
Zeitschrift Fur Naturforschung Section B-a Journal of Chemical Sciences, (63): 1199-1203 2008.
- Flores-Gallegos, N.; Esquivel, R. O.
von Neumann Entropies Analysis in Hilbert Space for the Dissociation Processes of Homonuclear and Heteronuclear Diatomic Molecules
Journal of the Mexican Chemical Society, (52): 19-30 2008.
- Florez, E.; Mondragon, F.; Fuentealba, P.; Illas, F.
Effect of surface site on the spin state of first-row transition metals adsorbed on MgO: Embedded cluster model and hybrid density functional theory calculations
Physical Review B, (78) 2008.
- Fowe, E. P.; Therrien, B.; Suss-Fink, G.; Daul, C.
Electron-structure calculations and bond order analysis using density functional theory of cationic dinuclear arene ruthenium complexes
Inorganic Chemistry, (47): 42-48 2008.
- Fracaroli, A. M.; Silva, O. F.; Granados, A. M.; de Rossi, R. H.
3H-1,2-Dithiole-3-thione derivatives as novel solvatochromic dyes
Journal of Physical Organic Chemistry, (21): 1007-1013 2008.
- Freeman, F.; Lau, D. J.; Patel, A. R.; Pavia, P. R.; Willey, J. D.
Substituent effects on singlet-triplet gaps and mechanisms of 1,2-rearrangements of 1,3-oxazol-2-ylidenes to 1,3-oxazoles
Journal of Physical Chemistry A, (112): 8775-8784 2008.
- Freeman, F.; Po, H. N.; Ho, T. S.; Wang, X.
Electrochemical oxidation of 2-pyrimidinethiols and theoretical study of their dimers, disulfides, sulfenyl radicals, and tautomers
Journal of Physical Chemistry A, (112): 1643-1655 2008.
- Freitas, M. P.; Rittner, R.; Tormena, C. F.; Abraham, R. J.

- The role of stereoelectronic interactions in the conformational isomerism of some phosphorus-containing model compounds*
Journal of Physical Organic Chemistry, (21): 505-509 2008.
- Fu, Y.; Shen, W.; Li, M.
Theoretical analysis on the electronic structures and properties of PPV fused with electron-withdrawing unit: Monomer, oligomer and polymer
Polymer, (49): 2614-2620 2008.
- Fu, Y. W.; Shen, W.; Li, M.
Geometries and Electronic Structures of Co-Oligomers and Co-Polymers Based on Tricyclic Nonclassical Thiophene: A Theoretical Study
Macromolecular Theory and Simulations, (17): 385-392 2008.
- Fuente, S. A.; Belelli, P. G.; Ferullo, R. M.; Castellani, N. J.
Adsorption of NO on Au atoms and dimers supported on MgO(100): DFT studies
Surface Science, (602): 1669-1676 2008.
- Fukui, H.; Kishi, R.; Minami, T.; Nagai, H.; Takahashi, H.; Kubo, T.; Kamada, K.; Ohta, K.; Champagne, B.; Botek, E.; Nakano, M.
Theoretical study on second hyperpolarizabilities of singlet diradical square planar nickel complexes involving o-semiquinonato type ligands
Journal of Physical Chemistry A, (112): 8423-8429 2008.
- Gajewski, M.; Tuszynski, J.; Mori, H.; Miyoshi, E.; Klobukowski, M.
DFT studies of the electronic structure and geometry of 18-crown-6, hexaaza[18]annulene, and their complexes with cations of the heavier alkali and alkaline earth metals
Inorganica Chimica Acta, (361): 2166-2171 2008.
- Galabov, B.; Ilieva, S.; Hadjieva, B.; Atanasov, Y.; Schaefer, H. F., III
Predicting reactivities of organic molecules. Theoretical and experimental studies on the aminolysis of phenyl acetates
Journal of Physical Chemistry A, (112): 6700-6707 2008.
- Galamba, N.; Cabral, B. J. C.
The Changing Hydrogen-Bond Network of Water from the Bulk to the Surface of a Cluster: A Born-Oppenheimer Molecular Dynamics Study
Journal of the American Chemical Society, (130): 17955-17960 2008.
- Gao, G.; Kang, H. S.
C-60 as a chemical Faraday cage for three ferromagnetic Fe atoms
Chemical Physics Letters, (462): 72-74 2008.
- Gao, J. G.; Wang, F.; Meng, Q. X.; Li, M.
DENSITY FUNCTIONAL COMPUTATIONS OF Rh(I)-CATALYZED HYDROACYLATION OF ETHENE OR ETHYNE
Journal of Theoretical & Computational Chemistry, (7): 1041-1053 2008.

- Garcia, F.; Less, R. J.; Naseri, V.; McPartlin, M.; Rawson, J. M.; Tomas, M. S.; Wright, D. S.
Direct synthesis of the 1,2,3-[C6H4P-P](-) anion, isoelectronic with the indenyl anion [C6H4CH-CH-CH](-)
Chemical Communications: 859-861 2008.
- Garzon, A.; Albaladejo, J.; Notario, A.; Pena-Ruiz, T.; Fernandez-Gomez, M.
Kinetic and theoretical study of the reaction of Cl atoms with a series of linear thiols
Journal of Chemical Physics, (129) 2008.
- Gaunt, A. J.; Reilly, S. D.; Enriquez, A. E.; Scott, B. L.; Ibers, J. A.; Sekar, P.; Ingram, K. I. M.; Kaltsoyannis, N.; Neu, M. P.
Experimental and theoretical comparison of actinide and lanthanide bonding in $M[N(EPR_2)(2)](3)$ complexes ($M = U, Pu, La, Ce$; $E = S, Se, Te$; $R = Ph, iPr, H$)
Inorganic Chemistry, (47): 29-41 2008.
- Gayatri, G.; Soujanya, Y.; Fernandez, I.; Frenking, G.; Sastry, G. N.
Further Shortening of the C-C Single Bond in Substituted Tetrahedranyl Tetrahedrane Systems: An Energy Decomposition Analysis
Journal of Physical Chemistry A, (112): 12919-12924 2008.
- Geier, J.
Radial exchange density and electron delocalization in molecules
Journal of Physical Chemistry A, (112): 5187-5197 2008.
- Geng, C.-Y.; Li, J.-L.; Huang, X.-R.; Liu, H.-L.; Li, Z.; Sun, C.-C.
Theoretical elucidation of the rhodium-catalyzed [4+2] annulation reactions
Journal of Computational Chemistry, (29): 686-693 2008.
- Gerken, J. B.; Badger, C.; Bisbee, C.; Gardner, S.; Qi, Y.; Vila, V. D.; Roberts, J. D.
Solution conformational preferences of glutaric, 3-hydroxyglutaric, 3-methylglutaric acid, and their mono- and dianions
Journal of Physical Organic Chemistry, (21): 193-197 2008.
- Ghiasi, R.
Theoretical study of classical isomers tropylium, azatropylium, phosphatropylium, and arsatropylium cations: structure, properties and aromaticity
Main Group Chemistry, (7): 147-154 2008.
- Ghiasi, R.; Monajjemi, M.
Theoretical study of the dihydrogen bonded $HMH \cdots HB \cdots NH$ and $HMH \cdots HN \cdots BH$ complexes ($M=Be, Mg$ and Ca): properties and structures
Main Group Chemistry, (7): 123-131 2008.
- Ghiasi, R.; Monajjemi, M.; Mokarram, E. E.; Makkipour, P.
Theoretical studies on the structures, properties, and aromaticities of fluorinated arsabenzenes
Journal of Structural Chemistry, (49): 600-605 2008.

- Ghiasi, R.; Yadegari, N.
Substitute Effect on the Structure, Stability of Valence Isomers and Aromaticity of 1-H-Boratabenzene
Journal of the Chinese Chemical Society, (55): 1308-1312 2008.
- Ghosh, R.; Emge, T. J.; Krogh-Jespersen, K.; Goldman, A. S.
Combined experimental and computational studies on carbon-carbon reductive elimination from bis(hydrocarbyl) complexes of (PCP)Ir
Journal of the American Chemical Society, (130): 11317-11327 2008.
- Gicquel, M.; Heully, J.-L.; Lepetit, C.; Chauvin, R.
Carbo-[3] oxocarbon and its isomers: evaluation of the stability and of the electron delocalization
Physical Chemistry Chemical Physics, (10): 3578-3589 2008.
- Gil, A.; Simon, S.; Sodupe, M.; Bertran, J.
How the site of ionisation influences side-chain fragmentation in histidine radical cation
Chemical Physics Letters, (451): 276-281 2008.
- Gillon, B.; Larionova, J.; Ruiz, E.; Nau, Q.; Goujon, A.; Bonadio, F.; Decurtins, S.
Experimental and theoretical study of the spin ground state of the high-spin molecular cluster [Ni-II{Ni-II(CH3OH)(3)}(8)(mu-CN)(30){W-V(CN)(3)}(6)] center dot 15CH(3)OH by polarised neutron diffraction and density functional theory calculations
Inorganica Chimica Acta, (361): 3609-3615 2008.
- Giordana, A.; Maranzana, A.; Ghigo, G.; Causa, M.; Tonachini, G.
Soot platelets and PAHs with an odd number of unsaturated carbon atoms and pi electrons: Theoretical study of their spin properties and interaction with ozone
Journal of Physical Chemistry A, (112): 973-982 2008.
- Glaser, R.; Sui, Y.; Sarkar, U.; Gates, K. S.
Electronic structures and spin topologies of gamma-picoliniumyl radicals. a study of the homolysis of N-methyl-gamma-picolinium and of benzo-, dibenzo-, and naphthoannulated analogs
Journal of Physical Chemistry A, (112): 4800-4814 2008.
- Gnaser, H.; Golser, R.; Pernpointner, M.; Forstner, O.; Kutschera, W.; Priller, A.; Steier, P.; Wallner, A.
Identification of the Sih(6)(2-) dianion by accelerator mass spectrometry and a fully relativistic computation of its photodetachment spectrum
Physical Review A, (77) 2008.
- Goel, S.; Masunov, A. E.
Potential energy curves and electronic structure of 3d transition metal hydrides and their cations
Journal of Chemical Physics, (129) 2008.
- Goldsmith, R. H.; Vura-Weis, J.; Scott, A. M.; Borkar, S.; Sen, A.; Ratner, M. A.; Wasielewski, M. R.
Unexpectedly similar charge transfer rates through benzo-annulated bicyclo[2.2.2]octanes
Journal of the American Chemical Society, (130): 7659-7669 2008.

- Goll, E.; Leininger, T.; Manby, F. R.; Mitrushchenkov, A.; Werner, H.-J.; Stoll, H.
Local and density fitting approximations within the short-range/long-range hybrid scheme: application to large non-bonded complexes
Physical Chemistry Chemical Physics, (10): 3353-3357 2008.
- Goll, E.; Werner, H.-J.; Stoll, H.
Short-range density functionals in combination with local long-range ab initio methods: Application to non-bonded complexes
Chemical Physics, (346): 257-265 2008.
- Gomes, J. R. B.; Cordeiro, M. N. D. S.; Jorge, M.
Gas-phase molecular structure and energetics of anionic silicates
Geochimica et Cosmochimica Acta, (72): 4421-4439 2008.
- Gomez Castano, J. A.; Romano, R. M.; Willner, H.; Della Vedova, C. O.
Preparation of the novel XC(O)SeX species (X = Cl, Br) through matrix photochemical reactions of OCS_e with Cl-2 and Br-2 at cryogenic temperatures
Inorganica Chimica Acta, (361): 540-550 2008.
- Gomez-Bengoia, E.; Linden, A.; Lopez, R.; Mugica-Mendiola, I.; Oiarbide, M.; Palomo, C.
Asymmetric aza-henry reaction under phase transfer catalysis: An experimental and theoretical study
Journal of the American Chemical Society, (130): 7955-7966 2008.
- Gomez-Ruiz, S.; Zahn, S.; Kirchner, B.; Bohlmann, W.; Hey-Hawkins, E.
P-P Bond Cleavage of Tetraphenyltetraphosphane-1,4-diide Facilitated by Nickel(0)
Chemistry-a European Journal, (14): 8980-8985 2008.
- Gomez-Sanchez, E.; Soriano, E.; Marco-Contelles, J.
Synthesis of heterocyclic analogues of epibatidine via 7-azabicyclo[2.2.1]hept-2-yl radical intermediates. 1. Intermolecular reactions
Journal of Organic Chemistry, (73): 6784-6792 2008.
- Gould, M. D.; Taylor, C.; Wolff, S. K.; Chandler, G. S.; Jayatilaka, D.
A definition for the covalent and ionic bond index in a molecule
Theoretical Chemistry Accounts, (119): 275-290 2008.
- Gourlaouen, C.; Parisel, O.
Competitive coordination between lead and oligoelements with respect to some therapeutic heavy-metal chelators
International Journal of Quantum Chemistry, (108): 1888-1897 2008.
- Grabowski, S. J.
Hydrogen bonds assisted by pi-electron delocalization - the influence of external intermolecular interactions on dimer of formic acid
Journal of Physical Organic Chemistry, (21): 694-702 2008.
- Grabowski, S. J.

- Hydrogen bonds assisted by pi-electron delocalization - the influence of external intermolecular interactions on dimer of formic acid*
Journal of Physical Organic Chemistry, (21): 694-702 2008.
- Gracia, L.; Polo, V.; Sambrano, J. R.; Andres, J.
Theoretical study on the reaction mechanism of VO₂⁺ with propyne in gas phase
Journal of Physical Chemistry A, (112): 1808-1816 2008.
- Gribanova, T. N.; Minyaev, R. M.; Minkin, V. I.
Nonclassical systems with two hypercoordinate atoms in a polyhedral cage
Doklady Chemistry, (418): 10-14 2008.
- Gridin, M. K.; Milov, A. A.; Starikov, A. G.; Minyaev, R. M.
Steric and electronic structure of complexes of pyrylium and thiopyrylium cations with borabenzene anion
Russian Journal of General Chemistry, (78): 1354-1360 2008.
- Gruber, S.; Zaitsev, A. B.; Woerle, M.; Pregosin, P. S.; Veiros, L. F.
Facile ruthenium(IV)-catalyzed single and double allylation of indole compounds using alcohols as substrates: Aspects of ruthenium(IV) allyl chemistry
Organometallics, (27): 3796-3805 2008.
- Gruber-Woelfler, H.; Flock, M.
Structure-Function-Performance Relationship of Bis(cyclopentadienyl)-Based Group 4 Metallocenes: A DFT Study
Organometallics, (27): 5196-5202 2008.
- Guirado, A.; Martiz, B.; Andreu, R.; Galvez, J.
On the selective electrogeneration of 1-aryl-4,4-dichlorobut-3-en-1-ones from 2,2,2-trichloroethylideneacetophenones - A combined experimental and HF and B3LYP computational study
Electrochimica Acta, (53): 7138-7145 2008.
- Guo, C.-H.; Jia, J.-F.; Zhang, F.-Q.; Wu, H.-S.
Density functional theory studies on the structure, electronic state and photoelectron spectroscopy of (GaP)(n)(-) (n=7-9) clusters
Journal of Molecular Structure-Theochem, (851): 167-174 2008.
- Guo, P.; Chen, W.; Song, J.; Cao, W.; Tian, C.
A DFT study of the interaction between butein anion and metal cations (M = Mg²⁺, Cr²⁺, Fe²⁺, and Cu²⁺): Taking an insight into its chelating property
Journal of Molecular Structure-Theochem, (849): 33-36 2008.
- Guo, Y.; Li, S.
A novel addition mechanism for the reaction of "Frustrated Lewis Pairs" with olefins
European Journal of Inorganic Chemistry: 2501-2505 2008.
- Guo, Y.; Li, S.

- Unusual concerted Lewis acid-Lewis base mechanism for hydrogen activation by a phosphine-borane compound*
Inorganic Chemistry, (47): 6212-6219 2008.
- Gurubasavaraj, P. M.; Roesky, H. W.; Nekoueshahraki, B.; Pal, A.; Herbst-Irmer, R.
From unstable to stable: Half-metallocene catalysts for olefin polymerization
Inorganic Chemistry, (47): 5324-5331 2008.
- Gutsev, G. L.; Johnson, E.; Mochena, M. D.; Bauschlicher, C. W., Jr.
The structure and energetics of (GaAs)(n), (GaAs)(n)(-), and (GaAs)(n)(+) (n=2-15)
Journal of Chemical Physics, (128) 2008.
- Gutsev, G. L.; Mochena, M. D.; Bauschlicher, C. W., Jr.; Zheng, W. J.; Thomas, O. C.; Bowen, K. H.
Electronic and geometrical structure of Mn-13 anions, cations, and neutrals
Journal of Chemical Physics, (129) 2008.
- Gutsev, G. L.; O'Neal, R. H.; Saha, B. C.; Mochena, M. D.; Johnson, E.; Bauschlicher, C. W.
Optical Properties of (GaAs)(n) Clusters (n=2-16)
Journal of Physical Chemistry A, (112): 10728-10735 2008.
- Haberhauer, G.; Drosdow, E.; Oeser, T.; Rominger, F.
Structural investigation of westiellamide analogues
Tetrahedron, (64): 1853-1859 2008.
- Hafied, M.; Belloum, M.
Density Functional Theory Study of Structural Properties and Charge Delocalization in Carbonium Ions(C-3 to C-5)
Journal of Computational and Theoretical Nanoscience, (5): 1420-1427 2008.
- Haqghu, M.; Irani, M.; Gholami, M. R.
Theoretical study of solvent and substituent effects on the reactions of 1,4-benzoquinone with cyclopentadiene and cyclohexadiene
Progress in Reaction Kinetics and Mechanism, (33): 191-206 2008.
- Hare, P. M.; Middleton, C. T.; Mertel, K. I.; Herbert, J. M.; Kohler, B.
Time-resolved infrared spectroscopy of the lowest triplet state of thymine and thymidine
Chemical Physics, (347): 383-392 2008.
- Hashemianzadeh, M.; Safarpour, M. A.; Gholamjani-Moghaddam, K.; Mehdipour, A. R.
DFT-based QSAR study of valproic acid and its derivatives
Qsar & Combinatorial Science, (27): 469-474 2008.
- Hawkes, K. J.; Yates, B. F.
The Mechanism of the Stetter Reaction - A DFT Study
European Journal of Organic Chemistry: 5563-5570 2008.
- Hayakawa, S.; Matsubara, H.; Panja, S.; Hvelplund, P.; Nielsen, S. B.; Chen, X.; Turecek, F.
Experimental evidence for an inverse hydrogen migration in arginine radicals

- Journal of the American Chemical Society, (130): 7645-7654 2008.
- He, N.; Xie, H. B.; Ding, Y. H.
One-Electron Metal-Metal Bond Stabilized in Dinuclear Metallocenes: Theoretical Prediction of DBe-LiCp (D = C5H5 or C5Me5)
Journal of Physical Chemistry A, (112): 12463-12468 2008.
- He, X. M.; Yang, P. X.; Chen, Z. N.; Fu, G.; Xu, X.
Density Functional Method Studies on Configuration and Electronic Structure of R-ReO3
Chemical Journal of Chinese Universities-Chinese, (29): 2267-2272 2008.
- Helgaker, T.; Jaszunski, M.
The quantum-chemical calculation of NMR indirect spin-spin coupling constants
Progress in Nuclear Magnetic Resonance Spectroscopy, (53): 249-268 2008.
- Herrmann, H.; Fillol, J. L.
Bonding and Bending in Zirconium(IV) and Hafnium(IV) Hydrazides
Chemistry-a European Journal, (14): 8131-8146 2008.
- Hofer, T. S.; Randolf, B. R.; Rode, B. M.
Al(III) hydration revisited. An ab initio quantum mechanical charge field molecular dynamics study
Journal of Physical Chemistry B, (112): 11726-11733 2008.
- Holm, A. I. S.; Larsen, M. K.; Panja, S.; Hvelplund, P.; Nielsen, S. B.; Leib, R. D.
Electron capture, femtosecond electron transfer and theory: A study of noncovalent crown ether 1,n-diammonium alkane complexes
International Journal of Mass Spectrometry, (276): 116-126 2008.
- Holtzl, T.; Janssens, E.; Veldeman, N.; Veszpremi, T.; Lievens, P.; Nguyen, M. T.
The Cu7Sc cluster is a stable sigma-aromatic seven-membered ring
Chemphyschem, (9): 833-838 2008.
- Horvath, S.; McCoy, A. B.; Roscioli, J. R.; Johnson, M. A.
Vibrationally Induced Proton Transfer in F-(H2O) and F-(D2O)
Journal of Physical Chemistry A, (112): 12337-12344 2008.
- Hou, R.-B.; Li, W.-W.; Shen, X.-C.
Ring-opening reaction mechanism of 8-hydroxyguanine radical
Acta Physico-Chimica Sinica, (24): 269-274 2008.
- Hrobarik, P.; Kaupp, M.; Riedel, S.
Is Allred's [Hg(cyclam)](3+) a True Mercury(III) Complex?
Angewandte Chemie-International Edition, (47): 8631-8633 2008.
- Hsu, W.-Y.; Lee, H.-Y.; Wang, S.-P.; Chang, T.-C.
The Fock matrix analysis for atomic orbitals in molecular orbitals II. The electronic structure of N-2 molecules

- Journal of the Chinese Chemical Society, (55): 97-102 2008.
- Hua, W. J.; Fang, T.; Li, W.; Yu, J. G.; Li, S. H.
Geometry Optimizations and Vibrational Spectra of Large Molecules from a Generalized Energy-Based Fragmentation Approach
Journal of Physical Chemistry A, (112): 10864-10872 2008.
- Huang, X. X.; Xu, X.; Xie, M. X.
Theoretical Studies on the Fe-M Interactions and P-31 NMR in Fe(CO)(3)(EtPhPpy)(2)MX2 (X=NCS, SCN, Cl; M=Zn, Cd, Hg)
Chinese Journal of Chemical Physics, (21): 438-444 2008.
- Huang, Y.; Zhong, A.; Rong, C.; Xiao, X.; Liu, S.
Structure, spectroscopy, and reactivity properties of porphyrin pincers: A conceptual density functional theory and time-dependent density functional theory study
Journal of Physical Chemistry A, (112): 305-311 2008.
- Huan-Mei, G.; Jing, M.; Pu-Su, Z.; Fang-Fang, J.
Synthesis, Crystal Structure Characterization and Quantum Chemical Studies on 1N-Acetyl-3-(2,4-dichloro-5-fluoro-phenyl)-5-(p-methyl-phenyl)-2-pyrazol ine
Chinese Journal of Structural Chemistry, (27): 1491-1498 2008.
- Hughes, T. F.; Bartlett, R. J.
Transferability in the natural linear-scaled coupled-cluster effective Hamiltonian approach: Applications to dynamic polarizabilities and dispersion coefficients
Journal of Chemical Physics, (129) 2008.
- Hughes, T. F.; Flocke, N.; Bartlett, R. J.
Natural linear-scaled coupled-cluster theory with local transferable triple excitations: Applications to peptides
Journal of Physical Chemistry A, (112): 5994-6003 2008.
- Hull, K. L.; Carmichael, I.; Noll, B. C.; Henderson, K. W.
Homo- and heterodimetallic geminal dianions derived from the bis(phosphinimine) {Ph2P(NSiMe3)}2CH2 and the alkali metals Li, Na, and K
Chemistry-a European Journal, (14): 3939-3953 2008.
- Huschek, G.; Hollmann, D.; Kurowski, N.; Kaupenjohann, M.; Vereecken, H.
Re-evaluation of the conformational structure of sulfadiazine species using NMR and ab initio DFT studies and its implication on sorption and degradation
Chemosphere, (72): 1448-1454 2008.
- Hyla-Kryspin, I.; Grimme, S.; Hruschka, S.; Haufe, G.
Conformational preferences and basicities of mono fluorinated cyclopropyl amines in comparison to cyclopropylamine and 2-fluoroethylamine
Organic & Biomolecular Chemistry, (6): 4167-4175 2008.
- Imamura, Y.; Baba, T.; Nakai, H.

