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- Acosta-Silva, C.; Branchadell, V.
Comparison of density functionals for reactions of sulfur ylides with aldehydes and Olefins
Journal of Physical Chemistry A, (111): 12019-12025 2007.
- Adcock, W.; Trout, N. A.
The nature of the electronic factor governing diastereofacial selectivity in remotely substituted (X) 2-adamantyl cations: 5-X versus 4-X substitution
Journal of Physical Organic Chemistry, (20): 791-798 2007.
- Adrover, M.; Vilanova, B.; Munoz, F.; Donoso, J.
Pyridoxamine, a scavenger agent of carbohydrates
International Journal of Chemical Kinetics, (39): 154-167 2007.
- Ahlquist, M.; Norrby, P. O.
Oxidative addition of aryl chlorides to monoligated palladium(0): A DFT-SCRF study
Organometallics, (26): 550-553 2007.
- Ahlrichs, R.; Eichhofer, A.; Fenske, D.; May, K.; Sommer, H.
Molecular structure and theoretical studies of (PPh₄)₂[Bi₁₀Cu₁₀(SPh)₂₄]
Angewandte Chemie-International Edition, (46): 8254-8257 2007.
- Akilandeswari, L.; Venuvanalingam, P.
Computational insights on the lone pair induced barrier modulation in the thermal rearrangement of 6-halo-2-pyrones
Journal of Theoretical & Computational Chemistry, (6): 233-243 2007.
- Alabugin, I. V.; Manoharan, M.
Rehybridization as a general mechanism for maximizing chemical and supramolecular bonding and a driving force for chemical reactions
Journal of Computational Chemistry, (28): 373-390 2007.
- Alabugin, I. V.; Manoharan, M.; Buck, M.; Clark, R. J.
Substituted anilines: The tug-of-war between pyramidalization and resonance inside and outside of crystal cavities
Journal of Molecular Structure-Theochem, (813): 21-27 2007.
- Albrecht, M.; Triyanti; Schiffers, S.; Osetska, O.; Raabe, G.; Wieland, T.; Russo, L.; Rissanen, K.
Anion receptors based on a quinoline backbone
European Journal of Organic Chemistry: 2850-2858 2007.
- Alexandrova, A. N.; Jorgensen, W. L.
Why urea eliminates ammonia rather than hydrolyzes in aqueous solution
Journal of Physical Chemistry B, (111): 720-730 2007.

- Alia, J. D.
Molecular structural formulas as one-electron density and hamiltonian operators: The VIF method extended
Journal of Physical Chemistry A, (111): 2307-2318 2007.
- Alia, J. M.; Edwards, H. G. M.
Vibrational dynamics of hydrogen-bonded HCN complexes with OH and NH acids: Computational DFT systematic study
International Journal of Quantum Chemistry, (107): 1170-1180 2007.
- Anderson, J. S. M.; Melin, J.; Ayers, P. W.
Conceptual density-functional theory for general chemical reactions, including those that are neither charge- nor frontier-orbital-controlled. 2. Application to molecules where frontier molecular orbital theory fails
Journal of Chemical Theory and Computation, (3): 375-389 2007.
- Anderson, R. D.; Milletti, M. C.
Structural and electronic characteristics of a series of glycosidase inhibitors
Letters in Drug Design & Discovery, (4): 587-595 2007.
- Andrada, D. M.; Michoff, M. E. Z.; Fernandez, I.; Granados, A. M.; Sierra, M. A.
Steric versus electronic effects in the structure of heteroatom (S and O)-substituted free and metal (Cr and W)-complexed carbenes
Organometallics, (26): 5854-5858 2007.
- Andre, E.; Lapouge, C.; Cornard, J. P.
Metal complexation of protocatechuic acid and its derivatives: Determination of the optimal computational conditions for the simulation of electronic spectra
Journal of Molecular Structure-Theochem, (806): 131-140 2007.
- Antonioti, P.; Borocci, S.; Bronzolino, N.; Cecchi, P.; Grandinetti, F.
Noble gas anions: A theoretical investigation of FNgBN(-) (Ng = He-Xe)
Journal of Physical Chemistry A, (111): 10144-10151 2007.
- Antonioti, P.; Carra, C.; Maranzana, A.; Tonachini, G.
Germyl mesolytic dissociations in the allylgermane and penta-2,4-dienylgermane radical anions. A theoretical study
Theoretical Chemistry Accounts, (118): 253-264 2007.
- An-Yong, L.; Xiu-Hua, Y.; Su-Wen, W.
Theoretical study of the CH3 center dot center dot center dot Y trifurcated blue-shifted hydrogen bonds
Acta Chimica Sinica, (65): 2809-2816 2007.
- Aragoni, M. C.; Arca, M.; Demartin, F.; Devillanova, F. A.; Gelbrich, T.; Garau, A.; Hursthouse, M. B.; Isaia, F.; Lippolis, V.
Charge-transfer adducts of N-methylthiazolidine-2-thione with IBr and I-2: An example of polymorphism featuring interpenetrating three-dimensional subcomponent assemblies and

halogen center dot center dot center dot pi center dot center dot center dot halogen weak interactions

Crystal Growth & Design, (7): 1284-1290 2007.

Aragoni, M. C.; Arca, M.; Devillanova, F. A.; Hursthouse, M. B.; Huth, S. L.; Isaia, F.; Lippolis, V.; Mancini, A.; Soddu, S.; Verani, G.

Investigation into the reactivity of the coordinatively unsaturated phosphonodithioato [Ni(MeOpdt)(2)] towards 2,4,6-tris(2-pyridyl)-1,3,5-triazine: goals and achievements
Dalton Transactions: 2127-2134 2007.

Arlt, V. M.; Glatt, H.; da Costa, G. G.; Reynisson, J.; Takamura-Enya, T.; Phillips, D. H.

Mutagenicity and DNA adduct formation by the urban air pollutant 2-nitrobenzanthrone
Toxicological Sciences, (98): 445-457 2007.

Arnaiz, A. M.; Carbayo, A.; Cuevas, J. V.; Diez, V.; Garcia-Herbosa, G.; Gonzalez, R.; Martinez, A.; Munoz, A.

Methylation of a terdentate Schiff base ligand NNO-coordinated to palladium with nitromethane
European Journal of Inorganic Chemistry: 4637-4644 2007.

Arno, M.; Zaragoza, R. J.; Domingo, L. R.

A DFT study of the asymmetric (S)-5-(pyrrolidin-2-yl)-1H-tetrazole catalyzed Michael addition of carbonyl compounds to nitroalkenes
Tetrahedron-Asymmetry, (18): 157-164 2007.

Arrieta, A.; Otaegui, D.; Zubia, A.; Cossio, F. P.; Diaz-Ortiz, A.; de la Hoz, A.; Herrero, M. A.; Prieto, P.; Foces-Foces, C.; Pizarro, J. L.; Arriortua, M. I.

Solvent-free thermal and microwave-assisted [3+2] cycloadditions between stabilized azomethine ylides and nitrostyrenes. An experimental and theoretical study
Journal of Organic Chemistry, (72): 4313-4322 2007.

Atesin, T. A.; Li, T.; Lachaize, S.; Brennessel, W. W.; Garcia, J. J.; Jones, W. D.

Experimental and theoretical examination of C-CN and C-H bond activations of acetonitrile using zerovalent nickel
Journal of the American Chemical Society, (129): 7562-7569 2007.

Auer, B.; Kumar, R.; Schmidt, J. R.; Skinnert, J. L.

Hydrogen bonding and Raman, IR, and 2D-IR spectroscopy of dilute HOD in liquid D2O
Proceedings of the National Academy of Sciences of the United States of America, (104): 14215-14220 2007.

Autschbach, J.

Analyzing molecular properties calculated with two-component relativistic methods using spin-free natural bond orbitals: NMR spin-spin coupling constants
Journal of Chemical Physics, (127) 2007.

Avenoza, A.; Busto, J. H.; Canal, N.; Garcia, J. I.; Jimenez-Oses, G.; Peregrina, J. M.; Perez-Fernandez, M.

Mechanistic study of the ring-size modulation in Michael-Dieckmann type reactions of 2-acylaminoacrylates with ketene diethyl acetal

- New Journal of Chemistry, (31): 224-229 2007.
- Aydillo, C.; Jimenez-Oses, G.; Busto, J. H.; Peregrina, J. M.; Zurbano, M. M.; Avenoza, A.
Theoretical evidence for pyramidalized bicyclic serine enolates in highly diastereoselective alkylations
Chemistry-a European Journal, (13): 4840-4848 2007.
- Ayers, P. W.
On the electronegativity nonlocality paradox
Theoretical Chemistry Accounts, (118): 371-381 2007.
- Azzouzi, S.; Jala, R.; El Messaoudi, M.; Domingo, L. R.; Esseffar, W.; Aurell, M. J.
Experimental and theoretical push-pull chemo- and regioselectivity in 1,3-dipolar cycloaddition reactions: The case of benzotriazepin-5-one with mesitylnitrile oxide
Journal of Physical Organic Chemistry, (20): 245-254 2007.
- Bach, M. A.; Parameswaran, P.; Jemmis, E. D.; Rosenthal, U.
Bimetallic complexes of metallacyclopentynes: cis versus trans and planarity versus nonplanarity
Organometallics, (26): 2149-2156 2007.
- Bachler, V.
Orthogonal natural atomic orbitals form an appropriate one-electron basis for expanding CASSCF wave functions into localized bonding schemes and their weights
Journal of Computational Chemistry, (28): 2013-2019 2007.
- Bagheri, A.
Structural study and investigation of NMR tensors in interaction of dopamine with Adenine and guanine
Bulletin of the Chemical Society of Ethiopia, (21): 427-435 2007.
- Bandeira, N. A. G.; Corminboeuf, C.; Calhorda, M. J.
Can five-membered Te₂N₂S rings be considered aromatic?
Structural Chemistry, (18): 841-847 2007.
- Bao, P.; Yu, Z. H.
Restricted geometry optimization: A different way to estimate stabilization energies for aromatic molecules of various types
Journal of Physical Chemistry A, (111): 5304-5313 2007.
- Bao, X. G.; Liang, G. M.; Wong, N. B.; Gu, J. D.
Microsolvation pattern of the hydrated radical anion of uracil: U-(H₂O)(n) (n=3-5)
Journal of Physical Chemistry A, (111): 666-672 2007.
- Barrientos-Salcedo, C.; Arenas-Aranda, D.; Salamanca-Gomez, F.; Ortiz-Muniz, R.; Soriano-Correa, C.
Electronic structure and physicochemical properties characterization of the amino acids 12-26 of TP53: A theoretical study
Journal of Physical Chemistry A, (111): 4362-4369 2007.

- Barros, N.; Maynau, D.; Maron, L.; Eisenstein, O.; Zi, G. F.; Andersen, R. A.
Single but stronger UO, double but weaker UNMe bonds: The tale told by Cp₂UO and Cp₂UNR
Organometallics, (26): 5059-5065 2007.
- Bayse, C. A.
DFT study of the glutathione peroxidase-like activity of phenylselenol incorporating solvent-assisted proton exchange
Journal of Physical Chemistry A, (111): 9070-9075 2007.
- Bayse, C. A.; Antony, S.
Molecular modeling of bioactive selenium compounds
Main Group Chemistry, (6): 185-200 2007.
- Bayse, C. A.; Antony, S.
Molecular modeling of bioactive selenium compounds: 185-200 2007.
- Beckmann, J.; Grabowsky, S.
Supramolecular silanol chemistry in the gas phase. Topological (AIM) and population (NBO) analyses of hydrogen-bonded complexes between H₃SiOH and selected O- and N-acceptor molecules
Journal of Physical Chemistry A, (111): 2011-2019 2007.
- Belelli, P. G.; Ferullo, R. M.; Branda, M. M.; Castellani, N. J.
Theoretical modeling of photocatalytic active species on illuminated TiO₂
Applied Surface Science, (254): 32-35 2007.
- Belkova, N. V.; Griбанова, T. N.; Gutsul, E. I.; Minyaev, R. M.; Bianchini, C.; Peruzzini, M.; Zanobini, F.; Shubina, E. S.; Epstein, L. M.
Specific and non-specific influence of the environment on dihydrogen bonding and proton transfer to [RuH₂{P(CH₂CH₂PPh₂)₃}]
Journal of Molecular Structure, (844): 115-131 2007.
- Bell, M. J.; Lau, K. C.; Krisch, M. J.; Bennett, D. I. G.; Butler, L. J.; Weinhold, F.
Characterization of the methoxy carbonyl radical formed via photolysis of methyl chloroformate at 193.3 nm
Journal of Physical Chemistry A, (111): 1762-1770 2007.
- Benmeddah, A.; Mekelleche, S. M.; Benchouk, W.; Mostefa-Kara, B.; Villemin, D.
Prediction of the reactivity of 2(5H)-furanones as potential dienophiles in Diels-Alder reactions using philicity indexes
Journal of Molecular Structure-Theochem, (821): 42-46 2007.
- Berente, I.; Czinki, E.; Naray-Szabo, G.
A combined electronegativity equalization and electrostatic potential fit method for the determination of atomic point charges
Journal of Computational Chemistry, (28): 1936-1942 2007.
- Berestovitskaya, V. M.; Pabolkova, E. A.; Belyakov, A. V.; Trukhin, E. V.

- beta,beta-dinitrostyrenes: Specificity of synthesis and structure*
Russian Journal of General Chemistry, (77): 1912-1918 2007.
- Berryman, O. B.; Bryantsev, V. S.; Stay, D. P.; Johnson, D. W.; Hay, B. P.
Structural criteria for the design of anion receptors: The interaction of halides with electron-deficient arenes
Journal of the American Chemical Society, (129): 48-58 2007.
- Berryman, O. B.; Bryantsev, V. S.; Stay, D. P.; Johnson, D. W.; Hay, B. P.
Structural criteria for the design of anion receptors: The interaction of halides with electron-deficient arenes
Journal of the American Chemical Society, (129): 48-58 2007.
- Bettinger, H. F.
BN-analogues of vinylidene transition metal complexes: The borylnitrene isomer
Inorganic Chemistry, (46): 5188-5195 2007.
- Bhabak, K. P.; Mugesh, G.
Synthesis, characterization, and antioxidant activity of some selenium analogues
Chemistry-a European Journal, (13): 4594-4601 2007.
- Bhirud, V. A.; Uzun, A.; Kletnieks, P. W.; Craciun, R.; Haw, J. F.; Dixon, D. A.; Olmstead, M. M.; Gates, B. C.
Synthesis and crystal structure of Ir(C₂H₄)(2)(C₅H₇O₂)
Journal of Organometallic Chemistry, (692): 2107-2113 2007.
- Bialek, M.; Trzesowska, A.; Kruszynski, R.
The 3-[3 alpha(2 alpha-hydroxy)pinane]-4,5-(pinan)-1,3-oxazolidine synthesis, structure and properties
Bulletin of the Korean Chemical Society, (28): 89-94 2007.
- Bil, A.; Berski, S.; Latajka, Z.
On three-electron bonds and hydrogen bonds in the open-shell complexes [H₂X₂](+) for X = F, Cl, and Br
Journal of Chemical Information and Modeling, (47): 1021-1030 2007.
- Billes, F.; Mohammed-Ziegler, I.; Mikosch, H.; Tyihak, E.
Vibrational spectroscopy of resveratrol
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (68): 669-679 2007.
- Blake, T. A.; Glendening, E. A.; Sams, R. L.; Sharpe, S. W.; Xantheas, S. S.
High-resolution infrared Spectroscopy in the 1200-1300 cm⁻¹ region and accurate theoretical estimates for the structure and ring-puckering barrier of perfluorocyclobutane
Journal of Physical Chemistry A, (111): 11328-11341 2007.
- Blake, T. A.; Glendening, E. A.; Sams, R. L.; Sharpe, S. W.; Xantheas, S. S.
High-resolution infrared Spectroscopy in the 1200-1300 cm⁻¹ region and accurate theoretical estimates for the structure and ring-puckering barrier of perfluorocyclobutane
Journal of Physical Chemistry A, (111): 11328-11341 2007.

- Bleiholder, C.; Gleiter, R.; Werz, D. B.; Koppel, H.
Theoretical investigations on heteronuclear chalcogen-chalcogen interactions: On the nature of weak bonds between chalcogen centers
Inorganic Chemistry, (46): 2249-2260 2007.
- Bolink, H. J.; Cappelli, L.; Cheylan, S.; Coronado, E.; Costa, R. D.; Lardies, N.; Nazeeruddin, M. K.; Orti, E.
Origin of the large spectral shift in electroluminescence in a blue light emitting cationic iridium(III) complex
Journal of Materials Chemistry, (17): 5032-5041 2007.
- Boo, B. H.; Cho, H.; Kang, D. E.
Ab initio and DFT investigation of structures and energies of low-lying isomers of Zn_xSe_x (x=1-4) clusters
Journal of Molecular Structure-Theochem, (806): 77-83 2007.
- Borocci, S.; Bronzolino, N.; Grandinetti, F.
Noble-gas complexes: Theoretical investigation of multicenter polynuclear species
Helvetica Chimica Acta, (90): 1335-1352 2007.
- Bortoluzzi, M.; Bordignon, E.; Paolucci, G.; Pitteri, B.
A computational study on mixed-ligand N₂P₃ donor-set iron(II) and ruthenium(II) classical and non-classical hydrides
Polyhedron, (26): 4936-4940 2007.
- Boyukata, M.; Ozdogan, C.; Guvenc, Z. B.
An investigation of hydrogen bonded neutral B₄H_n (n=1-11) and anionic B₄H₁₁(-1) clusters: Density functional study
Journal of Molecular Structure-Theochem, (805): 91-100 2007.
- Bradley, C. A.; Veiros, L. F.; Chirik, P. J.
C-O and C-S bond cleavage in chelating diethers and thioethers promoted by eta(9),eta(5)-bis(indenyl)zirconium sandwich complexes: A combined experimental and computational study
Organometallics, (26): 3191-3200 2007.
- Brand, H.; Schulz, A.; Villinger, A.
Modern aspects of pseudohalogen chemistry: News from CN- and PN-chemistry
Zeitschrift fur Anorganische und Allgemeine Chemie, (633): 22-35 2007.
- Brandan, S. A.; Diaz, S. B.; Gonzalez, J. J. L.; Disalvo, E. A.; Ben Altabef, A.
Experimental and theoretical study of the hydration of phosphate groups in esters of biological interest
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (66): 884-897 2007.
- Brandan, S. A.; Diaz, S. B.; Picot, R. C.; Disalvo, E. A.; Ben Altabef, A.
Hydration of inorganic phosphates in crystal lattices and in aqueous solution - An experimental and theoretical study
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (66): 1152-1164 2007.

Bren, V. A.; Dubonosov, A. D.; Minkin, V. I.; Tsukanov, A. V.; Gribanova, T. N.; Shepelenko, E. N.; Revinsky, Y. V.; Rybalkin, V. P.

Photochromic crown-containing molecular switches of chemosensor activity
Journal of Physical Organic Chemistry, (20): 917-928 2007.

Breunig, H. J.; Borrmann, T.; Lork, E.; Rat, C. I.

Syntheses, structures and DFT study of [W(CO)(5)(Ph2SbX)] X = Cl, Br, I
Journal of Organometallic Chemistry, (692): 2593-2598 2007.

Breza, M.; Majek, P.

DFT studies of copper complexes with biphenyldiimino dithioether. Part III: AIM analysis
Polyhedron, (26): 4156-4160 2007.

Brock, D. S.; Bilir, V.; Mercier, H. P. A.; Schrobilgen, G. J.

XeOF2, F2OXeN equivalent to CCH3, and XeOF2 center dot nHF: Rare examples of Xe(IV) oxide fluorides
Journal of the American Chemical Society, (129): 3598-3611 2007.

Brownridge, S.; Crawford, M. J.; Du, H. B.; Harcourt, R. D.; Knapp, C.; Laitinen, R. S.; Passmore, J.; Rautiainen, J. M.; Suontamo, R. J.; Valkonen, J.

Accounting for the differences in the structures and relative energies of the highly homoatomic np(pi)-np(pi) (n >= 3)-bonded S2I42+, the Se-I pi-bonded Se2I42+, and their higher-energy isomers by AIM, MO, NBO, and VB methodologies
Inorganic Chemistry, (46): 681-699 2007.