- Natural bond orbital-based energy density analysis for correlated methods: Second-order Moller-Plesset perturbation and coupled-cluster singles and doubles*
International Journal of Quantum Chemistry, (108): 1316-1325 2008.
- Improta, R.; Berisio, R.; Vitagliano, L.
Contribution of dipole-dipole interactions to the stability of the collagen triple helix
Protein Science, (17): 955-961 2008.
- Indrakanti, V. P.; Kubicki, J. D.; Schobert, H. H.
Quantum chemical modeling of ground states of CO₂ chemisorbed on anatase (001), (101), and (010) TiO₂ surfaces
Energy & Fuels, (22): 2611-2618 2008.
- Infante, I.; Gagliardi, L.; Scuseria, G. E.
Is fullerene C-60 large enough to host a multiply bonded dimetal?
Journal of the American Chemical Society, (130): 7459-7465 2008.
- Ingram, K. I. M.; Tassell, M. J.; Gaunt, A. J.; Kaltsoyannis, N.
Covalency in the f element-chalcogen bond. Computational studies of M[N(EPR₂)(2)](3) (M = La, Ce, Pr, Pm, Eu, U, Np, Pu, Am, Cm; E = O, S, Se, Te; R = H, Pr-i, Ph)
Inorganic Chemistry, (47): 7824-7833 2008.
- Iriarte, A. G.; Robles, N. L.; Cutin, E. H.; Della Vedova, C. O.
Vibrational spectra and theoretical calculations of [(trifluoromethyl)sulfonyl] phosphorimidic trichloride (CF₃SO₂N-PCl₃)
Journal of Molecular Structure, (888): 7-12 2008.
- Irikura, K. K.
Sigma stellation: A design strategy for electron boxes
Journal of Physical Chemistry A, (112): 983-988 2008.
- Irshaidat, T.
Some physical organic aspects of salicylaldehydes oximes, a theoretical study
Tetrahedron Letters, (49): 631-635 2008.
- Itzhaki, L.; Rozenal, E.; Altus, E.; Basch, H.; Hoz, S.
Conjugation in Polyene Rods: To What Extent Is Charge Delocalization Coupled to Geometrical Changes?
Journal of Physical Chemistry A, (112): 12812-12815 2008.
- Ivanic, J.; Atchity, G. J.; Ruedenberg, K.
Intrinsic local constituents of molecular electronic wave functions. I. Exact representation of the density matrix in terms of chemically deformed and oriented atomic minimal basis set orbitals
Theoretical Chemistry Accounts, (120): 281-294 2008.
- Ivanic, J.; Atchity, G. J.; Ruedenberg, K.
Intrinsic local constituents of molecular electronic wave functions. I. Exact representation of the density matrix in terms of chemically deformed and oriented atomic minimal basis set orbitals

- Theoretical Chemistry Accounts, (120): 281-294 2008.
- Ivashin, N.; Larsson, S.
Trapped water molecule in the charge separation of a bacterial reaction center
Journal of Physical Chemistry B, (112): 12124-12133 2008.
- Iwano, K.; Shimoi, Y.
Large electric-potential bias in an EDO-TTF tetramer as a major mechanism of charge ordering observed in its PF6 salt: A density functional theory study
Physical Review B, (77) 2008.
- Izod, K.; McFarlane, W.; Wills, C.; Clegg, W.; Harrington, R. W.
Agostic-type B-H...Pb interactions stabilize a dialkylplumbylene. Structure of and bonding in $[\{nPr(2)P(BH_3)\}(Me_3Si)C(CH_2)](2)Pb$
Organometallics, (27): 4386-4394 2008.
- Jahn, B. O.; Eger, W. A.; Anders, E.
Allene as the Parent Substrate in Zinc-Mediated Biomimetic Hydration Reactions of Cumulenes
Journal of Organic Chemistry, (73): 8265-8278 2008.
- Jalbout, A. F.; Contreras-Torres, F. F.; Hameed, A. J.; Trzaskowski, B.; Basiuk, V. A.
Structure and properties of a series of arylselenium [60]fulleropyrrolidine derivatives
Journal of Computational and Theoretical Nanoscience, (5): 554-562 2008.
- Jamalizadeh, E.; Jafari, A. H.; Hosseini, S. M. A.
Semi-empirical and ab initio quantum chemical characterisation of pyridine derivatives as HCl inhibitors of aluminium surface
Journal of Molecular Structure-Theochem, (870): 23-30 2008.
- James, C.; Pettit, G. R.; Nielsen, O. F.; Jayakumar, V. S.; Joe, I. H.
Vibrational spectra and ab initio molecular orbital calculations of the novel anti-cancer drug combretastatin A-4 prodrug
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (70): 1208-1216 2008.
- James, C.; Ravikumar, C.; Sundius, T.; Krishnakumar, V.; Kesavamoorthy, R.; Jayakumar, V. S.; Joe, I. H.
FT-Raman and FTIR spectra, normal coordinate analysis and ab initio computations of (2-methylphenoxy) acetic acid dimer
Vibrational Spectroscopy, (47): 10-20 2008.
- Janardanan, D.; Sunoj, R. B.
Enantio- and Diastereoselectivities in Chiral Sulfur Ylide Promoted Asymmetric Aziridination Reactions
Journal of Organic Chemistry, (73): 8163-8174 2008.
- Jarmelo, S.; Reva, I. D.; Lapinski, L.; Nowak, M. J.; Fausto, R.
Matrix-Isolated Diglycolic Anhydride: Vibrational Spectra and Photochemical Reactivity
Journal of Physical Chemistry A, (112): 11178-11189 2008.

- Jaronczyk, M.; Dobrowolski, J. C.
On isomers and tautomers of Nitro-1-deazapurine: A DFT study
Journal of Molecular Structure-Theochem, (858): 77-84 2008.
- Jesus, A. J. L.; Rosado, M. T. S.; Reva, I.; Fausto, R.; Eusebio, A. E. S.; Redinha, J. S.
Structure of isolated 1,4-butanediol: Combination of MP2 calculations, NBO analysis, and matrix-isolation infrared spectroscopy
Journal of Physical Chemistry A, (112): 4669-4678 2008.
- Jian, F. F.; Li, Y. F.; Yang, X. Y.; Zhao, P. S.; Xiao, H. L.
Crystal structure and quantum chemical calculations on o-hydroxyacetophenone phenylhydrazone
Polish Journal of chemistry, (82): 1597-1609 2008.
- Jian, F. F.; Zhao, P. S.; Li, Y. F.; Wang, X.; Yu, Q.
A combined computational and experimental approach for investigating a hydrogen-bonded supermolecular compound comprising benzimidazole and malonic acid
International Journal of Quantum Chemistry, (108): 521-531 2008.
- Jian, F.-F.; Zhao, P.-S.; Li, Y.-F.; Wang, X.; Yu, Q.
A combined computational and experimental approach for investigating a hydrogen-bonded supermolecular compound comprising benzimidazole and malonic acid
International Journal of Quantum Chemistry, (108): 521-531 2008.
- Jiang, L.; Zhang, X.-B.; Han, S.; Xu, Q.
Unique structural trends in the lanthanoid oxocarbonyl complexes
Inorganic Chemistry, (47): 4826-4831 2008.
- Jiang, Z.-Y.; Cao, X.-W.; Lee, K.-H.; Chu, S.-Y.
Structure and stability of high-spin Lin-1X (n=2-8, X = Li, Na, and K) clusters
International Journal of Mass Spectrometry, (274): 1-7 2008.
- Jimenez-Fabian, I.; Jalbout, A. F.; Moshfeghi, E.; Raissi, H.
beta-aminoacrolein: An ab initio, AIM and NBO study
International Journal of Quantum Chemistry, (108): 383-390 2008.
- John, A.; Shaikh, M. M.; Ghosh, P.
Structural and functional mimic of galactose oxidase by a copper complex of a sterically demanding [N2O2] ligand
Dalton Transactions: 2815-2824 2008.
- Johnson, L. E.; DuPre, D. B.
Topological and orbital-based mechanisms of the electronic stabilization of bis(diisopropylamino)cyclopropenyliene
Journal of Physical Chemistry A, (112): 7448-7454 2008.
- Joshi, Y. V.; Ghosh, P.; Daage, M.; Delgass, W. N.

- Support effects in HDS catalysts: DFT analysis of thiolysis and hydrolysis energies of metal-support linkages*
Journal of Catalysis, (257): 71-80 2008.
- Juarez, M. F.; Soria, F. A.; Patrio, E. M.; Paredes-Olivera, P.
Influence of subsurface oxidation on the structure, stability, and reactivity of grafted Si(111) surfaces
Journal of Physical Chemistry C, (112): 14867-14877 2008.
- Kakimoto, K.; Takekoshi, S.; Miyajima, K.; Osamura, R. Y.
Hypothesis for the mechanism for heat-induced antigen retrieval occurring on fresh frozen sections without formalin-fixation in immunohistochemistry
Journal of Molecular Histology, (39): 389-399 2008.
- Kalinina, D.; Dares, C.; Kaluarachchi, H.; Potvin, P. G.; Lever, A. B. P.
Spectroscopic, Electrochemical, and Computational Aspects of the Charge Distribution in Ru(acac)(2)(R-o-benzoquinonediimine) Complexes
Inorganic Chemistry, (47): 10110-10126 2008.
- Kameo, H.; Nakajima, Y.; Suzuki, H.
Drastic Acceleration of Phosphine/Phosphate Incorporation into a Tetrahydrido Ruthenium/Osmium Complex, and One-way Ruthenium to Osmium Migration of a Phosphorus Ligand
Angewandte Chemie-International Edition, (47): 10159-10162 2008.
- Kaminsky, J.; Mata, R. A.; Werner, H. J.; Jensen, F.
The accuracy of local MP2 methods for conformational energies
Molecular Physics, (106): 1899-1906 2008.
- Kandemirli, F.; Hoscan, M.; Dimoglo, A.; Esen, S.
Theoretical study and comparison of Bent's rule with hardness and polarizability for SF₄, SF₄O, PCI₄F, PCI₃F₂, PCI₂F₃, PCI₂F₄ molecules
Phosphorus Sulfur and Silicon and the Related Elements, (183): 1954-1967 2008.
- Kang, Y. K.; Scheraga, H. A.
An efficient method for calculating atomic charges of peptides and proteins from electronic populations
Journal of Physical Chemistry B, (112): 5470-5478 2008.
- Kao, H.-M.; Ho, S.-M.; Chen, I. C.; Kuo, P.-C.; Lin, C.-Y.; Tu, C.-Y.; Hu, C.-H.; Huang, J.-H.; Lee, G.-H.
Synthesis and structures of three, four, and six-coordinate monomeric tin(II) and tin(IV) compounds containing eta(2)-ketiminate ligands
Inorganica Chimica Acta, (361): 2792-2798 2008.
- Karabiyik, H.; Kilincarslan, R.; Aygun, M.; Cetinkaya, B.; Gardia-Granda, S.
The 1 : 1 co-crystallization of enantiomers of an arene-tethered and ortho-metallated N-heterocyclic carbene ruthenium(II) half-sandwich complex: Synthesis, structural characterization and theoretical study

Solid State Sciences, (10): 104-113 2008.

Karipidis, P. A.; Tsipis, C. A.

The dramatic effect of NH₃ co-ligation on the Fe⁺-assisted activation of carbon dioxide in the gas phase: From bare metal ions to complexes

Journal of Computational Chemistry, (29): 2382-2396 2008.

Karpichev, B.; Reisler, H.

Effect of hyperconjugation on ionization energies of hydroxyalkyl radicals

Journal of Physical Chemistry A, (112): 9965-9969 2008.

Karttunen, A. J.; Linnolahti, M.; Pakkanen, T. A.

Structural and Electronic Characteristics of Diamondoid Analogues of Group 14 Elements

Journal of Physical Chemistry C, (112): 16324-16330 2008.

Karttunen, A. J.; Linnolahti, M.; Pakkanen, T. A.

Structural characteristics of perhydrogenated boron nitride fullerenes

Journal of Physical Chemistry C, (112): 10032-10037 2008.

Kassaee, M. Z.; Arefrad, H.; Ghambarian, M.

Novel silicon nanorings: Persilacyclacenes at DFT

International Journal of Quantum Chemistry, (108): 696-707 2008.

Kassaee, M. Z.; Buazar, F.

Triplet germynes with separable minima at ab initio and DFT levels

Journal of Molecular Structure-Theochem, (866): 52-57 2008.

Kassaee, M. Z.; Ghambarian, M.; Musavi, S. M.

Halogen switching of azacarbenes C₂NH ground states at ab initio and DFT levels

Heteroatom Chemistry, (19): 377-388 2008.

Kassaee, M. Z.; Musavi, S. M.; Jalalimanesh, N.

A new generation of intermediates at ab initio and DFT levels: Allylic carbenonitrenes, C=(X)C-N (X = H, CH₃, COOH, F, OH, OCH₃, CF₃, CN, and NH₂)

Journal of Theoretical & Computational Chemistry, (7): 367-379 2008.

Kassaee, M. Z.; Soleimani-Amiri, S.; Ghambarian, M.; Boazar, F.; Motamedi, E.

Divalency switch from carbenes to germynes at theoretical levels

Journal of Molecular Structure-Theochem, (849): 37-45 2008.

Kataoka, Y.; Paul, D.; Miyake, H.; Yaita, T.; Miyoshi, E.; Mori, H.; Tsukamoto, S.; Tatewaki, H.; Shinoda, S.; Tsukube, H.

Experimental and theoretical approaches toward anion-responsive tripod-lanthanide complexes: Mixed-donor ligand effects on lanthanide complexation and luminescence sensing profiles

Chemistry-a European Journal, (14): 5258-5266 2008.

Kaur, D.; Kohli, R.

- A comparative study on hydrogen bonding ability of thioformohydroxamic acid and formohydroxamic acid*
Journal of Molecular Structure-Theochem, (864): 72-79 2008.
- Kaur, D.; Kohli, R.
Intra and intermolecular hydrogen bonding in formohydroxamic acid
International Journal of Quantum Chemistry, (108): 119-134 2008.
- Kenawi, I. M.; Kamel, A. H.; Hilal, R. H.
BSSE effects on the static dipole polarizability and first dipole hyperpolarizability of diclofenac sodium
Journal of Molecular Structure-Theochem, (851): 46-53 2008.
- Kessar, S. V.; Singh, P.; Singh, K. N.; Bharatam, P. V.; Sharma, A. K.; Lata, S.; Kaur, A.
A study of BF₃-promoted ortho lithiation of anilines and DFT calculations on the role of fluorine-lithium interactions
Angewandte Chemie-International Edition, (47): 4703-4706 2008.
- Khalimon, A. Y.; Holland, J. P.; Kowalczyk, R. M.; McInnes, E. J. L.; Green, J. C.; Mountford, P.; Nikonov, G. I.
Synthesis and molecular and electronic structure of an unusual paramagnetic borohydride complex Mo(NAr)(2)(PMe₃)(2)(eta(2)-BH₄)(dagger)
Inorganic Chemistry, (47): 999-1006 2008.
- Khaliullin, R. Z.; Bell, A. T.; Head-Gordon, M.
Analysis of charge transfer effects in molecular complexes based on absolutely localized molecular orbitals
Journal of Chemical Physics, (128) 2008.
- Khartabil, H. K.; Gros, P. C.; Fort, Y.; Ruiz-Lopez, M. F.
A Theoretical Study on nBuLi/Lithium Aminoalkoxide Aggregation in Hexane and THF
Journal of Organic Chemistry, (73): 9393-9402 2008.
- Khilifi, A.; Raouafi, N.; Tapsoba, I.; Boujlel, K.; Benkhoud, M. L.
Reactivity of N-thioamido amidines with halogenated alkyl derivatives: synthesis of 4,5-disubstituted 2-alkylaminothiazoles
Journal of Sulfur Chemistry, (29): 593-605 2008.
- Kholod, Y.; Kosenkov, D.
CL-20 photodecomposition: Ab initio foundations for identification of products
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (71): 230-237 2008.
- Khongpracha, P.; Probst, M.; Limtrakul, J.
The interaction of a gold atom with carbon nanohorn and carbon nanotube tips and their complexes with a CO molecule: A first principle calculation
European Physical Journal D, (48): 211-219 2008.
- Kikuchi, Y.; Ishii, M.; Akiba, K.-y.; Nakai, H.

- Discovery of hexacoordinate hypervalent carbon compounds: Density functional study*
Chemical Physics Letters, (460): 37-41 2008.
- Kim, C. K.; Lee, K. A.; Chen, J.; Lee, H. W.; Lee, B.-S.; Kim, C. K.
Theoretical studies on the addition reactions of ketene with NH₃ in the gas phase and in non-aqueous solutions
Bulletin of the Korean Chemical Society, (29): 1335-1343 2008.
- Kim, D. Y.; Singh, N. J.; Lee, J. W.; Kim, K. S.
Solvent-driven structural changes in anion- π complexes
Journal of Chemical Theory and Computation, (4): 1162-1169 2008.
- Kim, J. C.; Kim, K. H.; Jung, J.; Han, Y.-K.
Reaction mechanisms of dissociative chemisorption of HI, I-2, and CH₃I on a magic cluster Al-13(-)
Journal of Computational Chemistry, (29): 1626-1631 2008.
- Kim, S.; Lind, M. C.; Schaefer, H. F., III
Structures and energetics of the deprotonated adenine-uracil base pair, including proton-transferred systems
Journal of Physical Chemistry B, (112): 3545-3551 2008.
- Kimmel, A. V.; Sushko, P. V.; Shluger, A. L.; Kuklja, M. M.
Effect of molecular and lattice structure on hydrogen transfer in molecular crystals of diamino-dinitroethylene and triamino-trinitrobenzene
Journal of Physical Chemistry A, (112): 4496-4500 2008.
- Kleinpeter, E.; Boelke, U.
Polar substituent effect of the ester group on conformational equilibria of O-mono-substituted cyclohexanes - the para-substituent effect in cyclohexyl benzoates
Tetrahedron, (64): 10014-10017 2008.
- Kleinpeter, E.; Fettke, A.
Quantification of the (anti) aromaticity of fulvenes subject to ring size
Tetrahedron Letters, (49): 2776-2781 2008.
- Kleinpeter, E.; Holzberger, A.; Wacker, P.
Quantification of the (anti)aromaticity of fulvalenes subjected to π -electron cross-delocalization
Journal of Organic Chemistry, (73): 56-65 2008.
- Kluefers, P.; Reichvilser, M. M.
Toward carbohydrate derivatives with a markedly acidic centre: Structures and reactions of selenium(IV) diolates
European Journal of Inorganic Chemistry: 384-396 2008.
- Kobychev, V. B.; Vitkovskaya, N. M.; Trofimov, B. A.
Theoretical study of the [1,3]-prototropic rearrangements of oximes and their
Journal of Structural Chemistry, (49): 216-223 2008.

- Kolmann, S. J.; Chan, B.; Jordan, M. J. T.
Modelling the interaction of molecular hydrogen with lithium-doped hydrogen storage materials
Chemical Physics Letters, (467): 126-130 2008.
- Kolodziejczak, J.; Jezierska, A.; Panek, J. J.; De Borggraeve, W. M.; Kochel, A.; Jose, R. A.; Koll, A.
Structural property investigations of 1-[2-(2-methoxyphenyl)ethyl]piperidinium chloride: An experimental and computational study
Journal of Molecular Structure, (891): 184-191 2008.
- Koput, J.
Ab initio study on the structure and vibration-rotation energy levels of dilithium monofluoride
Journal of Chemical Physics, (129) 2008.
- Kosa, M.; Krack, M.; Cheetham, A. K.; Parrinello, M.
Modeling the Hydrogen Storage Materials with Exposed M²⁺ Coordination Sites
Journal of Physical Chemistry C, (112): 16171-16173 2008.
- Koshevoy, I. O.; Karttunen, A. J.
Supramolecular Luminescent Gold(I)-Copper(I) Complexes: Self-Assembly of the AuxCuy Clusters inside the [Au-3(diphosphine)(3)](3+) Triangles
Inorganic Chemistry, (47): 9478-9488 2008.
- Kozlov, A. V.; Semenov, V. E.; Mikhailov, A. S.; Aganov, A. V.; Smith, M. B.; Reznik, V. S.; Latypov, S. K.
Preferential protonation and methylation site of thiopyrimidine derivatives in solution: NMR data
Journal of Physical Chemistry B, (112): 3259-3267 2008.
- Kraka, E.; Cremer, D.
Bonding in mercury-alkali molecules: Orbital-driven van der Waals complexes
International Journal of Molecular Sciences, (9): 926-942 2008.
- Kramer, M. U.; Robert, D.
Cationic Methyl Complexes of the Rare-Earth Metals: An Experimental and Computational Study on Synthesis, Structure, and Reactivity
Inorganic Chemistry, (47): 9265-9278 2008.
- Kramos, B.; Kovacs, A.
Metal-ligand interactions in Fe(II)-dioxime complexes
Journal of Molecular Structure-Theochem, (867): 1-4 2008.
- Krapp, A.; Frenking, G.; Uggerud, E.
Nonpolar dihydrogen bonds - On a gliding scale from weak dihydrogen interaction to covalent H-H in symmetric radical cations [HnE-H-H-EHn](+)
Chemistry-a European Journal, (14): 4028-4038 2008.
- Krawczyk, H.; Albrecht, L.; Wojciechowski, J.; Wolf, W. M.
Synthesis and crystal structure of 1-(aminomethyl)vinylphosphonic acid
Tetrahedron, (64): 5051-5054 2008.