Buhl, M.; Hnyk, D.; Machacek, J.

Computational studies of structures and properties of metallaboranes. Part 3: Protonated iron bis(dicarbollide), [3-Fe-(1,2-C2B9H11)(2)H](-)
Inorganic Chemistry, (46): 1771-1777 2007.

Buhl, M.; Vrcek, I. V.; Kabrede, H.

Dehalogenation of chloroalkenes at cobalt centers. A model density functional study
Organometallics, (26): 1494-1504 2007.

Buis, N.; French, S. A.; Ruggiero, G. D.; Stengel, B.; Tulloch, A. A. D.; Williams, I. H.

Computational investigation of mechanisms for ring-opening polymerization of epsilon-caprolactone: Evidence for bifunctional catalysis by alcohols
Journal of Chemical Theory and Computation, (3): 146-155 2007.

Bultinck, P.; Ayers, P. W.; Fias, S.; Tiels, K.; Van Alsenoy, C.

Uniqueness and basis set dependence of iterative Hirshfeld charges
Chemical Physics Letters, (444): 205-208 2007.

Bultinck, P.; Van Alsenoy, C.; Ayers, P. W.; Carbo-Dorca, R.

Critical analysis and extension of the Hirshfeld atoms in molecules
Journal of Chemical Physics, (126) 2007.

- Bytheway, I.; Griffith, C. S.; Koutsantonis, G. A.; Skelton, B. W.; White, A. H.
A linear Ru-Tl-Ru complex obtained from halide abstraction: An example of metal-dative bonding
European Journal of Inorganic Chemistry, 3240-3246 2007.
- Bzhezovskii, V. M.; Chura, M. B.
An ab initio quantum-chemical study of C₆H₅SO₂CH₃ and C₆H₅SO₂CF₃ in the MP2(full)/6-31+G Approximation with NBO analysis of wave functions*
Russian Journal of General Chemistry, (77): 1780-1786 2007.
- Cabaleiro-Lago, E. M.; Rodriguez-Otero, J.; Pena-Gallego, A.
A computational study of the electrocyclization of o-divinylbenzene and derivatives
Journal of Molecular Structure-Theochem, (811): 141-151 2007.
- Cabrera, S.; Arrayas, R. G.; Martin-Matute, B.; Cossio, F. P.; Carretero, J. C.
Cu-I-fesulphos complexes: efficient chiral catalysts for asymmetric 1,3-dipolar cycloaddition of azomethine ylides
Tetrahedron, (63): 6587-6602 2007.
- Cadoni, E.; Arca, M.; De Montis, S.; Fattuoni, C.; Perra, E.; Cabiddu, M. G.; Usai, M.; Cabiddu, S.
Lithium 2,3-dihydro-1-benzothiophene-1,1-dioxide: synthesis, characterization, DFT calculations, and reactivity toward aldehydes and azomethines
Tetrahedron, (63): 11122-11134 2007.
- Cai, X.; Zhang, Y. X.; Zhang, X. X.; Jiang, J. Z.
Structures and properties of metal-free and copper tetrakis(thiadiazole) porphyrine and metal-free tetrakis(selenodiazole) porphyrine based on density functional theory calculations
Journal of Molecular Structure-Theochem, (812): 63-70 2007.
- Calhorda, M. J.; Krapp, A.; Frenking, G.
A new look at the ylidic bond in phosphorus ylides and related compounds: Energy decomposition analysis combined with a domain-averaged fermi hole analysis
Journal of Physical Chemistry A, (111): 2859-2869 2007.
- Calichman, M.; Derecskei-Kovacs, A.; Allen, C. W.
The origin of endocyclic bond length variations in disubstituted cyclotriphosphazenes
Inorganic Chemistry, (46): 2011-2016 2007.
- Campomanes, P.; Menedez, M. I.; Cadenas-Jiro, G. I.; Sordo, T. L.
Molecular magnetic properties of heteroporphyrins: a theoretical analysis
Physical Chemistry Chemical Physics, (9): 5644-5648 2007.
- Campomanes, P.; Menendez, M. I.; Sordo, T. L.
Structure, aromaticity, and bonding in subporphyrins: theoretical study of [14]tribenzosubporphine(1.1.1)hydroxyboron(III) and [14]subporphine(1.1.1)hydroxyboron(III) complexes
Journal of Porphyrins and Phthalocyanines, (11): 815-821 2007.
- Cao, D. L.; Ren, F. D.; Wang, J. L.; Wang, W. L.

- Theoretical study on intermolecular interactions of 2,4-dinitroimidazole with methanol*
Journal of Molecular Structure-Theochem, (805): 53-60 2007.
- Carabineiro, S. A.; Gomes, P. T.; Veiros, L. F.; Freire, C.; Pereira, L. C. J.; Henriques, R. T.; Warren, J. E.; Pascu, S. I.
Bis(ketopyrrolyl) complexes of Co(II) stabilised by trimethylphosphine ligands
Dalton Transactions: 5460-5470 2007.
- Caramori, G. F.; de Oliveira, K. T.; Galembeck, S. E.; Bultinck, P.; Constantino, M. G.
Aromaticity and homoaromaticity in methano[10]annulenes
Journal of Organic Chemistry, (72): 76-85 2007.
- Caramori, G. F.; Frenking, G.
The nature of the Ru-NO bond in ruthenium tetraammine nitrosyl complexes
Organometallics, (26): 5815-5825 2007.
- Caramori, G. F.; Galembeck, S. E.
Computational study about through-bond and through-space interactions in [2.2]cyclophanes
Journal of Physical Chemistry A, (111): 1705-1712 2007.
- Cardey, B.; Foley, S.; Enescu, M.
Mechanism of thiol oxidation by the superoxide radical
Journal of Physical Chemistry A, (111): 13046-13052 2007.
- Carrasco, R.; Morgenstern-Badarau, I.; Cano, J.
Two proton-one electron coupled transfer in iron and manganese superoxide dismutases: A density functional study
Inorganica Chimica Acta, (360): 91-101 2007.
- Carvalho, M.; Ferreira, A. S. D.; Da Silva, J. L. F.; Veiros, L. F.
E/Z isomerization of 3-hydrizonocamphor promoted by coordination to palladium or platinum
Collection of Czechoslovak Chemical Communications, (72): 649-665 2007.
- Castano, J. A. G.; Picone, A. L.; Romano, R. M.; Willner, H.; Vedova, C. O.
Early barriers in the matrix photochemical formation of syn-anti randomized FC(O)SeF from the OCS_e : F-2 complex
Chemistry-a European Journal, (13): 9355-9361 2007.
- Castellar, R. J.; Lorono, M.; Cordova, T.; Chuchani, G.
Theoretical studies on the gas-phase elimination kinetics of 2-arylethyl N,N-dimethylcarbamates [(CH₃)₂NCOOCH(2)CH(2)Z, Z=4-CH₃C₆H₄, 4-CH₃OC₆H₄, 4-NO₂C₆H₄]
Journal of Molecular Structure-Theochem, (811): 109-115 2007.
- Ceacero-Vega, A. A.; Ruiz, T. P.; Gomez, M. F.; Roldan, J. M. G.; Navarro, A.; Fernandez-Lienres, M. P.; Jayasooriya, U. A.
Molecular structure, vinyl rotation barrier, and vibrational dynamics of 2,6-dichlorostyrene. A theoretical and experimental research
Journal of Physical Chemistry A, (111): 6406-6419 2007.

- Celik, M. A.; Yurtsever, M.; Tuzun, N. S.; Gungor, F. S.; Sezer, O.; Anac, O.
Metal-catalyzed cyclization reactions of carbonyl ylides: Synthesis and DFT study of mechanisms
Organometallics, (26): 2978-2985 2007.
- Chamot-Rooke, J.; Malosse, C.; Frison, G.; Turecek, F.
Electron capture in charge-tagged peptides. Evidence for the role of excited electronic states
Journal of the American Society for Mass Spectrometry, (18): 2146-2161 2007.
- Chandra, A. K.; Parveen, S.; Zeegers-Huyskens, T.
Anomeric effects in the symmetrical and asymmetrical structures of triethylamine. Blue-shifts of the C-H stretching vibrations in complexed and protonated triethylamine
Journal of Physical Chemistry A, (111): 8884-8891 2007.
- Chandra, A. K.; Zeegers-Huyskens, T.
Theoretical study of the acidity and basicity of uric acid and its interaction with water
Journal of Molecular Structure-Theochem, (811): 215-221 2007.
- Charif, I. E.; Mekelleche, S. M.; Villemin, D.; Mora-Diez, N.
Correlation of aqueous pK(a) values of carbon acids with theoretical descriptors: A DFT study
Journal of Molecular Structure-Theochem, (818): 1-6 2007.
- Chaudhuri, P.; Ganguly, B.; Bhattacharya, S.
An experimental and computational analysis on the differential role of the positional isomers of symmetric bis-2-(pyridyl)-1H-benzimidazoles as DNA binding agents
Journal of Organic Chemistry, (72): 1912-1923 2007.
- Chen, D. L.; Tian, W. Q.; Feng, J. K.; Sun, C. C.
Evidence for d-orbital aromaticity in Sn- and Pb-based clusters: Is Sn-12(2-) aromatic?
Journal of Physical Chemistry A, (111): 8277-8280 2007.
- Chen, D. L.; Tian, W. Q.; Feng, J. K.; Sun, C. C.
Search for more stable C58X18 isomers: Stabilities and electronic properties of seven-membered ring C58X18 fullerene derivatives (X = H, F, and Cl)
Journal of Physical Chemistry B, (111): 5167-5173 2007.
- Chen, D. L.; Tian, W. Q.; Feng, J. K.; Sun, C. C.
Structures and electronic properties of C56Cl8 and C56Cl10 fullerene compounds
Chemphyschem, (8): 2386-2390 2007.
- Chen, D. L.; Tian, W. Q.; Feng, J. K.; Sun, C. C.
Structures, stabilities, and electronic and optical properties of C-52 fullerene, ions, and metallofullerenes
Journal of Chemical Physics, (126) 2007.
- Chen, D. L.; Tian, W. Q.; Feng, J. K.; Sun, C. C.
Structures, stabilities, and electronic and optical properties of C-58 fullerene isomers, ions, and metallofullerenes

- Chemphyschem, (8): 1029-1036 2007.
- Chen, D. L.; Tian, W. Q.; Sun, C. C.
First-principles studies of AlPbn and AlPbn+ clusters (n=1-12): Search for Al-doped clusters with large stabilities
Physical Review A, (75) 2007.
- Chen, J. C.; Chen, L. M.; Liao, S. Y.; Zheng, K.; Ji, L. N.
The hydrolysis process of the anticancer complex [ImH][trans-RuCl4(Im)(2)]: a theoretical study
Dalton Transactions: 3507-3515 2007.
- Chen, J. C.; Chen, L. M.; Liao, S. Y.; Zheng, K. C.; Ji, L. N.
A theoretical study on the hydrolysis process of the antimetastatic ruthenium(III) complex NAMI-A
Journal of Physical Chemistry B, (111): 7862-7869 2007.
- Chen, J. C.; Shen, Y.; Liao, S. Y.; Chen, L. M.; Zheng, K. C.
DFT-based QSAR study and molecular design of AHMA derivatives as potent anticancer agents
International Journal of Quantum Chemistry, (107): 1468-1478 2007.
- Chen, J. M.; Wei, W.; Feng, X. L.; Lu, T. B.
CO2 fixation and transformation by a dinuclear copper cryptate under acidic conditions
Chemistry-an Asian Journal, (2): 710-719 2007.
- Chen, X. F.; Guo, W. Y.; Zhao, L. M.; Fu, Q. T.; Ma, Y.
Reaction of acetaldehyde with Ni+: An extended theoretical study of the decarbonylation mechanism of acetaldehyde by first-row transition metal ions
Journal of Physical Chemistry A, (111): 3566-3570 2007.
- Chen, X. H.; Bu, Y. X.
Cation-modulated electron-transfer channel: H-atom transfer vs proton-coupled electron transfer with a variable electron-transfer channel in acylamide units
Journal of the American Chemical Society, (129): 9713-9720 2007.
- Cheng, J. G.; Gong, Z.; Zhu, W. L.; Tang, Y.; Li, W. H.; Li, Z.; Jiang, H. L.
Cation sitting in aromatic cages: ab initio computational studies on tetra methylammonium-(benzene)(n) (n=3-4) complexes
Journal of Physical Organic Chemistry, (20): 448-453 2007.
- Cheng, L. P.; Cao, W. Q.
Theoretical study of N4X (X = O, S, Se) systems
Journal of Molecular Modeling, (13): 1073-1080 2007.
- Chermahini, A. N.; Nasr-Esfahani, M.; Dalirnasab, Z.; Dabbagh, H. A.; Telmouri, A.
Theoretical studies on tautomerism of tetrazole derivatives by polarisable continuum method (PCM)
Journal of Molecular Structure-Theochem, (820): 7-11 2007.

- Chiu, C. W.; Gabbai, F. R.
Structural changes accompanying the stepwise population of a B-C pi bond
Angewandte Chemie-International Edition, (46): 6878-6881 2007.
- Cho, H. G.; Andrews, L.
Formation of HC ReH3 in methane activation by rhenium atoms: Observation of the elusive methylidyne C-H stretching absorption
Organometallics, (26): 4098-4101 2007.
- Choe, Y. K.; Nagase, S.; Nishimoto, K.
Theoretical study of the electronic spectra of oxidized and reduced states of lumiflavin and its derivative
Journal of Computational Chemistry, (28): 727-739 2007.
- Cimino, P.; Pavone, M.; Barone, V.
Halogen bonds between 2,2,6,6-Tetramethylpiperidine-N-oxyl radical and CxHyFzI species: DFT calculations of physicochemical properties and comparison with hydrogen bonded adducts
Journal of Physical Chemistry A, (111): 8482-8490 2007.
- Ciofini, I.; Laine, P. P.; Adamo, C.
Quantifying electron delocalization in orthogonal channels: Theoretical investigation of sigma and pi aromaticity in [C6I6](2+) and [C6Cl6](2+)
Chemical Physics Letters, (435): 171-175 2007.
- Clark, T.; Hennemann, M.; Murray, J. S.; Politzer, P.
Halogen bonding: the sigma-hole
Journal of Molecular Modeling, (13): 291-296 2007.
- Clennan, E. L.; Hightower, S. E.
Conformationally induced electrostatic stabilization (CIES) of persulfoxides. A comparison to homologous sulfoxides
Heteroatom Chemistry, (18): 591-599 2007.
- Cohen, R.; Stokbro, K.; Martin, J. M. L.; Ratner, M. A.
Charge transport in conjugated aromatic molecular junctions: Molecular conjugation and molecule-electrode coupling
Journal of Physical Chemistry C, (111): 14893-14902 2007.
- Contreras, J. G.; Gerli, L. A.
"conformational preference of 4-ethyl-6-methyl-1,3-dithianes"
Journal of the Chilean Chemical Society, (52): 1271-1275 2007.
- Contreras, R. H.; Esteban, A. L.; Diez, E.; Lochert, I. J.; Della, E. W.; Tormena, C. F.
Experimental and DFT studies on the transmission mechanisms of analogous NMR J(CH) and J(CC) couplings in 1-X- and 1-X-3-methylbicyclo[1.1.1]-pentanes
Magnetic Resonance in Chemistry, (45): 572-577 2007.
- Cordeiro, M.; Pinto, A. S. S.; Gomes, J.

- A DFT study of the chemisorption of methoxy on clean and low oxygen precovered Ru(0001) surfaces*
Surface Science, (601): 2473-2485 2007.
- Cornard, J. P.; Lapouge, C.; Merlin, J. C.
A DFT/TDDFT study of the structural and spectroscopic properties of Al(III) complexes with 4-nitrocatechol in acidic aqueous solution
Chemical Physics, (340): 273-282 2007.
- Corzana, F.; Busto, J. H.; Jimenez-Oses, G.; de Luis, M. G.; Asensio, J. L.; Jimenez-Barbero, J.; Peregrina, J. M.; Avenoza, A.
Serine versus threonine glycosylation: The methyl group causes a drastic alteration on the carbohydrate orientation and on the surrounding water shell
Journal of the American Chemical Society, (129): 9458-9467 2007.
- Costa, P. J.; Calhorda, M. J.; Pregosin, P. S.
Remote metal-arene pi bonding in organometallic complexes: A DFT study
Collection of Czechoslovak Chemical Communications, (72): 703-714 2007.
- Cremer, D.; Grafenstein, J.
Calculation and analysis of NMR spin-spin coupling constants
Physical Chemistry Chemical Physics, (9): 2791-2816 2007.
- Cui, S. H.; Li, Y.; Wang, F. F.; Wu, D.; Li, Z. R.
Prediction and characterization of a new kind of alkali-superhalogen species with considerable stability: MBeX₃ (M = Li, Na; X = F, Cl, Br)
Physical Chemistry Chemical Physics, (9): 5721-5726 2007.
- Cui, Y. H.; Tian, W. Q.; Feng, J. K.; Liu, Z. Z.; Li, W. Q.
Theoretical studies on the aromaticity of eta 5-cyclopentadienyl cobalt dithiolene complexes
Journal of Molecular Structure-Theochem, (810): 65-72 2007.
- Czerski, I.; Kamienska-Trela, K.; Kozminski, W.; Ratajczyk, T.; Szymanski, S.; Wojcik, J.
J(F,H), J(C,H) and J(H,H) couplings involving the individual methyl group protons in 1,2,3,4-tetrachloro-5,6,7,8-tetrafluoro-9-methyltripitycene. Evidence of blue-shifting hydrogen bond
Magnetic Resonance in Chemistry, (45): 1040-1044 2007.
- Dakkouri, M.; Typke, V.
Theoretical analysis of bonding properties in 1,1-dicyanocyclopentane and 1,1-dichlorocyclopentane by applying the AIM and NBO approaches
Structural Chemistry, (18): 357-372 2007.
- Danielsson, J.; Meuwly, M.
Energetics and dynamics in MbCN: CN--vibrational relaxation from molecular dynamics simulations
Journal of Physical Chemistry B, (111): 218-226 2007.
- De, S.; Parameswaran, P.; Jemmis, E. D.