- Krawczyk, H.; Albrecht, L.; Wojciechowski, J.; Wolf, W. M.
Synthesis and crystal structure of 1-(aminomethyl)vinylphosphonic acid
Tetrahedron, (64): 5051-5054 2008.
- Kruszynski, R.
Intermolecular interactions in 2,4-dinitrophenylhydrazine hydrochloride hydrate: X-ray structural and quantum mechanical study
Central European Journal of Chemistry, (6): 542-548 2008.
- Kuiper, D. S.; Wolczanski, P. T.; Lobkovsky, E. B.; Cundari, T. R.
Four-Coordinate Mo(II) as (silox)(2)Mo(PMe3)(2) and Its W(IV) Congener (silox)(2)HW(eta(2)-CH2PMe2)(PMe3) (silox = (Bu3SiO)-Bu-t)
Inorganic Chemistry, (47): 10542-10553 2008.
- Kuiper, D. S.; Wolczanski, P. T.; Lobkovsky, E. B.; Cundari, T. R.
Four-Coordinate Mo(II) as (silox)(2)Mo(PMe(3))(2) and Its W(IV) Congener (silox)(2)HW(eta(2)-CH(2)PMe(2))(PMe(3)) (silox = (t)Bu(3)SiO)
Inorganic Chemistry, (47): 10542-10553 2008.
- Kuiper, D. S.; Wolczanski, P. T.; Lobkovsky, E. B.; Cundari, T. R.
Low coordinate, monomeric molybdenum and tungsten(III) complexes: Structure, reactivity and calculational studies of (silox)(3)Mo and (silox)(3)ML (M = Mo, W; L = PMe3, CO; silox = (Bu3SiO)-Bu-t)
Journal of the American Chemical Society, (130): 12931-12943 2008.
- Kuiper, D. S.; Wolczanski, P. T.; Lobkovsky, E. B.; Cundari, T. R.
Low coordinate, monomeric molybdenum and tungsten(III) complexes: Structure, reactivity and calculational studies of (silox)(3)Mo and (silox)(3)ML (M = Mo, W; L = PMe3, CO; silox = (Bu3SiO)-Bu-t)
Journal of the American Chemical Society, (130): 12931-12943 2008.
- Kumar, R.; Skinner, J. L.
Water simulation model with explicit three-molecule interactions
Journal of Physical Chemistry B, (112): 8311-8318 2008.
- Kuznetsov, M. L.; Kukushkinc, V. Y.; Pombeiro, A. J. L.
Reactivity of Pt- and Pd-bound nitriles towards nitrile oxides and nitrones: substitution vs. cycloaddition
Dalton Transactions: 1312-1322 2008.
- Kyne, S. H.; Schiesser, C. H.; Matsubara, H.
Multiorbital interactions during acyl radical addition reactions involving Imines and electron-rich olefins
Journal of Organic Chemistry, (73): 427-434 2008.
- La Macchia, G.; Aquilante, F.; Veryazov, V.; Roos, B. O.; Gagliardi, L.
Bond Length and Bond Order in One of the Shortest Cr-Cr Bonds

- Inorganic Chemistry, (47): 11455-11457 2008.
- Laali, K. K.; Arrica, M. A.; Okazaki, T.; Bunge, S. D.
Synthesis and Stable-Ion Studies of Regioisomeric Acetylnitropyrenes and Nitropyrenyl Carbinols and GIAO-DFT Study of Nitro Substituent Effects on alpha-Pyrenyl Carbocations
European Journal of Organic Chemistry: 6093-6105 2008.
- Lage, M. L.; Fernandez, I.; Mancheno, M. J.; Sierra, M. A.
Electronic structure of alkoxychromium(0) carbene complexes: A joint TD-DFT/experimental study
Inorganic Chemistry, (47): 5253-5258 2008.
- Lahiri, S.; Yadav, S.; Banerjee, S.; Patil, M. P.; Sunoj, R. B.
Face-selective Diels-Alder reactions between unsymmetrical cyclohexadienes and symmetric trans-dienophile: An experimental and computational investigation
Journal of Organic Chemistry, (73): 435-444 2008.
- Lai, C. H.; Chou, P. T.
The theoretical comparison between two model NO carriers, MeSNO and MeSeNO
Journal of Molecular Modeling, (14): 1-9 2008.
- Lamsabhi, A. M.; Mo, O.; Yanez, M.; Guillemin, J.-C.; Haldys, V.; Tortajada, J.; Salpin, J.-Y.
Ni+ reactions with aminoacetonitrile, a potential prebiological precursor of glycine
Journal of Mass Spectrometry, (43): 317-326 2008.
- Lange, A. W.; Rohrdanz, M. A.; Herbert, J. M.
Charge-transfer excited states in a pi-stacked adenine dimer, as predicted using long-range-corrected time-dependent density functional theory
Journal of Physical Chemistry B, (112): 6304-6308 2008.
- Lapkowski, M.; Plewa, S.; Stolarczyk, A.; Doskocz, J.; Soloducho, J.; Cabaj, J.; Bartoszek, M.; Sulkowski, W. W.
Electrochemical synthesis of polymers with alternate phenothiazine and bithiophene units
Electrochimica Acta, (53): 2545-2552 2008.
- Larkin, J. D.; Bhat, K. L.; Markham, G. D.; James, T. D.; Brooks, B. R.; Bock, C. W.
A computational characterization of boron-oxygen multiple bonding in HN=CH-CH=CH-NH-BO
Journal of Physical Chemistry A, (112): 8446-8454 2008.
- Larkin, J. D.; Milkevitch, M.; Bhat, K. L.; Markham, G. D.; Brooks, B. R.; Bock, C. W.
Dimers of boroglycine and methylamine boronic acid: A computational comparison of the relative importance of dative versus hydrogen bonding
Journal of Physical Chemistry A, (112): 125-133 2008.
- Latelli, N.; Zeroual, S.; Ouddai, N.; Mokhtari, M.; Ciofini, I.
Reactivity of nitrobenzofurazan towards nucleophiles: Insights from DFT
Chemical Physics Letters, (461): 16-20 2008.

Le, T. D.; Weyland, M.-C.; El-Harouch, Y.; Arquier, D.; Vendier, L.; Miqueu, K.; Sotiropoulos, J.-M.; Bastin, S.; Igau, A.

N-phosphanylformamidines (phosfam) R-2 ' N-C(H)=N-PR2: One-pot synthesis and versatile protonation reaction

European Journal of Inorganic Chemistry: 2577-2583 2008.

Lechtken, A.; Neiss, C.; Stairs, J.; Schooss, D.

Comparative study of the structures of copper, silver, and gold icosamers: Influence of metal type and charge state

Journal of Chemical Physics, (129) 2008.

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

Structural and vibrational study of 2-(2'-furyl)-1H-imidazole

Journal of Physical Organic Chemistry, (21): 1086-1097 2008.

Lee, D.-K.; Lim, I. S.; Lee, Y. S.; Jeung, G.-H.

Relativistic effects on the ground state properties of group 1 and group 11 cyanides estimated from quantum chemical calculations

International Journal of Mass Spectrometry, (271): 22-29 2008.

Lee, H. M.; Kim, K. S.

Hydrogen detachment of the hydrated hydrohalogen acids upon attaching an excess electron

Journal of Chemical Physics, (128) 2008.

Lee, W.; Jang, S.; Kim, M. J.; Myoung, J.-M.

Interfacial interactions and dispersion relations in carbon-aluminium nanocomposite systems

Nanotechnology, (19) 2008.

Lee, Y.-m.; Lim, C.

Physical basis of structural and catalytic Zn-binding sites in proteins

Journal of Molecular Biology, (379): 545-553 2008.

Lei, X. L.; Zhu, H. J.; Wang, X. M.; Luo, Y. H.

Equilibrium geometries and electronic properties of BenLi (n=2-15) clusters from first principles

Chinese Physics B, (17): 3687-3695 2008.

Leovac, V. M.; Markovic, S.; Divjakovic, V.; Szecsenyi, K. M.; Joksovic, M. D.; Leban, I.

Structural and DFT Studies on Molecular Structure of Ni(II) Chloride Complex with Pyridoxal Semicarbazone (PLSC). Unusual Coordination Mode of PLSC

Acta Chimica Slovenica, (55): 850-860 2008.

Leovac, V. M.; Tomic, Z. D.; Kovacs, A.; Joksovic, M. D.; Jovanovic, L. S.; Szecsenyi, K. M.

Cobalt(II) complexes with disubstituted 3-aminopyrazole derivative: Mononuclear Co(II) complex with in situ prepared formamidine ligand

Journal of Organometallic Chemistry, (693): 77-86 2008.

Lessing, J.; Li, X.; Lee, T.; Rose-Petruck, C. G.

Structure of solvated Fe(CO)(5): Complex formation during solvation in alcohols

- Journal of Physical Chemistry A, (112): 2282-2292 2008.
- Li, A.
Theoretical study of bifurcated bent blue-shifted hydrogen bonds CH₂ center dot center dot center dot Y
Science in China Series B-Chemistry, (51): 623-631 2008.
- Li, H.; Li, W.; Li, S.; Ma, J.
Fragmentation-based QM/MM simulations: Length dependence of chain dynamics and hydrogen bonding of polyethylene oxide and polyethylene in aqueous solutions
Journal of Physical Chemistry B, (112): 7061-7070 2008.
- Li, H. B.; Tian, S. X.
Chemical bonds and electronic structures of the methonium cations CH₆²⁺ and CH₇³⁺
Journal of Theoretical & Computational Chemistry, (7): 139-156 2008.
- Li, H. B.; Tian, S. X.
Chemical bonds and electronic structures of the methonium cations CH₆²⁺ and CH₇³⁺
Journal of Theoretical & Computational Chemistry, (7): 139-156 2008.
- Li, H. B.; Tian, S. X.; Yang, J. L.
Theoretical Study of the Stepwise Protonation of the Dioxo Manganese(V) Porphyrin
Journal of Physical Chemistry B, (112): 15807-15812 2008.
- Li, H. B.; Tian, S. X.; Yang, J. L.
Theoretical Study of the Stepwise Protonation of the Dioxo Manganese(V) Porphyrin
Journal of Physical Chemistry B, (112): 15807-15812 2008.
- Li, H.-Z.; Wang, Y.-C.
The theoretical investigation on gas-phase chemistry of YNH⁺ with propene
Journal of Molecular Structure-Theochem, (866): 5-10 2008.
- Li, J.; Huang, H.; Huang, Y.; Dong, H.
A theoretical study of highly nitrated azacubanes
Journal of Energetic Materials, (26): 230-245 2008.
- Li, J.; Jia, G.; Lin, Z.
Theoretical studies on coupling reactions of carbon dioxide with alkynes mediated by nickel(0) complexes
Organometallics, (27): 3892-3900 2008.
- Li, J. S.
An Ab Initio Theoretical Study of 2,4,6-Trinitro-1,3,5-Triazine, 3,6-Dinitro-1,2,4,5-Tetrazine, and 2,5,8-Trinitro-Tri-s-Triazine
Propellants Explosives Pyrotechnics, (33): 443-447 2008.
- Li, M.-X.; Zhu, M.-L.; Lu, L.-P.
Ethyl [(2-hydroxyphenyl)(pyridinium-2-ylamino)methyl]phosphonate methanol solvate

Acta Crystallographica Section E-Structure Reports Online, (64): O1178-U1098 2008.

Li, P.; Xie, X.; Bu, Y.; Wang, W.; Wang, N.; Shi, J.; Mou, Z.

Theoretical studies on the coupling interactions and self-exchange reaction mechanisms in the complexes of NO with ONH and NOH

Journal of Theoretical & Computational Chemistry, (7): 435-446 2008.

Li, Q.; An, M.; Luan, F.; Li, W.; Gong, B.; Cheng, J.

Regulating function of methyl group in strength of CH center dot center dot center dot O hydrogen bond: A high-level ab initio study

Journal of Physical Chemistry A, (112): 3985-3990 2008.

Li, Q.; An, X.

Non-additivity of methyl group in the single-electron halogen bond of CH₃-BrH complex

Journal of Molecular Structure-Theochem, (866): 11-14 2008.

Li, Q.; An, X.; Luan, F.; Li, W.; Gong, B.; Cheng, J.; Sun, J.

The effect of methyl group on the cooperativity between three types of hydrogen bond: O-H center dot center dot center dot O, C-H center dot center dot center dot O, and O-H center dot center dot center dot pi

International Journal of Quantum Chemistry, (108): 558-566 2008.

Li, Q.; Liu, H.; An, X.; Gong, B.; Cheng, J.

Effect of methyl group on the cooperativity of CH center dot center dot center dot O blue-shifted hydrogen bond in HCHO-HCHO-HCHO cyclic complex

Journal of Molecular Structure-Theochem, (861): 14-17 2008.

Li, Q.; Wang, N.; Yu, Z.

Solvent effect on the role of methyl groups in formation of O center dot center dot center dot HO hydrogen bond in dimethyl ether-methanol complex

Journal of Molecular Structure-Theochem, (862): 74-79 2008.

Li, Q. G.; Deng, C.; Ren, Y.; Wong, N. B.; Chu, S. Y.; Wang, X.

Tautomerism of monochalcogenosilanoic acids CH₃Si(=O)XH (X = s, se, te) in the gas phase and in the polar and aprotic solution: An ab initio computational investigation

International Journal of Quantum Chemistry, (108): 142-150 2008.

Li, Q. Z.; An, X. L.; Luan, F.; Li, W. Z.; Gong, B. A.; Cheng, J. B.; Sun, J. Z.

The effect of methyl group on the cooperativity between three types of hydrogen bond: O-H center dot center dot center dot O, C-H center dot center dot center dot O, and O-H center dot center dot center dot pi

International Journal of Quantum Chemistry, (108): 558-566 2008.

Li, R. J.; Zhang, Y. X.; Zhou, Y.; Dong, S. A.; Zhang, X. Y.; Bian, Y. Z.; Jiang, J. Z.

H₂O-Involved Hydrogen Bonds in Pseudo-Double-Decker Supramolecular Structure of 1,8,15,22-Tetrasubstituted Phthalocyaninato Zinc Complex

Crystal Growth & Design, (8): 4454-4459 2008.

- Li, W. Q.; Liu, L. L.; Feng, J. K.; Liu, Z. Z.; Ren, A. M.; Zhang, G.; Sun, C. C.
PYRAMIDALITY AND AROMATICITY IN POLYPHOSPHAPHOSPHOLES
Journal of Theoretical & Computational Chemistry, (7): 1203-1214 2008.
- Li, X.; Shi, X.
A theoretical investigation on the Ti(CH₃)₄(0,-1) clusters by density functional theory methods
Journal of Molecular Structure-Theochem, (864): 62-67 2008.
- Li, X.; Ye, S.; He, C.; Yu, Z.-X.
Mechanisms of bronsted acid catalyzed additions of phenols and protected amines to olefins: A DFT study
European Journal of Organic Chemistry: 4296-4303 2008.
- Li, Y.; Wu, D.; Li, Z. R.
Compounds of Superatom Clusters: Preferred Structures and Significant Nonlinear Optical Properties of the BLi₆-X (X = F, LiF₂, BeF₃, BF₄) Motifs
Inorganic Chemistry, (47): 9773-9778 2008.
- Li, Z.; Wang, C.; Fu, Y.; Guo, Q.-X.; Liu, L.
Substituent effect on the efficiency of desulfurizative rearrangement of allylic disulfides
Journal of Organic Chemistry, (73): 6127-6136 2008.
- Li, Z.; Zhu, Y.; Yang, S.; Lu, X.
Quantum chemical and topological study on the insertion reaction of dichlorocarbene with acetaldehyde
Chinese Science Bulletin, (53): 2287-2296 2008.
- Li, Z.-F.; Lue, L.-L.
Theoretical study on the mechanism of CF₂ reaction with CH₂O
Chinese Journal of Structural Chemistry, (27): 1039-1044 2008.
- Li, Z.-W.; Ren, A.-M.
Color-tuning mechanism in firefly luminescence: Theoretical studies on fluorescence of oxyluciferin in aqueous solution using time dependent density functional theory
Journal of Physical Chemistry A, (112): 9796-9800 2008.
- Liang, G. M.; Bao, X. G.; Gu, J. D.
The Possibility of the Decomposition of 2'-Deoxyribose Moiety of Thymidine Induced by the Low Energy Electron Attachment
Journal of Computational Chemistry, (29): 2648-2655 2008.
- Liang, J.-X.; Geng, Z.-Y.; Wang, Y.-C.; Han, Y.-X.; Yan, P.-J.
Theoretical study on reaction of C₆H₅⁻ with N₂O in gas phase
Journal of Molecular Structure-Theochem, (859): 79-85 2008.
- Liang, Q.; Wang, Q.; Xu, S.-F.; Sun, Y.-X.
Experimental and theoretical studies on bis[μ-2-methoxy-N⁻(2-oxidobenzoyl)benzohydrazidato(3-)]dipyridinetricopper(II)

- Structural Chemistry, (19): 279-284 2008.
- Liang, X.; Pu, X.; Liao, X.; Wong, N.-B.; Tian, A.
Theoretical study of structures and properties of cyclobutadiene, cyclopentadiene and benzene and their nitrogen isoelectronic equivalents
Journal of Molecular Structure-Theochem, (860): 86-94 2008.
- Liang, X.-Q.; Pu, X.-M.; Tian, A.-M.
Structures and properties of s-triazine derivations substituted by substituent groups containing nitrogen
Acta Physico-Chimica Sinica, (24): 639-645 2008.
- Liao, S. Y.; Chen, J. C.; Qian, L.; Shen, Y.; Zheng, K. C.
QSAR, action mechanism and molecular design of flavone and isoflavone derivatives with cytotoxicity against HeLa
European Journal of Medicinal Chemistry, (43): 2159-2170 2008.
- Liao, S. Y.; Qian, L.; Chen, J. C.; Lu, H. L.; Zheng, K. C.
2D and 3D-QSAR studies on antiproliferative thiazolidine analogs
International Journal of Quantum Chemistry, (108): 1380-1390 2008.
- Liao, S. Y.; Qian, L.; Lu, H. L.; Shen, Y.; Zheng, K. C.
Combined 2D-and 3D-QSAR study on analogues of ARC-111 with antitumor activity
Qsar & Combinatorial Science, (27): 740-749 2008.
- Liao, Y.; Ma, J.
Stacking and solvent effects on the electronic and optical properties of gold and mercury acetylide aggregations: A theoretical study
Organometallics, (27): 4636-4648 2008.
- Librando, V.; Alparone, A.; Tomaselli, G.
Electronic properties of some nitrobenzo[a]pyrene isomers: a possible relationship to mutagenic activity
Journal of Molecular Modeling, (14): 489-497 2008.
- Lill, S. O. N.
Computational note on the dimerisation of lithium alkoxides
Journal of Molecular Structure-Theochem, (866): 81-81 2008.
- Lillestolen, T. C.; Wheatley, R. J.
Redefining the atom: atomic charge densities produced by an iterative stockholder approach
Chemical Communications: 5909-5911 2008.
- Liu, F. L.; Li, J.; Zhang, H.
DFT study of a heterofullerene molecule containing fifty-eight carbon atoms and one sulphur atom
Chemical Physics, (353): 19-24 2008.

- Liu, F.-L.; Jalbout, A. F.
Structural, electronic, and magnetic properties of heterofullerene C58Si with odd number of atoms and a near planar tetracoordinate Si atom
Journal of Molecular Graphics and Modelling, (26): 1327-1332 2008.
- Liu, F.-L.; Wang, C.-H.
DFT study of structural, electronic, vibrational, and magnetic properties of the chirality cage-like molecule C24O12
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (70): 1141-1145 2008.
- Liu, F.-L.; Wang, C.-H.
Structural, electronic, and magnetic properties of two isomers of C40O10 with cage-like structure
Journal of Molecular Graphics and Modelling, (26): 893-899 2008.
- Liu, H.-Y.
DFT calculations on manganese(III)5,10,15-tris(pentafluorophenyl)-corrole
Acta Physico-Chimica Sinica, (24): 1602-1608 2008.
- Liu, S.; Govind, N.
Toward understanding the nature of internal rotation barriers with a new energy partition scheme: Ethane and n-butane
Journal of Physical Chemistry A, (112): 6690-6699 2008.
- Liu, S.; Govind, N.; Pedersen, L. G.
Exploring the origin of the internal rotational barrier for molecules with one rotatable dihedral angle
Journal of Chemical Physics, (129) 2008.
- Liu, T.; Li, H.; Huang, M.-B.; Duan, Y.; Wang, Z.-X.
Two-way effects between hydrogen bond and intramolecular resonance effect: An ab initio study on complexes of formamide and its derivatives with water
Journal of Physical Chemistry A, (112): 5436-5447 2008.
- Liu, W.-L.; Wang, Z.-G.
Effect of beta-Ring Rotation on the Structures and Vibrational Spectra of beta-Carotene: Density Functional Theory Analysis
Journal of Physical Chemistry A, (112): 10580-10585 2008.
- Liu, Y.
Hydrogen bonding characterization of XH2NH2 center dot center dot center dot HNO(X = B, Al, Ga) complexes: A theoretical investigation
International Journal of Quantum Chemistry, (108): 1123-1129 2008.
- Liu, Y.
Theoretical study on the multi-channel reaction of CH3S with ClO
Journal of Molecular Structure-Theochem, (866): 46-51 2008.
- Liu, Y.; Villamena, F. A.; Sun, J.; Xu, Y.; Dhimitruka, I.; Zweier, J. L.

- Synthesis and characterization of ester-derivatized tetrathiatriarylmethyl radicals as intracellular oxygen probes*
Journal of Organic Chemistry, (73): 1490-1497 2008.
- Liu, Y.-Z.; He, L.-H.
Structures and electronic properties of HOCl center dot center dot center dot HCOCl complexes
Acta Physico-Chimica Sinica, (24): 1625-1630 2008.
- Long, H.; Chang, C. H.
Brownian dynamics and molecular dynamics study of the association between hydrogenase and ferredoxin from Chlamydomonas reinhardtii
Biophysical Journal, (95): 3753-3766 2008.
- Lopes, J. F.; Rocha, W. R.; Dos Santos, H. F.; De Almeida, W. B.
Theoretical study of the potential energy surface for the interaction of cisplatin and their aquated species with water
Journal of Chemical Physics, (128) 2008.
- Lto, K.; Pu, Z.; Li, Q. S.; Schleyer, P. V. R.
Cyclic Boron Clusters Enclosing Planar Hypercoordinate Cobalt, Iron, and Nickel
Inorganic Chemistry, (47): 10906-10910 2008.
- Lu, H.; Wang, Y.
Hydrogen-bond network and local structure of liquid water: An atoms-in-molecules perspective
Journal of Chemical Physics, (129) 2008.
- Lu, Q.-X.; Tan, H.-W.; Chen, G.-J.; Wang, Y.
Theoretical studies on electronic structures and catalytic activities of superoxide dismutase mimetics of imidazolate-bridged dinuclear Cu(II) complexes
Chemical Journal of Chinese Universities-Chinese, (29): 1635-1640 2008.
- Lu, T.-T.; Xiang, M.; Wang, H.-L.; He, T. J.; Chen, D.-M.
Density functional theory studies of N-protonation of the free base phthalocyanine
Journal of Molecular Structure-Theochem, (860): 141-149 2008.
- Lucas, M. F.; Michelini, M. C.; Russo, N.; Sicilia, E.
On the nature of the CP bond in phosphalkynes
Journal of Chemical Theory and Computation, (4): 397-403 2008.
- Lucena, J. R.; Sharma, A.; Reva, I. D.; Araujo, R.; Ventura, E.; do Monte, S. A.; Braga, C. F.; Ramos, M. N.; Fausto, R.
Matrix Isolation FTIR Spectroscopic and Theoretical Study of 3,3-Dichloro-1,1,1-Trifluoropropane (HCFC-243)
Journal of Physical Chemistry A, (112): 11641-11648 2008.
- Lue, L.; Wang, X.; Wang, Y.; Dai, G.
A theoretical study of the proton transfer process in the spin-forbidden reaction (HNO)-H-1((1)A') + OH- -> (NO-)-N-3((3)Sigma(-))+H2O