- A theoretical study on the mechanism of boron metathesis*
Inorganic Chemistry, (46): 6091-6098 2007.
- De Vleeschouwer, F.; Van Speybroeck, V.; Waroquier, M.; Geerlings, P.; De Proft, F.
Electrophilicity and nucleophilicity index for radicals
Organic Letters, (9): 2721-2724 2007.
- Deakynne, C. A.; Norton, L. K.; Abele, A. M.; Ludden, A. K.; Liebman, J. F.
Thermochemical considerations and bond enthalpy ratios involving triatomic 16-valence electron neutrals and ions and some isoelectronically related pentaatomics
International Journal of Mass Spectrometry, (267): 324-337 2007.
- DeChancie, J.; Houk, K. N.
The origins of femtomolar protein-ligand binding: Hydrogen-bond cooperativity and desolvation energetics in the biotin-(strept)avidin binding site
Journal of the American Chemical Society, (129): 5419-5429 2007.
- Denehy, E.; White, J. M.; Williams, S. J.
Electronic structure of the sulfonyl and phosphonyl groups: A computational and crystallographic study
Inorganic Chemistry, (46): 8871-8886 2007.
- Derrah, E. J.; Pantazis, D. A.; McDonald, R.; Rosenberg, L.
A highly reactive ruthenium phosphido complex exhibiting Ru-P pi-bonding
Organometallics, (26): 1473-1482 2007.
- Despotovic, I.; Kovacevic, B.; Maksic, Z. B.
Hyperstrong neutral organic bases: Phosphazeno azacalix[3](2,6)pyridines
Organic Letters, (9): 4709-4712 2007.
- Despotovic, I.; Maksic, Z. B.
The structure and stability of [3]-radialenes and their dianions - A DFT study
Journal of Molecular Structure-Theochem, (811): 313-322 2007.
- Dey, A.; Green, K. N.; Jenkins, R. M.; Jeffrey, S. P.; Darensbourg, M.; Hodgson, K. O.; Hedman, B.; Solomon, E. I.
SK-Edge XAS and DFT calculations on square-planar NiII-thiolate complexes: Effects of active and passive H-bonding
Inorganic Chemistry, (46): 9655-9660 2007.
- Di Salvo, F.; Escola, N.; Scherlis, D. A.; Estrin, D. A.; Bondia, C.; Murgida, D.; Ramallo-Lopez, J. M.; Requejo, F. G.; Shimon, L.; Doctorovich, F.
Electronic perturbation in a molecular nanowire of [IrCl5(NO)](-) units
Chemistry-a European Journal, (13): 8428-8436 2007.
- Diao, K.-S.; Wang, H.-J.; Ge, Q.-Y.
Structures and bonding of the complexes [M(eta(5)-E-5)] and [M(eta(5)-E-5)(2)] (M = Sc, Y, E = N, P): a DFT study

- Structural Chemistry, (18): 875-882 2007.
- Dmitrenko, O.; Thorpe, C.; Bach, R. D.
Mechanism of SN2 disulfide bond cleavage by phosphorus nucleophiles. Implications for biochemical disulfide reducing agents
Journal of Organic Chemistry, (72): 8298-8307 2007.
- Domingo, L. R.; Aurell, M. J.; Arno, M.; Saez, J. A.
Toward an understanding of the 1,3-dipolar cycloaddition between diphenylnitrene and a maleimide : bisamide complex. A DFT analysis of the reactivity of symmetrically substituted dipolarophiles
Journal of Molecular Structure-Theochem, (811): 125-133 2007.
- Domingo, L. R.; Benchouk, W.; Mekelleche, S. M.
Understanding the role of the Lewis acid catalyst on the 1,3-dipolar cycloaddition of N-benzylideneaniline N-oxide with acrolein: a DFT study
Tetrahedron, (63): 4464-4471 2007.
- Dong, W. B.; Wang, H. J.; Ren, X. H.; Shan, Y. Y.; Ge, Q. Y.
A theoretical study of the interaction between cytosine and BX3 (X = F, Cl) systems
Journal of Solution Chemistry, (36): 549-561 2007.
- dos Santos, F. P.; Ducati, L. C.; Tormena, C. F.; Rittner, R.
Effects of hyperconjugative interactions on (1)J(CH) coupling constant for hexamethylenetetramine and adamantane: Theoretical and experimental study
Quimica Nova, (30): 1681-1685 2007.
- Doux, M.; Thuery, P.; Blug, M.; Ricard, L.; Le Floch, P.; Arliguie, T.; Mezailles, N.
Anions of tridentate SPS ligands: Syntheses, X-ray structures and DFT calculations
Organometallics, (26): 5643-5653 2007.
- Du, J. A.; Wang, H. Y.; Jiang, G.
Structures of the small Ti-n (n=2-5) clusters: A DFT study
Journal of Molecular Structure-Theochem, (817): 47-53 2007.
- Dupre, D. B.; Wong, J. L.
Thiamin deprotonation mechanism. Carbanion development stabilized by the LUMOs of thiazolium and pyrimidylimine working in tandem and release governed by a H-bond switch
Journal of Physical Chemistry A, (111): 2172-2181 2007.
- Ebrahimi, A.; Habibi, M.; Masoodi, H. R.
Theoretical study of the influence of para- and meta-substituents on X-pyridine center dot center dot center dot HF hydrogen bonding
Chemical Physics, (340): 85-92 2007.
- Ellis, B. D.; Macdonald, C. L. B.
Cycloaddition and electron transfer: On a synthetically useful aspect of pnictogen(I) reactivity
Inorganica Chimica Acta, (360): 329-344 2007.

- El-Nahas, A. M.; El-Demerdash, S. H.; El-Shereefy, E. S. E.
Quantum chemical calculations on the structure and stability of Mg₂+XH₃OH complexes in the gas phase (X = C, Si, and Ge)
International Journal of Mass Spectrometry, (263): 267-275 2007.
- Elsener, A.; Samson, C. C. M.; Brandle, M. P.; Buhlmann, P.; Luthl, H. P.
Statistical analysis of quantum chemical data using generalized XML/CML archives for the derivation of molecular design rules
Chimia, (61): 165-168 2007.
- Ermakov, A. I.; Belousov, V. V.
*Relaxation of STO-3G and 6-31G*basis set functions in the series of LiF isoelectronic molecules of second row elements*
Journal of Structural Chemistry, (48): 6-15 2007.
- Esteban-Gomez, D.; Platas-Iglesias, C.; Avecilla, F.; de Blas, A.; Rodriguez-Blas, T.
Effect of protonation and interaction with anions on a lead(II) complex with a lateral macrobicycle containing a phenol Schiff-base spacer
European Journal of Inorganic Chemistry: 1635-1643 2007.
- Fabian, W. M. F.; Bakulev, V. A.; Janoschek, R.
Cyclisation of alpha-diazonitriles to 5-halo-1,2,3-triazoles: A computational study
Journal of Molecular Structure-Theochem, (821): 89-94 2007.
- Fan, W. J.; Zhang, R. Q.; Liu, S. B.
Computation of large systems with an economic basis set: Structures and reactivity indices of nucleic acid base pairs from density functional theory
Journal of Computational Chemistry, (28): 967-974 2007.
- Fanfrlik, J.; Hnyk, D.; Lepsik, M.; Hobza, P.
Interaction of heteroboranes with biomolecules - Part 2. The effect of various metal vertices and exo-substitutions
Physical Chemistry Chemical Physics, (9): 2085-2093 2007.
- Feng, X. J.; Luo, Y. H.
Structure and stability of Al-doped boron clusters by the density-functional theory
Journal of Physical Chemistry A, (111): 2420-2425 2007.
- Fernandez, I.; Cossio, F. P.; Sierra, M. A.
Mechanism of the generation of ketenimine-M(CO)(n) complexes (M = Cr, W, Fe) from Fischer carbenes and isocyanides
Organometallics, (26): 3010-3017 2007.
- Fernandez, I.; Uggerud, E.; Frenking, G.
Stable pentacoordinate carbocations: Structure and bonding
Chemistry-a European Journal, (13): 8620-8626 2007.

- Fernandez, L.; Viruela-Martin, P.; Latorre, J.; Guillem, C.; Beltran, A.; Amoros, P.
Molecular precursors of mesostructured silica materials in the atrane route: A DFT/GIAO/NBO theoretical study
Journal of Molecular Structure-Theochem, (822): 89-102 2007.
- Fernandez, L. E.; Varetti, E. L.
A quantum chemistry approach to the force fields of the thionyl and selenyl halides, SOX₂ and SeOX₂
Zeitschrift Fur Naturforschung Section B-a Journal of Chemical Sciences, (62): 1491-1496 2007.
- Fernandez, L. E.; Varetti, E. L.
Scaled quantum mechanical force fields for the isoelectronic molecules CF₃X (X = SiH₃, PH₂, SH, Cl)
Zeitschrift fur Anorganische und Allgemeine Chemie, (633): 2678-2682 2007.
- Ferro, V. R.; Lopez, R.; Omar, S.; de la Vega, J. M. G.
On the molecular electron structure of three phosphinine-containing macrocycles
Journal of Computational Chemistry, (28): 958-966 2007.
- Filho, E. B. A.; Ventura, E.; do Monte, S. A.; Oliveira, B. G.; Junior, C. G. L.; Rocha, G. B.; Vasconcellos, M.
Synthesis and conformational study of a new class of highly bioactive compounds
Chemical Physics Letters, (449): 336-340 2007.
- Filho, E. B. A.; Ventura, E.; do Monte, S. A.; Oliveira, B. G.; Junior, C. G. L.; Rocha, G. B.; Vasconcellos, M. L. A. A.
Synthesis and conformational study of a new class of highly bioactive compounds
Chemical Physics Letters, (449): 336-340 2007.
- Fiorucci, S.; Golebiowski, J.; Cabrol-Bass, D.; Antonczak, S.
DFT study of quercetin activated forms involved in antiradical, antioxidant, and prooxidant biological processes
Journal of Agricultural and Food Chemistry, (55): 903-911 2007.
- Fleming, G. J.; McGill, P. R.; Idriss, H.
Gas phase interaction of (L)-proline with Be²⁺, Mg²⁺ and Ca²⁺ ions: a computational study
Journal of Physical Organic Chemistry, (20): 1032-1042 2007.
- Freitas, M. P.; Rittner, R.
Is there a general rule for the gauche effect in the conformational isomerism of 1,2-disubstituted ethanes?
Journal of Physical Chemistry A, (111): 7233-7236 2007.
- Frenking, G.; Cossio, F. P.; Sierra, M. A.; Fernandez, I.
Double group transfer reactions as indicators of aromatic stabilization
European Journal of Organic Chemistry: 5410-5415 2007.
- Furtado, N.; Vescicchi, R.; Tomaz, J. C.; Galembeck, S. E.; Bastos, J. K.; Lopes, N. P.; Crotti, A. E. M.

Fragmentation of diketopiperazines from Aspergillus fumigatus by electrospray ionization tandem mass spectrometry (ESI-MS/MS)

Journal of Mass Spectrometry, (42): 1279-1286 2007.

Gagnepain, J.; Castet, F.; Quideau, W.

Total synthesis of (+)-aquaticol by biomimetic phenol dearomatization: Double diastereofacial differentiation in the Diels-Alder dimerization of orthoquinols with a C-2-symmetric transition state

Angewandte Chemie-International Edition, (46): 1533-1535 2007.

Gai, D. G.; Ren, Y.

Theoretical study of the gas-phase ion pairs S(N)2 reactions of LiX with CH3SY (X, Y=F, Cl, Br, I)

International Journal of Quantum Chemistry, (107): 1487-1494 2007.

Gai, J. G.; Ren, Y.

Theoretical study of the gas-phase S(N)2 reactions of X- with CH3OY (X, Y=Cl, Br, I)

International Journal of Quantum Chemistry, (107): 1142-1149 2007.

Galano, A.; Alvarez-Idaboy, J. R.; Vivier-Bunge, A.

Non-alkane behavior of cyclopropane and its derivatives: characterization of unconventional hydrogen bond interactions

Theoretical Chemistry Accounts, (118): 597-606 2007.

Galvez, O.; Gomez, P. C.

An ab initio study on the structure and energetics of the ClO hydrates

Chemical Physics Letters, (448): 16-23 2007.

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

Hypercoordinate atoms of second-row elements in dodecahedrane endohedral complexes

Russian Chemical Bulletin, (56): 856-862 2007.

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

Octacoordinate carbon atom in tetra(metalloamino)methanes CN4M4 (M = Be, Mg, Ca): Quantum-chemical investigation

Russian Journal of Organic Chemistry, (43): 685-690 2007.

Garcia, M. E.; Garcia-Vivo, D.; Ruiz, M. A.; Alvarez, S.; Aullon, G.

Chemistry of unsaturated group 6 metal complexes with bridging hydroxy and methoxycarbyne ligands. 1. Synthesis, structure, and bonding of 30-electron complexes

Organometallics, (26): 4930-4941 2007.

Garcia, M. E.; Garcia-Vivo, D.; Ruiz, M. A.; Alvarez, S.; Aullon, G.

Chemistry of unsaturated group 6 metal complexes with bridging hydroxy- and methoxycarbyne ligands. 2. Synthesis, structure, and bonding of 32- and 34-electron complexes

Organometallics, (26): 5912-5921 2007.

Garcia, M. E.; Ramos, A.; Ruiz, M. A.; Lanfranchi, M.; Marchio, L.

- Structure and bonding in the unsaturated hydride- and hydrocarbyl-bridged complexes [Mo-2(eta(5)-C5H5)(2)(mu-X)(mu-PCy2)(CO)(2)] (X = h, CH3, CH2Ph, ph). Evidence for the presence of alpha-agostic and pi-bonding interactions*
Organometallics, (26): 6197-6212 2007.
- Garcia Ruano, J. L.; Martin-Castro, A. M.; Tato, F.; Alonso, I.
Stereoselective quaternization of alpha-amino phenylacetonitriles mediated by a remote sulfinyl group
Journal of Organic Chemistry, (72): 5994-6005 2007.
- Garcia-Fandino, R.; Castedo, L.; Granja, J. R.; Cardenas, D. J.
Feasibility of associative mechanism in enyne metathesis catalyzed by grubbs complexes
Dalton Transactions: 2925-2934 2007.
- Gennari, M.; Lanfranchi, M.; Cammi, R.; Pellinghelli, M. A.; Marchio, L.
Mononuclear and polynuclear copper(I) complexes with a new N,N',S-donor ligand and with structural analogies to the copper thionein core
Inorganic Chemistry, (46): 10143-10152 2007.
- George, L.; Wong, M. W.; Wentrup, C.
Carboxyketenes, methyleneketenes, vinylketenes, oxetanediones, ynols, and ylidic ketenes from Meldrum's acid derivatives
Organic & Biomolecular Chemistry, (5): 1437-1441 2007.
- Georgieva, I.; Trendafilova, N.
Bonding analyses, formation energies, and vibrational properties of M-R(2)dtc complexes (M = Ag(I), Ni(II), Cu(III), or Zn(II))
Journal of Physical Chemistry A, (111): 13075-13087 2007.
- Georgieva, I.; Trendafilova, N.; Aquino, A. J. A.; Lischka, H.
Excited-state proton transfer in 7-hydroxy-4-methylcoumarin along a hydrogen-bonded water wire
Journal of Physical Chemistry A, (111): 127-135 2007.
- Georgieva, L.; Trendafilova, N.; Aquino, A. J. A.; Lischka, H.
Theoretical study of metal-ligand interaction in Sm(III), Eu(III), and Tb(III) complexes of coumarin-3-carboxylic acid in the gas phase and solution
Inorganic Chemistry, (46): 10926-10936 2007.
- Ghiasi, M.; Tafazzoli, M.; Safari, N.
Role of axial ligand on the electronic structures of active intermediates in cytochrome P-450, peroxidase and catalase
Journal of Molecular Structure-Theochem, (820): 18-25 2007.
- Ghiasi, R.
Theoretical study of Borazanaphthalene and its mono-Fluorinated derivatives: structure and properties
Main Group Chemistry, (6): 43-51 2007.

Ghosh, S.; Gorelsky, S. I.; George, S. D.; Chan, J. M.; Cabrito, I.; Dooley, D. M.; Moura, J. J. G.; Moura, I.; Solomon, E. I.

Spectroscopic, computational, and kinetic studies of the $\mu(4)$ -sulfide-bridged tetranuclear Cu-Z cluster in N2O reductase: pH effect on the edge ligand and its contribution to reactivity
Journal of the American Chemical Society, (129): 3955-3965 2007.

Gil, A.; Simon, S.; Rodriguez-Santiago, L.; Bertran, J.; Sodupe, M.

Influence of the side chain in the structure and fragmentation of amino acids radical cations
Journal of Chemical Theory and Computation, (3): 2210-2220 2007.

Gil, A.; Simon, S.; Sodupe, M.; Bertran, J.

Gas-phase proton-transport self-catalysed isomerisation of glutamine radical cation: The important role of the side-chain
Theoretical Chemistry Accounts, (118): 589-595 2007.

Gilbert, T. M.; Bachrach, S. M.

Computational studies of [2+2] and [4+2] pericyclic reactions between phosphinoboranes and alkenes. Steric and electronic effects in identifying a reactive phosphinoborane that should avoid dimerization
Organometallics, (26): 2672-2678 2007.

Gillon, B.; Goujon, A.; Willemin, S.; Larionova, J.; Desplanches, C.; Ruiz, E.; Andre, G.; Stride, J. A.; Guerin, C.

Neutron diffraction and theoretical DFT studies of two dimensional molecular-based magnet $K-2[Mn(H_2O)(2)](3)[Mo(CN)(7)](2) \cdot 6H(2)O$
Inorganic Chemistry, (46): 1090-1099 2007.

Gomez-Bengoa, E.; Helm, M. D.; Plant, A.; Harrity, J. P. A.

The participation of alkynylboronates in inverse electron demand [4+2] cycloadditions: A mechanistic study
Journal of the American Chemical Society, (129): 2691-2699 2007.

Gong, Y.; Zhou, M. F.; Tian, S. X.; Yang, J. L.

Interconvertible side-on- and end-on-bonded oxo-superoxo titanium ozonide complexes
Journal of Physical Chemistry A, (111): 6127-6130 2007.

Gong, Y.; Zhou, M. F.; Tian, S. X.; Yang, J. L.

Interconvertible side-on- and end-on-bonded oxo-superoxo titanium ozonide complexes
Journal of Physical Chemistry A, (111): 6127-6130 2007.

Goodman, L.; Sauers, R. R.

Diffuse functions in natural bond orbital analysis
Journal of Computational Chemistry, (28): 269-275 2007.

Gopakumar, G.; Lievens, P.; Nguyen, M. T.

Interaction of triatomic germanium with lithium atoms: Electronic structure and stability of Ge_3Li_n clusters

- Journal of Physical Chemistry A, (111): 4353-4361 2007.
- Grabowski, S. J.
Covalent character of three-center, two-electron systems - C₂H₃⁺ and C₂H₅⁺
Chemical Physics Letters, (436): 63-67 2007.
- Grigorenko, B. L.; Nemukhin, A. V.; Shadrina, M. S.; Topol, I. A.; Burt, S. K.
Mechanisms of guanosine triphosphate hydrolysis by Ras and Ras-GAP proteins as rationalized by ab initio QM/MM simulations
Proteins-Structure Function and Bioinformatics, (66): 456-466 2007.
- Grobe, J.; Lutke-Brochtrup, K.; Krebs, B.; Lage, M.; Niemeyer, H. H.; Wurthwein, E. U.
Alternative ligands XXXVIII. Further attempts to synthesize Pd(0) and Pt(0) complexes with the tripod phosphane ligand FSi(CH₂CH₂PMe₂)₃
Zeitschrift Fur Naturforschung Section B-a Journal of Chemical Sciences, (62): 55-65 2007.
- Grosso, V.; Previtali, C.; Chesta, C. A.; Mariano, D.; Vera, A.; Pierini, A. B.
An experimental and theoretical study on the electrostatic effect of an appended cationic group on electronic properties of aromatic systems
Physical Chemistry Chemical Physics, (9): 5988-5996 2007.
- Grubisic, S.; Radanovic, D. D.; Rychlewska, U.; Warzajtis, B.; Draskovic, N. S.; Djuran, M. I.; Niketic, S. R.
Conformational study of Co(II), Ni(II), and Cr(III) complexes of the edta-type: Crystal structure of 1D polymeric trans(O-6)-Ba[Co(1,3-pddadp)]-8H₂O complex stabilized by infinite water tapes
Polyhedron, (26): 3437-3447 2007.
- Gu, J. D.; Xie, Y. M.; Schaefer, H. F.
Electron attachment induced proton transfer in a DNA nucleoside pair: 2'-deoxyguanosine-2'-deoxycytidine
Journal of Chemical Physics, (127) 2007.
- Gu, J. D.; Xie, Y. M.; Schaefer, H. F.
Electron attachment to DNA single strands: gas phase and aqueous solution
Nucleic Acids Research, (35): 5165-5172 2007.
- Guirado, A.; Martiz, B.; Andreu, R.; Bautista, D.; Galvez, J.
First synthesis of 1-aryl-4,4-dichlorobut-3-en-1-ones. The electrochemical reduction of 1-aryl-4,4,4-trichlorobut-2-en-1-ones as a key step
Tetrahedron, (63): 1175-1182 2007.
- Gupta, N.; Garg, R.; Shah, K. K.; Tanwar, A.; Pal, S.
Deprotonation of 1,2-dialkylpyridinium ions: A DFT study of reactivity and site selectivity
Journal of Physical Chemistry A, (111): 8823-8828 2007.
- Gurubasavaraj, P. M.; Mandal, S. K.; Roesky, H. W.; Oswald, R. B.; Pal, A.; Noltemeyer, M.
Synthesis, structural characterization, catalytic properties, and theoretical study of compounds containing an Al-O-M (M = Ti, Hf) core
Inorganic Chemistry, (46): 1056-1061 2007.