- Chinese Science Bulletin, (53): 1489-1496 2008.
- Lue, L.-L.; Yan, E.-D.; Wang, X.-F.; Wang, Y.-C.; Dai, G.-L.
Theoretical study on the photochemical ring opening process of 2H-pyran
Chinese Journal of Chemistry, (26): 1195-1200 2008.
- Lukes, V.; Matuszna, K.; Rapta, P.; Solc, R.; Dunsch, L.; Aquino, A. J. A.; Lischka, H.
Experimental and theoretical study of model ladder fluoranthenopyracylene with two-dimensional pi-conjugation upon charging: Structure and optical properties
Journal of Physical Chemistry C, (112): 3949-3958 2008.
- Luo, Q.
Theoretical observation of hexatomic molecules containing pentacoordinate planar carbon
Science in China Series B-Chemistry, (51): 1030-1035 2008.
- Lyakhov, A. S.; Matulis, V. E.; Gaponik, P. N.; Voitekhovich, S. V.; Ivashkevich, O. A.
1-Vinyl-5-amino-1H-tetrazole: X-ray molecular and crystal structures and quantum-chemical DFT calculations
Journal of Molecular Structure, (876): 260-267 2008.
- Lyon, J. T.; Andrews, L.; Hu, H.-S.; Li, J.
Infrared spectra and electronic structures of agostic uranium methyldene molecules
Inorganic Chemistry, (47): 1435-1442 2008.
- Lyubimova, O.; Sizova, O. V.
The nature of the metal-nitric oxide bond in the $[M(CN)(5)(NO)](q)$ ($M = Cr, Mn, Fe, Ru, Os, and Co$) and $trans-[Ru(NH_3)(4)L(NO)](q)$ ($L = pyrazine, pyridine, N-2, H_2O, Cl-, CN-, NO_2-$) complexes: A bond-energy decomposition analysis
Journal of Molecular Structure-Theochem, (865): 28-35 2008.
- Ma, C.-P.; Yao, L.; Ge, M.-F.
Substituent effects of halopyridines
Journal of Molecular Structure, (881): 123-131 2008.
- Ma, F.; Li, Z. R.; Xu, H. L.; Li, Z. J.; Li, Z. S.; Aoki, Y.; Gu, F. L.
Lithium Salt Electride with an Excess Electron Pair-A Class of Nonlinear Optical Molecules for Extraordinary First Hyperpolarizability
Journal of Physical Chemistry A, (112): 11462-11467 2008.
- Ma, H.; Xiao, H.; Song, J.; Ju, X.; Zhu, W.; Yu, K.
Molecular structure of 4-amino-1,2,4-triazol-5-one and a density-functional theoretical investigation of its dimers and crystal band structure
Chemical Physics, (344): 79-89 2008.
- Machura, B.; Kusz, J.
Reactivity of oxorhenium(V) complexes towards 8-hydroxyquinoline-2-carboxylic acid: X-ray structure of $[ReOCl_2(hquin-2-COOH)(AsPh_3)] \cdot MeCN$ and $[ReOCl_2(hquin-2-$

- COOH)(PPh3)]center dot MeCN complexes. DFT and TDDFT calculations for [ReOCl2(hquin-2-COOH)(AsPh3)]*
Polyhedron, (27): 366-374 2008.
- Machura, B.; Milek, J.; Kusz, J.; Nycz, J.; Tabak, D.
Reactivity of oxorhenium(V) complexes towards quinoline carboxylic acids. X-ray structure of [ReOCl2(hquin-7-COOH)(PPh3)]center dot OPPh3, [ReOBr2(hquin-7-COOH)(PPh3)] and [ReOX2(hmquin-7-COOH)(PPh3)]. DFT and TD-DFT calculations for [ReOCl2(hquin-7-COOH)(PPh3)]
Polyhedron, (27): 1121-1130 2008.
- Maciel, G. S.; Cappelletti, D.; Grossi, G.; Pirani, F.; Aquilanti, V.
Elementary processes in atmospheric chemistry: Quantum studies of intermolecular dimer formation and intramolecular dynamics
Advances in Quantum Chemistry: Applications of Theoretical Methods to Atmospheric Science: 311-332 2008.
- Mak, A. M.; Steudel, R.; Wong, M. W.
Homolytic S-S bond dissociation of 11 bis(thiocarbonyl)disulfides R-C(S)-S-S-C(=S)R and prediction of a novel rubber vulcanization accelerator
Chemistry-an Asian Journal, (3): 1026-1034 2008.
- Makiabadi, B.; Roohi, H.
Interaction between O-3 and H2O2: A theoretical study
Chemical Physics Letters, (460): 72-78 2008.
- Mallick, D.; Parameswaran, P.; Jemmis, E. D.
Structure and Bonding in Cyclic Isomers of B2AlHnm (n=3-6, m =-2 to+1): A Comparative Study with B3Hnm, BAl2Hnm and Al3Hnm
Journal of Physical Chemistry A, (112): 13080-13087 2008.
- Mani, P.; Umamaheswari, H.; Joshua, B. D.; Sundaraganesan, N.
Molecular structure, vibrational spectra and NBO analysis of phenylisothiocyanate by density functional method
Journal of Molecular Structure-Theochem, (863): 44-49 2008.
- Mansfield, N. E.; Coles, M. P.; Hitchcock, P. B.
A Structural and Theoretical Study of the Thiophosphinite and Dithiophosphinate Anions
Phosphorus Sulfur and Silicon and the Related Elements, (183): 2685-2702 2008.
- Manz, T. A.; Sharma, S.; Phomphrai, K.; Novstrup, K. A.; Fenwick, A. E.; Fanwick, P. E.; Medvedev, G. A.; Abu-Omar, M. M.; Delgass, W. N.; Thomson, K. T.; Caruthers, J. M.
Quantitative Effects of Ion Pairing and Sterics on Chain Propagation Kinetics for 1-Hexene Polymerization Catalyzed by Mixed Cp'/ArO Complexes
Organometallics, (27): 5504-5520 2008.
- Mao, S.; Pu, X.; Li, L.; Wong, N.-B.; Tian, A.
Theoretical predictive study on N7H7 hydronitrogen compounds

- Journal of Molecular Structure-Theochem, (858): 12-17 2008.
- Mao, S.; Tan, Y.-X.; Pu, X.-M.; Li, L.-C.; Tian, A.-M.
Isomerization and conformation transformation of triazane
Acta Physico-Chimica Sinica, (24): 981-986 2008.
- Marcos, E.; Crehuet, R.; Anglada, J. M.
Inductive and external electric field effects in pentacoordinated phosphorus compounds
Journal of Chemical Theory and Computation, (4): 49-63 2008.
- Markad, S. D.; Xia, S.; Snyder, N. L.; Surana, B.; Morton, M. D.; Hadad, C. M.; Peczu, M. W.
Stereoselectivity in the epoxidation of carbohydrate-based oxepines
Journal of Organic Chemistry, (73): 6341-6354 2008.
- Markovic, S.; Durovic, I.; Markovic, Z.
Formation of sodium 6-hydroxy-2-naphthoate in the Kolbe-Schmitt reaction
Monatshefte fur Chemie, (139): 1169-1174 2008.
- Markovic, S.; Stankovic, S.; Radenkovic, S.; Gutman, I.
Electronic Structure Study of Thermal Intraconversions of Some Dicyclopenta-Fused Polycyclic Aromatic Compounds
Journal of Chemical Information and Modeling, (48): 1984-1989 2008.
- Markovic, Z.; Markovic, S.
Last step of the para route of the Kolbe-Schmitt reaction
Journal of Chemical Information and Modeling, (48): 143-147 2008.
- Markovic, Z.; Markovic, S.
Last step of the para route of the Kolbe-Schmitt reaction
Journal of Chemical Information and Modeling, (48): 143-147 2008.
- Markovic, Z.; Markovic, S.; Durovic, I.
Kolbe-Schmitt reaction of sodium 2-naphthoxide
Monatshefte fur Chemie, (139): 329-335 2008.
- Mata, R. A.; Stoll, H.
Incremental expansions for SCF interaction energies: A comparison for hydrogen-bonded clusters
Chemical Physics Letters, (465): 136-141 2008.
- Mata, R. A.; Werner, H.-J.; Schuetz, M.
Correlation regions within a localized molecular orbital approach
Journal of Chemical Physics, (128) 2008.
- Matano, Y.; Miyajima, T.; Ochi, N.; Nakabuchi, T.; Shiro, M.; Nakao, Y.; Sakaki, S.; Imahori, H.
Syntheses, structures, and coordination chemistry of phosphole-containing hybrid calixphyrins: Promising macrocyclic P,N-2,X-mixed donor ligands for designing reactive transition-metal complexes
Journal of the American Chemical Society, (130): 990-1002 2008.

- Matos, M. A. R.; Sousa, C. C. S.; Morais, V. M. F.
Experimental and theoretical thermochemistry of beta-tetralone
Journal of Chemical Thermodynamics, (40): 1552-1557 2008.
- Mawhinney, R. C.; Goddard, J. D.
A theoretical study of H(S₂N₂)(Y)H (Y = 1, 2, 3, 4, 5): Modeling the superconducting polymer (SN)(X)
Journal of Molecular Structure-Theochem, (856): 16-29 2008.
- Mayr, M.; Bataille, C. J. R.; Gosiewska, S.; Raskatov, J. A.; Brown, J. M.
Synthesis and rhodium complexation of enantiomerically enriched bicyclo[3.3.1]nona-2,6-diene
Tetrahedron-Asymmetry, (19): 1328-1332 2008.
- Mazzone, G.; Michelihi, M. d. C.; Russo, N.; Sicilia, E.
Mechanistic aspects of the reaction of Th⁺ and Th²⁺ with water in the gas phase
Inorganic Chemistry, (47): 2083-2088 2008.
- McDowell, S. A. C.
A computational study of some structural analogues of the lowest energy structure of periodane
Molecular Physics, (106): 141-146 2008.
- Meng, Q.; Wang, F.; Li, M.
Density functional computations of alkynylation of ethanimine catalyzed by chiral zinc (II)-complexes
International Journal of Quantum Chemistry, (108): 362-369 2008.
- Meng, Q. X.; Wang, F.; Li, M.
Density functional computations of alkynylation of ethanimine catalyzed by chiral zinc (II)-complexes
International Journal of Quantum Chemistry, (108): 362-369 2008.
- Michalak, A.; DeKock, R. L.; Ziegler, T.
Bond multiplicity in transition-metal complexes: Applications of two-electron valence indices
Journal of Physical Chemistry A, (112): 7256-7263 2008.
- Michalak, A.; Mitoraj, M.; Ziegler, T.
Bond orbitals from chemical valence theory
Journal of Physical Chemistry A, (112): 1933-1939 2008.
- Michalik, D.; Schulz, A.; Villinger, A.
Lewis-Acid-Assisted Methyl Exchange Reactions In Silylated Aminodichloroarsanes
Inorganic Chemistry, (47): 11798-11806 2008.
- Michalik, S.; Machura, B.; Kruszynski, R.; Kusz, J.
Crystal, molecular and electronic structure of [ReCl₂(eta(2)-N₂COPh-N', O)(PPh₃)(2)]
Journal of Coordination Chemistry, (61): 1066-1077 2008.

Michalska, D.; Bienko, D. C.; Czarnik-Matusewicz, B.; Wierzeiewska, M.; Sandorfy, C.; Zeegers-Huyskens, T.

Theoretical and experimental studies of enflurane. Infrared spectra in solution, in low-temperature argon matrix and blue shifts resulting from dimerization (vol 111, pg 12228, 2007)
Journal of Physical Chemistry B, (112): 2755-2755 2008.

Michelini, M. C.; Rivalta, I.; Sicilia, E.

Theoretical study of the gas-phase ethane C-H and C-C bonds activation by bare niobium cation
Theoretical Chemistry Accounts, (120): 395-403 2008.

Michl, J.

Chemistry of the three-dimensionally aromatic CB11 cage
Pure and Applied Chemistry, (80): 429-446 2008.

Minasian, S. G.; Krinsky, J. L.; Williams, V. A.; Arnold, J.

A heterobimetallic complex with an unsupported Uranium(III)-Aluminum(I) bond: (CpSiMe₃)(3)U-AlCp star (Cp-star = C₅Me₅)
Journal of the American Chemical Society, (130): 10086-+ 2008.

Mitoraj, M.; Michalak, A.

Applications of natural orbitals for chemical valence in a description of bonding in conjugated molecules
Journal of Molecular Modeling, (14): 681-687 2008.

Moc, J.

Hydrogenation of aluminium hexamer: Ab initio molecular orbital theory and density functional theory study
Chemical Physics Letters, (466): 116-121 2008.

Moc, J.; Musaev, D. G.; Morokuma, K.

Zeolite-supported palladium tetramer and its reactivity toward H₂ molecules: Computational studies
Journal of Physical Chemistry A, (112): 5973-5983 2008.

Mohajeri, A.; Nobandegani, F. F.

Detection and evaluation of hydrogen bond strength in nucleic acid base pairs
Journal of Physical Chemistry A, (112): 281-295 2008.

Molnar, V.; Billes, F.; Tyihak, E.; Mikosch, H.

Theoretical study on the vibrational spectra of methoxy- and formyl-dihydroxy-trans-stilbenes and their hydrolytic equilibria
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (69): 542-558 2008.

Montejo, M.; Urena, F. P.; Marquez, F.; Lopez Gonzalez, J. J.

Triethylsilanol: Molecular conformations and role of the hydrogen-bonding oligomerization in its vibrational spectra
Journal of Physical Chemistry A, (112): 1545-1551 2008.

- Montiel-Palma, V.; Piechaczyk, O.
Bonding mode of a bifunctional P similar to Si-H ligand in the ruthenium complex "Ru(PPh₂CH₂OSiMe₂H)₃"
Inorganic Chemistry, (47): 8601-8603 2008.
- Mora, J. R.; Cordova, T.; Chuchani, G.
Ab initio and DFT calculations of benzaldoxime elimination kinetics in the gas phase
International Journal of Quantum Chemistry, (108): 1735-1741 2008.
- Moran, J.; Gorelsky, S. I.; Dimitrijevic, E.; Lebrun, M. E.; Bedard, A. C.; Seguin, C.; Beauchemin, A. M.
Intermolecular Cope-Type Hydroamination of Alkenes and Alkynes using Hydroxylamines
Journal of the American Chemical Society, (130): 17893-17906 2008.
- Moreno, A.; Pregosin, P. S.; Veiros, L. E.; Albinati, A.; Rizzato, S.
PGSE NMR diffusion overhauser studies on [Ru(Cp)(eta(6)-arene)][PF₆], plus a variety of transition-metal, inorganic, and organic salts: An overview of ion pairing in dichloromethane*
Chemistry-a European Journal, (14): 5617-5629 2008.
- Moreno, Y.; Belmar, J.; Brovelli, F.; Buljan, A.; Pena, O.; Moreno, L.
ELECTROCHEMICAL AND COMPUTATIONAL STUDY OF COPPER (II) ALKYLPIRAZOLONE BASED ENAMINE COMPLEX
Journal of the Chilean Chemical Society, (53): 1689-1693 2008.
- Mori, Y.; Shirase, H.
Substituent and Solvent Effects on Square-Planar-Tetrahedral Equilibria of Bis[4-(arylimino)pentan-2-onato]nickel(II) and Bis[1-aryl-3-(phenylimino)butan-1-onato]nickel(II) Complexes
Bulletin of the Chemical Society of Japan, (81): 1108-1115 2008.
- Muchaill, H. M.
Changes in the isotropic shielding of the O-17 nucleus upon torsion in terminal oxygen systems: A computational study on their origin
Journal of Physical Chemistry A, (112): 9118-9127 2008.
- Mutseneck, E. V.; Wadepohl, H.; Kudinov, A. R.; Siebert, W.
Cationic triple-decker complexes with a bridging 4-borataborepine ligand: Synthesis, structure, and bonding
European Journal of Inorganic Chemistry: 3320-3329 2008.
- Nabavizadeh, S. M.; Hoseini, S. J.; Momeni, B. Z.; Shahabadi, N.; Rashidi, M.; Pakiari, A. H.; Eskandari, K.
Oxidative addition of n-alkyl halides to diimine-dialkylplatinum(II) complexes: a closer look at the kinetic behaviors
Dalton Transactions: 2414-2421 2008.
- Nachtigalova, D.; Vrbka, L.; Bludsky, O.; Nachtigall, P.
Interaction of acetonitrile with Na-zeolites: adsorption modes and vibrational dynamics in the zeolite channels and cavities
Physical Chemistry Chemical Physics, (10): 4189-4198 2008.

- Nagahora, N.; Sasamori, T.; Tokitoh, N.
A ferrocenyldiphosphene-platinum complex: Structural features and theoretical calculations
Organometallics, (27): 4265-4268 2008.
- Nagase, H.; Yamamoto, N.
Synthesis of a stable iminium salt and propellane derivatives
Journal of Organic Chemistry, (73): 8093-8096 2008.
- Nagendran, S.; Roesky, H. W.
The chemistry of aluminum(I), silicon(II), and germanium(II)
Organometallics, (27): 457-492 2008.
- Nagendran, S.; Roesky, H. W.
The chemistry of aluminum(I), silicon(II), and germanium(II)
Organometallics, (27): 457-492 2008.
- Nagendran, S.; Sen, S. S.; Roesky, H. W.; Koley, D.; Grubmuller, H.; Pal, A.; Herbst-Irmer, R.
RGe(I)Ge(I)R Compound (R = PhC(NtBu)(2))with a Ge-Ge Single Bond and a Comparison with the Gauche Conformation of Hydrazine
Organometallics, (27): 5459-5463 2008.
- Nahum, T. L.; Mamlok-Naaman, R.; Hofstein, A.; Kronik, L.
A New "Bottom-Up" Framework for Teaching Chemical Bonding
Journal of Chemical Education, (85): 1680-1685 2008.
- Nakai, H.; Suzuki, J.; Kikuchi, Y.
Determination of active sites based on unified analysis of potential energy profile in chemical reaction: Application to C-H activation of methane by Ti(IV)-imido complex
Chemical Physics Letters, (460): 347-351 2008.
- Nakamura, S.; Hirata, N.; Yamada, R.; Kita, T.; Shibata, N.; Toru, T.
Catalytic and highly enantioselective reactions of alpha-sulfonyl carbanions with chiral bis(oxazoline)s
Chemistry-a European Journal, (14): 5519-5527 2008.
- Nakanishi, W.; Hayashi, S.; Morinaka, S.; Sasamori, T.; Tokitoh, N.
Extended hypervalent E 'center dot center dot center dot E-E center dot center dot center dot E ' 4c-6e (E, E ' = Se, S) interactions: structure, stability and reactivity of 1-(8-PhE ' C10H6)EE(C10H6E ' Ph-8 ')-1 '
New Journal of Chemistry, (32): 1881-1889 2008.
- Nakanishi, W.; Hayashi, S.; Narahara, K.; Hada, M.
Contributions from Atomic p(Se), d(Se), and f(Se) Orbitals to Absolute Paramagnetic Shielding Tensors in Neutral and Charged SeHn and Some Oxides Including the Effect of Methyl and Halogen Substitutions on sigma(P)(Se)
Chemistry-a European Journal, (14): 9647-9655 2008.

- Namorado, S.; Antunes, M. A.; Veiros, L. F.; Ascenso, J. R.; Duarte, M. T.; Martins, A. M.
Ionic hydrogenation of ketones with molybdenum pentabenzylcyclopentadienyl hydride catalysts
Organometallics, (27): 4589-4599 2008.
- Naota, T.; Tanna, A.; Kamuro, S.; Hieda, M.; Ogata, K.; Murahashi, S.-I.; Takaya, H.
Switchable C- and N-bound isomers of transition-metal cyanocarbanions: Synthesis and interconversions of cyclopentadienyl ruthenium complexes of phenylsulfonylacetonitrile anions
Chemistry-a European Journal, (14): 2482-2498 2008.
- Nayek, H. P.; Massa, W.
A Heterometallic, Heterovalent Cu-I/Sn-II/IV/S Cluster with an Unprecedented Cu₄Sn Core and Stannacyclopentane Units
Inorganic Chemistry, (47): 9146-9148 2008.
- Nazmutdinov, R. R.; Roznyatovskaya, N. V.; Glukhov, D. V.; Manyurov, I.; Mazin, V. M.; Tsirlina, G. A.; Probst, M.
Medium and interfacial effects in the multistep reduction of binuclear complexes with Robson-type ligand
Inorganic Chemistry, (47): 6659-6673 2008.
- Nematollahi, D.; Azizian, J.; Sargordan-Arani, M.; Hesari, M.; Jameh-Bozorghi, S.; Alizadeh, A.; Fotouhi, L.; Mirza, B.
Electrochemical Synthesis of 4-(Dihydroxyphenylthio)-2H-chromen-2-one Derivatives
Chemical and Pharmaceutical Bulletin, (56): 1562-1566 2008.
- Neto, A. C.; dos Santos, F. P.; Contreras, R. H.; Rittner, R.; Tormena, C. F.
Analysis of the Electronic Origin of the (1)J(CH) Spin-Spin Coupling Trend in 1-X-Cyclopropanes: Experimental and DFT Study
Journal of Physical Chemistry A, (112): 11956-11959 2008.
- Neuvonen, H.; Fueleop, F.; Neuvonen, K.; Koch, A.; Kleinpeter, E.
Electronic effects of heterocyclic ring systems as evaluated with the aid of C-13 and N-15 NMR chemical shifts and NBO analysis
Journal of Physical Organic Chemistry, (21): 173-184 2008.
- Nguyen, D.; Xu, T.
The expanding role of mouse genetics for understanding human biology and disease
Disease Models & Mechanisms, (1): 56-66 2008.
- Nguyen, S. C.; Vilster Hansen, B. K.
Electronic states of emodin and its conjugate base. Synchrotron linear dichroism spectroscopy and quantum chemical calculations
Chemical Physics, (352): 167-174 2008.
- Ni, B.-Q.; Shan, Y.-Y.; Wang, H.-J.; Liu, W.-L.
A DFT study on the interactions between sulfolane and aromatic hydrocarbons
Journal of Solution Chemistry, (37): 1343-1354 2008.

- Ni, D.; Zhou, D.; Zhang, J.
Study of ethylene and benzene adsorption on Bronsted acid sites in MCM-22 zeolites by theoretical calculation
Chinese Journal of Catalysis, (29): 366-372 2008.
- Ni, J.; Li, A. Y.; Yan, X. H.
Blue- and Red-Shifted Hydrogen Bonds between HNO and (HF)_n 1 ≤ n ≤ 3
Acta Physico-Chimica Sinica, (24): 2000-2006 2008.
- Nikiforov, G. B.; Roesky, H. W.; Heisen, B. C.; Grosse, C.; Oswald, R. B.
Formation of a titanium complex with a Ti=CHAl₂ structural unit from LTiMe₃ and trimethylaluminum
Organometallics, (27): 2544-2548 2008.
- Ning, L. X.; Zhang, Y. F.; Cui, Z. F.; Trioni, M. I.; Brivio, G. P.
Density Functional Theory Study of Magnetic Coupling in the Gd₁₂O₁₈ Cluster
Journal of Physical Chemistry A, (112): 13650-13654 2008.
- Nordlund, D.; Odellius, M.; Bluhm, H.; Ogasawara, H.; Pettersson, L. G. M.; Nilsson, A.
Electronic structure effects in liquid water studied by photoelectron spectroscopy and density functional theory
Chemical Physics Letters, (460): 86-92 2008.
- Nori-Shargh, D.
Stereoelectronic effects on the conformational properties of 1,3-dioxane, 1,3-dithiane, and 1,3-diselenane: An ab initio study and NBO analysis
Phosphorus Sulfur and Silicon and the Related Elements, (183): 2399-2409 2008.
- Nsangou, M.; Dhaouadi, Z.; Jaidane, N.; Ben Lakhdar, Z.
DFT study of the structure of hydroxybenzoic acids and their reactions with (OH)-O-center dot and O-center dot(2)- radicals
Journal of Molecular Structure-Theochem, (850): 135-143 2008.
- Nsangou, M.; Fifen, J. J.; Dhaouadi, Z.; Lahmar, S.
Hydrogen atom transfer in the reaction of hydroxycinnamic acids with (OH)-O-center dot and (HO₂)-H-center dot radicals: DFT study
Journal of Molecular Structure-Theochem, (862): 53-59 2008.
- Nunes, S. C. C.; Eusebio, M. E. S.; Jesus, A. J. L.; Rosado, M. T. S.; Redinha, J. S.
Structure of the 2-isopropylaminoethanol isolated molecule: Conformational analysis and intramolecular interactions
Journal of Molecular Structure-Theochem, (863): 73-78 2008.
- Oezen, C.; Tuezuen, N. S.
A DFT study on the mechanism of cyclopropanation via Cu(acac)₂-catalyzed diazo ester decomposition
Organometallics, (27): 4600-4610 2008.

- Ohman, K. T.; Sagstuen, E.
Free radical conformations and conversions in X-irradiated single crystals of L-cysteic acid by electron magnetic resonance and density functional theory studies
Journal of Physical Chemistry A, (112): 4284-4293 2008.
- Olah, G. A.; Prakash, G. K. S.; Rasul, G.
Comparative ab initio/GIAO-CCSD(T) study of protonated propionaldehyde, isobutyraldehyde and pivalaldehyde cations and their superelectrophilic diprotonated dication
Journal of Molecular Structure, (890): 9-17 2008.
- Olah, G. A.; Prakash, G. K. S.; Rasul, G.
Protonated tert-pentyl dication (C₅H₁₂²⁺, isopentane dication)
Dalton Transactions: 521-526 2008.
- Olsen, M. T.; Bruschi, M.; De Gioia, L.; Rauchfuss, T. B.; Wilson, S. R.
Nitrosyl derivatives of diiron(I) dithiolates mimic the structure and Lewis acidity of the [FeFe]-hydrogenase active site
Journal of the American Chemical Society, (130): 12021-12030 2008.
- Ortiz, A.; Insuasty, B.; Torres, M. R.; Herranz, M. A.; Martin, N.; Viruela, R.; Orti, E.
Aminopyrimidine-based donor-acceptor chromophores: Push-pull versus aromatic behaviour
European Journal of Organic Chemistry: 99-108 2008.
- Otero-Calvi, A.; Montero, L. A.; Stohrer, W.-D.
DFT modelling of cobalt and nickel complexes with dithiophosphinic acid
Journal of Molecular Structure-Theochem, (859): 93-97 2008.
- O'Toole, M. G.; Kreso, M.; Kozlowski, P. M.; Mashuta, M. S.; Grapperhaus, C. A.
Spin-state-dependent oxygen sensitivity of iron dithiolates: sulfur oxygenation or disulfide formation
Journal of Biological Inorganic Chemistry, (13): 1219-1230 2008.
- Ott, H.; Matthes, C.; Schmatz, S.; Klingebiel, U.; Stalke, D.
First trichloroaluminum adducts of silyliminoborenes
Zeitschrift Fur Naturforschung Section B-a Journal of Chemical Sciences, (63): 1023-1026 2008.
- Otyepka, M.; Banas, P.; Magistrato, A.; Carloni, P.; Damborsky, J.
Second step of hydrolytic dehalogenation in haloalkane dehalogenase investigated by QM/MM methods
Proteins-Structure Function and Bioinformatics, (70): 707-717 2008.
- Padilla-Campos, L.
Theoretical study of the adsorption of carbon monoxide on small copper clusters
Journal of Molecular Structure-Theochem, (851): 15-21 2008.
- Padmaja, L.
Analysis of vibrational spectra of L-alanylglycine based on density functional theory calculations
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (71): 252-262 2008.

- Pakal'nis, V. V.; Borovitev, M. E.
Heteroligand Bipyridyl-Pyridylbenzimidazole Ru(II) Complexes. Synthesis, Structural Characterization, and Investigation of Electronic Structure
Russian Journal of General Chemistry, (78): 1594-1605 2008.
- Pakiari, A. H.; Azami, S. M.
Coherent superposition of resonance wave function in terms of weighted orthogonalized natural localized configurations
International Journal of Quantum Chemistry, (108): 219-228 2008.
- Pakiari, A. H.; Fakfiraee, S.; Azami, S. M.
Decomposition of deformation density into orbital components
International Journal of Quantum Chemistry, (108): 415-422 2008.
- Pakiari, A. H.; Jamshidi, Z.
Interaction of coinage metal clusters with chalcogen dihydrides
Journal of Physical Chemistry A, (112): 7969-7975 2008.
- Panda, M. K.; John, A.; Shaikh, M. M.; Ghosh, P.
Mimicking the Intradiol Catechol Cleavage Activity of Catechol Dioxygenase by High-Spin Iron(III) Complexes of a New Class of a Facially Bound [N₂O] Ligand
Inorganic Chemistry, (47): 11847-11856 2008.
- Pandey, K. K.
Stretched sigma-borane complexes of rhodium: A theoretical study
Inorganic Chemistry Communications, (11): 288-292 2008.
- Panja, S.; Nielsen, S. B.; Hvelplund, P.; Turecek, F.
Inverse Hydrogen Migration in Arginine-Containing Peptide Ions upon Electron Transfer
Journal of the American Society for Mass Spectrometry, (19): 1726-1742 2008.
- Pantazis, D. A.; Chen, X.-Y.; Landis, C. R.; Neese, F.
All-electron scalar relativistic basis sets for third-row transition metal atoms
Journal of Chemical Theory and Computation, (4): 908-919 2008.
- Pantazis, D. A.; McGrady, J. E.; Besora, M.; Maseras, F.; Etienne, M.
On the origin of alpha- and beta-agostic distortions in early-transition-metal alkyl complexes
Organometallics, (27): 1128-1134 2008.
- Papanikolaou, P.; Karafiloglou, P.
Extracting covalent and ionic structures from usual delocalized wave functions: The electron-expansion methodology
Journal of Physical Chemistry A, (112): 8839-8848 2008.
- Parandekar, P. V.; Hratchian, H. P.
Applications and assessment of QM:QM electronic embedding using generalized asymmetric Mulliken atomic charges

- Journal of Chemical Physics, (129) 2008.
- Pardo, E.; Carrasco, R.; Ruiz-Garcia, R.; Julve, M.; Lloret, F.; Munoz, M. C.; Journaux, Y.; Ruiz, E.; Cano, J.
Structure and magnetism of dinuclear Copper(II) metallacyclophanes with oligoacenebis(oxamate) bridging ligands: Theoretical predictions on wirelike magnetic coupling
Journal of the American Chemical Society, (130): 576-585 2008.
- Park, Y. S.; Little, R. D.
Redox electron-transfer reactions: Electrochemically mediated rearrangement, mechanism, and a total synthesis of daucene
Journal of Organic Chemistry, (73): 6807-6815 2008.
- Parthasarathi, R.; Subramanian, V.; Sathyamurthy, N.
Electron density topography, NMR, and NBO analysis of water clusters
Synthesis and Reactivity in Inorganic Metal-Organic and Nano-Metal Chemistry, (38): 18-26
2008.
- Partyka, D. V.
A porphyrin complex of gold(I): (Phosphine)gold(I) azides as cation precursors
Proceedings of the National Academy of Sciences of the United States of America, (105): 14293-14297 2008.
- Parveen, S.; Das, S.; Chandra, A. K.; Zeegers-Huyskens, T.
THEORETICAL STUDIES OF HYDROGEN BONDING INTERACTION BETWEEN TRIMETHYLAMINE AND SUBSTITUTED PHENOLS, INFLUENCE OF THE SUBSTITUENTS ON THE HYDROGEN BOND PROPERTIES AND THE VIBRATIONAL SPECTRUM
Journal of Theoretical & Computational Chemistry, (7): 1171-1186 2008.
- Pasha, F. A.; Chung, H. W.; Kang, S. B.; Cho, S. J.
3D-quantitative structure activity analysis and quantum chemical analysis of pyrido-di-indoles
International Journal of Quantum Chemistry, (108): 391-400 2008.
- Patil, M. P.; Sunoj, R. B.
The Role of Noninnocent Solvent Molecules in Organocatalyzed Asymmetric Michael Addition Reactions
Chemistry-a European Journal, (14): 10472-10485 2008.
- Paton, R. S.; Goodman, J. M.; Pellegrinet, S. C.
Theoretical study of the asymmetric conjugate alkenylation of enones catalyzed by binaphthols
Journal of Organic Chemistry, (73): 5078-5089 2008.
- Pavelka, M.; Burda, J. V.
Computational study of redox active centres of blue copper proteins: a computational DFT study
Molecular Physics, (106): 2733-2748 2008.
- Pavelka, M.; Shukla, M. K.; Leszczynski, J.; Burda, J. V.
Theoretical study of hydrated copper(II) interactions with guanine: A computational density functional theory study

- Journal of Physical Chemistry A, (112): 256-267 2008.
- Pedersoli, S.; Tormena, C. F.; dos Santos, F. P.; Contreras, R. H.; Rittner, R.
Stereochemical behavior of (1)J(CH) and (2)J(CH) NMR coupling constants in alpha-substituted acetamides
Journal of Molecular Structure, (891): 508-513 2008.
- Peng, C.-C.; Rushmore, T.; Crouch, G. J.; Jones, J. P.
Modeling and synthesis of novel tight-binding inhibitors of cytochrome P4502C9
Bioorganic & Medicinal Chemistry, (16): 4064-4074 2008.
- Perez, C.; Suardiaz, R.; Ortiz, P. J.; Crespo-Otero, R.; Bonetto, G. M.; Gavin, J. A.; Garcia de la Vega, J. M.; Fabian, J. S.; Contreras, R. H.
On the unusual (2)J(C2-Hf) coupling dependence on syn/anti CHO conformation in 5-X-furan-2-carboxaldehydes
Magnetic Resonance in Chemistry, (46): 846-850 2008.
- Perez, J. R.; Lorono, M.; Dominguez, R. M.; Cordova, T.; Chuchani, G.
MP2 study of the gas phase elimination mechanism of some neutral amino acids and their ethyl esters
Journal of Physical Organic Chemistry, (21): 402-408 2008.
- Perez-Juste, I.; Carballeira, L.
Theoretical study of the electronic and hyperfine structures of the HSO and SOH radicals
Journal of Molecular Structure-Theochem, (855): 27-33 2008.
- Pichierri, F.
Effect of fluorine substitution in calix[4]pyrrole: A DFT study
Journal of Molecular Structure-Theochem, (870): 36-42 2008.
- Pichierri, F.
Geometries and Electronic Structures of Alkaline Earth Auride Clusters, Au₄M (M = Mg, Ca, Sr, Ba)
Materials Transactions, (49): 2437-2440 2008.
- Pichierri, F.
Molecular structure of the octatetrayl anion, C₈H⁻: A computational study
Journal of Physical Chemistry A, (112): 7717-7722 2008.
- Pinjari, R. V.; Joshi, K. A.; Gejji, S. R.
Theoretical studies on the electronic structure, charge distribution and vibrational spectra of diglyme-M⁺-AsF₆⁻ (M = Li, Na, K)
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (71): 1056-1062 2008.
- Pinter, B.; Veszpremi, T.
Synthesizability of the Heavy Analogues of Disubstituted Cyclopropenylidene: A Theoretical Study
Organometallics, (27): 5571-5576 2008.

Piquemal, J. P.; Pilme, J.; Parisel, O.; Gerard, H.; Fourre, I.; Berges, J.; Gourlaouen, C.; De La Lande, A.; Van Severen, M. C.; Silvi, B.

What can be learnt on biologically relevant systems from the topological analysis of the electron localization function?

International Journal of Quantum Chemistry, (108): 1951-1969 2008.

Podewitz, M.; Herrmann, C.; Malassa, A.; Westerhausen, M.; Reiher, M.

Spin-Spin interactions in polynuclear transition-metal complexes

Chemical Physics Letters, (451): 301-308 2008.

Pogany, P.; Kovacs, A.; Szecsenyi, K. M.; Leovac, V. M.

FT-IR and theoretical study of 3,5-dimethyl-1H-pyrazole-1-carboxamide (L) and the complexes CoL₂(H₂O)₂(NO₃)₂, NiL₂(H₂O)₂(NO₃)₂

Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (71): 1466-1473 2008.

Polo, V.; Andres, J.; Berskit, S.; Domingo, L. R.; Silvi, B.

Understanding reaction mechanisms in organic chemistry from catastrophe theory applied to the electron localization function topology

Journal of Physical Chemistry A, (112): 7128-7136 2008.

Ponec, R.; Cooper, D. L.; Savin, A.

Analytic models of domain-averaged fermi holes: A new tool for the study of the nature of chemical bonds

Chemistry-a European Journal, (14): 3338-3345 2008.

Prestianni, A.; Martorana, A.; Ciofini, I.; Labat, F.; Adamo, C.

CO Oxidation on Cationic Gold Clusters: A Theoretical Study

Journal of Physical Chemistry C, (112): 18061-18066 2008.

Prikryl, J.; Machacek, V.; Jansa, P.; Svobodova, M.; Ruzicka, A.; Nachtigall, P.; Cerny, M.

Stable triazenes derived from 2-alkylaminonaphthalenes and 5-nitrobenzo[c]-1,2-thiazole-3-diazonium hydrogensulfate

European Journal of Organic Chemistry: 3272-3278 2008.

Qi, X.-J.; Li, Z.; Fu, Y.; Guo, Q.-X.; Liu, L.

anti-spin-delocalization effect in Co-C bond dissociation enthalpies

Organometallics, (27): 2688-2698 2008.

Qi, Y.; Feng, D.; Feng, S.

Theoretical study on the addition reactions of silylenoids H₂SiLiX (X = F, Cl) to formaldehyde

Journal of Molecular Structure-Theochem, (856): 96-104 2008.

Qiu, Y. F.; Cao, Z. X.

Effect of Intramolecular Structural Environment on Bond Dissociation Energies

Chemical Journal of Chinese Universities-Chinese, (29): 2489-2491 2008.

Quinonero, D.; Frontera, A.; Deya, P. M.; Alkorta, I.; Elguero, J.

- Interaction of positively and negatively charged aromatic hydrocarbons with benzene and triphenylene: Towards a model of pure organic insulators*
Chemical Physics Letters, (460): 406-410 2008.
- Ramirez-Solis, A.; Kirtman, B.; Bernal-Jaquez, R.; Zicovich-Wilson, C. M.
Periodic density functional theory calculations for Na-doped quasi-one-dimensional polyacetylene chains
Journal of Physical Chemistry C, (112): 9493-9500 2008.
- Ravikumar, C.; Joe, I. H.; Jayakumar, V. S.
Charge transfer interactions and nonlinear optical properties of push-pull chromophore benzaldehyde phenylhydrazone: A vibrational approach
Chemical Physics Letters, (460): 552-558 2008.
- Ray, L.; Barman, S.; Shaikh, M. M.; Ghosh, P.
Highly convenient amine-free Sonogashira coupling in air in a polar mixed aqueous medium by trans- and cis-[(NHC)(2)PdX2] (X = Cl, Br) complexes of N/O-functionalized N-heterocyclic carbenes
Chemistry-a European Journal, (14): 6646-6655 2008.
- Ray, L.; Shaikh, M. M.; Ghosh, P.
Shorter argentophilic interaction than aurophilic interaction in a pair of dimeric {(NHC)MCl}(2) (M= Ag, Au) complexes supported over a N/O-functionalized N-heterocyclic carbene (NHC) ligand
Inorganic Chemistry, (47): 230-240 2008.
- Rayon, V. M.; Valdes, H.; Diaz, N.; Suarez, D.
Monoligand Zn(II) complexes: Ab initio benchmark calculations and comparison with density functional theory methodologies
Journal of Chemical Theory and Computation, (4): 243-256 2008.
- Reinhardt, P.; Piquemal, J. P.; Savin, A.
Fragment-Localized Kohn-Sham Orbitals via a Singles Configuration-interaction Procedure and Application to Local Properties and Intermolecular Energy Decomposition Analysis
Journal of Chemical Theory and Computation, (4): 2020-2029 2008.
- Remacle, F.; Grandjean, F.; Long, G. J.
A density functional theory calculation of the electronic properties of several high-spin and low-spin iron(II) pyrazolylborate complexes
Inorganic Chemistry, (47): 4005-4014 2008.
- Ren, F. D.; Cao, D. L.; Wang, W. L.; Hou, S. Q.; Chen, S. S.
Can B=B double bond be as potential proton acceptor: A UB3LYP and UMP2 theoretical study on unusual intermolecular T-shaped X-H center dot center dot center dot pi interactions between the triplet state HB=BH ((3)Sigma(-)(g)) and HF, HCl, HCN or H2C2
Journal of Molecular Structure-Theochem, (870): 43-48 2008.
- Ren, Y.; Wang, X.; Chu, S.-Y.; Wong, N.-B.

- Counter-ion effect in the nucleophilic substitution reactions at silicon: a G2M(+) level theoretical investigation*
Theoretical Chemistry Accounts, (119): 407-411 2008.
- Requena, A.; Ceron-Carrasco, J. P.; Bastida, A.; Zuniga, J.; Miguel, B.
Density functional theory study of the structure and vibrational spectra of beta-carotene, capsanthin, and capsorubin
Journal of Physical Chemistry A, (112): 4815-4825 2008.
- Rinaldo, D.; Tian, L.; Harvey, J. N.; Friesner, R. A.
Density functional localized orbital corrections for transition metals
Journal of Chemical Physics, (129) 2008.
- Rinaldo, D.; Tian, L.; Harvey, J. N.; Friesner, R. A.
Density functional localized orbital corrections for transition metals
Journal of Chemical Physics, (129) 2008.
- Rivera-Jimenez, S. M.; Hernandez-Maldonado, A. J.
Nickel(II) grafted MCM-41: A novel sorbent for the removal of Naproxen from water
Microporous and Mesoporous Materials, (116): 246-252 2008.
- Robles, N. L.; Cutin, E. H.; Alvarez, R. M. S.; Oberhammer, H.
Structure and conformations of N-(chloroformyl) iminosulfur dichloride, ClC(O)N=SCl₂
Journal of Molecular Structure, (891): 40-44 2008.
- Ronchin, L.; Bortoluzzi, M.; Vavasori, A.
A DFT study on secondary reaction pathways in the acid-catalysed Beckmann rearrangement of cyclohexanone oxime in aprotic solvent
Journal of Molecular Structure-Theochem, (858): 46-51 2008.
- Roohi, H.
DFT study of the biphenylene-NO₂⁺ complexes formed in nitration mechanism
Journal of Physical Organic Chemistry, (21): 971-978 2008.
- Roohi, H.; Azarpour, M.
Adsorption of methanol on the nanocrystalline H-zeolite and alkali metal exchanged M-zeolites: Energetic, NBO and QTAIM analyses
Microporous and Mesoporous Materials, (113): 240-251 2008.
- Roohi, H.; Bagheri, S.
Atomic and electronic structures of finite single-walled BN nanotubes: Hybrid DFT calculations
Journal of Molecular Structure-Theochem, (856): 46-58 2008.
- Roohi, H.; Bagheri, S.; Hosseini, S. G.
Effect of Hydration and Self-Association on the Reaction Mechanism of Proton Transfer in Methimazole: A Theoretical Study
Bulletin of the Chemical Society of Japan, (81): 1402-1414 2008.

- Roohi, H.; Gholipour, Y.
Characterization of the N-H center dot center dot center dot O = N and N-H center dot center dot center dot N = O H-bonds in nitrosamine dimers
International Journal of Quantum Chemistry, (108): 462-471 2008.
- Roohi, H.; Noruozi, A. R.; Salemi, S.; Sharaki, J.
Theoretical study of solvent effects on the conformational preference in CH₂FWH (W=O, S) using PCM and IPCM methods
Journal of Molecular Liquids, (143): 119-124 2008.
- Roy, D.; Patel, C.; Liebman, J. F.; Sunoj, R. B.
Probing intramolecular interactions in arylselenides using a property descriptor based approach
Journal of Physical Chemistry A, (112): 8797-8803 2008.
- Roy, D. R.; Chattaraj, P. K.
Reactivity, selectivity, and aromaticity of Be-3(2-) and its complexes
Journal of Physical Chemistry A, (112): 1612-1621 2008.
- Rozas, I.; Alkorta, I.; Elguero, J.
Hydrogen bonds and ionic interactions in Guanidine/Guanidinium complexes: a computational case study
Structural Chemistry, (19): 923-933 2008.
- Ruben, E. A.; Plumley, J. A.; Chapman, M. S.; Evanseck, J. D.
Anomeric effect in "High energy" phosphate bonds. Selective destabilization of the scissile bond and modulation of the exothermicity of hydrolysis
Journal of the American Chemical Society, (130): 3349-3358 2008.
- Ruiz, J. M.; Regas, D.; Afonso, M. M.; Palenzuela, J. A.
Study of an unexpected rearrangement of the alpha-phenyl pyrane derivatives prepared via hetero-Diels-Alder reaction of acyclic vinyl allenes and aldehydes
Journal of Organic Chemistry, (73): 7246-7254 2008.
- Rupar, P. A.; Staroverov, V. N.; Baines, K. M.
A Cryptand-Encapsulated Germanium(II) Dication
Science, (322): 1360-1363 2008.
- Sadlej-Sosnowska, N.; Murlowska, K.
Similarity based on atomic electrostatic potential in heterocyclic molecules: Acidity of tetrazoles
Journal of Physical Chemistry A, (112): 10017-10022 2008.
- Safarpour, M. A.; Hashemianzadeh, S. M.; Kasaeian, A.
The theoretical investigation of one of the derivatives of 1,2-dithienylcyclopentene as a molecular switch
Journal of Molecular Modeling, (14): 315-323 2008.
- Sajan, D.; Sockalingum, G. D.; Manfait, M.; Joel, I. H.; Jayakumar, V. S.

- NIR-FT Raman, FT-IR and surface-enhanced Raman scattering spectra, with theoretical simulations on chloramphenicol*
Journal of Raman Spectroscopy, (39): 1772-1783 2008.
- Sakata, K.; Fujimoto, H.
Quantum chemical study of Lewis acid catalyzed allylboration of aldehydes
Journal of the American Chemical Society, (130): 12519-12526 2008.
- Sakota, K.; Kageura, Y.; Sekiya, H.
Cooperativity of hydrogen-bonded networks in 7-azaindole(CH₃OH)(n) (n=2,3) clusters evidenced by IR-UV ion-dip spectroscopy and natural bond orbital analysis
Journal of Chemical Physics, (129) 2008.
- Sakota, K.; Kageura, Y.; Sekiya, H.
Cooperativity of hydrogen-bonded networks in 7-azaindole(CH₃OH)(n) (n=2,3) clusters evidenced by IR-UV ion-dip spectroscopy and natural bond orbital analysis
Journal of Chemical Physics, (129) 2008.
- Samantaray, M. K.; Pang, K.; Shaikh, M. M.; Ghosh, P.
From large 12-membered macrometallacycles to ionic (NHC)(2)M+Cl- type complexes of gold and silver by modulation of the N-substituent of amido-functionalized N-heterocyclic carbene (NHC) Ligands
Inorganic Chemistry, (47): 4153-4165 2008.
- Sammelson, R. E.; Najafi, A.; Azizkhani, M.; Lorestani, F.; Tayyari, S. F.
Hydrogen bond strength and vibrational assignment of the enol form of 3-(phenylthio)pentane-2,4-dione
Journal of Molecular Structure, (889): 165-176 2008.
- Sanderson, J.; Bayse, C. A.
The Lewis acidity of bismuth(III) halides: a DFT analysis
Tetrahedron, (64): 7685-7689 2008.
- Santos, S. G.; Santana, J. V.; Maia, F. F.; Lemos, V.; Freire, V. N.; Caetano, E. W. S.; Cavada, B. S.; Albuquerque, E. L.
Adsorption of Ascorbic Acid on the C-60 Fullerene
Journal of Physical Chemistry B, (112): 14267-14272 2008.
- Sanz, P.; Mo, O.; Yanez, M.; Elguero, J.
Bonding in tropolone, 2-aminotropone, and aminotropoimine: No evidence of resonance-assisted hydrogen-bond effects
Chemistry-a European Journal, (14): 4225-4232 2008.
- Sapse, D. S.; Champeil, E.; Maddaluno, J.; Fressigne, C.; Sapse, A. M.
An ab initio study of the interaction of DNA fragments with methyl lithium
Comptes Rendus Chimie, (11): 1262-1270 2008.