- Gurubasavaraj, P. M.; Roesky, H. W.; Sharma, P. M. V.; Oswald, R. B.; Dolle, V.; Herbst-Irmer, R.; Pal, A.
Oxygen effect in heterobimetallic catalysis: The Zr-O-Ti system as an excellent example for olefin polymerization
Organometallics, (26): 3346-3351 2007.
- Gutowski, K. E.; Cocalia, V. A.; Griffin, S. T.; Bridges, N. J.; Dixon, D. A.; Rogers, R. D.
Interactions of 1-methylimidazole with $UO_2(CH_3CO_2)_2$ and $UO_2(NO_3)_2$: Structural, spectroscopic, and theoretical evidence for imidazole binding to the uranyl ion
Journal of the American Chemical Society, (129): 526-536 2007.
- Haberhauer, G.; Pinter, A.; Oeser, T.; Rominger, F.
Synthesis and structural investigation of C-4- and C-2-symmetric molecular scaffolds based on imidazole peptides
European Journal of Organic Chemistry: 1779-1792 2007.
- Hackett, J. C.; Sanan, T. T.; Hadad, C. M.
Oxidative dehalogenation of perhalogenated benzenes by cytochrome P450 Compound I
Biochemistry, (46): 5924-5940 2007.
- Hagebaum-Reignier, D.; Girardi, R.; Carissan, Y.; Humbel, S.
Huckel theory for Lewis structures: Huckel-lewis configuration interaction (HL-CI)
Journal of Molecular Structure-Theochem, (817): 99-109 2007.
- Hamzehlooian, M.; Yeganegi, S.
Structural and NBO studies of anomeric effects in polyoxa, polyaza and polycyclics compounds
Asian Journal of Chemistry, (19): 4395-4406 2007.
- Handzlik, J.
Properties and metathesis activity of monomeric and dimeric Mo centres variously located on gamma-alumina - A DFT study
Surface Science, (601): 2054-2065 2007.
- Hanusek, J.; Russell, M. A.; Laws, A. P.; Jansa, P.; Atherton, J. H.; Fettes, K.; Page, M. I.
Mechanism of the sulfurisation of phosphines and phosphites using 3-amino-1,2,4-dithiazole-5-thione (xanthane hydride)
Organic & Biomolecular Chemistry, (5): 478-484 2007.
- Haqghu, M.; Irani, M.; Gholami, M. R.
Theoretical study of kinetics and mechanism of reactions of hydroxylamine and amineoxide anion with methyl iodide in gas and aqueous phases
Progress in Reaction Kinetics and Mechanism, (32): 29-50 2007.
- Harb, M.; Rabilloud, F.; Simon, D.
Density functional study of structural and electronic properties of small bimetallic silver-nickel clusters
Journal of Physical Chemistry A, (111): 7726-7731 2007.

- Hassall, K.; Lobachevsky, S.; Schiesser, C. H.; White, J. M.
Carbon-silicon hyperconjugation and strain-enhanced hyperconjugation: Structures of N-methyl 2-and 4-tert-butyldimethylsilylmethyl pyridinium cations
Organometallics, (26): 1361-1364 2007.
- Haubenstock, H.; Sauers, R. R.
NBO analysis of halogen bridging in 4-halo-1-buten-3-yl cations
Journal of Molecular Structure-Theochem, (822): 8-11 2007.
- Havenith, R. W. A.; van Walree, C. A.; Marsman, A. W.; van Lenthe, J. H.; Jenneskens, L. W.
Weak distance dependence of through-bond interactions in tetrahydro-4H-thiopyran-4-ylidene end-capped oligo(cyclohexylidenes); a computational survey
Physical Chemistry Chemical Physics, (9): 1312-1317 2007.
- Hayakawa, S.; Hashimoto, M.; Matsubara, H.; Turecek, F.
Dissecting the proline effect: Dissociations of proline radicals formed by electron transfer to protonated pro-gly and gly-pro dipeptides in the gas phase
Journal of the American Chemical Society, (129): 7936-7949 2007.
- Hayashi, S.; Nakanishi, W.
Structures in 8-(methylselanyl)-1-(methylseleninyl)- and 1,8-bis(methylseleninyl)naphthalenes: Transition states involving simultaneous rotation around Se-C bonds, together with stable structures
Journal of Molecular Structure-Theochem, (811): 293-301 2007.
- Hazra, S.; Naskar, S.; Mishra, D.; Gorelsky, S. I.; Figgie, H. M.; Sheldrick, W. S.; Chattopadhyay, S. K.
Synthesis, X-ray crystal structure and DFT calculations of bis(N-(2-picolyl) picolinamido) Mn(III) hexafluorophosphate
Dalton Transactions: 4143-4148 2007.
- Henn, J.; Leusser, D.; Stalke, D.
Chemical interpretation of molecular electron density distributions
Journal of Computational Chemistry, (28): 2317-2324 2007.
- Hernandez-Garcia, L.; Quintero, L.; Sanchez, M.; Sartillo-Piscil, F.
Beneficial effect of internal hydrogen bonding interactions on the beta-fragmentation of primary alkoxy radicals. Two-step conversion of D-Xylo- and D-ribofuranoses into L-threose and D-erythrose, respectively
Journal of Organic Chemistry, (72): 8196-8201 2007.
- Hernandez-Gruel, M. A. F.; Lahoz, F. J.; Dobrinovich, I. T.; Modrego, F. J.; Oro, L. A.; Perez-Torrente, J. J.
Reversible opening of the triangular structure of a sulfido-bridged ZrRh₂ early-late heterobimetallic complex induced by bis-(diphenylphosphino)methane
Organometallics, (26): 2616-2622 2007.
- Hernandez-Soto, H.; Weinhold, F.; Francisco, J. S.
Radical hydrogen bonding: Origin of stability of radical-molecule complexes
Journal of Chemical Physics, (127) 2007.

- Herrero, R.; Davalos, J. Z.; Abboud, J. L. M.; Alkorta, I.; Koppel, I.; Koppel, I. A.; Sonoda, T.; Mishima, M.
The intrinsic (gas-phase) acidities of bridgehead alcohols - An experimental (FT-ICR) and computational study
International Journal of Mass Spectrometry, (267): 302-307 2007.
- Hiberty, P. C.; Shaik, S.
A survey of recent developments in ab initio valence bond theory
Journal of Computational Chemistry, (28): 137-151 2007.
- Hiberty, P. C.; Shaik, S.
A survey of recent developments in ab initio valence bond theory
Journal of Computational Chemistry, (28): 137-151 2007.
- Hirao, H.
Reactive bond orbitals: A localized resonance-structure approach to charge transfer
Chemical Physics Letters, (443): 141-146 2007.
- Hirsch, W.; Kobra, M.
Lewis structure representation of free radicals similar to ClO
Journal of Chemical Education, (84): 1360-1363 2007.
- Hnyk, D.; Brain, P. T.; Rankin, D. W. H.; Robertson, H. E.; Smart, B. A.; Banks, R. E.; Murtagh, V.
The molecular structure of N-fluorobis(trifluoromethanesulfonyl)imide, NF(SO₂CF₃)(₂), as studied in the gas phase by electron diffraction restrained by ab initio calculations
Dalton Transactions: 265-271 2007.
- Holt, A.; Karlstrom, G.; Lindh, R.
The charge capacity of the chemical bond
Chemical Physics Letters, (436): 297-301 2007.
- Holtz, T.; Nguyen, M. T.; Veszpremi, T.
Mono-, di-, tri- and tetraphosphatrafulvenes: Electronic structure and aromaticity
Journal of Molecular Structure-Theochem, (811): 27-35 2007.
- Hoque, M. E. U.; Dey, S.; Guha, A. K.; Kim, C. K.; Lee, B. S.; Lee, H. W.
Kinetics and mechanism of the aminolysis of aryl phenyl chlorothiophosphates with anilines
Journal of Organic Chemistry, (72): 5493-5499 2007.
- Horrillo-Martinez, P.; Hultsch, K. C.; Gil, A.; Branchadell, V.
Base-catalyzed anti-Markovnikov hydroamination of vinylarenes - Scope, limitations and computational studies
European Journal of Organic Chemistry: 3311-3325 2007.
- Hou, J. Q.; Kang, H. S.
A DFT study of the heterofullerenes Sc₃N@C₇₉B, Sc₃N@C₇₉N, and Sc₃N@C₇₈BN
Chemical Physics, (334): 29-35 2007.

- Hou, J. Q.; Kang, H. S.
A DFT study on the dimerization of C-62, H-2-C-62, and F-2-C-62
Journal of Computational Chemistry, (28): 1417-1426 2007.
- Hou, J. Q.; Kang, H. S.
DFT study on the stabilities of the heterofullerenes Sc3N@C67B, Sc3N@C67N, and Sc3N@C66BN
Journal of Physical Chemistry A, (111): 1111-1116 2007.
- Houriez, C.; Ferre, N.; Flament, J. P.; Masella, M.; Siri, D.
Electronic basis of the comparable hydrogen bond properties of small H2CO/(H2O)(n) and H2NO/(H2O)n systems (n=1, 2)
Journal of Physical Chemistry A, (111): 11673-11682 2007.
- Hrobarik, P.; Horvath, B.; Sigmundova, I.; Zahradnik, P.; Malkina, O. L.
The impact of pi-electron conjugation on N-15, C-13 and H-1 NMR chemical shifts in push-pull benzothiazolium salts. Experimental and theoretical study
Magnetic Resonance in Chemistry, (45): 942-953 2007.
- Hsu, W.-Y.; Lee, H.-Y.; Wang, S.-P.; Chang, T.-C.
The Fock matrix analysis for atomic orbitals in molecular orbitals I. A new look on the covalent bond in H-2?
Journal of the Chinese Chemical Society, (54): 1463-1470 2007.
- Hsueh, P.; Lukowski, M.; Lindsay, H. A.; Milletti, M. C.
Factors affecting the relative stability of a series of iminium cation stereoisomers
Journal of Molecular Structure-Theochem, (806): 223-230 2007.
- Hu, B.; Gahungu, G.; Zhang, J. P.
Optical properties of the phosphorescent trinuclear copper(I) complexes of pyrazolates: Insights from theory
Journal of Physical Chemistry A, (111): 4965-4973 2007.
- Hu, H.; Lu, Z. Y.; Yang, W. T.
Fitting molecular electrostatic potentials from quantum mechanical calculations
Journal of Chemical Theory and Computation, (3): 1004-1013 2007.
- Hu, Q. S.; Liu, J. L.; Li, L. C.; Tian, A. M.
Reaction mechanism of the activation of ethane via cobalt atom catalysis
Acta Physico-Chimica Sinica, (23): 916-920 2007.
- Hu, Z.; Turner, C. H.
Atomic layer deposition of TiO2 from Ti(4) and H2O onto SiO2 surfaces: Ab initio calculations of the initial reaction mechanisms
Journal of the American Chemical Society, (129): 3863-3878 2007.
- Hu, Z. Q.; Shi, S. M.; He, H. W.; Ding, Y.; Jia, B.
Synthesis, crystal structure and theoretical study of one-dimensional binuclear zinc complex [Zn-2(SHSH)(2)(2-Me-py)(2)]

- Chinese Journal of Inorganic Chemistry, (23): 323-328 2007.
- Huang, M. Q.; Wang, Z. Y.; Yang, Y.; Hao, L. Q.; Zhao, W. W.; Gao, X. M.; Fang, L.; Zhang, W. J.
Intramolecular hydrogen bond in the hydroxycyclohexadienyl peroxy radicals
International Journal of Quantum Chemistry, (107): 1092-1098 2007.
- Hubrich, C.; Schulz, A.; Villinger, A.
Adducts of gallium trichloride and bis(trimethylsilyl)sulfur diimide
Zeitschrift für Anorganische und Allgemeine Chemie, (633): 2362-2366 2007.
- Humbel, S.
Getting the weights of Lewis structures out of Huckel theory: Huckel-Lewis configuration interaction (HL-CI)
Journal of Chemical Education, (84): 1056-1061 2007.
- Hunt, P. A.
Why does a reduction in hydrogen bonding lead to an increase in viscosity for the 1-butyl-2,3-dimethyl-imidazolium-based ionic liquids?
Journal of Physical Chemistry B, (111): 4844-4853 2007.
- Hunt, P. A.; Gould, I. R.; Kirchner, B.
The structure of imidazolium-based ionic liquids: Insights from ion-pair interactions
Australian Journal of Chemistry, (60): 9-14 2007.
- Hurn, D. M.; Cosford, N. D. P.
The Molecular Libraries Screening Center Network (MLSCN): Identifying Chemical Probes of Biological Systems
Annual Reports in Medicinal Chemistry, Vol 42, (42): 401-416 2007.
- Iche-Tarrat, N.; Ruiz-Lopez, M.; Barthelat, J. C.; Vigroux, A.
Theoretical evaluation of the substrate-assisted catalysis mechanism for the hydrolysis of phosphate monoester dianions
Chemistry—a European Journal, (13): 3617-3629 2007.
- Ignatyev, I. S.; Sundius, T. R.; Vrazhnov, D. V.; Kochina, T. A.; Voronkov, M. G.
Bonding in germatranyl cation and germatranes
Journal of Organometallic Chemistry, (692): 5697-5700 2007.
- Ikeda, A.; Nakao, Y.; Sato, H.; Sakaki, S.
Binding energy of transition-metal complexes with large pi-conjugate systems. Density functional theory vs post-hartree-fock methods
Journal of Physical Chemistry A, (111): 7124-7132 2007.
- Ikeda, A.; Yokogawa, D.; Sato, H.; Sakaki, S.
Solvation effect on the interaction between sodium and chloride ions in aqueous solution: An analysis based on the new resonance theory
International Journal of Quantum Chemistry, (107): 3132-3136 2007.

- Illa, O.; Rodriguez-Garcia, C.; Acosta-Silva, C.; Favier, I.; Picurelli, D.; Oliva, A.; Gomez, M.; Branchadell, V.; Ortuno, R. M.
Cyclopropanation of cyclohexenone by diazomethane catalyzed by palladium diacetate: Evidence for the formation of palladium(0) nanoparticles
Organometallics, (26): 3306-3314 2007.
- Imamura, Y.; Takahashi, A.; Nakai, H.
Grid-based energy density analysis: Implementation and assessment
Journal of Chemical Physics, (126) 2007.
- Ingram, K. I. M.; Kaltsoyannis, N.; Gaunt, A. J.; Neu, M. P.
Covalency in the f-element-chalcogen bond computational studies of [M(N(EPH₂)(₂))(₃)] (M = La, U, Pu; E = O, S, Se, Te)
Journal of Alloys and Compounds, (444): 369-375 2007.
- Ionescu, A. R.; Whitfield, D. M.; Zglerski, M. Z.
O-2 Substituted pyranosyl oxacarbenium ions are C-2-O-2 2-fold rotors with a strong syn preference
Carbohydrate Research, (342): 2793-2800 2007.
- Iqbal, P.; Patel, D. S.; Bharatam, P. V.
Ab initio study on N,N',N''-triaminoguanidine
Journal of Physical Organic Chemistry, (20): 1072-1080 2007.
- Iriarte, A. G.; Cutin, E. H.; Ulic, S. E.; Jios, J.; Della Vedova, C. O.
Spectroscopic and theoretical studies of N-trichlorophosphazotrifluoroacetyl, CF₃C(O)NPCl₃ and N-trichlorophosphazotrichloroacetyl, CCl₃C(O)NPCl₃
Vibrational Spectroscopy, (43): 290-296 2007.
- Islas, R.; Heine, T.; Ito, K.; Schleyer, P. V. R.; Merino, G.
Boron rings enclosing planar hypercoordinate group 14 elements
Journal of the American Chemical Society, (129): 14767-14774 2007.
- Jalili, S.; Akhavan, M.
Study of hydrogen-bonded clusters of 2-methoxyphenol-water
Theoretical Chemistry Accounts, (118): 947-957 2007.
- James, C.; Jayakumar, V. S.; Joe, I. H.
Natural bond orbital analysis and vibrational spectroscopic studies of H-bonded N,N'-diphenylguanidinium nitrate
Journal of Molecular Structure, (830): 156-166 2007.
- Jansma, A.; Zhang, Q.; Li, B.; Ding, Q.; Uno, T.; Bursulaya, B.; Liu, Y.; Furet, P.; Gray, N. S.; Geierstanger, B. H.
Verification of a designed intramolecular hydrogen bond in a drug scaffold by nuclear magnetic resonance spectroscopy
Journal of Medicinal Chemistry, (50): 5875-5877 2007.

- Jemmis, E. D.; Parameswaran, P.
Structure and bonding in cyclic isomers of $BAI(2)H(n)(m)$ ($n=3-6$, $m=-2$ to $+1$): Preference for planar tetracoordination, pyramidal tricoordination, and divalency
Chemistry-a European Journal, (13): 2622-2631 2007.
- Jimenez, F.; Jalbout, A. F.
The origin of the rotational barrier in dimethyl ether and dimethyl sulfide. A theoretical study
Journal of Theoretical & Computational Chemistry, (6): 421-434 2007.
- Jin, L. X.; Wang, W. L.; Wu, D. B.; Wang, W. N.
Theoretical study on the structures and isomerization mechanisms of 5-methylcytosine-BH3 complexes
Acta Chimica Sinica, (65): 1012-1018 2007.
- Johnson, L. E.; Dupre, D. B.
Mechanism of the electronic stabilization of the 3MR and divalent carbon of bis(diisopropylamino)cyclopropenylidene
Journal of Physical Chemistry A, (111): 11066-11073 2007.
- Joo, H.; Kraka, E.; Quapp, W.; Cremer, D.
The mechanism of a barrierless reaction: hidden transition state and hidden intermediates in the reaction of methylene with ethene
Molecular Physics, (105): 2697-2717 2007.
- Joseph, J.; Jemmis, E. D.
Red-, blue-, or no-shift in hydrogen bonds: A unified explanation
Journal of the American Chemical Society, (129): 4620-4632 2007.
- Jothy, V. B.; Vijayakumar, T.; Jayakumar, V. S.; Udayalekshmi, K.; Ramamoorthy, K.; Joe, I. H.
NIR-FT Raman and FT-IR spectral investigations of the nonlinear optical chromophore p-bromoacetanilide
Journal of Raman Spectroscopy, (38): 1148-1158 2007.
- Jung, Y. S.; Marcus, R. A.
On the nature of organic catalysis "on water"
Journal of the American Chemical Society, (129): 5492-5502 2007.
- Junior, V.; de Oliveira, K. T.; Silva, R. C. E.; Constantino, M. G.; da Silva, G. V. J.
Reactivity in Diels-Alder reactions: a computational experiment
Quimica Nova, (30): 727-730 2007.
- Justringo, V.; Pellegrinet, S. C.; Colombo, M. I.
Studies on the intramolecular cyclizations of bicyclic delta-hydroxynitriles promoted by triflic anhydride
Journal of Organic Chemistry, (72): 3702-3712 2007.
- Kalaiselvan, A.; Venuvanalingam, P.
Ring opening of boriranes vis-a-vis aziridines: An ab initio and DFT probe on the mechanisms

International Journal of Quantum Chemistry, (107): 1590-1597 2007.

Kang, H. S.

A theoretical study of Fullerene-Ferrocene hybrids

Journal of Computational Chemistry, (28): 594-600 2007.

Karafiloglou, P.; Papanikolaou, P.

The role of ionic structures in the response of a non-polar molecule to an electric field

Chemical Physics, (342): 288-296 2007.

Kassaee, M. Z.; Buazar, F.; Musavi, S. M.; Motamedi, E.

Detours for reaching at new germylenes, silylenes, carbenes, and carbenogermynes through substituted cyclopropenylidenes at Ab initio and DFT levels

Monatshefte für Chemie, (138): 833-848 2007.

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

A theoretical study on C₂HXS_i silylenes (X = H, CN, NH₂, and OMe)

Heteroatom Chemistry, (18): 283-293 2007.

Katritzky, A. R.; Akhmedov, N. G.; Doskocz, J.; Mohapatra, P. P.; Hall, C. D.; Guven, A.

NMR spectra, GIA and charge density calculations of five-membered aromatic heterocycles

Magnetic Resonance in Chemistry, (45): 532-543 2007.

Kaur, D.; Sharma, P.; Bharatam, P. V.

A comparative study on the nature and strength of O-O, S-S, and Se-Se bond

Journal of Molecular Structure-Theochem, (810): 31-37 2007.

Kaur, D.; Sharma, P.; Kaur, R. P.; Kaur, M.; Bharatam, P. V.

Substituent effects on the proton affinities of selenoamides: A theoretical study

Journal of Molecular Structure-Theochem, (805): 119-125 2007.

Kavitha, V.; Viswanathan, K. S.

Conformations of dimethoxydimethylsilane: Matrix isolation infrared and ab initio studies

Journal of Physical Chemistry A, (111): 1879-1886 2007.