Sarangi, R.; Gorelsky, S. I.; Basumallick, L.; Hwang, H. J.; Pratt, R. C.; Stack, T. D. P.; Lu, Y.; Hodgson, K. O.; Hedman, B.; Solomon, E. I.

Spectroscopic and density functional theory studies of the blue-copper site in M121SeM and C112SeC azurin: Cu-Se versus Cu-S bonding

Journal of the American Chemical Society, (130): 3866-3877 2008.

Sarangi, R.; York, J. T.; Helton, M. E.; Fujisawa, K.; Karlin, K. D.; Tolman, W. B.; Hodgson, K. O.; Hedman, B.; Solomon, E. I.

X-ray absorption spectroscopic and theoretical studies on (L)(2)[Cu-2(S-2)n](2+) complexes: Disulfide versus disulfide(center dot 1-) bonding

Journal of the American Chemical Society, (130): 676-686 2008.

Saric, A.; Vrcek, V.; Buehl, M.

Density functional study of protonated formylmetallocenes

Organometallics, (27): 394-401 2008.

Sarkar, B.; Patra, S.; Fiedler, J.; Sunoj, R. B.; Janardanan, D.; Lahiri, G. K.; Kaim, W.

Mixed-valent metals bridged by a radical ligand: Fact or fiction based on structure-oxidation state correlations

Journal of the American Chemical Society, (130): 3532-3542 2008.

Sarkar, M.; Samanta, A.

Mechanism of interaction of a flavone derivative with halides: Basis set dependence of the theoretical results

Journal of Molecular Structure-Theochem, (863): 111-116 2008.

Sarma, B. K.; Mugesh, G.

Thiol cofactors for selenoenzymes and their synthetic mimics

Organic & Biomolecular Chemistry, (6): 965-974 2008.

Sarma, B. K.; Mugeshii, G.

Antioxidant Activity of the Anti-Inflammatory Compound Ebselen: A Reversible Cyclization Pathway via Selenenic and Seleninic Acid Intermediates

Chemistry-a European Journal, (14): 10603-10614 2008.

Sasanuma, Y.; Watanabe, A.; Tamura, K.

Structure-property relationships of polyselenoethers $[-(\text{CH}_2)_y\text{Se}]_x$ ($y=1, 2, \text{ and } 3$) and related polyethers and polysulfides

Journal of Physical Chemistry B, (112): 9613-9624 2008.

Schulz, A.

Staudinger Reaction as a Way Out To Avoid Cyclization in the Reaction of Silylated Dichloro(hydrazino)phosphane with Trimethylsilyl Azide

European Journal of Inorganic Chemistry: 4199-4203 2008.

Schulz, A.; Villinger, A.

Tetrazarsoles - A new class of binary arsenic-nitrogen heterocycles

Angewandte Chemie-International Edition, (47): 603-606 2008.

- Schuquel, I. T. A.; Ducati, L. C.; Custodio, R.; Rittner, R.; Klapstein, D.
An investigation of the electronic structure of some 3-monosubstituted-2-methylpropenes through computational chemistry and photoelectron spectroscopy
Chemical Physics, (349): 263-268 2008.
- Selby, J. D.; Manley, C. D.; Schwarz, A. D.; Clot, E.; Mountford, P.
Titanium Hydrazides Supported by Diamide-Amine and Related Ligands: A Combined Experimental and DFT Study
Organometallics, (27): 6479-6494 2008.
- Semnani, A.; Pouretedal, H. R.; Keshavarz, M. H.; Firooz, A. R.; Oftadeh, M.
Interaction between 1,3,5-Trithiane and Iodine Monobromide in Halomethane Solutions
Heterocyclic Communications, (14): 205-213 2008.
- Senthilkumar, K.; Mujika, J. I.; Ranaghan, K. E.; Manby, F. R.; Mulholland, A. J.; Harvey, J. N.
Analysis of polarization in QM/MM modelling of biologically relevant hydrogen bonds
Journal of the Royal Society Interface, (5): S207-S216 2008.
- Serafin, M. M.; Peebles, S. A.
Dimers of Fluorinated Methanes with Carbonyl Sulfide: The Rotational Spectrum and Structure of Difluoromethane-OCS
Journal of Physical Chemistry A, (112): 12616-12621 2008.
- Serrano, A. J.; Lorono, M.; Cordova, T.; Chuchani, G.
Theoretical calculations of the thermal decomposition kinetics of several tert-nitroalkanes in the gas phase
Journal of Molecular Structure-Theochem, (859): 69-72 2008.
- Shaik, S.; Kumar, D.; de Visser, S. P.
Valence bond modeling of trends in hydrogen abstraction barriers and transition states of hydroxylation reactions catalyzed by cytochrome P450 enzymes
Journal of the American Chemical Society, (130): 10128-10140 2008.
- Shainyan, B. A.; Fettke, A.; Kleinpeter, E.
Push-Pull vs Captodative Aromaticity
Journal of Physical Chemistry A, (112): 10895-10903 2008.
- Shainyan, B. A.; Ushakov, I. A.; Meshcheryakov, V. I.; Koch, A.; Kleinpeter, E.
Variable temperature NMR and theoretical study of the stereodynamics of 5-trifluoromethylsulfonyl-1,3,5-dioxazinanone: Perlin effect subject to heteroatom substitution
Tetrahedron, (64): 5379-5383 2008.
- Shainyan, B. A.; Ushakov, I. A.; Tolstikova, L. L.; Koch, A.; Kleinpeter, E.
N-triflyl substituted 1,4-diheterocyclohexanes-stereodynamics and the Perlin effect
Tetrahedron, (64): 5208-5216 2008.
- Sharma, P.; Mitra, A.; Sharma, S.; Singh, H.; Bhattacharyya, D.

Quantum chemical studies of structures and binding in noncanonical RNA base pairs: The trans Watson-Crick : Watson-Crick family

Journal of Biomolecular Structure and Dynamics, (25): 709-732 2008.

Shi, F.-Q.; Song, B.-A.

Effect of Al-H center dot center dot center dot H-O dihydrogen bond on the reaction between diphenylmethanol and pyrazolate-bridged dialuminum complex. An ONIOM DFT/AM1 study

International Journal of Quantum Chemistry, (108): 1107-1113 2008.

Shibahara, M.; Watanabe, M.; Iwanaga, T.; Matsumoto, T.; Ideta, K.; Shinmyozu, T.

Synthesis, structure, and transannular pi-pi interaction of three- and four-layered [3.3]paracyclophanes

Journal of Organic Chemistry, (73): 4433-4442 2008.

Shieh, M.; Miu, C. Y.; Lee, C. J.; Chen, W. C.; Chu, Y. Y.; Chen, H. L.

Construction of Copper Halide-Triiron Selenide Carbonyl Complexes: Synthetic, Electrochemical, and Theoretical Studies

Inorganic Chemistry, (47): 11018-11031 2008.

Shindo, M.; Mori, S.

Torquoselective olefination of carbonyl compounds with ynolates: Highly efficient stereoselective synthesis of tetrasubstituted alkenes

Synlett: 2231-2243 2008.

Shindo, M.; Mori, S.

Torquoselective olefination with ynolates

Journal of Synthetic Organic Chemistry Japan, (66): 28-38 2008.

Shishkov, I. F.; Khristenko, L. V.; Rykov, A. N.; Vilkov, L. V.; Giricheva, N. I.; Shlykov, S. A.; Girichev, G. V.; Oberhammer, H.

Structure and conformation of (trifluoromethyl)thiobenzene, C₆H₅SCF₃: Gas electron diffraction and quantum chemical calculations

Journal of Molecular Structure, (876): 147-153 2008.

Shiu, B.-Y.; Huang, P.-C.; Huang, Y.-L.; Hong, F.-E.

Preparation of cobalt-containing bulky monodentate phosphines with electron-withdrawing/donating substituents on bridged arylolefinyl and their applications in Suzuki coupling reactions

Tetrahedron, (64): 6221-6229 2008.

Shlykov, S. A.; Oberhammer, H.; Titov, A. V.; Giricheva, N. I.; Girichev, G. V.

A Combined Gas-Phase Electron Diffraction/Mass Spectrometric Study of the Sublimation Processes of TeBr₄ and TeI₄: The Molecular Structure of Tellurium Dibromide and Tellurium Diiodide

European Journal of Inorganic Chemistry: 5220-5227 2008.

Shlykov, S. A.; Titov, A. V.; Oberhammer, H.; Giricheva, N. I.; Giricheva, G. V.

The molecular structure of selenium dibromide as determined by combined gas-phase electron diffraction-mass spectrometric experiments and quantum chemical calculations

Physical Chemistry Chemical Physics, (10): 6438-6445 2008.

Shulga, Y. M.; Martynenko, V. M.; Open'ko, V. V.; Kulikov, A. V.; Michtchenko, A.; Johnson, E.; Mochena, M. D.; Gutsev, G. L.

Oxidation of C-60 fullerite by interstitial oxygen

Journal of Physical Chemistry C, (112): 12096-12103 2008.

Siboulet, B.; Marsden, C. J.; Vitorge, P.

What can quantum chemistry tell us about Pa(v) hydration and hydrolysis?

New Journal of Chemistry, (32): 2080-2094 2008.

Sierra, M. A.

Computational and experimental tools in solving some mechanistic problems in the chemistry of Fischer carbene complexes

Chemical Communications: 4671-4682 2008.

Simon, L.; Goodman, J. M.

Theoretical study of the mechanism of Hantzsch ester hydrogenation of imines catalyzed by chiral BINOL-phosphoric acids

Journal of the American Chemical Society, (130): 8741-8747 2008.

Singh, P. C.; Patwari, G. N.

IR-UV double resonance spectroscopic investigation of phenylacetylene-alcohol complexes. Alkyl group induced hydrogen bond switching

Journal of Physical Chemistry A, (112): 5121-5125 2008.

Sinha, R. K.; Singh, B. P.; Kundu, T.

Origin of threefold methyl torsional potential in methylindoles

Theoretical Chemistry Accounts, (121): 59-70 2008.

Siu, C. K.; Ke, Y.; Orlova, G.; Hopkinson, A. C.; Siu, K. W. M.

Dissociation of the N-C-alpha Bond and Competitive Formation of the [z(n) - H](center dot+) and [c(n)+2H](+) Product Ions in Radical Peptide Ions Containing Tyrosine and Tryptophan: The Influence of Proton Affinities on Product Formation

Journal of the American Society for Mass Spectrometry, (19): 1799-1807 2008.

Siu, C.-K.; Ke, Y.; Guo, Y.; Hopkinson, A. C.; Siu, K. W. M.

Dissociations of copper(II)-containing complexes of aromatic amino acids: radical cations of tryptophan, tyrosine, and phenylalanine

Physical Chemistry Chemical Physics, (10): 5908-5918 2008.

Sizova, O. V.; Lubimova, O. O.; Sizov, V. V.; Ivanova, N. V.

DFT study of metastable linkage isomers of six-coordinate ruthenium nitrosyl complexes

Zeitschrift Fur Kristallographie, (223): 343-355 2008.

Sizova, O. V.; Skripnikov, L. V.; Sokolov, A. Y.

Calculation of sigma-, pi-, and delta-components of quantum-chemical bond orders
Russian Journal of General Chemistry, (78): 2146-2147 2008.

Sizova, O. V.; Skripnikov, L. V.; Sokolov, A. Y.

Symmetry decomposition of quantum chemical bond orders
Journal of Molecular Structure-Theochem, (870): 1-9 2008.

Snehalatha, M.; Ravikumar, C.; Sekar, N.; Jayakumar, V. S.; Joe, I. H.

FT-Raman, IR and UV-visible spectral investigations and ab initio computations of a nonlinear food dye amaranth
Journal of Raman Spectroscopy, (39): 928-936 2008.

Snehalatha, M.; Sekar, N.; Jayakumar, V. S.; Joe, I. H.

Quantum chemical computations and Fourier transform infrared spectral studies of a nonlinear food dye E110
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (69): 82-90 2008.

Snyder, J. A.; Madura, J. D.

Interaction of the phospholipid head group with representative quartz and aluminosilicate structures: An ab initio study
Journal of Physical Chemistry B, (112): 7095-7103 2008.

Soderhjelm, P.; Ohrn, A.; Ryde, U.; Karlstrom, G.

Accuracy of typical approximations in classical models of intermolecular polarization
Journal of Chemical Physics, (128) 2008.

Song, Q.; Niu, T.; Wang, H.

Theoretical study of the reaction of 2,4-dichlorophenol with O-1(2)
Journal of Molecular Structure-Theochem, (861): 27-32 2008.

Song, Y.; Cushman, M.

The binding orientation of a norindenoisoquinoline in the topoisomerase I-DNA cleavage complex is primarily governed by pi-pi stacking interactions
Journal of Physical Chemistry B, (112): 9484-9489 2008.

Sordo, T. L.; Ardura, D.

On the mechanism of gold(I)-catalyzed ring expansion of cyclopropanols: Theoretical calculations uncover a bottle-neck 1,4-H shift and suggest adequate reaction conditions
European Journal of Organic Chemistry: 3004-3013 2008.

Soriano, E.; Marco-Contelles, J.

New insights on the mechanism of the transition-metal stereoselective olefin cyclopropanation
Chemistry-a European Journal, (14): 6771-6779 2008.

Sornmer, H.; Eichhofer, A.; Drebov, N.; Ahlrichs, R.; Fenske, D.

Preparation, Geometric and Electronic Structures of [Bi₂Cu₄(SPh)₈(PPh₃)₄] with a Bi-2 Dumbbell, [Bi₄Ag₃(SePh)₆Cl-3(PPh₃)₃](2) and [Bi₄Ag₃(SePh)₆X-3(PPh₃)₃](2) (X = Cl, Br) with a Bi-4 Unit

- European Journal of Inorganic Chemistry: 5138-5145 2008.
- Spichty, M.; Kulicke, K. J.; Neuburger, M.; Schaffner, S.; Mueller, J. F. K.
Heterobimetallic Bisphosphonate Titanium Complexes: Carbene-Like Carbanions?
European Journal of Inorganic Chemistry: 5024-5028 2008.
- Spickermann, C.; Felder, T.; Schalley, C. A.; Kirchner, B.
How can rotaxanes be modified by varying functional groups at the axle? A combined theoretical and experimental analysis of thermochemistry and electronic effects
Chemistry-a European Journal, (14): 1216-1227 2008.
- Spickermann, C.; Thar, J.
Why are ionic liquid ions mainly associated in water? A Car-Parrinello study of 1-ethyl-3-methylimidazolium chloride water mixture
Journal of Chemical Physics, (129) 2008.
- Sponer, J. E.; Sumpter, B. G.; Leszczynski, J.; Sponer, J.; Fuentes-Cabrera, M.
Theoretical Study on the Factors Controlling the Stability of the Borate Complexes of Ribose, Arabinose, Lyxose, and Xylose
Chemistry-a European Journal, (14): 9990-9998 2008.
- Sproviero, E. M.; Gascon, J. A.; McEvoy, J. P.; Brudvig, G. W.; Batista, V. S.
Computational studies of the O₂-evolving complex of photosystem II and biomimetic oxomanganese complexes
Coordination Chemistry Reviews, (252): 395-415 2008.
- Sproviero, E. M.; Shinopoulos, K.; Gascon, J. A.; McEvoy, J. P.; Brudvig, G. W.; Batista, V. S.
QM/MM computational studies of substrate water binding to the oxygen-evolving centre of photosystem II
Philosophical Transactions of the Royal Society B-Biological Sciences, (363): 1149-1156 2008.
- Standard, J. M.; Copack, B. A.; Johnson, T. K.; Przybyla, D. E.; Graham, S. R.; Steidl, R. J.
An ab initio and density functional theory study of the structure and bonding of sulfur ylides
Journal of Physical Chemistry A, (112): 336-341 2008.
- Stashenko, E. E.; Martinez, J. R.; Tafurt-Garcia, G.; Palma, A.; Bofill, J. M.
A computational study and valence bond approach to the intramolecular electrophilic aromatic substitution mechanism of ortho-allyl-N-benzylanilines
Tetrahedron, (64): 7407-7418 2008.
- Staubitz, A.; Besora, M.; Harvey, J. N.; Manners, I.
Computational analysis of amine-borane adducts as potential hydrogen storage materials with reversible hydrogen uptake
Inorganic Chemistry, (47): 5910-5918 2008.
- Stecko, S.; Pasniczek, K.; Michel, C.; Milet, A.; Perez, S.; Chmielewski, M.
A DFT study of 1,3-dipolar cycloaddition reactions of 5-membered cyclic nitrones with alpha,beta-unsaturated lactones and with cyclic vinyl ethers: Part 1

- Tetrahedron-Asymmetry, (19): 1660-1669 2008.
- Stecko, S.; Pasniczek, K.; Michel, C.; Milet, A.; Perez, S.; Chmielewski, M.
A DFT study of 1,3-dipolar cycloadditions of cyclic nitrones to unsaturated lactones. Part II
Tetrahedron-Asymmetry, (19): 2140-2148 2008.
- Stuedel, R.; Stuedel, Y.; Wong, M. W.
Complexation of the vulcanization accelerator tetramethylthiuram disulfide and related molecules with zinc compounds including zinc oxide clusters (Zn₄O₄)
Chemistry-a European Journal, (14): 919-932 2008.
- Streitwieser, A.; Jayasree, E. G.; Hasanayn, F.; Leung, S. S. H.
A Theoretical Study Of S(N)2 ' Reactions of Allylic Halides: Role of Ion Pairs
Journal of Organic Chemistry, (73): 9426-9434 2008.
- Su, J. W.; Burnette, R. R.
First principles investigation of noncovalent complexation: A 2.2.2 -cryptand ion-binding selectivity study
Chemphyschem, (9): 1989-1996 2008.
- Su, J. W.; Burnette, R. R.
First principles investigation of noncovalent complexation: A [2.2.2]-cryptand ion-binding selectivity study
Chemphyschem, (9): 1989-1996 2008.
- Sukhanov, O. S.; Shishkin, O. V.; Gorb, L.; Leszczynski, J.
Structure and hydrogen bonding in polyhydrated complexes of guanine
Structural Chemistry, (19): 171-180 2008.
- Sun, S.; Chen, W.; Cao, W.; Zhang, F.; Song, J.; Tian, C.
Research on the chelation between quercetin and Cr(III) ion by Density Functional Theory (DFT) method
Journal of Molecular Structure-Theochem, (860): 40-44 2008.
- Sun, Y.-Y.; Zhang, C.-H.; Xue, Y.; Yan, G.-S.
Theoretical study on the stability of anionic tetrazolate complexes with amidiniums
Acta Chimica Sinica, (66): 751-756 2008.
- Sung, C.-Y.; Broadbelt, L. J.; Snuft, R. Q.
A DFT study of adsorption of intermediates in the NO_x reduction pathway over BaNaY zeolites
Catalysis Today, (136): 64-75 2008.
- Sung, D. D.; Jang, H. M.; Il Jung, D.; Lee, I.
Kinetics and mechanism of the anilinolysis of S-aryl N-arylthiocarbamates in acetonitrile
Journal of Physical Organic Chemistry, (21): 1014-1019 2008.
- Suzuki, T.
The hydration of glucose: the local configurations in sugar-water hydrogen bonds

- Physical Chemistry Chemical Physics, (10): 96-105 2008.
- Svozil, D.; Sponer, J. E.; Marchan, I.; Perez, A.; Cheatham, T. E., III; Forti, F.; Luque, F. J.; Orozco, M.; Sponer, J.
Geometrical and electronic structure variability of the sugar-phosphate backbone in nucleic acids
Journal of Physical Chemistry B, (112): 8188-8197 2008.
- Szarek, P.; Sueda, Y.; Tachibana, A.
Electronic stress tensor description of chemical bonds using nonclassical bond order concept
Journal of Chemical Physics, (129) 2008.
- Szatylowicz, H.; Krygowski, T. M.
H-bonded complexes of aniline with HF/F- and anilide with HF in terms of symmetry-adapted perturbation, atoms in molecules, and natural bond orbitals theories
Journal of Physical Chemistry A, (112): 9895-9905 2008.
- Takahashi, M.; Kawazoe, Y.
Metal-substituted disilynes with linear forms
Organometallics, (27): 4829-4832 2008.
- Tanaka, M.; Siehl, H.-U.
An application of the consistent charge equilibration (CQEq) method to guanidinium ionic liquid systems
Chemical Physics Letters, (457): 263-266 2008.
- Tanskanen, J. T.; Linnolahti, M.; Karttunen, A. J.; Pakkanen, T. A.
Structural Characteristics of Hydrogenated Carbon and Boron Nitride Nanotubes: Impact of H-H Interactions
Chemphyschem, (9): 2390-2396 2008.
- Taubert, S.; Straka, M.; Pennanen, T. O.; Sundholm, D.; Vaara, J.
Dynamics and magnetic resonance properties of Sc3C2@C-80 and its monoanion
Physical Chemistry Chemical Physics, (10): 7158-7168 2008.
- Taylor, C. J.; Wu, B.
On the intrinsic stability of the isolated dichromate dianion: Collision activated dissociation of a multiply charged anion via electron detachment
International Journal of Mass Spectrometry, (276): 31-36 2008.
- Tayyari, S. F.; Moosavi-Tekyeh, Z.; Soltanpour, M.; Berenji, A. R.; Sammelson, R. E.
Structure and vibrational assignment of 3-nitro-2,4-pentanedione: A density functional theoretical study
Journal of Molecular Structure, (892): 32-38 2008.
- Tayyari, S. F.; Najafi, A.; Lorestani, F.; Sammelson, R. E.
Hydrogen bond strength and vibrational assignment of the enol form of 3-(methylthio)pentane-2,4-dione
Journal of Molecular Structure-Theochem, (854): 54-62 2008.

- Tayyari, S. F.; Zahedi-Tabrizi, M.; Afzali, R.; Laleh, S.; Mirshahi, H.-A.; Wang, Y. A.
Structure and vibrational assignment of the enol form of 3-chloro-pentane-2,4-dione
Journal of Molecular Structure, (873): 79-88 2008.
- Tejerina, B.; Gordon, M. S.
Addition of POSS-T8 to the Si(100) surface
Journal of Physical Chemistry C, (112): 754-761 2008.
- Temprado, M.; Roux, M. V.
Thermochemistry of 2-and 3-Thiopheneacetic Acids: Calorimetric and Computational Study
Journal of Physical Chemistry A, (112): 10378-10385 2008.
- Thar, J.; Zahn, S.; Kirchner, B.
When is a molecule properly solvated by a continuum model or in a cluster ansatz? A first-principles simulation of alanine hydration
Journal of Physical Chemistry B, (112): 1456-1464 2008.
- Thompson, D.; Hodnett, B. K.
Hydrocarbon Selective Oxidation on Vanadium Phosphorus Oxide Catalysts: Insights from Electronic Structure Calculations
Topics in Catalysis, (50): 116-123 2008.
- Thompson, D.; Miller, C.; McCarthy, F. O.
Computer simulations reveal a novel nucleotide-type binding orientation for ellipticine-based anticancer c-kit kinase inhibitors
Biochemistry, (47): 10333-10344 2008.
- Tian, F.-Y.; Wang, Y.-X.
The competition of double-, four-, and three-ring tubular B-3n (n=8-32) nanoclusters
Journal of Chemical Physics, (129) 2008.
- Tian, S. X.; Li, H. B.; Bai, Y. B.; Yang, J. L.
Unique interactions between diborane and pi orbitals: Blue- or red-shifted hydrogen bonding?
Journal of Physical Chemistry A, (112): 8121-8128 2008.
- Tian, S. X.; Li, H.-B.; Bai, Y.; Yang, J.
Unique interactions between diborane and pi orbitals: Blue- or red-shifted hydrogen bonding?
Journal of Physical Chemistry A, (112): 8121-8128 2008.
- Tian, Z.-N.; Xu, X.
Theoretical study on the isomers of [M(CO)(3)(PPh(2)py)(2)] (M=Fe, Ru) complex
Acta Physico-Chimica Sinica, (24): 1481-1486 2008.
- Tiwari, S.; Shukla, P. K.; Mishra, P. C.
Improved electrostatic properties using combined Mulliken and hybridization-displaced charges for radicals
Journal of Molecular Modeling, (14): 631-640 2008.

- Tobita, M.; Ho, S.
Electronic structure calculation of MgO (001) surface with aggregated oxygen vacancies
Journal of Chemical Theory and Computation, (4): 1057-1064 2008.
- Tomura, M.
Theoretical study for a complex of 1,2,5-thiadiazole with formic acid
Journal of Molecular Structure-Theochem, (868): 1-5 2008.
- Tomura, M.; Ono, K.; Yamashita, Y.
Crystallographic and theoretical studies of 4,4'-dimethyl-7,7'-bi[[1,2,5]thiadiazolo[3,4-b]pyridylidene)-chloranilic acid (1/1) with intermolecular O-H center dot center dot center dot N hydrogen bonds and S center dot center dot center dot O heteroatom interactions
Structural Chemistry, (19): 967-974 2008.
- Tong, G. S. M.; Wong, E. L.-M.; Che, C.-M.
Density functional theory study of trans-dioxo complexes of iron, ruthenium, and osmium with saturated amine ligands, trans-[M(O)(2)(NH3)(2)(NMeH2)(2)](2+) (M = Fe, Ru, Os), and detection of [Fe(qpy)(O)(2)](n+) (n=1, 2) by high-resolution ESI mass spectrometry
Chemistry-a European Journal, (14): 5495-5506 2008.
- Tong, S.; Du, L.; Yao, L.; Ge, M.; Della Vedova, C. O.
Gas-phase generation, structure, spectroscopy, and quantum chemical calculations of fluorocarbonylsulfur thiocyanate, FC(O)SSCN
European Journal of Inorganic Chemistry: 3987-3995 2008.
- Tongraar, A.; Hannongbua, S.
Solvation structure and dynamics of ammonium (NH4+) in liquid ammonia studied by HF/MM and B3LYP/MM molecular dynamics simulations
Journal of Physical Chemistry B, (112): 885-891 2008.
- Tonner, R.; Frenking, G.
Divalent carbon(0) chemistry, part 1: Parent compounds
Chemistry-a European Journal, (14): 3260-3272 2008.
- Tonner, R.; Frenking, G.
Divalent carbon(0) chemistry, part 2: Protonation and complexes with main group and transition metal lewis acids
Chemistry-a European Journal, (14): 3273-3289 2008.
- Tonner, R.; Heydenrych, G.; Frenking, G.
First and second proton affinities of carbon bases
Chemphyschem, (9): 1474-1481 2008.
- Toomey, H. E.; Pun, D.; Veiros, L. F.; Chirik, P. J.
1,2-addition versus sigma-bond metathesis reactions in transient bis(cyclopentadienyl)zirconium imides: Evidence for a d(0) dihydrogen complex
Organometallics, (27): 872-879 2008.

- Torrent-Sucarrat, M.; De Proft, F.
Do the Local Softness and Hardness Indicate the Softest and Hardest Regions of a Molecule?
Chemistry-a European Journal, (14): 8652-8660 2008.
- Torrent-Sucarrat, M.; Salvador, P.; Sola, M.; Geerlings, P.
The hardness kernel as the basis for global and local reactivity indices
Journal of Computational Chemistry, (29): 1064-1072 2008.
- Toth, F.; Olah, J.; Kalas, G.; Greiner, I.; Szollosy, A.; Goemoery, A.; Hazai, L.; Szantay, C.
Synthesis of vinca alkaloids and related compounds. Part 110: A new synthetic method for the preparation of pandoline-type alkaloid-like molecules
Tetrahedron, (64): 7949-7955 2008.
- Trindade, A. F.; Gois, P. M. P.; Veiros, L. F.; Andre, V.; Duarte, M. T.; Afonso, C. A. M.; Caddick, S.; Cloke, F. G. N.
Axial coordination of NHC ligands on dirhodium(II) complexes: Generation of a new family of catalysts
Journal of Organic Chemistry, (73): 4076-4086 2008.
- Trujillo, C.; Lamsabhi, A. M.
Interaction of Ca²⁺ with uracil and its thio derivatives in the gas phase
Organic & Biomolecular Chemistry, (6): 3695-3702 2008.
- Trujillo, C.; Lamsabhi, A. M.; Mo, O.; Yanez, M.
The importance of the oxidative character of doubly charged metal cations in binding neutral bases. [Urea-M](²⁺) and [thiourea-M](²⁺) (M = Mg, Ca, Cu) complexes
Physical Chemistry Chemical Physics, (10): 3229-3235 2008.
- Trujillo, C.; Mo, O.
On the Bonding of Selenocyanates and Isoselenocyanates and Their Protonated Derivatives
Journal of Chemical Theory and Computation, (4): 1593-1599 2008.
- Trujillo, C.; Mo, O.; Yanez, M.
Why are selenouracils as basic as but stronger acids than uracil in the gas phase?
Chemphyschem, (9): 1715-1720 2008.
- Trung, N. T.; Hue, T. T.; Nguyen, M. T.; Zeegers-Huyskens, T.
Theoretical study of the interaction between HN_Z (Z = O, S) and H₂XNH₂ (X = B, Al). Conventional and dihydrogen bonds
Physical Chemistry Chemical Physics, (10): 5105-5113 2008.
- Tsai, W. H.; Ho, J. J.
Reaction HFCO+2H(2)O - Calculated Mechanisms
Journal of the Chinese Chemical Society, (55): 1011-1021 2008.
- Tsai, W.-H.; Ho, J.-J.
Theoretical study on the reaction pathways of HFCO+H₂O

- Journal of Molecular Structure-Theochem, (858): 88-93 2008.
- Tsaryk, N. V.; Kozachkova, A. N.; Trachevskii, V. V.; Rozhenko, A. B.; Pekhnyo, V. I.
Palladium(II) complexes with 1-hydroxyethylidene-1,1-diphosphonic acid
Russian Journal of Coordination Chemistry, (34): 493-498 2008.
- Tsipis, A. C.
Upright or in-plane conformational preference: Dilemma of eta(2)-coordinated C = C double bond in PtX₂(CO)(eta(2)-ene) (X = H, Cl, or C₆F₅) complexes
Organometallics, (27): 3701-3713 2008.
- Tsipis, A. C.; Kefalidis, C. E.; Tsipis, C. A.
The role of the 5f orbitals in bonding, aromaticity, and reactivity of planar Isocyclic and heterocyclic uranium clusters
Journal of the American Chemical Society, (130): 9144-9155 2008.
- Tsvion, E.; Zilberg, S.; Gerber, R. B.
Predicted stability of the organo-xenon compound HXeCCH above the cryogenic range
Chemical Physics Letters, (460): 23-26 2008.
- Turecek, F.; Chen, X.; Hao, C.
Where does the electron go? Electron distribution and reactivity of peptide cation radicals formed by electron transfer in the gas phase
Journal of the American Chemical Society, (130): 8818-8833 2008.
- Turecek, F.; Jones, J. W.; Towle, T.; Panja, S.; Nielsen, S. B.; Hvelplund, P.; Paizs, B.
Hidden Histidine Radical Rearrangements upon Electron Transfer to Gas-Phase Peptide Ions. Experimental Evidence and Theoretical Analysis
Journal of the American Chemical Society, (130): 14584-14596 2008.
- Tuzun, N. S.; Bayata, F.; Sarac, A. S.
An experimental and quantum mechanical study on electrochemical properties of N-substituted pyrroles
Journal of Molecular Structure-Theochem, (857): 95-104 2008.
- Uzunova, E. L.; Mikosch, H.; Nikolov, G. S.
Electronic structure of oxide, peroxide, and superoxide clusters of the 3d elements: A comparative density functional study
Journal of Chemical Physics, (128) 2008.
- Valencia, H.; Kohyama, M.; Tanaka, S.; Matsumoto, H.
Ab initio study of EMIM-BF₄ molecule adsorption on Li surfaces as a model for ionic liquid/Li interfaces in Li-ion batteries
Physical Review B, (78) 2008.
- Valencia, I.; Chavez, V.; Castro, M.
Bonding of benzene with excited states of Fe-7
Journal of Physical Chemistry A, (112): 5028-5033 2008.

- Van Doren, J. M.; Miller, T. M.; Viggiano, A. A.
G3 and density functional theory investigations of the structures and energies of SF_nCl (n=0-5) and their anions
Journal of Chemical Physics, (128) 2008.
- Varadwaj, P. R.
DFT-UX3LYP Studies on the Coordination Chemistry of Ni²⁺. Part 1: Six Coordinate [Ni(NH₃)(n)(H₂O)(6-n)](2+) Complexes
Journal of Physical Chemistry A, (112): 10657-10666 2008.
- Varga, Z.; Hargittai, M.
Structures and thermodynamic properties of aluminum oxyhalides: a computational study
Structural Chemistry, (19): 595-602 2008.
- Vargas-Baca, I.; Findlater, M.; Powell, A.; Vasudevan, K. V.; Cowley, A. H.
Boron di- and tri-cations
Dalton Transactions: 6421-6426 2008.
- Velcheva, E. A.; Vassileva-Boyadjieva, P. J.; Binev, I. G.
Experimental and DFT studies on IR spectral and structural changes arising from the conversion of 1H-indole-2,3-dione (isatin) into azanion
Bulgarian Chemical Communications, (40): 433-439 2008.
- Velez, E.; Quijano, J.; Notario, R.; Murillo, J.; Ramirez, J. F.
Computational study of the mechanism of thermal decomposition of xanthates in the gas phase (the Chugaev reaction)
Journal of Physical Organic Chemistry, (21): 797-807 2008.
- Venkataramanan, N. S.
Structures of small Ni_xTi_y (x+y ≤ 5) clusters: A DFT study
Journal of Molecular Structure-Theochem, (856): 9-15 2008.
- Venter, G. A.; Matthews, R. P.; Naidoo, K. J.
Conformational flexibility of sulphur linked saccharides a possible key to their glycosidase inhibitor activity
Molecular Simulation, (34): 391-401 2008.
- Vessally, E.; Nikoorazm, M.
Singlet-triplet energy gaps in divalent C₂H₂M and C₂H₆M (M = C, Si, Ge, Sn and Pb)
Asian Journal of Chemistry, (20): 1121-1129 2008.
- Vessecchi, R.; Galembeck, S. E.; Lopes, N. P.; Nascimento, P. G. B. D.; Crotti, A. E. M.
Application of computational quantum chemistry to chemical processes involved in mass spectrometry
Quimica Nova, (31): 840-853 2008.
- Victoria Roux, M.; Temprado, M.; Notario, R.; Foces-Foces, C.; Emel'yanenko, V. N.; Verevkin, S. P.

- Structure-energy relationship in barbituric acid: A calorimetric, computational, and crystallographic study*
Journal of Physical Chemistry A, (112): 7455-7465 2008.
- Vijayakumar, T.; Joe, I. H.; Nair, C. P. R.; Jayakumar, V. S.
Non-bonded interactions and its contribution to the NLO activity of Glycine Sodium Nitrate - A vibrational approach
Journal of Molecular Structure, (877): 20-35 2008.
- Vishnevskiy, Y. V.; Vogt, N.; Vogt, J.; Rykov, A. N.; Kuznetsov, V. V.; Makhova, N. N.; Vilkov, L. V.
Molecular structure of 1,5-diazabicyclo[3.1.0]hexane as determined by gas electron diffraction and quantum-chemical calculations
Journal of Physical Chemistry A, (112): 5243-5250 2008.
- Vrcek, I. V.; Kos, I.; Weitner, T.; Birus, M.
Acido-Base Behavior of Hydroxamic Acids: Experimental and Ab Initio Studies on Hydroxyureas
Journal of Physical Chemistry A, (112): 11756-11768 2008.
- Vueba, M. L.; Pina, M. E.; De Carvalho, L. A. E. B.
Conformational stability of ibuprofen: Assessed by DFT calculations and optical vibrational spectroscopy
Journal of Pharmaceutical Sciences, (97): 845-859 2008.
- Vujkovic, N.; Fillol, J. L.; Ward, B. D.; Wadepohl, H.; Mountford, P.; Gade, L. H.
Insertions into azatitanacyclobutenes: New insights into three-component coupling reactions involving imidotitanium intermediates
Organometallics, (27): 2518-2528 2008.
- Vyboishchikov, S. F.
Partitioning of atomization energy
International Journal of Quantum Chemistry, (108): 708-718 2008.
- Vyboishchikov, S. F.; Krapp, A.
Two complementary molecular energy decomposition schemes: The Mayer and Ziegler-Rauk methods in comparison
Journal of Chemical Physics, (129) 2008.
- Wagner, G.; Danks, T. N.; Desai, B.
Theoretical study of the cycloaddition of nitrones to cinnamionitrile: effect of Lewis acid coordination on the selectivity of the reaction
Tetrahedron, (64): 477-486 2008.
- Wahl, B.; Kloo, L.; Ruck, M.
The molecular cluster [Bi₁₀Au₂](SbBi₃Br₉)(₂)
Angewandte Chemie-International Edition, (47): 3932-3935 2008.
- Wahl, B.; Ruck, M.

The Molecular Clusters [Bi₁₀Au₂](EBi₃X₉)(₂) (E = As, Bi; X = Cl, Br) -Synthesis, Crystal Structures, Twinning and Chemical Bonding

Zeitschrift für Anorganische und Allgemeine Chemie, (634): 2267-2275 2008.

Waller, M. P.; Geethalakshmi, K. R.; Buehl, M.

V-51 NMR chemical shifts from quantum-mechanical/molecular-mechanical models of vanadium bromoperoxidase

Journal of Physical Chemistry B, (112): 5813-5823 2008.

Wander, M. C. F.; Clark, A. E.

Hydration properties of aqueous Pb(II) ion

Inorganic Chemistry, (47): 8233-8241 2008.

Wang, A. D.; Bi, C. F.; Fan, Y. H.; Zou, Y. N.; Xu, J. K.; Kan, Y. H.

Structure and coordination environment of the zinc complex with vanillin of double-stranded helix

Russian Journal of Coordination Chemistry, (34): 475-479 2008.

Wang, F.; Izvekov, S.; Voth, G. A.

Unusual "Amphiphilic" association of hydrated protons in strong acid solution

Journal of the American Chemical Society, (130): 3120-3126 2008.

Wang, F.; Meng, Q.; Li, M.

Density functional computations of Rh(I)-catalysed hydroacylation of acetic aldehyde and ethene

Molecular Simulation, (34): 515-523 2008.

Wang, F.; Meng, Q.; Li, M.

Density functional computations of the cyclopropanation of ethene catalyzed by iron(II) carbene complexes Cp(CO)(L)Fe = CHR, L=CO, PMe₃, R=Me, OMe, ph, Co₂Me

International Journal of Quantum Chemistry, (108): 945-953 2008.

Wang, H. L.; Lu, T. T.; He, T. J.; Chen, D. M.

Theoretical Studies on the Structure and Spectrum of Imidazole-Chloranil Charge Transfer Complex

Chinese Journal of Chemical Physics, (21): 560-568 2008.

Wang, M. Y.; Cheng, L.; Wu, Z. J.

Theoretical Studies on the Reaction Mechanism of Platinum-Catalyzed Diboration of Allenes

Organometallics, (27): 6464-6471 2008.

Wang, W.; Hobza, P.

Origin of the X-Hal (Hal = Cl, Br) bond-length change in the halogen-bonded complexes

Journal of Physical Chemistry A, (112): 4114-4119 2008.

Wang, W.; Hobza, P.

Theoretical study on the complexes of benzene with isoelectronic nitrogen-containing heterocycles

Chemphyschem, (9): 1003-1009 2008.

- Wang, W.; Wang, N.; Li, P.; Bu, Y.; Xie, X.; Song, R.
Theoretical studies on the properties of uracil and its dimer upon thioketo substitution
Theoretical Chemistry Accounts, (121): 21-31 2008.
- Wang, W. Z.; Hobza, P.
Application of Berlin's Theorem to Bond-Length Changes in Isolated Molecules and Red- and Blue-Shifting H-Bonded Clusters
Collection of Czechoslovak Chemical Communications, (73): 862-872 2008.
- Wang, X.; Andrews, L.
Infrared spectra, structure, and bonding of the GeH₃-CrH, HGe MoH₃, and HGe WH₃ molecules in solid neon and argon
Inorganic Chemistry, (47): 8159-8166 2008.
- Wang, X.; Andrews, L.
Infrared spectra, structure, and bonding of the group 6 and ammonia M : NH₃, H₂N-MH, and N MH₃ reaction products in solid argon
Organometallics, (27): 4885-4891 2008.
- Wang, X.; Andrews, L.
Silylidyne, HSi MoH₃ and HSi WH₃, and silyl metal hydride, SiH₃-CrH, products in silane reactions
Journal of the American Chemical Society, (130): 6766-6773 2008.
- Wang, X.; Andrews, L.; Gagliardi, L.
Infrared spectra of ThH₂, ThH₄, and the hydride bridging ThH₄(H-2)(x) (x=1-4) complexes in solid neon and hydrogen
Journal of Physical Chemistry A, (112): 1754-1761 2008.
- Wang, X.; Yang, L.; Tian, A.-M.; Wong, N.-B.
Theoretical investigation on reactivity of Ag and Au atoms toward CS₂ in gas phase
International Journal of Mass Spectrometry, (269): 177-186 2008.
- Wang, X. F.; Andrews, L.; Marsden, C. J.
Reactions of Uranium Atoms with Ammonia: Infrared Spectra and Quasi-Relativistic Calculations of the U:NH₃, H₂N-UH, and HN=UH₂ Complexes
Chemistry-a European Journal, (14): 9192-9201 2008.
- Wang, X. L.; Wan, H.; Guan, G. F.
Structure and Interaction of Ion-Pairs of [EPy]Cl and [EPy]Br in Gas and Liquid Phases
Acta Physico-Chimica Sinica, (24): 2077-2082 2008.
- Wang, Y.; Huang, Y.; Yin, B.; Yang, B.; Liu, R.
Octacoordinate carbons encaged inside carborane clusters: A density functional theory investigation
Journal of Physical Chemistry A, (112): 7643-7651 2008.
- Wang, Y.; Truong, T. N.

- Cluster formation model in vapor deposition of Pd atoms on the perfect MgO(100) surface and on its surface oxygen vacancy*
Journal of Physical Chemistry C, (112): 13674-13680 2008.
- Wang, Y.; Wang, C.
Difference for SO₂ and CO₂ in TGML ionic liquids: a theoretical investigation
Physical Chemistry Chemical Physics, (10): 5976-5982 2008.
- Wang, Y.-C.; Chen, D.-P.; Geng, Z.-Y.; Zhang, J.-H.
Theoretical study of activation Fe-O bond of FeO⁺ by CO in the gas phase
Journal of Molecular Structure-Theochem, (858): 26-30 2008.
- Wang, Y. H.; Lu, Y. X.; Zou, J. W.; Yu, Q. S.
Theoretical investigation on charge-assisted halogen bonding interactions in the complexes of bromocarbons with some anions
International Journal of Quantum Chemistry, (108): 90-99 2008.
- Wang, Y.-H.; Lu, Y.-X.; Zou, J.-W.; Yu, Q.-S.
Use of ab initio calculations to provide insights into the strength and nature of interfluorine interactions
International Journal of Quantum Chemistry, (108): 1083-1089 2008.
- Wang, Y.-P.; Leu, H.-L.; Cheng, H.-Y.; Lin, T.-S.; Wang, Y.; Lee, G.-H.
Cyclopentadienyl chromium and tungsten complexes with halide, methyl and sigma-phenylethynyl ligands: Structures of (eta(5)-C₅H₅)Cr(NO)(2)(-C-C₆H₅), (eta(5)-C₅H₅)Cr(NO)(2)I and [(eta(5)-C₅H₄)-COOCH₃]W(CO)(3)Cl
Journal of Organometallic Chemistry, (693): 2615-2623 2008.
- Wang, Y.-P.; Pang, S.-R.; Cheng, H.-Y.; Lin, T.-S.; Wang, Y.; Lee, G.-H.
Syntheses and spectra of chromium-titanium complexes bridged by carboxylate substituted cyclopentadienyl group: The structure of CP₂Ti(CH₃){[OC(O)C₅H₄]Cr(NO)(2)Cl}
Journal of Organometallic Chemistry, (693): 329-337 2008.
- Wang, Z.-X.; Zhang, C.-G.; Chen, Z.; von Ragu Schleyer, P.
Planar tetracoordinate carbon species involving beryllium substituents
Inorganic Chemistry, (47): 1332-1336 2008.
- Wang, Z.-X.; Zheng, B.-S.; Yu, X.-Y.; Yi, P.-G.
Characteristics and nature of the intermolecular interactions between thiophene and XY(X, Y=F, Cl, Br): A theoretical study
Journal of Molecular Structure-Theochem, (857): 13-19 2008.
- Watts, C. R.; Badenhoop, J. K.
Steric and hyperconjugative contributions to rotation barriers in diboron analogs B₂L₄ (L=F, OH, NH₂, CH₃, and H)
Journal of Chemical Physics, (129) 2008.
- Wedel, T.; Gehring, T.; Podlech, J.; Kordel, E.; Bihlmeier, A.; Klopper, W.

Nucleophilic additions to alkylidene bis(sulfoxides)-stereoelectronic effects in vinyl sulfoxides
Chemistry-a European Journal, (14): 4631-4639 2008.

Wenska, G.; Filipiak, P.; Asmus, K.-D.; Bobrowski, K.; Koput, J.; Marciniak, B.
Formation of a sandwich-structure assisted, relatively long-lived sulfur-centered three-electron bonded radical anion in the reduction of a bis(1-substituted-uracilyl) disulfide in aqueous solution
Journal of Physical Chemistry B, (112): 10045-10053 2008.

Werz, D. B.; Dufert, A.
sigma/pi versus pi/pi Conjugation: DFT Studies on Oligocyclopropanones and Related Systems
Organic Letters, (10): 5231-5234 2008.

Wheelock, C. E.; Colvin, M. E.; Sanborn, J. R.; Hammock, B. D.
Substituted 3-phenylpropenoates and related analogs: electron ionization mass spectral fragmentation and density functional theory calculations
Journal of Mass Spectrometry, (43): 1053-1062 2008.

Wielgus, P.; Roszak, S.; Majumdar, D.; Saloni, J.; Leszczynski, J.
Theoretical studies on the bonding and thermodynamic properties of GenSim (m+n=5) clusters: The precursors of germanium/silicon nanomaterials
Journal of Chemical Physics, (128) 2008.