Ke, Z. F.; Zhao, C. Y.; Phillips, D. L.

Methylene transfer or carbometalation? A theoretical study to determine the mechanism of lithium carbenoid-promoted cyclopropanation reactions in aggregation and solvation states

Journal of Organic Chemistry, (72): 848-860 2007.

Kemnitz, C. R.; Loewen, M. J.

"Amide resonance" correlates with a breadth of C-N rotation barriers

Journal of the American Chemical Society, (129): 2521-2528 2007.

Keshtova, S. V.; Keshtova, F. M.

Investigation of influence of electrical induction on electrostatic interaction of atoms and

molecules in solution. 1. Dependence of atomic charges in molecule from environment based on the model of FQ theory

- International Journal of Quantum Chemistry, (107): 1126-1141 2007.
- Khaliullin, R. Z.; Cobar, E. A.; Lochan, R. C.; Bell, A. T.; Head-Gordon, M.
Unravelling the origin of intermolecular interactions using absolutely localized molecular orbitals
Journal of Physical Chemistry A, (111): 8753-8765 2007.
- Kim, C. K.; Kim, D. J.; Hsieh, Y.; Lee, H. W.; Lee, B. S.
Effects of entropy on the gas-phase pyrolysis of ethyl N,N-dimethylcarbamate
Journal of Computational Chemistry, (28): 625-631 2007.
- Kim, C. K.; Kim, D. J.; Hsieh, Y.; Lee, H. W.; Lee, B. S.; Kim, C. K.
Effects of entropy on the gas-phase pyrolysis of ethyl N,N-dimethylcarbamate
Journal of Computational Chemistry, (28): 625-631 2007.
- Kim, C. K.; Kim, D. J.; Zhang, H.; Hsieh, Y. H.; Lee, B. S.; Lee, H. W.
Substituent effects on the gas-phase pyrolyses of 2-substituted ethyl N,N-dialkylcarbamates: A theoretical study
Bulletin of the Korean Chemical Society, (28): 1031-1034 2007.
- Kim, D.; Lee, E. C.; Kim, K. S.; Tarakeshwar, P.
Cation- π -anion interaction: A theoretical investigation of the role of induction energies
Journal of Physical Chemistry A, (111): 7980-7986 2007.
- Kim, J.; Kim, T. K.; Kim, J.; Lee, Y. S.; Ihee, H.
Density functional and ab initio study of Cr(CO)(n) (n=1-6) complexes
Journal of Physical Chemistry A, (111): 4697-4710 2007.
- Kim, J.; Kim, T. K.; Lee, Y. S.; Ihee, H.
Density functional and ab initio study of Cr(CO)(n) (n=1-6) complexes
Journal of Physical Chemistry A, (111): 4697-4710 2007.
- Kingsbury, C. A.; Weinhold, J.; Winter, J.
Addition, elimination, exchange, and epimerization in nitro sulfones
Journal of Physical Organic Chemistry, (20): 161-166 2007.
- Kirsten, M.; Rehbein, J.; Hiersemann, M.; Strassner, T.
Organocatalytic Claisen rearrangement: Theory and experiment
Journal of Organic Chemistry, (72): 4001-4011 2007.
- Knippenberg, S.; Hajgato, B.; Francois, J.-P.; Deleuze, M. S.
Theoretical study of the fragmentation pathways of norbornane in its doubly ionized ground state
Journal of Physical Chemistry A, (111): 10834-10848 2007.
- Koehler, F.; Herges, R.; Stanger, A.
Comment on "Origin of the nonplanarity of tetrafluoro cyclobutadiene, C₄F₄"
Journal of Physical Chemistry A, (111): 5116-5118 2007.

Kokatam, S.; Ray, K.; Pap, J.; Bill, E.; Geiger, W. E.; LeSuer, R. J.; Rieger, P. H.; Weyhermuller, T.; Neese, F.; Wieghardt, K.

Molecular and electronic structure of square-planar gold complexes containing two 1,2-di(4-tert-butylphenyl)ethylene-1,2-dithiolato ligands: [Au(L-2)(2)](1+/0/1-/2-). A combined experimental and computational study

Inorganic Chemistry, (46): 1100-1111 2007.

Koltunov, K. Y.; Prakash, G. K. S.; Rasu, G.; Olah, G. A.

Superacidic activation of quinoline and isoquinoline; Their reactions with cyclohexane and benzene

Journal of Organic Chemistry, (72): 7394-7397 2007.

Kovacs, A.

Theoretical study of the strong intramolecular hydrogen bond and metal-ligand interactions in group 10 (Ni, Pd, Pt) bis(dimethylglyoximate) complexes

Journal of Organometallic Chemistry, (692): 5383-5389 2007.

Kovacs, A.; Szecsenyi, K. M.; Leovac, V. M.; Tomic, Z. D.; Pokol, G.

Synthesis under self-controlled reaction conditions: Reaction of tetraamminezinc(II) chloride with 3,5-dimethyl-1-thiocarboxamide pyrazole

Journal of Organometallic Chemistry, (692): 2582-2592 2007.

Kowalewski, M.; Krumm, B.; Mayer, P.; Schulz, A.; Villinger, A.

Transition-metal-free boron-carbon bond activation: Insertion of an NNP fragment into a boron-carbon bond

European Journal of Inorganic Chemistry: 5319-5322 2007.

Krapp, A.; Frenking, G.

Is this a chemical bond? A theoretical study of Ng(2)@C-60 (Ng = He, Ne, Ar, Kr, Xe)

Chemistry-a European Journal, (13): 8256-8270 2007.

Krapp, A.; Pandey, K. K.; Frenking, G.

Transition metal-carbon complexes. A theoretical study

Journal of the American Chemical Society, (129): 7596-7610 2007.

Kreisel, K. A.; Yap, G. P. A.; Dmitrenko, O.; Landis, C. R.; Theopold, K. H.

The shortest metal-metal bond yet: Molecular and electronic structure of a dinuclear chromium diazadiene complex

Journal of the American Chemical Society, (129): 14162-+ 2007.

Krishtal, S.; Kiselev, M.; Kolker, A.; Idrissi, A.

Study of H-bond characteristics in sub- and supercritical methanol

Theoretical Chemistry Accounts, (117): 297-304 2007.

Krivdin, L. B.; Contreras, R. H.

Recent advances in theoretical calculations of indirect spin-spin coupling constants

Annual Reports on Nmr Spectroscopy, Vol 61: 133-245 2007.

- Kumar, R.; Schmidt, J. R.; Skinner, J. L.
Hydrogen bonding definitions and dynamics in liquid water
Journal of Chemical Physics, (126) 2007.
- Kusama, H.; Sugihara, H.
Theoretical studies of charge-transfer complexes of I-2 with pyrazoles, and implications on the dye-sensitized solar cell performance
Journal of Photochemistry and Photobiology a-Chemistry, (187): 233-241 2007.
- Kuznetsov, M. L.; Nazarov, A. A.; Kozlova, L. V.; Kukushkin, V. Y.
Theoretical study of chemo-, regio-, and stereoselectivity in 1,3-dipolar cycloadditions of nitrones and nitrile oxides to free and Pt-bound bifunctional dipolarophiles
Journal of Organic Chemistry, (72): 4475-4485 2007.
- Kyne, S. H.; Schiesser, C. H.; Matsubara, H.
Multi-component orbital interactions during oxyacyl radical addition reactions involving imines and electron-rich olefins
Organic & Biomolecular Chemistry, (5): 3938-3943 2007.
- Lai, C. H.; Chou, P. T.
Can an OH radical form a strong hydrogen bond? a theoretical comparison with H₂O
Journal of Computational Chemistry, (28): 1357-1363 2007.
- Lai, C. H.; Li, E. Y.; Chou, P. T.
Isomerization reactions of RSNO (R=H, C_nH_{2n+1} n <= 4)
Theoretical Chemistry Accounts, (117): 145-152 2007.
- Lammers, S.; Meuwly, M.
Investigating the relationship between infrared spectra of shared protons in different chemical environments: A comparison of protonated diglyme and protonated water dimer
Journal of Physical Chemistry A, (111): 1638-1647 2007.
- Landis, C. R.; Weinhold, F.
Valence and extra-valence orbitals in main group and transition metal bonding
Journal of Computational Chemistry, (28): 198-203 2007.
- Langer, V.; Scholtzova, E.; Gyepesova, D.; Luston, J.; Kronek, J.
2-(2-Oxazolin-2-yl)benzene-1,4-diol: X-ray and density functional theory studies
Acta Crystallographica Section C-Crystal Structure Communications, (63): O187-O189 2007.
- Langer, V.; Scholtzova, E.; Koos, M.
3-(4-bromophenyl)-5-(4-dimethylaminophenyl)-1-phenyl-2-pyrazoline: X-ray and density functional theory (DFT) studies
Acta Crystallographica Section C-Crystal Structure Communications, (63): O340-O342 2007.
- Langer, V.; Scholtzova, E.; Milata, V.; Solcan, T.
(E)-Methyl 2-anilinomethylene-3-oxobutanoate: X-ray and density functional theory studies
Acta Crystallographica Section C-Crystal Structure Communications, (63): O552-O554 2007.

- Lapouge, C.; Cornard, J. P.
Reaction pathways involved in the mechanism of Al-III chelation with caffeic acid: Catechol and carboxylic functions competition
Chemphyschem, (8): 473-479 2007.
- Larin, A. V.; Mortier, W. J.; Vercauteren, D. P.
Quick scheme for evaluation of atomic charges in arbitrary aluminophosphate sieves on the basis of electron densities calculated with DFT methods
Journal of Computational Chemistry, (28): 1695-1703 2007.
- Lauderbach, F.; Prakash, R.; Gotz, A. W.; Munoz, M.; Heinemann, F. W.; Nickel, U.; Hess, B. A.; Sellmann, D.
Alternative synthesis, density functional calculations and proton reactivity study of a trinuclear [NiFe] hydrogenase model compound
European Journal of Inorganic Chemistry: 3385-3393 2007.
- Lavoie, N.; Ong, T. G.; Gorelsky, S. I.; Korobkov, I.; Yap, G. P. A.; Richeson, D. S.
Bis(imido) W(VI) complexes chelated by N,N'-Disubstituted 1,8-diamidonaphthalene: An analysis of bonding, isocyanate insertion, and Al-Me transfer
Organometallics, (26): 6586-6590 2007.
- Lecea, B.; Ayerbe, M.; Arrieta, A.; Cossio, F. P.; Branchadell, V.; Ortuno, R. M.; Baceiredo, A.
Theoretical study on the mechanism of the [2+1] thermal cycloaddition between alkenes and stable singlet (phosphino)(silyl)carbenes
Journal of Organic Chemistry, (72): 357-366 2007.
- Lee, H. M.; Kim, D.; Singh, N. J.; Kolaski, M.; Kim, K. S.
Hydrated hydride anion clusters
Journal of Chemical Physics, (127) 2007.
- Lein, M.; Hammerl, A.; Hermann, H. L.; Schwerdtfeger, P.
Theoretical investigations into trioxo group 7 compounds LRO3 with perfluorated ligands
Polyhedron, (26): 486-492 2007.
- Leopoldini, M.; Russo, N.; Toscano, M.
A comparative study of the antioxidant power of flavonoid catechin and its planar analogue
Journal of Agricultural and Food Chemistry, (55): 7944-7949 2007.
- Lepsik, M.; Field, M. J.
Binding of calcium and other metal ions to the EF-Hand loops of calmodulin studied by quantum chemical calculations and molecular dynamics simulations
Journal of Physical Chemistry B, (111): 10012-10022 2007.
- Leysens, T.; Peeters, D.; Orpen, A. G.; Harvey, J. N.
How important is metal-ligand back-bonding toward YX3 ligands (Y = N, P, C, Si)? an NBO analysis
Organometallics, (26): 2637-2645 2007.

- Li, A. Y.
Chemical origin of blue- and redshifted hydrogen bonds: Intramolecular hyperconjugation and its coupling with intermolecular hyperconjugation
Journal of Chemical Physics, (126) 2007.
- Li, A. Y.; Wang, S. W.
Ab initio investigation of hydrogen bonds between pyridine and HCl, CHCl₃
Journal of Molecular Structure-Theochem, (807): 191-199 2007.
- Li, A. Y.; Yan, X. H.
Electronic properties of multifurcated bent hydrogen bonds CH₃ center dot center dot center dot Y and CH₂ center dot center dot center dot Y
Physical Chemistry Chemical Physics, (9): 6263-6271 2007.
- Li, F.; Huang, X. R.; Yu, G. T.; Sun, C. C.
Theoretical study on structures and stability of triplet SiC₃O isomers
Theoretical Chemistry Accounts, (118): 383-397 2007.
- Li, H. Q.; Sun, G. Q.; Li, N.; Sun, S. G.; Su, D. S.; Xin, Q.
Design and preparation of highly active Pt-Pd/C catalyst for the oxygen reduction reaction
Journal of Physical Chemistry C, (111): 5605-5617 2007.
- Li, J.; Hu, H. S.; Lyon, J. T.; Andrews, L.
Chirality, agostic interactions, and pyramidalities in actinide methylidene complexes
Angewandte Chemie-International Edition, (46): 9045-9049 2007.
- Li, J. L.; Geng, C. Y.; Huang, X. R.; Sun, C. C.
Atomic radical-molecule reactions F+CH₃CCH: mechanistic study
Theoretical Chemistry Accounts, (117): 417-429 2007.
- Li, J. L.; Geng, C. Y.; Huang, X. R.; Zhang, X.; Sun, C. C.
Theoretical elucidation of the platinum-mediated arene C-H activation reactions
Organometallics, (26): 2203-2210 2007.
- Li, L. C.; Liu, J. L.; Shang, J.; Wang, X.; Wong, N. B.
Theoretical investigation on the activation of ethane via nickel atom catalysis
Journal of Theoretical & Computational Chemistry, (6): 323-330 2007.
- Li, Q. G.; Liang, G. M.; Wang, X.; Chu, S. Y.; Ren, Y.
Ab initio computational modeling on the tautomerism of monochalcogenocarboxylic acids CH₃C(=O)XH (X = S, Se, and Te) in the polar and aprotic solution
International Journal of Quantum Chemistry, (107): 921-929 2007.
- Li, Q. S.; Xu, Y.
A quantum chemistry study: A new kind of boron nitrides
Journal of Computational Chemistry, (28): 1446-1455 2007.

- Li, Q. S.; Zhang, Y.
Density functional theoretical study of A series of pentazolide compounds A(n)(N-5)(q)(6-n) (A=B, Al, Si, P, and S; n=1-3; q=+1, 0, -1, -2, and -3)
Theoretical Chemistry Accounts, (118): 399-405 2007.
- Li, W.; Li, S. H.; Jiang, Y. S.
Generalized energy-based fragmentation approach for computing the ground-state energies and properties of large molecules
Journal of Physical Chemistry A, (111): 2193-2199 2007.
- Li, W. Q.; Tian, W. Q.; Feng, J. K.; Cui, Y. H.; Liu, Z. Z.
Tri-coordinated nitrogen and phosphorus in planar eight pi electron systems: Intriguing conformational differences
Journal of Molecular Structure-Theochem, (823): 1-5 2007.
- Li, W. Q.; Tian, W. Q.; Feng, J. K.; Liu, Z. Z.
Does the planar aromatic phosphorus analogue of pyridone exist?
European Journal of Organic Chemistry: 1669-1677 2007.
- Li, W. Q.; Tian, W. Q.; Feng, J. K.; Liu, Z. Z.; Ren, A. M.; Sun, C. C.; Aoki, Y.
Electronic properties of tricoordinated phosphorus in hexagonal phosphininium compounds and molecular aromaticity
Journal of Computational Chemistry, (28): 1467-1475 2007.
- Li, W.-Q.; Tian, W. Q.; Feng, J.-K.; Cui, Y.-H.; Liu, Z.-Z.
Tri-coordinated nitrogen and phosphorus in planar eight pi electron systems: Intriguing conformational differences
Journal of Molecular Structure-Theochem, (823): 1-5 2007.
- Li, X. B.; Song, Q. H.
Theoretical study of the reaction mechanism and solvent effect on the regioselectivity of 1,3-dipolar cycloaddition reaction between azide and acetylene derivatives
Heteroatom Chemistry, (18): 203-207 2007.
- Li, X. S.; Tully, J. C.
Ab initio time-resolved density functional theory for lifetimes of excited adsorbate states at metal surfaces
Chemical Physics Letters, (439): 199-203 2007.
- Li, Z. F.; Lu, L. L.; Yuan, K.; Kang, J. W.
TD-DFT study on electronic spectrum properties of bis(2-phenyl-8-hydroxyquinolato)zinc and its derivatives
Chinese Journal of Inorganic Chemistry, (23): 659-663 2007.
- Li, Z. H.; Geng, Z. Y.; Zhao, C. Y.; Wang, Y. C.; Liu, L. Y.
The influence of the leaving group X (X = F, Cl, Br, I) on the carbenoid nature of the carbenoids X₂AlCH₂X - A theoretical study
Journal of Molecular Structure-Theochem, (807): 173-178 2007.

- Li, Z. W.; Zhao, C. Y.; Chen, L. P.
Spectroscopic properties of aromatic heterocyclic systems: XAl3 (X = Si, Ge, Sn, Pb) and their anions and cations
Journal of Molecular Structure-Theochem, (809): 45-54 2007.
- Liao, S. Y.; Xu, L. C.; Qian, L.; Zheng, K. C.
QSAR and action mechanism of troxacitabine prodrugs with antitumor activity
Journal of Theoretical & Computational Chemistry, (6): 947-958 2007.
- Linares, M.; Humbel, S.; Braida, B.
Quantifying resonance through a Lewis Valence Bond approach: application to haloallyl and carbonyl cations
Faraday Discussions, (135): 273-283 2007.
- Linder, D. P.; Rodgers, K. R.
Computational modeling of factors that modulate the unique FeNO bonding in {FeNO}(6) heme-thiolate model complexes
Journal of Biological Inorganic Chemistry, (12): 721-731 2007.
- Liu, C. H.; Tang, M. S.; Wang, H. M.
The conversion among various B4C clusters: A density functional theoretical study
Journal of Physical Chemistry A, (111): 704-709 2007.
- Liu, F. L.
[5,6]-Heterofullerene-like C(58)Ge: odd atoms assembling a cage
Physical Chemistry Chemical Physics, (9): 3872-3876 2007.
- Liu, F. L.; Song, Z. M.
Structural and vibrational frequencies determination of the molecule C18H12O12 with double cages sharing the same hexagon of carbon atoms
Journal of Molecular Structure-Theochem, (804): 77-80 2007.
- Liu, F. L.; Wang, C. H.
C-114: Two intact C-60 cages share the same hexagon
Journal of Molecular Structure-Theochem, (819): 130-135 2007.
- Liu, F. L.; Zhao, X. X.
Two intact C-60 cages linked by six carbon-carbon single bonds
Journal of Molecular Structure-Theochem, (804): 117-121 2007.
- Liu, H. L.; Huang, X. R.; Ding, Y. H.; Sun, C. C.
Theoretical study on the potential energy surface of NC3P isomers
Theoretical Chemistry Accounts, (117): 501-520 2007.
- Liu, H. L.; Huang, X. R.; Sun, C. C.
Theoretical study on the potential energy surface of SiC2O
Journal of Molecular Structure-Theochem, (802): 59-65 2007.

- Liu, H. T.; Wang, S. Y.; Zhou, G.; Wu, J.; Duan, W. H.
Structures and stabilities of small lead oxide clusters $PbmOn$ ($m=1-4, n=1-2m$)
Journal of Chemical Physics, (126) 2007.
- Liu, Y.; Drew, M. G. B.
The crucial importance of agostic interactions in intermediates formed in propylene polymerization using neutral salicyladiminato palladium(II) and nickel complexes as catalysts
Journal of Molecular Structure-Theochem, (821): 30-41 2007.
- Liu, Y.; Liu, W. Q.; Li, H. Y.; Yang, Y.; Cheng, S.
Hydrogen bonding interaction of formic acid-, formaldehyde-, formylfluoride-nitrosyl hydride: Theoretical study on the geometries, interaction energies and blue- or red-shifted hydrogen bonds
Chinese Journal of Chemistry, (25): 44-52 2007.
- Liu, Y.; Liu, W. Q.; Li, H. Y.; Yang, Y.; Cheng, S.
Theoretical study of hydrogen bonding interaction of 1 : 1 dimer of HNO with HARF
Chinese Journal of Chemical Physics, (20): 37-42 2007.
- Liu, Y. L.; Chang, Y. H.; Li, T. H.; Chen, H. R.; Hu, W. P.
Theoretical study on the noble-gas anions $F-(NgO)(n)$ ($Ng = He, Ar, and Kr$)
Chemical Physics Letters, (439): 14-17 2007.
- Li, Q. Y.; Xu, X.
Fe-Hg Interactions and P-31 Chemical Shifts in $[Fe(CO)(3)(PPh_2R)(2)(HgCl_2)]$ ($R=pym, fur, py, thi$)
Acta Physico-Chimica Sinica, (23): 1875-1880 2007.
- Li, Q.-Y.; Xu, X.
Fe-Hg Interactions and P-31 Chemical Shifts in $[Fe(CO)(3)(PPh_2R)(2)(HgCl_2)]$ ($R=pym, fur, py, thi$)
Acta Physico-Chimica Sinica, (23): 1875-1880 2007.
- Loginov, D. A.; Vinogradov, M. M.; Starikova, Z. A.; Petrovskaya, E. A.; Zanello, P.; Laschi, F.; Rossi, F.; Cinqantini, A.; Kudinov, A. R.
(1,2,3,4,7-Pentamethylindenyl)rhodium complexes with arene ligands
Journal of Organometallic Chemistry, (692): 5777-5787 2007.
- Londesborough, M. G. S.; Janousek, Z.; Stibr, B.; Hnyk, D.; Plesek, J.; Cisarova, I.
The $[2,5,12-C_3B_8H_{15}](-)$ anion, the first representative of the eleven-vertex hypoph family of tricarboranes
Dalton Transactions: 1221-1228 2007.
- Loos, P. F.; Assfeld, X.
Self-consistent strictly localized orbitals
Journal of Chemical Theory and Computation, (3): 1047-1053 2007.
- Lopez, C. S.; Faza, O. N.; Souto, J. A.; Alvarez, R.; de Lera, A. R.

Pseudopericyclic design drives antara-antara [1,5] methylene sigmatropic shifts from a stepwise to a concerted mechanism

Journal of Computational Chemistry, (28): 1411-1416 2007.

Lopez-Vallejo, F.; Medina-Franco, J. L.; Hernandez-Campos, A.; Rodriguez-Morales, S.; Yepez, L.; Cedillo, R.; Castillo, R.

Molecular modeling of some 1H-benzimidazole derivatives with biological activity against Entamoeba histolytica: A comparative molecular field analysis study

Bioorganic & Medicinal Chemistry, (15): 1117-1126 2007.

Lu, D. N.; Nadas, J.; Zhang, G. S.; Johnson, W.; Zweier, J. L.; Cardounel, A. J.; Villamena, F. A.; Wang, P. G.
4-aryl-1,3,2-oxathiazolylum-5-olates as pH-controlled NO-donors: The next generation of S-nitrosothiols

Journal of the American Chemical Society, (129): 5503-5514 2007.

Lu, R.; Ma, H.; Liu, W.; Yan, B.; Song, J.

A quantum chemical and statistical study of benzoic acid derivatives with inhibiting tyrosinase activity

Journal of Computational and Theoretical Nanoscience, (4): 1311-1315 2007.

Lu, X. Q.; Guo, W. Y.; Zhao, L. M.; Chen, X. F.; Fu, Q. T.; Ma, Y.

Hydride abstraction of methylamine with Cu+(S-1) in the gas phase: A density functional theory study

Journal of Organometallic Chemistry, (692): 3796-3803 2007.

Lu, Y. X.; Zou, J. W.; Wang, Y. H.; Yu, Q. S.

Substituent effects on noncovalent halogen/pi interactions: Theoretical study

International Journal of Quantum Chemistry, (107): 1479-1486 2007.

Lu, Y. X.; Zou, J. W.; Wang, Y. H.; Yu, Q. S.

Theoretical investigations of the C-X/pi interactions between benzene and some model halocarbons

Chemical Physics, (334): 1-7 2007.

Lu, Y. X.; Zou, J. W.; Yu, Q. S.; Jiang, Y. J.; Zhao, W. N.

Ab initio investigation of halogen bonding interactions involving fluorine as an electron acceptor

Chemical Physics Letters, (449): 6-10 2007.

Lu, Y.-X.; Zou, J.-W.; Wang, Y.-H.; Jiang, Y.-J.; Yu, Q.-S.

Ab initio investigation of the complexes between bromobenzene and several electron donors: Some insights into the magnitude and nature of halogen bonding interactions

Journal of Physical Chemistry A, (111): 10781-10788 2007.

Lu, Y.-X.; Zou, J.-W.; Yu, Q.-S.; Jiang, Y.-J.; Zhao, W.-N.

Ab initio investigation of halogen bonding interactions involving fluorine as an electron acceptor

Chemical Physics Letters, (449): 6-10 2007.

Lucassen, A. C. B.; Karton, A.; Leitus, G.; Shimon, L. J. W.; Martin, J. M. L.; van der Boom, M. E.

- Co-crystallization of sym-triiodo-trifluorobenzene with bipyridyl donors: Consistent formation of two instead of anticipated three N center dot center dot center dot I halogen bonds*
Crystal Growth & Design, (7): 386-392 2007.
- Lue, R.; Cao, Z.; Shen, G.
Ab initio calculation of room temperature ionic liquid 1-ethyl-3-methyl-imidazolium and AlCl₃
China Petroleum Processing & Petrochemical Technology: 51-56 2007.
- Lue, R.; Cao, Z.; Shen, G.
Theoretical study on ionic liquid based on 1-ethyl-3-methyl-imidazolium cation and hexafluorophosphate or tetrafluoroborate
Journal of Natural Gas Chemistry, (16): 428-436 2007.
- Lukes, V.; Matuszna, K.; Rapta, P.; Dunsch, L.; Aquino, A. J. A.; Lischka, H.
Electronic excitations in a ladder type fluoranthenopyracylene in its neutral and charged states: A theoretical and experimental study
Zeitschrift Fur Physikalische Chemie-International Journal of Research in Physical Chemistry & Chemical Physics, (221): 911-928 2007.
- Luna, A.; Mo, O.; Yanez, M.; Guillemin, J. C.; Gal, J. F.; Maria, P. C.
Cyano substituent effects on enol and enethiol acidity and basicity: The protonation and deprotonation of 3-hydroxy-2-propenenitrile and its thio analogue
International Journal of Mass Spectrometry, (267): 125-133 2007.
- Luo, Q.; Zhang, X. H.; Huang, K. L.; Liu, S. Q.; Yu, Z. H.; Li, Q. S.
Theoretical studies on novel main group metallocene-like complexes involving planar hexacoordinate carbon eta(6)-B6C2- ligand
Journal of Physical Chemistry A, (111): 2930-2934 2007.
- Lyon, J. T.; Andrews, L.; Malmqvist, P. A.; Roos, B. O.; Yang, T. X.; Bursten, B. E.
Infrared spectrum and bonding in uranium methylidene dihydride, CH₂=UH₂
Inorganic Chemistry, (46): 4917-4925 2007.
- Lyon, J. T.; Cho, H. G.; Andrews, L.
Methylidyne XC MX₃ (M = Cr, Mo, W; X = H, F, Cl) diagnostic C-H and C-X stretching absorptions and methylidene CH₂ = MX₂ analogues
Organometallics, (26): 6373-6387 2007.
- Lyon, J. T.; Cho, H. G.; Andrews, L.; Hu, H. S.; Li, J.
Infrared and DFT investigations of the XC ReX₃ and HC ReX₃ complexes: Jahn-Teller distortion and the methylidyne C-X(H) stretching absorptions
Inorganic Chemistry, (46): 8728-8738 2007.
- Lyon, J. T.; Hu, H. S.; Andrews, L.; Li, J.
Formation of unprecedented actinide carbon triple bonds in uranium methylidyne molecules
Proceedings of the National Academy of Sciences of the United States of America, (104): 18919-18924 2007.

- Ma, W. J.; Wang, Y. B.; Zhang, J.; Wu, H. S.
Structure characteristics and stability of BmN (m=2-9) clusters
Acta Physico-Chimica Sinica, (23): 169-172 2007.
- Ma, Y.; Guo, W. Y.; Zhao, L. M.; Hu, S. Q.; Zhang, J.; Fu, Q. T.; Chen, X. F.
Theoretical survey of the gas-phase reactions of allylamine with Co+
Journal of Physical Chemistry A, (111): 6208-6216 2007.
- Ma, Y. G.; Balbuena, P. B.
Catalytic activity tuning of a biomimetic HO-Fe-V=O oxidant for methane hydroxylation by substituents on aromatic rings: Theoretical study
Journal of Physical Chemistry B, (111): 2711-2718 2007.
- Machura, B.; Kruszynski, R.
New oxorhenium complexes with the 8-quinolinolato ligand: X-ray structure and DFT calculations for [ReOBr(hqn)(2)]
Polyhedron, (26): 2957-2963 2007.
- Machura, B.; Kruszynski, R.
Synthesis, crystal, molecular and electronic structure of the [Re(NO)(0.87)Br-2.13(PPh3)(PPh(2)py-P,N)] complex and DFT calculations of [Re(NO)Br-2(PPh3)(PPh(2)py-P,N)]
Journal of Molecular Structure, (837): 92-100 2007.
- Machura, B.; Kruszynski, R.; Kusz, J.
New oxorhenium complexes with 2-(2'-hydroxyphenyl)-2-benzoxazolinato ligand. X-ray structure and DFT calculations for [ReOX2(hbo)(AsPh3)] and [ReOX2(hbo)(PPh3)] complexes
Polyhedron, (26): 3455-3464 2007.
- Machura, B.; Kruszynski, R.; Kusz, J.
A novel tricarbonyl rhenium complex of 2-thienyl-N, N-bis(2-thienylmethylene)methanediamine - X-ray structure, spectroscopic characterisation and DFT calculations
Polyhedron, (26): 2543-2549 2007.
- Machura, B.; Kruszynski, R.; Kusz, J.
X-ray structure, spectroscopic characterisation and DFT calculations of the [Re(CO)(3)(dppt)Cl] complex
Polyhedron, (26): 1590-1596 2007.
- Machura, B.; Kruszynski, R.; Mrozinski, J.
An unusual oxo-bridged rhenium complex with the Re centers in different coordination environments
Polyhedron, (26): 1259-1268 2007.
- Machura, B.; Michalik, S.; Kruszynski, R.; Kusz, J.
Oxorhenium complexes with the 8-quinolinolato ligand. X-ray structure and DFT calculations for [ReOX2(hqn)(AsPh3)] and [ReOX2(hqn)(PPh3)] complexes
Polyhedron, (26): 2837-2844 2007.

- Machura, B.; Penczek, R.; Kruszynski, R.; Kusz, J.
Synthesis, crystal, molecular, and electronic structure of [ReOCl₃(bpzm)] complex
Polyhedron, (26): 2581-2588 2007.
- Maity, A. N.; Schwederski, B.; Sarkar, B.; Zalis, S.; Fiedler, J.; Kar, S.; Lahiri, G. K.; Duboc, C.; Grunert, M.; Gutlich, P.; Kaim, W.
Tetranuclear complexes of [Fe(CO)₂(C₅H₅)](+) with TCNX ligands (TCNX = TCNE, TCNQ, TCNB): Intramolecular electron transfer alternatives in compounds (μ₄-TCNX)[ML_n](4)
Inorganic Chemistry, (46): 7312-7320 2007.
- Makedonas, C.; Mitsopoulou, C. A.
W(CO)₄(diimine) structure revised - Correlating structure to π back-bonding*
European Journal of Inorganic Chemistry: 110-119 2007.
- Malde, A. K.; Khedkar, S. A.; Coutinho, E. C.
The B(OH)-NH analog is a surrogate for the amide bond (CO-NH) in peptides: An ab initio study
Journal of Chemical Theory and Computation, (3): 619-627 2007.
- Malde, A. K.; Khedkar, S. A.; Coutinho, E. C.
Isosteres of peptides: boron analogs as dipolar forms of alpha-amino acids - a theoretical study
Journal of Physical Organic Chemistry, (20): 151-160 2007.
- Mandal, S. K.; Gurubasavaraj, P. M.; Roesky, H. W.; Oswald, R. B.; Magull, J.; Ringe, A.
Synthesis, structural characterization, and theoretical investigation of compounds containing an Al-O-M-O-Al (M = Ti, Zr) Core
Inorganic Chemistry, (46): 7594-7600 2007.
- Mandal, S. K.; Gurubasavaraj, P. M.; Roesky, H. W.; Schwab, G.; Stalke, D.; Swald, R. B.; Dolle, V.
Oxygen-bridged hybrid metallocene - Nonmetallocene polymetallic catalysts of group 4 metals for bimodal activity in olefin polymerization: Synthesis, characterization, and theoretical investigation
Inorganic Chemistry, (46): 10158-10167 2007.
- Marenich, A. V.; Olson, R. M.; Chamberlin, A. C.; Cramer, C. J.; Truhlar, D. G.
Polarization effects in aqueous and nonaqueous solutions
Journal of Chemical Theory and Computation, (3): 2055-2067 2007.
- Markgraf, J. H.; Hong, L.; Richardson, D. P.; Schofield, M. H.
Substituent effects on N-15 and C-13 NMR chemical shifts of 5-phenyl-1,3,4-oxathiazol-2-ones: a theoretical and spectroscopic study
Magnetic Resonance in Chemistry, (45): 985-988 2007.
- Markovic, S.; Markovic, Z.; Begovic, N.; Manojlovic, N.
Mechanism of the Kolbe-Schmitt reaction with lithium and sodium phenoxides
Russian Journal of Physical Chemistry A, (81): 1392-1397 2007.
- Markovic, Z.; Markovic, S.; Manojlovic, N.; Predojevic-Simovic, J.

- Mechanism of the Kolbe-Schmitt reaction. Structure of the intermediate potassium phenoxide-CO₂ complex*
Journal of Chemical Information and Modeling, (47): 1520-1525 2007.
- Maron, L.; Bourissou, D.
Lanthanide complexes of amino-carbenes: On the samarium-carbene bond from DFT calculations
Organometallics, (26): 1100-1103 2007.
- Marsella, M. J.; Rahbarnia, S.; Wilmot, N.
Molecular springs, muscles, rheostats, and precessing gyroscopes: from review to preview
Organic & Biomolecular Chemistry, (5): 391-400 2007.
- Martin, N. H.; Main, K. L.; Pyles, A. K.
Computation of through-space NMR shielding effects by aromatic ring-cation complexes: Substantial synergistic effect of complexation
Journal of Molecular Graphics and Modelling, (25): 806-812 2007.
- Martinek, T. A.; Varga, T.; Fulop, F.; Bartok, M.
NMR spectroscopic and theoretical evidence of cinchona alkaloid-ketopantolactone complex formation in aprotic solvents: Implications for the mechanism of Pt-catalyzed enantioselective hydrogenation of activated ketones
Journal of Catalysis, (246): 266-276 2007.
- Martiniano, H.; Cabral, B. J. C.; Simoes, J. A.
Substituent effects on water-assisted proton transfer in [p-XC₆H₄OH-(H₂O)(1-3)](.) clusters
Chemical Physics Letters, (442): 451-459 2007.
- Mata, R. A.; Werner, H.-J.
Local correlation methods with a natural localized molecular orbital basis
Molecular Physics, (105): 2753-2761 2007.
- Mata, R. A.; Werner, H. J.
Local correlation methods with a natural localized molecular orbital basis
Molecular Physics, (105): 2753-2761 2007.
- Matos, M. A. R.; Sousa, C. C. S.; Morais, V. M. F.
Experimental and computational thermochemistry of 1,3-benzodioxole derivatives
Journal of Chemical and Engineering Data, (52): 1089-1094 2007.
- Matxain, J. M.; Ristilla, M.; Strid, A.; Eriksson, L. A.
Theoretical study of the reaction of vitamin B-6 with O-1(2)
Chemistry-a European Journal, (13): 4636-4642 2007.
- Mauleon, P.; Alonso, I.; Rivero, M. R.; Carretero, J. C.
Enantioselective synthesis of chiral sulfones by Rh-catalyzed asymmetric addition of boronic acids to alpha,beta-unsaturated 2-pyridyl sulfones
Journal of Organic Chemistry, (72): 9924-9935 2007.

- Mayer, I.
Energy partitioning schemes: a dilemma
Faraday Discussions, (135): 439-450 2007.
- Mayer, P.; Schulz, A.; Villinger, A.
GaCl₃-assisted [3+2] cycloaddition: A route to new binary PN-heterocycles
Journal of Organometallic Chemistry, (692): 2839-2842 2007.
- McKee, M. L.
Modeling hydrogen evolution from the Fe₄S₄ and Fe₈S₉X (X = N, C) clusters. Can a Fe-S high-spin cluster serve as a surrogate for the FeMo cofactor?
Journal of Computational Chemistry, (28): 1796-1808 2007.
- McKee, M. L.
Modeling the nitrogenase FeMo cofactor with high-spin Fe₈S₉X⁺ (X=N, C) clusters. Is the first step for N₂ reduction to NH₃ a concerted dihydrogen transfer?
Journal of Computational Chemistry, (28): 1342-1356 2007.
- Megyes, T.; Balint, S.; Grosz, T.; Radnai, T.; Bako, I.; Almasy, L.
Structure of liquid nitromethane: Comparison of simulation and diffraction studies
Journal of Chemical Physics, (126) 2007.
- Melero, C.; Guijarro, A.; Baumann, V.; Perez-Jimenez, A. J.; Yus, M.
Carbolithiation of simple terminal and strained internal alkenes by the naphthalene and the biphenyl dianion: New modes of reactivity of highly reduced organic species in solution
European Journal of Organic Chemistry: 5514-5526 2007.
- Melin, J.; Ayers, P. W.; Ortiz, J. V.
Removing electrons can increase the electron density: A computational study of negative Fukui functions
Journal of Physical Chemistry A, (111): 10017-10019 2007.
- Memarian, H. R.; Sabzyan, H.; Abdoli-Senejani, M.
Conformational analysis of some unsymmetrically substituted 1,4-dihydropyridines
Journal of Molecular Structure-Theochem, (813): 39-47 2007.
- Mendizabal, F.; Donoso, D.; Olea-Azar, C.; Mera, R.
Theoretical study of the interaction d(10)-s(2) between Pt(0) and metals on the [Pt(PH₃)(3)M] complexes (M = Hg(0), Au(-I))
Journal of Molecular Structure-Theochem, (803): 39-44 2007.
- Mendizabal, F.; Olea-Azar, C.; Miranda, S.
Theoretical study of the interaction d(10)-d(8) between Pt(0) and M(I) on the [Pt(PH₃)-MPH₃](+) complexes (M = Cu, Ag, Au)
International Journal of Quantum Chemistry, (107): 1454-1458 2007.
- Meng, Q. X.; Wang, F.; Qu, X. J.; Zhou, J.; Li, M.
Theoretical insights of copper(I)-nitrene complexes

- Journal of Molecular Structure-Theochem, (815): 111-118 2007.
- Meng, Q. X.; Wang, F.; Qu, X. J.; Zhou, J.; Li, M.
Theoretical insights of iron(II)-carbene complexes Cp(CO)(L)Fe=CHR, L = CO, PMe₃
Journal of Molecular Structure-Theochem, (815): 157-163 2007.
- Merino, P.; Tejero, T.; Chiacchio, U.; Romeo, G.; Rescifina, A.
A DFT study on the 1,3-dipolar cycloaddition reactions of C-(hetaryl) nitrones with methyl acrylate and vinyl acetate
Tetrahedron, (63): 1448-1458 2007.
- Michalska, D.; Bienko, D. C.; Czarnik-Matusiewicz, B.; Wierzejewska, 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
Journal of Physical Chemistry B, (111): 12228-12238 2007.
- Michalska, D.; Hernik, K.; Wysokinski, R.; Morzyk-Ociepa, B.; Pietraszko, A.
Copper(II)-pi interaction in cis-[Cu(otolato)(NH₃)(2)] and the crystal structure of [Cu(otolato)(H₂O)(4)] center dot H₂O: X-ray, vibrational spectroscopy and density functional study
Polyhedron, (26): 4303-4313 2007.
- Michelini, M. D.; Russo, N.; Sicilia, E.
Gas-phase chemistry of actinides ions: New insights into the reaction of UO⁺ and UO₂⁺ with water
Journal of the American Chemical Society, (129): 4229-4239 2007.
- Mieusset, J. L.; Brinker, U. H.
Foiled carbenes revisited: When sigma-stabilization surpasses pi-stabilization
Journal of Organic Chemistry, (72): 263-268 2007.
- Mignon, P.; Geerlings, P.; Schoonheydt, R.
Oxygen basicity in alkaline cation-exchanged zeolite and the effect of isomorphous substitution. Use of hard descriptors
Journal of Physical Chemistry C, (111): 12376-12382 2007.
- Milov, A. A.; Starikov, A. G.; Gridin, M. K.; Minyaev, R. M.
Effect of the counterion on the steric and electronic structure of pyrylium cation
Russian Journal of General Chemistry, (77): 1373-1385 2007.
- Mitoraj, M.; Michalak, A.
Donor-acceptor properties of ligands from the natural orbitals for chemical valence
Organometallics, (26): 6576-6580 2007.
- Mo, O.; Yanez, M.; Pendas, A. M.; Del Bene, J. E.; Alkorta, I.; Elguero, J.
Unusual substituent effects on the bonding of iminoboranes
Physical Chemistry Chemical Physics, (9): 3970-3977 2007.