Wierzejewska, M.; Sompolski, D. J.
Ab initio MP2 and FTIR matrix isolation studies on tert-butanethiol complexes with water
Journal of Molecular Structure, (872): 166-175 2008.

Woldu, M. G.; Dillen, J.
A quantum mechanical study of the stability and structural properties of substituted acylthiourea compounds
Theoretical Chemistry Accounts, (121): 71-82 2008.

Wong, B. M.
Nuclear quadrupole hyperfine structure in (HCN)-N-14/(HNC)-N-14 and DC N-15/D-15 NC isomerization: a diagnostic tool for characterizing vibrational localization
Physical Chemistry Chemical Physics, (10): 5599-5606 2008.

Woodcock, H. L.; Brooks, B. R.; Pastor, R. W.
Pathways and populations: Stereoelectronic insights into the exocyclic torsion of 5-(hydroxymethyl)tetrahydropyran
Journal of the American Chemical Society, (130): 6345-+ 2008.

Wu, D.-Y.; Duani, S.; Liu, X.-M.; Xu, Y.-C.; Jiang, Y.-X.; Ren, B.; Xu, X.; Lin, S. H.; Tian, Z.-Q.
Theoretical study of binding interactions and vibrational Raman spectra of water in hydrogen-bonded anionic complexes: (H₂O)(n)(-) (n=2 and 3), H₂O center dot center dot center dot X (X = F, Cl, Br, and I), and H₂O center dot center dot center dot M- (M = Cu, Ag, and Au)
Journal of Physical Chemistry A, (112): 1313-1321 2008.

Wu, L.; Hernandez-Soto, H.; Liu, D. Q.; Vogt, F. G.; O'Neill-Slawecki, S. A.; Su, Q.

- Tandem mass spectrometry and hydrogen/deuterium exchange studies of protonated species of 1,1'-bis(diphenylphosphino)-ferrocene oxidative impurity generated during a Heck reaction*
Rapid Communications in Mass Spectrometry, (22): 314-320 2008.
- Wu, Y.; Feng, L.; Zhang, X.-D.
Theoretical calculation on the C₆H₅-H center dot center dot center dot X hydrogen-bonded complexes
Acta Physico-Chimica Sinica, (24): 653-658 2008.
- Xi, H. W.; Karni, M.; Apeloig, Y.
Silabutadienes. Internal Rotations and pi-Conjugation. A Density Functional Theory Study
Journal of Physical Chemistry A, (112): 13066-13079 2008.
- Xia, X.; Zhang, C.
DFT Study and Monte Carlo Simulation on the Aminolysis of XC(O)OCH₃ (X = NH₂, H, and CF₃) with Monomeric and Dimeric Ammonias
Journal of Chemical Theory and Computation, (4): 1643-1653 2008.
- Xia, Y.; Yin, D.
Impact of Lewis acids on Diels-Alder reaction reactivity: A conceptual density functional theory study
Journal of Physical Chemistry A, (112): 9970-9977 2008.
- Xie, H.; Wu, R.; Xia, F.; Cao, Z.
Effects of electron attachment on C-5'-O-5' and C-1'-N-1 bond cleavages of pyrimidine nucleotides: A theoretical study
Journal of Computational Chemistry, (29): 2025-2032 2008.
- Xing, D.; Bu, Y.; Tan, X.
Characterizing the properties of the N₇,N₉-dimethylguaninium chloride ion pairs: Prospecting for the design of a novel ionic liquid
Journal of Physical Chemistry A, (112): 106-116 2008.
- Xing, D.; Tan, X.; Chen, X.; Bu, Y.
Theoretical study on the gas-phase acidity of multiple sites of Cu⁺-adenine and Cu²⁺-adenine complexes
Journal of Physical Chemistry A, (112): 7418-7425 2008.
- Xiong, Z.; Liu, Y.; Sun, H.
Electrostatic and covalent contributions in the coordination bonds of transition metal complexes
Journal of Physical Chemistry A, (112): 2469-2476 2008.
- Xu, B. H.; Li, L. C.; Sun, L.; Tian, A. M.
Theoretical study on the structures and properties of the isomers of N-n(CH)_(8-n)H-8 (n=0-7)
Journal of Molecular Structure-Theochem, (870): 77-82 2008.
- Xu, W. G.; Zhang, R. C.
Structures and aromaticity of the planar Si₂BX (X = Li, K, O, S) clusters

- Journal of Molecular Structure-Theochem, (864): 1-5 2008.
- Xu, W. G.; Zhang, R. C.; Lu, S. X.; Zhang, Y. C.
Structures and aromaticity of the planar XSi_2Y ($X = Al, Ga$ and $Y = P, As$) clusters
Journal of Molecular Structure-Theochem, (859): 18-21 2008.
- Xu, X.; Li, Q. Y.; Fang, L.; Sun, S. L.; Su, Z. M.
Quantum Chemistry Studies on the Fe-Cu Interactions and P-31 NMR in $Fe(CO)_3(Ph)_2Ppy)_2(CuX_n)$ ($X-n = Cl-2(2-), Cl-, Br-$)
Chinese Journal of Structural Chemistry, (27): 1339-1348 2008.
- Xua, X.; Kang, H. S.
Ferromagnetic and half-metallic behaviors of fullerene-cobalt polymer chains
Journal of Chemical Physics, (128) 2008.
- Xue, W.; Wang, Z. C.; He, S. G.; Xie, Y.; Bernstein, E. R.
Experimental and Theoretical Study of the Reactions between Small Neutral Iron Oxide Clusters and Carbon Monoxide
Journal of the American Chemical Society, (130): 15879-15888 2008.
- Yakovenko, O.; Oliferenko, A. A.; Bdzhola, V. G.; Palyulin, V. A.; Zefirov, N. S.
Kirchhoff atomic charges fitted to multipole moments: Implementation for a virtual screening system
Journal of Computational Chemistry, (29): 1332-1343 2008.
- Yamakita, Y.; Okazaki, T.; Ohno, K.
Conformation-Specific Raman Bands and Electronic Conjugation in Substituted Thioanisoles
Journal of Physical Chemistry A, (112): 12220-12227 2008.
- Yamamoto, T.; Kaneno, D.; Tomoda, S.
The importance of lone pair delocalizations: Theoretical investigations on the stability of cis and trans isomers in 1,2-halodiazenes
Journal of Organic Chemistry, (73): 5429-5435 2008.
- Yamamoto, T.; Kaneno, D.; Tomoda, S.
The Origin of Cis Effect in 1,2-Dihaloethenes: The Quantitative Comparison of Electron Delocalizations and Steric Exchange Repulsions
Bulletin of the Chemical Society of Japan, (81): 1415-1422 2008.
- Yamane, K.; Hayashi, S.; Nakanishi, W.; Sasamori, T.; Tokitoh, N.
Fine structures of 8-G-1-(arylethynylselanyl)naphthalenes ($G = H, Cl, Br$): Factors to control the linear alignment of five G center dot center dot center dot Se-C C-C-Ar atoms in crystals and the behavior in solution
Polyhedron, (27): 3557-3566 2008.
- Yan, H.; Lu, J.
Theoretical study of the hexahydrated metal cations for the understanding of their template effects in the construction of layered double hydroxides

- Journal of Molecular Structure-Theochem, (866): 34-45 2008.
- Yan, S. H.; Cho, S. J.; Lee, S. J.; Kang, S.; Paek, K.; Lee, J. Y.
Molecular recognition of a fluoride anion receptor: the importance of C-H (N-H)center dot center dot center dot F- and "electropositive field space"center dot center dot center dot F- interactions
Physical Chemistry Chemical Physics, (10): 7079-7084 2008.
- Yanez, M.; Mo, O.; Alkorta, I.; Del Bene, J. E.
Structures, Bonding, and One-Bond B-N and B-H Spin-Spin Coupling Constants for a Series of Neutral and Anionic Five-Membered Rings Containing BN Bonds
Journal of Chemical Theory and Computation, (4): 1869-1876 2008.
- Yang, C.; Wang, H.
Ab initio and DFT theory studies of interaction of thymine with formaldehyde
Structural Chemistry, (19): 843-847 2008.
- Yang, J.; White, P. S.; Schauer, C. K.; Brookhart, M.
Structural and spectroscopic characterization of an unprecedented cationic transition-metal eta(1)-silane complex
Angewandte Chemie-International Edition, (47): 4141-4143 2008.
- Yang, P.; Tretiak, S.; Masunov, A. E.; Ivanov, S.
Quantum chemistry of the minimal CdSe clusters
Journal of Chemical Physics, (129) 2008.
- Yang, Z.; Rannulu, N. S.; Chu, Y.; Rodgers, M. T.
Bond dissociation energies and equilibrium structures of Cu+(MeOH)(x), x=1-6, in the gas phase: Competition between solvation of the metal ion and hydrogen-bonding interactions
Journal of Physical Chemistry A, (112): 388-401 2008.
- Yao, W.; Gang, F.; Ze-Ning, C.; Hm-Lin, W.
Theoretical Studies on the Reduction of N2O by CO on FeO+ ((6)Sigma(+))
Chemical Journal of Chinese Universities-Chinese, (29): 2365-2370 2008.
- Yao, Y.; Li, Z. S.
Inhibition Mechanism of Cholinesterases by Carbamate: A Theoretical Study
Chemical Research in Chinese Universities, (24): 778-781 2008.
- Yeguas, V.; Campomanes, P.; Lopez, R.
A Theoretical Study on the Reactivity of a Rhenium Hydroxo-Carbonyl Complex Towards beta-Lactams
European Journal of Inorganic Chemistry: 4547-4554 2008.
- Yeguas, V.; Diaz, N.; Campomanes, P.; Lopez, R.
Ring opening at N1-C2 bond of azetidin-2-ones by a molybdenum hydroxo-carbonyl complex: evidence from a computational study
Dalton Transactions: 6427-6434 2008.

- Yeung, C. S.; Liu, L. V.; Wang, Y. A.
Adsorption of small gas molecules onto Pt-doped single-walled carbon nanotubes
Journal of Physical Chemistry C, (112): 7401-7411 2008.
- Yi, G.-Q.; Zeng, Y.; Xia, X.-F.; Xue, Y.; Kim, C.-K.; Yan, G.-S.
The substituent effects of the leaving groups on the aminolysis of phenyl acetates: DFT studies
Chemical Physics, (345): 73-81 2008.
- Yin, B.; Wang, G.; Sa, N.; Huang, Y.
Bonding analysis and stability on alternant B16N16 cage and its dimers
Journal of Molecular Modeling, (14): 789-795 2008.
- Yong, Y.
Coexistence of S-H center dot center dot center dot O and N-H center dot center dot center dot O Blue-shifted Hydrogen Bonds in a Small System: HSO center dot center dot center dot HNO
Chemistry Letters, (37): 1070-1071 2008.
- Yoshikai, N.; Iida, R.; Nakamura, E.
Mechanism of the nucleophilic substitution of acyl electrophiles using lithium organocuprates
Advanced Synthesis & Catalysis, (350): 1063-1072 2008.
- Yu, H.; Jia, G.; Lin, Z.
Theoretical studies on O-insertion reactions of nitrous oxide with ruthenium hydride complexes
Organometallics, (27): 3825-3833 2008.
- Yu, J.; Yang, X. J.; Liu, Y. Y.; Pu, Z. F.; Li, Q. S.; Xie, Y. M.; Schaefer, H. F.; Wu, B. A.
Dinuclear versus Mononuclear Zinc Compounds from Reduction of LZnCl₂ (L = alpha-Diimine Ligands): Effects of the Ligand Substituent, Reducing Agent, and Solvent
Organometallics, (27): 5800-5814 2008.
- Yu, S.-P.; Yan, H.; Yuan, X.-X.; Wang, X.; Tian, A.-M.
Theoretical study on reaction mechanism of the C-H bond activation of methane by Br⁺
Acta Chimica Sinica, (66): 1518-1522 2008.
- Yu, Y.; Shen, W.; Zhang, J.; He, R.; Li, M.
Theoretical investigation of direct amination of beta-ketoesters catalyzed by copper(II)-bisoxazoline(BOX)
Journal of Molecular Modeling, (14): 237-247 2008.
- Yu, Y. Q.; Shen, W.; Zhang, J. S.; He, R. X.; Li, M.
DFT studies on the mechanism of Pd(II)-catalyzed intermolecular 1,2-diamination of conjugated dienes
Journal of Physical Organic Chemistry, (21): 979-987 2008.
- Yuan, K.; Liu, Y. Z.; Zhu, Y. C.; Zhang, J.
Hydrogen-Bonded Complex between Ozone and Thioperoxy Radical in Gas-Phase
Acta Physico-Chimica Sinica, (24): 2065-2070 2008.

- Yuan, K.; Liu, Y.-Z.; Lue, L.-L.
Red shift hydrogen bond of open-shell (CH₃)₂S(O) center dot center dot center dot HOO complexes in gas phase Structures and properties
Acta Physico-Chimica Sinica, (24): 861-867 2008.
- Yuan, K.; Liu, Y.-Z.; Lue, L.-L.; Ma, W.-C.
Halogen bond and hydrogen bond interactions between (CH₃)₂S and HOCl
Acta Physico-Chimica Sinica, (24): 1257-1263 2008.
- Yuan, K.; Lue, L.; Liu, Y.
Theoretical study on the lithium bond interaction of furan homologues C₄H₄Y (Y=O, S) with LiCH₃ via DFT and MP2
Chinese Science Bulletin, (53): 1315-1323 2008.
- Yuan, K.; Zhu, Y. C.; Liu, Y. Z.; Li, Z. F.; Dong, X. N.; Wang, X. F.; Li, H. X.; Zhang, J.
Lithium bond structures of H (n) Y (n=2, 3; Y=O, S, N) center dot center dot center dot LiNH₂ and the abnormal blue shift of N-Li bond
Chinese Science Bulletin, (53): 3151-3158 2008.
- Yuan, L.; Sumpter, B. G.; Abboud, K. A.; Castellano, R. K.
Links between through-bond interactions and assembly structure in simple piperidones
New Journal of Chemistry, (32): 1924-1934 2008.
- Zeng, T.; Klobukowski, M.
Relativistic model core potential study of the Au+Xe system
Journal of Physical Chemistry A, (112): 5236-5242 2008.
- Zeng, Y.; Xue, Y.; Yan, G.
Theoretical study of the acid-promoted hydrolysis of oxazolin-5-one: A microhydration model
Journal of Physical Chemistry B, (112): 10659-10667 2008.
- Zettergren, H.; Alcamí, M.; Martín, F.
Stable non-IPR C-60 and C-70 fullerenes containing a uniform distribution of pyrenes and adjacent pentagons
Chemphyschem, (9): 861-866 2008.
- Zhang, C.; Liang, W.; Chen, H.; Chen, Y.; Wei, Z.; Wu, Y.
Theoretical studies on the geometrical and electronic structures of N-methyle-3,4-fulleropyrrolidine
Journal of Molecular Structure-Theochem, (862): 98-104 2008.
- Zhang, C.; Xue, Y.
Theoretical study on the hydrolysis mechanism of N,N-dimethyl-N'-(2',3'-dideoxy-3'-thiacytidine)-formamidine
Science in China Series B-Chemistry, (51): 911-917 2008.
- Zhang, C.-R.; Chen, H.-S.; Chen, Y.-H.; Wei, Z.-Q.; Pu, Z.-S.
DFT study on methanofullerene derivative [6,6]-phenyl-C-61 butyric acid methyl ester

- Acta Physico-Chimica Sinica, (24): 1353-1358 2008.
- Zhang, C.-R.; Chen, Y.-H.; Wang, D.-B.; Wu, Y.-Z.; Chen, H.-S.
Structures and electronic properties of SimN8-m(0 < m < 8) clusters: a density functional theory study
Chinese Physics B, (17): 2938-2950 2008.
- Zhang, D. B.; Ren, Y. H.; Fu, D. W.; Yan, B.; Song, J. R.; Lue, X. Q.
Crystal Structure, Theoretical Calculation and Bioactivity of 1-(4-Methoxybenzoyl)-3-(4,6-dimethylpyrimidin-2-yl)thiourea
Acta Chimica Sinica, (66): 2409-2415 2008.
- Zhang, G.-L.; Zhang, H.
End-substitution effect on the geometry and electronic structure of oligoheterocyclics
Theoretical Chemistry Accounts, (121): 109-122 2008.
- Zhang, G. Q.; Wang, W.; Chen, D. Z.
Chemical origin of blue and red shifts of C-H stretching vibrations in M+-C2H2 (M = V, Fe, Co, Ni) and M+-C6H6 (M = V, Si, Ni) complexes
Chemical Physics, (354): 225-229 2008.
- Zhang, J.; Zhang, T.-L.; Yang, L.; Zhang, J.-G.; Cui, Y.
Preparation, crystal structure and thermal decomposition character of [Ni(CHZ)(3)]SO4 center dot 3H(2)O
Acta Physico-Chimica Sinica, (24): 760-766 2008.
- Zhang, J.; Zheng, H.; Zhang, T.; Feng, L.
Theoretical study for high-energy-density compounds from cyclophosphazene III. A quantum chemistry study: High nitrogen-contented energetic compound of 1,1,3,3,5,5,7,7-octaazido-cyclo-tetraphosphazene: N4P4(N-3)(8)
Inorganica Chimica Acta, (361): 4143-4147 2008.
- Zhang, J. D.; Chen, Z.; Schaefer, H. F.
Electron attachment to the hydrogenated Watson-Crick guanine cytosine base pair (GC+H): Conventional and proton-transferred structures
Journal of Physical Chemistry A, (112): 6217-6226 2008.
- Zhang, L. D.; Guo, H. J.; Pan, Y.; Qi, F.
Theoretical Study of the AlEt3-Promoted Tandem Reductive Rearrangement of Epoxides
Chinese Journal of Chemical Physics, (21): 547-554 2008.
- Zhang, S.-G.
Structures and properties of cytosine center dot center dot center dot CO complex
Acta Physico-Chimica Sinica, (24): 1637-1642 2008.
- Zhang, Y.; Huang, K.
DFT studies on the role of glutamate residue in the tyrosine nitration
Journal of Molecular Structure-Theochem, (864): 48-55 2008.

- Zhang, Z. Q.; Chow, R. K. K.; Zhou, H. W.; Li, J. L.; Cheung, H.-Y.
An ab initio study on the structure-cytotoxicity relationship of terpenoid lactones based on the Michael reaction between their pharmacophores and L-cysteine-methylester(-1)
Journal of Theoretical & Computational Chemistry, (7): 347-356 2008.
- Zhao, J.; Siu, K. W. M.; Hopkinson, A. C.
The cysteine radical cation: structures and fragmentation pathways
Physical Chemistry Chemical Physics, (10): 281-288 2008.
- Zhao, L.; Guo, W.; Yang, T.; Lu, X.
Theoretical survey of the potential energy surface of methyl nitrite + Cu⁺ reaction
Journal of Physical Chemistry A, (112): 533-541 2008.
- Zhao, L.; Wang, Y.; Guo, W.; Shan, H.; Lu, X.; Yang, T.
Theoretical investigation of the Fe⁺-catalyzed oxidation of acetylene by N₂O
Journal of Physical Chemistry A, (112): 5676-5683 2008.
- Zhao, P. S.; Li, R. Q.; Song, J.; Guo, M. P.
Quantum chemical studies on nicotinato lead(II) complex [Pb(II)(C₅H₄NCOO)(2)]
Bulletin of the Korean Chemical Society, (29): 546-550 2008.
- Zhao, P. S.; Qin, Y. Q.; Zhang, J.; Jian, F. F.
Synthesis, Characterization, Crystal Structure and Quantum Chemical Studies on N-Dimethyl-N'-phenyl-thiocarbamide
Polish Journal of chemistry, (82): 2153-2165 2008.
- Zhao, P. S.; Wang, H. Y.; Li, R. Q.; Guo, H. M.
Synthesis, crystal structure, electronic spectra and density functional studies on 1N-phenyl-3-(3,4-dichlorophenyl)-5-phenyl-2-pyrazoline
Indian Journal of Chemistry Section a-Inorganic Bio-Inorganic Physical Theoretical & Analytical Chemistry, (47): 986-991 2008.
- Zhao, P.-S.; Guo, H.-M.; Wang, X.; Jian, F.-F.
Synthesis, crystal structure and density functional studies on 1N-phenyl-3-(2,4-dichlorophenyl)-5-(4-chlorophenyl)-2-pyrazoline
Journal of the Chinese Chemical Society, (55): 183-188 2008.
- Zhao, Y.-Y.; Tao, F.-M.; Zeng, E. Y.
Theoretical study on the chemical properties of polybrominated diphenyl ethers
Chemosphere, (70): 901-907 2008.
- Zheng, S. Y.; Wang, J. Y.; Xiong, Y.
Theoretical investigation on isomerization of Et₂AlCN to Et₂AlNC and cyanation of aldimine
Journal of Molecular Structure-Theochem, (869): 83-88 2008.
- Zheng, Y.; Xue, Y.; Yan, G. S.

- The effects of oxidation and protonation on the N-glycosidic bond stability of 8-oxo-2'-deoxyguanosine: DFT study*
Journal of Molecular Structure-Theochem, (860): 52-57 2008.
- Zhou, X.; Hrovat, D. A.; Borden, W. T.
Very-low-lying electronic states result from $n \rightarrow \pi$ excitations in open-shell annulenes, annelated with alpha-dicarbonyl groups
Organic Letters, (10): 893-896 2008.
- Zhou, X.; Pan, Q.-J.; Liu, T.; Li, M.-X.; Zhang, H.-X.
Theoretical studies upon the electronic structures and spectroscopic properties for a series of luminescent terpyridyl platinum(II) phenylacetylide complexes
Journal of Molecular Structure-Theochem, (863): 91-98 2008.
- Zhou, Y.; Liu, X.; Yang, J.; Han, Q. B.; Song, J. Z.; Li, S. L.; Qiao, C. F.; Ding, L. S.; Xu, H. X.
*Analysis of caged xanthenes from the resin of *Garcinia hanburyi* using ultra-performance liquid chromatography/electrospray ionization quadrupole time-of-flight tandem mass spectrometry*
Analytica Chimica Acta, (629): 104-118 2008.
- Zhou, Z.-J.; Liu, H.-L.; Huang, X.-R.; Sun, C.-C.
Forecasting for the stable isomers of [C, O, S] system
Chemical Journal of Chinese Universities-Chinese, (29): 1641-1643 2008.
- Zhou, Z.-J.; Liu, H.-L.; Huang, X.-R.; Sun, C.-C.
Si2CS: A new sulfur-containing molecule with singlet cyclic ground state
Journal of Molecular Structure-Theochem, (848): 74-81 2008.
- Zhu, R.-X.; Zhang, D.-J.; Wang, R.-X.; Liu, C.-B.
Theoretical study on the ring-opening polymerization of D-lactide catalyzed by bifunctional thiourea catalyst
Acta Chimica Sinica, (66): 885-889 2008.
- Zielinski, M.; van Lenthe, J. H.
Spin Coupling and Resonance
Journal of Physical Chemistry A, (112): 13197-13202 2008.
- Zubarev, D. Y.; Boldyrev, A. I.
Developing paradigms of chemical bonding: adaptive natural density partitioning
Physical Chemistry Chemical Physics, (10): 5207-5217 2008.
- Zubarev, D. Y.; Boldyrev, A. I.
Revealing Intuitively Assessable Chemical Bonding Patterns in Organic Aromatic Molecules via Adaptive Natural Density Partitioning
Journal of Organic Chemistry, (73): 9251-9258 2008.