- Mo, Y. R.; Gao, J. L.
Theoretical analysis of the rotational barrier of ethane
Accounts of Chemical Research, (40): 113-119 2007.
- Mo, Y. R.; Song, L. C.; Lin, Y. C.
Block-localized wavefunction (BLW) method at the density functional theory (DFT) level
Journal of Physical Chemistry A, (111): 8291-8301 2007.
- Moens, J.; Roos, G.; Jaque, P.; Proft, F.; Geerlings, P.
Can electrophilicity act as a measure of the redox potential of first-row transition metal ions?
Chemistry-a European Journal, (13): 9331-9343 2007.
- Mohajeri, A.; Dasmeh, P.
Evaluating the nature of chemical bonds based on probabilistic models
International Journal of Modern Physics C, (18): 1795-1809 2007.
- Mola, J.; Romero, I.; Rodriguez, M.; Bozoglian, F.; Poater, A.; Sola, M.; Parella, T.; Benet-Buchholz, J.; Fontrodona, X.; Llobet, A.
Mechanistic insights into the chemistry of Ru(II) complexes containing Cl and DMSO ligands
Inorganic Chemistry, (46): 10707-10716 2007.
- Montagnon, L.; Spiegelman, F.
Self-consistent field tight-binding model for neutral and (multi-) charged carbon clusters
Journal of Chemical Physics, (127) 2007.
- Montejo, M.; Cabeza, A. J. C.; Urena, F. P.; Marquez, F.; Gonzalez, J. J. L.
Validation of the existence of tetrameric species of potassium trimethylsilanolate in the gas phase with a theoretical cluster model: Role of the counterion as charge localizer in the structure
Journal of Physical Chemistry A, (111): 2629-2633 2007.
- Moon, S.; Case, D. A.
A new model for chemical shifts of amide hydrogens in proteins
Journal of Biomolecular NMR, (38): 139-150 2007.
- Moores, A.; Cantat, T.; Ricard, L.; Mezailles, N.; Le Floch, P.
Experimental and theoretical study of phosphinine sulfides
New Journal of Chemistry, (31): 1493-1498 2007.
- Moosavi-Movahedi, Z.; Bahrami, H.; Zahedi, M.; Mahnam, K.; Chamani, J.; Safarian, S.; Saboury, A. A.; Moosavi-Movahedi, A. A.
A theoretical elucidation of bilirubin interaction with HSA's lysines: First electrostatic binding site in IIA subdomain
Biophysical Chemistry, (125): 375-387 2007.
- Mora, J. R.; Tosta, M.; Dominguez, R. M.; Herize, A.; Barroso, J.; Cordova, T.; Chuchani, G.

- Joint theoretical and experimental study of the gas-phase elimination kinetics of tert-butyl ester of carbamic, N,N-dimethylcarbamic, N-hydroxycarbamic acids and 1-(tert-butoxycarbonyl)-imidazole*
Journal of Physical Organic Chemistry, (20): 1021-1031 2007.
- Moran, M. D.; Mercier, H. P. A.; Schrobilgen, G. J.
Synthesis and structural characterization of C(OTeF5)(4) and a comparative structural study of the isoelectronic B(OTeF5)(4)(-) anion
Inorganic Chemistry, (46): 5034-5045 2007.
- Morzyk-Ociepa, B.
X-ray crystal structure and vibrational spectra of hydrazides and their metal complexes. Part I. Catena-poly[di- μ -aqua-(μ -maleic hydrazidato-O)sodium] hydrate
Journal of Molecular Structure, (833): 121-132 2007.
- Morzyk-Ociepa, B.
X-ray crystal structure and vibrational spectra of hydrazides and their metal complexes. Part II. Hexaaquacobalt(II)bis(phthalhydrazidato)tetrahydrate
Journal of Molecular Structure, (846): 74-86 2007.
- Muller, J.; Bohme, D.; Dupre, N.; Mehring, M.; Polonius, F. A.
Differential reactivity of alpha and beta 2'-deoxyribonucleosides towards protonation and metalation
Journal of Inorganic Biochemistry, (101): 470-476 2007.
- Muniz-Miranda, M.; Cardini, G.; Pagliai, M.; Schettino, V.
DFT investigation on the SERS band at similar to 1025 cm⁻¹ of pyridine adsorbed on silver
Chemical Physics Letters, (436): 179-183 2007.
- Murray, J. S.; Lane, P.; Clark, T.; Politzer, P.
sigma-hole bonding: molecules containing group VI atoms
Journal of Molecular Modeling, (13): 1033-1038 2007.
- Murray, J. S.; Lane, P.; Politzer, P.
A predicted new type of directional noncovalent interaction
International Journal of Quantum Chemistry, (107): 2286-2292 2007.
- Nakanishi, W.; Nakamoto, T.; Hayashi, S.; Sasamori, T.; Tokitoh, N.
Atoms-in-molecules analysis of extended hypervalent five-center, six-electron (5c-6e) C(2)Z(2)O interactions at the 1,8,9-positions of anthraquinone and 9-methoxyanthracene systems
Chemistry-a European Journal, (13): 255-268 2007.
- Nam, P. C.; Nguyen, M. T.; Zeegers-Huyskens, T.
Effects of fluorine-substitution on the molecular properties of dimethyl ethers: A theoretical investigation
Journal of Molecular Structure-Theochem, (821): 71-81 2007.
- Nazari, F.; Zali, F. R.

- Density functional study of the relative reactivity of the carbonyl group in substituted cyclohexanone*
Journal of Molecular Structure-Theochem, (817): 11-18 2007.
- Nazmutdinov, R. R.; Manyurov, I. R.; Zinkicheva, T. T.; Jang, J.; Ulstrup, J.
Cysteine adsorption on the Au(111) surface and the electron transfer in configuration of a scanning tunneling microscope: A quantum-chemical approach
Russian Journal of Electrochemistry, (43): 328-341 2007.
- Negri, F.; Saendig, N.
Tuning the physisorption of molecular hydrogen: binding to aromatic, hetero-aromatic and metal-organic framework materials
Theoretical Chemistry Accounts, (118): 149-163 2007.
- Nemirowski, A.; Schreiner, P. R.
Electronic stabilization of ground state triplet carbenes
Journal of Organic Chemistry, (72): 9533-9540 2007.
- Nguyen, M. T.; Nguyen, V. S.; Matus, M. H.; Gopakumar, G.; Dixon, D. A.
Molecular mechanism for H₂ release from BH₃NH₃, including the catalytic role of the lewis acid BH₃
Journal of Physical Chemistry A, (111): 679-690 2007.
- Nikolai, J.; Loe, O.; Dominiak, P. M.; Gerlitz, O. O.; Autschbach, J.; Davies, H. M. L.
Mechanistic studies of UV assisted [4+2] cycloadditions in synthetic efforts toward vibsantin E
Journal of the American Chemical Society, (129): 10763-10772 2007.
- Nirmala, V.; Kolandaivel, P.
Structure and electronic properties of armchair boron nitride nanotubes
Journal of Molecular Structure-Theochem, (817): 137-145 2007.
- Nockemann, P.; Thijs, B.; Driesen, K.; Janssen, C. R.; Van Hecke, K.; Van Meervelt, L.; Kossmann, S.; Kirchner, B.; Binnemans, K.
Choline saccharinate and choline acesulfamate: Ionic liquids with low toxicities
Journal of Physical Chemistry B, (111): 5254-5263 2007.
- Noguera, M.; Branchadell, V.; Constantino, E.; Rios-Font, R.; Sodupe, M.; Rodriguez-Santiago, L.
On the bonding of first-row transition metal cations to guanine and adenine nucleobases
Journal of Physical Chemistry A, (111): 9823-9829 2007.
- Noguera, M.; Sodupe, M.; Bertran, J.
Effects of protonation on proton transfer processes in Watson-Crick adenine-thymine base pair
Theoretical Chemistry Accounts, (118): 113-121 2007.
- Nori-Shargh, D.; Deyhimi, F.; Boggs, J. E.; Jameh-Bozorghi, S.; Shakibazadeh, R.
DFT study and NBO analysis of the mutual interconversion of cumulene compounds
Journal of Physical Organic Chemistry, (20): 355-364 2007.

- Nori-Shargh, D.; Ghanizadeh, F. R.; Hosseini, M. M.; Deyhimi, F.
Ab initio study and NBO analysis of configurational and conformational properties of cyclododeca-1,2,7,8-tetraene
Journal of Molecular Structure-Theochem, (808): 135-144 2007.
- Nori-Shargh, D.; Roohi, F.; Farajzadeh, J.; Deyhimi, F.
Structural and configurational properties of ethene, silaethene, germaethene, and stannaethene: A density functional theory study and natural bond orbital analysis
Phosphorus Sulfur and Silicon and the Related Elements, (182): 793-813 2007.
- Notni, J.; Gunther, W.; Anders, E.
Zinc thiolate complexes [ZnLn(SR)](+) with azamacrocyclic ligands, part III: The influence of the ligand L-n on the reactivity of zinc-bound thiolate
European Journal of Inorganic Chemistry: 985-993 2007.
- Novoa, J. N.; Ribas-Arino, J.; Shum, W. W.; Miller, J. S.
Control of two-electron four-center (2e(-)/4c) C-C bond formation observed for tetracyanoethenide dimerization, [TCNE](2)(2-)
Inorganic Chemistry, (46): 103-107 2007.
- Nowroozi-Isfahani, T.; Musaev, D. G.; Morokuma, K.; Gagne, M. R.
Density functional study of platinum(II)-mediated bicyclization of 1,6-dienylphenols
Organometallics, (26): 2540-2549 2007.
- Nsangou, M.; Dhaouadi, Z.; Jaidane, N.; Ben Lakhdar, Z.
DFT study of proton transfer, cooperativity, and tautomerization in 2-pyridineselenol and 2-pyridinethiol ammonia and water clusters
Journal of Molecular Structure-Theochem, (819): 142-152 2007.
- Nutt, D. R.; Meuwly, M.
Ferric and ferrous iron in nitroso-myoglobin: Computer simulations of stable and metastable states and their infrared spectra
Chemphyschem, (8): 527-536 2007.
- Occhipinti, G.; Bjorsvik, H. R.; Tornroos, K. W.; Jensen, V. R.
The first imidazolium-substituted metal alkylidene
Organometallics, (26): 4383-4385 2007.
- Ochi, N.; Nakao, Y.; Sato, H.; Sakaki, S.
Theoretical study of C-H and N-H sigma-bond activation reactions by titanium(IV)-imido complex. Good understanding based on orbital interaction and theoretical proposal for N-H sigma-bond activation of ammonia
Journal of the American Chemical Society, (129): 8615-8624 2007.
- Oehlke, A.; Auer, A. A.; Jahre, I.; Walfort, B.; Ruffer, T.; Zoufala, P.; Lang, H.; Spange, S.
Nitro-substituted stilbeneboronate pinacol esters and their fluoro-adducts. Fluoride ion induced polarity enhancement of arylboronate esters
Journal of Organic Chemistry, (72): 4328-4339 2007.

- Ohta, K.; Goto, T.; Yamazaki, H.; Pichierri, F.; Endo, Y.
Facile and efficient synthesis of C-hydroxycarboranes and C,C'-dihydroxycarboranes
Inorganic Chemistry, (46): 3966-3970 2007.
- Ohta, K.; Yamazaki, H.; Pichierri, F.; Kawahata, M.; Yamaguchi, K.; Endo, Y.
Solid-state supramolecular array through cooperative pi-pi interactions of 1-(2-methoxyphenyl)-o-carborane
Tetrahedron, (63): 12160-12165 2007.
- Ojala, C. R.; Ojala, W. H.; Britton, D.; Cramer, C. J.
Three polymorphs of 4,4'-diiodobenzalazine, and 4-chloro-4'-iodobenzalazine
Acta Crystallographica Section C-Crystal Structure Communications, (63): O518-O523 2007.
- Okiyama, Y.; Watanabe, H.; Fukuzawa, K.; Nakano, T.; Mochizuki, Y.; Ishikawa, T.; Tanaka, S.; Ebina, K.
Application of the fragment molecular orbital method for determination of atomic charges on polypeptides
Chemical Physics Letters, (449): 329-335 2007.
- Olah, J.; Veszpremi, T.; De Proft, F.; Geerlings, P.
Silylenes: A unified picture of their stability, acid-base and spin properties, nucleophilicity, and electrophilicity via computational and conceptual density functional theory
Journal of Physical Chemistry A, (111): 10815-10823 2007.
- Olbert, D.; Kalisch, A.; Herzer, N.; Górls, H.; Mayer, P.; Yu, L.; Reiher, M.; Westerhausen, M.
Syntheses of N-(diphenylphosphanyl)-2-pyridylmethylamine and its use as a ligand in magnesium and zinc complexes
Zeitschrift für Anorganische und Allgemeine Chemie, (633): 893-902 2007.
- Oliveira, B. G.; de Araujo, R.
Relationship between charge transfer and intermolecular interactions in heterocyclic hydrogen-bonded complexes
Quimica Nova, (30): 791-796 2007.
- Olson, R. M.; Marenich, A. V.; Cramer, C. J.; Trublarlc, D. G.
Charge model 4 and intramolecular charge polarization
Journal of Chemical Theory and Computation, (3): 2046-2054 2007.
- Ottosson, H.; Kilsa, K.; Chajara, K.; Piqueras, M.; Crespo, R.; Kato, H.; Muthas, D.
Scope and limitations of Baird's theory on triplet state aromaticity: Application to the tuning of singlet-triplet energy gaps in fulvenes
Chemistry-a European Journal, (13): 6998-7005 2007.
- Oulie, P.; Freund, C.; Saffon, N.; Martin-Vaca, B.; Maron, L.; Bourissou, D.
Enforced eta(1)-fluorenyl and indenyl coordination to zirconium: Geometrically constrained and sterically expanded complexes derived from the bifunctional (FluPPh(2)NAr)(-) and (IndPPh(2)NAr)(-) ligands
Organometallics, (26): 6793-6804 2007.

- Overgaard, J.; Waller, M. P.; Piltz, R.; Platts, J. A.; Emseis, P.; Leverett, P.; Williams, P. A.; Hibbs, D. E.
Experimental and theoretical charge density distribution in two ternary cobalt(III) complexes of aromatic amino acids
Journal of Physical Chemistry A, (111): 10123-10133 2007.
- Padilla-Campos, L.
Theoretical investigation of the adsorption of oxygen on small copper clusters
Journal of Molecular Structure-Theochem, (815): 63-69 2007.
- Padmanabhan, J.; Parthasarathi, R.; Elango, M.; Subramanian, V.; Krishnamoorthy, B. S.; Gutierrez-Oliva, S.; Toro-Labbe, A.; Roy, D. R.; Chattaraj, P. K.
Multiphilic descriptor for chemical reactivity and selectivity
Journal of Physical Chemistry A, (111): 9130-9138 2007.
- Pakiari, A. H.; Jamshidi, Z.
Interaction of amino acids with gold and silver clusters
Journal of Physical Chemistry A, (111): 4391-4396 2007.
- Palafox, M. A.; Tardajos, G.; Guerrero-Martinez, A.; Rastogi, V. K.; Mishra, D.; Ojha, S. P.; Kiefer, W.
FT-IR, FT-Raman spectra, density functional computations of the vibrational spectra and molecular geometry of biomolecule 5-aminouracil
Chemical Physics, (340): 17-31 2007.
- Pandey, K. K.
Structure and coordinate bonding nature of the manganese-sigma-borane complexes
Journal of Organometallic Chemistry, (692): 1997-2005 2007.
- Parra, R. D.; Arena, A.; Sankisa, S.
Conformational preferences of carbonic acid and its sulfur derivatives, H₂C(=X)O₂-nSn(X = O/S; n=0-2)
Journal of Molecular Structure-Theochem, (815): 31-40 2007.
- Parra, R. D.; Cedeno, D. L.
Preferred conformations of the gas phase complex between Li⁺ and a model macrocycle tetraamide
Journal of Molecular Structure-Theochem, (819): 79-87 2007.
- Parreira, R. L. T.; Galembeck, S. E.; Hobza, P.
On the origin of red and blue shifts of X-H and C-H stretching vibrations in formic acid (formate ion) and proton donor complexes
Chemphyschem, (8): 87-92 2007.
- Pasquini, M.; Schiccheri, N.; Piani, G.; Pietraperzia, G.; Becucci, M.; Biczysko, M.; Pavone, M.; Barone, V.
Isotopomeric conformational changes in the anisole-water complex: New insights from HR-UV spectroscopy and theoretical studies
Journal of Physical Chemistry A, (111): 12363-12371 2007.

- Pau, M. Y. M.; Davis, M. I.; Orville, A. M.; Lipscomb, J. D.; Solomon, E. I.
Spectroscopic and electronic structure study of the enzyme-substrate complex of intradiol dioxygenases: Substrate activation by a high-spin ferric non-heme iron site
Journal of the American Chemical Society, (129): 1944-1958 2007.
- Pavanello, M.; Jalbout, A. F.; Trzaskowski, B.; Adamowicz, L.
Fullerene as an electron buffer: Charge transfer in Li@C-60
Chemical Physics Letters, (442): 339-343 2007.
- Pavelka, M.; Burda, J. V.
Pt-bridges in various single-strand and double-helix DNA sequences. DFT and MP2 study of the cisplatin coordination with guanine, adenine, and cytosine
Journal of Molecular Modeling, (13): 367-379 2007.
- Pavelka, M.; Lucas, M. F. A.; Russo, N.
On the hydrolysis mechanism of the second-generation anticancer drug carboplatin
Chemistry-a European Journal, (13): 10108-10116 2007.
- Penka, E. F.; Schlaepfer, C. W.; Atanasov, M.; Albrecht, M.; Daul, C.
Theoretical investigation of the bonding properties of N-heterocyclic carbenes coordinated to electron-rich d(8) metal centers
Journal of Organometallic Chemistry, (692): 5709-5716 2007.
- Perez-Juste, I.; Carballeira, L.
Theoretical study of the electronic structure of HXY/XYH radicals (X = C,Si; Y = O,S)
Journal of Chemical Physics, (127) 2007.
- Periyasamy, G.; Burton, N. A.; Hillier, I. H.; Vincent, M. A.; Disley, H.; McMaster, J.; Garner, C. D.
The dithiolene ligand - 'innocent' or 'non-innocent'? A theoretical and experimental study of some cobalt-dithiolene complexes
Faraday Discussions, (135): 469-488 2007.
- Perpete, E. A.; Maurel, F.; Jacquemin, D.
TD-DFT investigation of diarylethene dyes with cyclopentene, dihydrothiophene, and dihydropyrrole bridges
Journal of Physical Chemistry A, (111): 5528-5535 2007.
- Pfletschinger, A.; Schneider, U.; Lex, J.; Schmalz, H. G.
Stereospecific side chain activation in Cyclobutadiene-Fe(CO)(3) chemistry: A theoretical and experimental study on the structure and configurational stability of cationic, radical and anionic intermediates
European Journal of Organic Chemistry: 3991-3998 2007.
- Phillips, J. A.; Cramer, C. J.
B-N distance potential of CH3CN-BF3 revisited: Resolving the experiment-theory structure discrepancy and modeling the effects of low-dielectric environments
Journal of Physical Chemistry B, (111): 1408-1415 2007.

- Picazo, O.; Alkorta, I.; Elguero, J.; Sundberg, M. R.; Valo, J.
Bonding properties related with chiral discrimination in dinuclear metal complexes of group 10
European Journal of Inorganic Chemistry: 324-332 2007.
- Pichierri, F.; Yamamoto, Y.
Mechanism and chemoselectivity of the Pd(II)-catalyzed allylation of aldehydes: A density functional theory study
Journal of Organic Chemistry, (72): 861-869 2007.
- Pino, T.; Parneix, P.; Calvo, F.; Brechignac, P.
Theoretical rates for the emission of atomic hydrogen from a naphthalene cation
Journal of Physical Chemistry A, (111): 4456-4463 2007.
- Pinter, B.; De Proft, F.; Van Speybroeck, V.; Hemelsoet, K.; Waroquier, M.; Chamorro, E.; Veszpremi, T.; Geerlings, P.
Spin-polarized conceptual density functional theory study of the regioselectivity in ring closures of radicals
Journal of Organic Chemistry, (72): 348-356 2007.
- Pitteri, B.; Bortoluzzi, M.
Displacement of neutral nitrogen donors by chloride in AuCl₃(am) (am = pyridines and amines): Kinetics and DFT calculations show the effects of basicity and pi-acceptor ability
European Journal of Inorganic Chemistry: 4456-4461 2007.
- Pluhackova, K.; Hobza, P.
On the nature of the surprisingly small (red) shift in the halothane ...acetone complex
Chemphyschem, (8): 1352-1356 2007.
- Plumley, J. A.; Evanseck, J. D.
Covalent and ionic nature of the dative bond and account of accurate ammonia borane binding enthalpies
Journal of Physical Chemistry A, (111): 13472-13483 2007.
- Plusquellic, D. F.; Pratt, D. W.
Probing the electronic structure of peptide bonds using methyl groups
Journal of Physical Chemistry A, (111): 7391-7397 2007.
- Poater, A.; Solans-Monfort, X.; Clot, E.; Coperet, C.; Eisenstein, O.
Understanding d(0)-olefin metathesis catalysts: Which metal, which ligands?
Journal of the American Chemical Society, (129): 8207-8216 2007.
- Ponec, R.
Anatomy of bond formation. domain-averaged fermi holes as a tool for the study of the nature of the chemical bonding in Li-2, Li-4, and F-2
Journal of Physical Chemistry A, (111): 11294-11301 2007.
- Popa, M. V.
Quantification of sites active in DNA and RNA bases using condensed Fukui functions

Revista Mexicana De Fisica, (53): 241-253 2007.

Popp, B. V.; Stahl, S. S.

Insertion of molecular oxygen into a palladium-hydride bond: Computational evidence for two nearly isoenergetic pathways

Journal of the American Chemical Society, (129): 4410-4422 2007.

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

Origin of methyl torsional barrier in 1-methyl-2(1H)-pyridinimine and 3-methyl-2(1H)-pyridone: II. Ground state

Journal of Chemical Physics, (126) 2007.

Pradines, V.; Potea, R.; Pimienta, V.

Amphiphilic organic ion pairs in solution: A theoretical study

Chemphyschem, (8): 1524-1533 2007.

Pradines, V.; Poteau, R.; Pimienta, V.

Amphiphilic organic ion pairs in solution: A theoretical study

Chemphyschem, (8): 1524-1533 2007.

Praveena, G.; Kolandaivel, P.

Interaction of hydrogen halides and water molecules with the isomers of C-20 fullerene - A theoretical study

Journal of Molecular Structure, (828): 154-161 2007.

Priego, E. M.; Sanchez, L.; Herranz, M. A.; Martin, N.; Viruela, R.; Orti, E.

Synthesis and radical coupling of pyridine-bridged pi-extended tetrathiafulvalene (TTF)-type donors and push-pull analogues

Organic & Biomolecular Chemistry, (5): 1201-1209 2007.

Puyad, A. L.; Raghunath, P.; Chaitanya, G. K.; Ramakrishna, K.; Bhanuprakash, K.

Structure and bonding differences in C₃N₄ and Si₃N₄ isomers - A comparative study of [Si-3,N-4] and [C-3,N-4] potential energy surfaces using DFT and MP2 methodologies

Journal of Molecular Structure-Theochem, (807): 73-85 2007.

Qingzhong, L.; Wang, N.; Zhiwu, Y.

Effect of hydration on the C-H center dot center dot center dot O hydrogen bond: A theoretical study

Journal of Molecular Structure-Theochem, (847): 68-74 2007.

Rademacher, P.; Mohr, P. C.

Transannular 1,5-hydride shift in 5-hydroxycyclooctanone: an experimental and theoretical investigation

Organic & Biomolecular Chemistry, (5): 2698-2703 2007.

Raissi, H.; Bakavol, M.; Jimenez-Fabian, I.; Tajabadi, J.; Mdoshfeghi, E.; Jalbout, A. F.

Effect of substitution on the intramolecular hydrogen bonding of 4-amino-3-penten-2-one: Ab initio, AIM and NBO studies

- Journal of Molecular Structure-Theochem, (847): 47-51 2007.
- Ramalingam, M.; Ramasam, K.; Venuvanalingam, P.
Insertion of singlet chlorocarbenes across C-H bonds in alkanes: Evidence for two phase mechanism
Journal of Chemical Sciences, (119): 467-473 2007.
- Ramirez, B. C.; Dominguez, R. M.; Herize, A.; Tosta, M.; Cordova, T.; Chuchani, G.
Experimental and theoretical study of the homogeneous, unimolecular gas-phase elimination kinetics of 2-furoic acid
International Journal of Chemical Kinetics, (39): 298-306 2007.
- Rannulu, N. S.; Rodgers, M. T.
Noncovalent interactions of Cu⁺ with N-donor ligands (pyridine, 4,4-dipyridyl, 2,2-dipyridyl, and 1,10-phenanthroline): Collision-induced dissociation and theoretical studies
Journal of Physical Chemistry A, (111): 3465-3479 2007.
- Rastogi, V. K.; Palafox, M. A.; Singhal, S.; Ojha, S. P.; Kiefer, W.
Geometrical parameters, vibrational wavenumbers, and relationships established with six difluorobenzonitriles
International Journal of Quantum Chemistry, (107): 1099-1114 2007.
- Ray, S.; Mohan, R.; Singh, J. K.; Samantaray, M. K.; Shaikh, M. M.; Panda, D.; Ghosh, P.
Anticancer and antimicrobial metallopharmaceutical agents based on palladium, gold, and silver N-heterocyclic carbene complexes
Journal of the American Chemical Society, (129): 15042-15053 2007.
- Rayon, C. M.; Redondo, P.; Valdes, H.; Barrientos, C.; Largo, A.
Cyanides and isocyanides of first-row transition metals: Molecular structure, bonding, and isomerization barriers
Journal of Physical Chemistry A, (111): 6334-6344 2007.
- Rayon, V. M.; Redondo, P.; Barrientos, C.; Largo, A.
Structure and bonding in first-row transition metal dicarbide cations MC₂⁺
Journal of Physical Chemistry A, (111): 6345-6353 2007.
- Reddy, A. R.; Fridman-Marueli, G.; Bendikov, M.
Kinetic and thermodynamic stability of acenes: Theoretical study of nucleophilic and electrophilic addition
Journal of Organic Chemistry, (72): 51-61 2007.
- Remenyi, C.; Reviakine, R.; Kaupp, M.
Density functional study of EPR parameters and spin-density distribution of azurin and other blue copper proteins
Journal of Physical Chemistry B, (111): 8290-8304 2007.
- Ren, Y.; Gai, J. G.; Xiong, Y.; Lee, K. H.; Chu, S. Y.

- Theoretical study on the identity ion pair S(N)2 reactions of LiX with CH3SX (X = Cl, Br, and I): Structure, mechanism, and potential energy surface*
Journal of Physical Chemistry A, (111): 6615-6621 2007.
- Ren, Y.; Yamataka, H.
G2(+) investigation on the alpha-effect in the S(N)2 reactions at saturated carbon
Chemistry-a European Journal, (13): 677-682 2007.
- Ren, Y. H.; Song, J. R.; Xu, K. Z.; Ma, H. X.; Huang, J.; Fu, D. W.; Hu, H. M.
Preparation, crystal structure and theoretical calculation of N-(pyrimidin-2-yl)-N'-methoxycarbonyl-thiourea
Chinese Journal of Chemistry, (25): 510-514 2007.
- Reveles, J. U.; Calaminici, P.; Beltran, M. R.; Koster, A. M.; Khanna, S. N.
H2O nucleation around Au+
Journal of the American Chemical Society, (129): 15565-15571 2007.
- Richard, R. M.; Ball, D. W.
B3LYP, G2, G3, and complete basis set calculations of the thermodynamic properties of small cyclic and chain hydroboranes
Journal of Molecular Structure-Theochem, (814): 91-98 2007.
- Rincon, E.; Toro-Labbe, A.
Reaction force and electron localization function analysis of the metal chelation process in Mg(II)-thymine complex
Chemical Physics Letters, (438): 93-98 2007.
- Rincon, E.; Yanez, M.; Toro-Labbe, A.; Mo, O.
Effect of Ni(II), Cu(II) and Zn(II) association on the keto-enol tautomerism of thymine in the gas phase
Physical Chemistry Chemical Physics, (9): 2531-2537 2007.
- Rios-Font, R.; Rodriguez-Santiago, L.; Bertran, J.; Sodupe, M.
Influence of N7 protonation on the mechanism of the N-glycosidic bond hydrolysis in 2'-deoxyguanosine. A theoretical study
Journal of Physical Chemistry B, (111): 6071-6077 2007.
- Robe, E.; Maria, S.; Richard, P.; Poli, R.
Mixed titanium-hafnium chloridometallate complexes
European Journal of Inorganic Chemistry: 2434-2442 2007.
- Robles, N. L.; Alvarez, R. M. S.; Cutin, E. H.; Della Vedova, C. O.; Erben, M. F.; Boese, R.; Willner, H.; Mews, R.
Anomeric interactions in pentafluoroethylimidodisulfurous dichloride, CF3CF2N=SCl2: Structural, conformational and configurational properties in the gaseous and condensed phases
European Journal of Inorganic Chemistry: 3535-3542 2007.
- Rodriguez, A. H.; Branda, M. M.; Castellani, N. J.

- Adsorption of n methanol molecules on MgO(100) with n=1 to 4: A theoretical study*
Journal of Physical Chemistry C, (111): 10603-10609 2007.
- Rodriguez-Dieguez, A.; Cano, J.; Kivekas, R.; Debdoubi, A.; Colacio, E.
Self-assembled cationic heterochiral honeycomb-layered metal complexes with the in situ generated pyrimidine-2-carboxylato bidentate ligand. Hydrothermal synthesis, crystal structures, magnetic properties, and theoretical study of [M-2(mu-pymca)(3)]OH center dot H2O (M = Fe-II, Co-II)
Inorganic Chemistry, (46): 2503-2510 2007.
- Rodriguez-Otero, J.; Cabaleiro-Lago, E. M.; Pena-Gallego, A.
Theoretical study of the walk rearrangement in perfluorotetramethyl (Dewar thiophene) exo-S-oxide
Tetrahedron, (63): 2191-2198 2007.
- Rogachev, A. Y.; Mironov, A. V.; Nemukhin, A. V.
Experimental and theoretical studies of the products of reaction between Ln(hfa)(3) and Cu(acac)(2) (Ln = La, Y; acac = acetylacetonate, hfa = hexafluoroacetylacetonate)
Journal of Molecular Structure, (831): 46-54 2007.
- Rogachev, A. Y.; Sevryugina, Y.; Filatov, A. S.; Petrukhina, M. A.
Corannulene vs. C-60-fullerene in metal binding reactions: A direct DFT and X-ray structural comparison
Dalton Transactions: 3871-3873 2007.
- Rogacheva, M. V.; Bochenkova, A. V.; Kuznetsova, S. A.; Saparbaev, M. K.; Nemukhin, A. V.
Impact of pyrophosphate and O-ethyl-substituted pyrophosphate groups on DNA structure
Journal of Physical Chemistry B, (111): 432-438 2007.
- Roldan, M. L.; Brandan, S. A.; Masters, S. L.; Wann, D. A.; Robertson, H. E.; Rankin, D. W. H.; Ben Altabef, A.
Molecular structure and vibrational spectra of iodotrimethylgermane (GeIme3) by theory and experiment
Journal of Physical Chemistry A, (111): 7200-7210 2007.
- Romao, C. C.; Veiros, L. F.
Haptotropic shifts and fluxionality of cyclopentadienyl in mixed-hapticity complexes: A DFT mechanistic study
Organometallics, (26): 1777-1781 2007.
- Romeo, R.; D'Amico, G.; Sicilia, E.; Russo, N.; Rizzato, S.
beta-hydrogen kinetic effect
Journal of the American Chemical Society, (129): 5744-5755 2007.
- Rondinelli, F.; Russo, N.; Toscano, M.
On the origin of the different performance of iron and manganese monocations in catalyzing the nitrous oxide reduction by carbon oxide
Inorganic Chemistry, (46): 7489-7493 2007.

- Roohi, H.; Habibi, S. M.
Generalized anomeric effect in CH₄-nClnS. Energetic and NBO analyses
Bulletin of the Chemical Society of Japan, (80): 1323-1330 2007.
- Roohi, H.; Machiabadi, B.
Blue-shifted H-bond in aromatic sulfines: An ab initio calculation
International Journal of Quantum Chemistry, (107): 1559-1565 2007.
- Roshal, A. D.; Sikorski, A.; Baumer, V. N.; Novikov, A. I.; Blazejowski, J.
Two polymorphs of 2-(4-chlorophenyl)-4-methylchromenium perchlorate
Acta Crystallographica Section C-Crystal Structure Communications, (63): O626-O630 2007.
- Rostkowski, M.; Paneth, P.
Charge localization in monothiophosphate monoanions
Polish Journal of chemistry, (81): 711-720 2007.
- Roux, M. V.; Temprado, M.; Jimenez, P.; Notario, R.
Thermochemistry of 2-and 3-acetylthiophenes: Calorimetric and computational study
Journal of Physical Chemistry A, (111): 11084-11092 2007.
- Roux, M. V.; Temprado, M.; Jimenez, P.; Notario, R.; Guzman-Mejia, R.; Juaristi, E.
Calorimetric and computational study of 1,3-and 1,4-oxathiane sulfones
Journal of Organic Chemistry, (72): 1143-1147 2007.
- Roux, M. V.; Temprado, M.; Notario, R.; Chickos, J. S.; Santos, A.; da Silva, M.
Experimental and computational thermochemical study of 2-and 3-thiopheneacetic acid methyl esters
Journal of Physical Chemistry A, (111): 5280-5286 2007.
- Roy, D.; Sunoj, R. B.
Intramolecular nonbonding interactions in organoseleniums: Quantification using a computational thermochemical approach
Journal of Molecular Structure-Theochem, (809): 145-152 2007.
- Roy, G.; Das, D.; Mugesh, G.
Bioinorganic chemistry aspects of the inhibition of thyroid hormone biosynthesis by anti-hyperthyroid drugs
Inorganica Chimica Acta, (360): 303-316 2007.
- Roy, T. K.; Ghanta, S.; Mondal, T.; Saritha, B.; Mahapatra, S.; Prasad, M. D.
Conformational preferences of mono-substituted cyclohydronitrogens: A theoretical study
Journal of Molecular Structure-Theochem, (822): 145-150 2007.
- Rozas, I.
On the nature of hydrogen bonds: an overview on computational studies and a word about patterns
Physical Chemistry Chemical Physics, (9): 2782-2790 2007.

- Ruan, C. H.; Yang, Z. B.; Rodgers, M. T.
Cation- π interactions with a π -excessive nitrogen heterocycle: Structures and absolute binding energies of alkali metal cation-pyrrole complexes
International Journal of Mass Spectrometry, (267): 233-247 2007.
- Ruan, C. H.; Yang, Z. B.; Rodgers, M. T.
Influence of the d orbital occupation on the nature and strength of copper cation- π interactions: threshold collision-induced dissociation and theoretical studies
Physical Chemistry Chemical Physics, (9): 5902-5918 2007.
- Ruano, J. L. G.; Aleman, J.; Alonso, I.; Parra, A.; Marcos, V.; Aguirre, J.
 π - π stacking versus steric effects in stereoselectivity control: Highly diastereoselective synthesis of syn-1,2-diarylpropylamines
Chemistry-a European Journal, (13): 6179-6195 2007.
- Ruben, E. A.; Chapman, M. S.; Evanseck, J. D.
Hydrogen bonding mediated by key orbital interactions determines hydration enthalpy differences of phosphate water clusters
Journal of Physical Chemistry A, (111): 10804-10814 2007.
- Ruben, E. A.; Chapman, M. S.; Evanseck, J. D.
Hydrogen bonding mediated by key orbital interactions determines hydration enthalpy differences of phosphate water clusters
Journal of Physical Chemistry A, (111): 10804-10814 2007.
- Ruiz-Garcia, R.; Pardo, E.; Munoz, M. C.; Cano, J.
High-valent bis(oxo)-bridged dinuclear manganese oxamates: Synthesis, crystal structures, magnetic properties, and electronic structure calculations of bis(μ -oxo)dimanganese(IV) complexes with a binucleating o-phenylenedioxamate ligand
Inorganica Chimica Acta, (360): 221-232 2007.
- Rupar, P. A.; Staroverov, V. N.; Ragogna, P. J.; Baines, K. M.
A germanium(II)-centered dication
Journal of the American Chemical Society, (129): 15138-+ 2007.
- Rusakov, Y. Y.; Krivdin, L. B.; Senotrusova, E. Y.; Schmidt, E. Y.; Vasiltssov, A. M.; Mikhaleva, A. I.; Trofimov, B. A.; Dyachenko, O. A.; Chekhlov, A. N.; Kazheva, O. N.
Conformational study of 2-aryloxy-1-vinylpyrroles
Magnetic Resonance in Chemistry, (45): 142-151 2007.
- Sablon, N.; De Proft, F.; Ayers, P. W.; Geerlings, P.
Computing Fukui functions without differentiating with respect to electron number. II. Calculation of condensed molecular Fukui functions
Journal of Chemical Physics, (126) 2007.
- Sabolovic, J.; Kaitner, B.

- The effects of steric aliphatic-aliphatic interactions in the coordination polymer of bis(N,N-diethylglycinato)copper(II): Experimental evidence and theoretical modeling*
Polyhedron, (26): 1087-1097 2007.
- Sabzyan, H.; Farmanzadeh, D.
Electric field effects on the performance of a candidate multipole molecular switch: A quantum computational study
Journal of Computational Chemistry, (28): 922-931 2007.
- Sadjadi, M. S.; Farhadyar, N.; Zare, K.
Ab initio and natural bond orbital (NBO) study on the strain energy of chlorocyclotrisilane and chlorocyclopropane
Journal of Molecular Structure-Theochem, (814): 141-145 2007.
- Sadjadi, M. S.; Sadeghi, B.; Zare, K.
Natural bond orbital (NBO) population analysis of cyclic thionylphosphazenes, [NSOX(NPC1(2))(2)]; X = F (1), X = Cl (2)
Journal of Molecular Structure-Theochem, (817): 27-33 2007.
- Sadlej-Sosnowska, N.
Molecular similarity based on atomic electrostatic potential
Journal of Physical Chemistry A, (111): 11134-11140 2007.
- Sadlej-Sosnowska, N.
On the way to physical interpretation of Hammett constants: How substituent active space impacts on acidity and electron distribution in p-substituted benzoic acid molecules
Polish Journal of chemistry, (81): 1123-1134 2007.
- Safi, Z.; Lamsabhi, A. M.
Gas-phase reactivity of 2,7-dimethyl-[1,2,4]-triazepine thio derivatives toward Cu⁺ cation: A DFT study
Journal of Physical Chemistry A, (111): 2213-2219 2007.
- Sahnoun, R.; Fujimura, Y.; Kabuto, K.; Takeuchi, Y.; Noyori, R.
Ab initio molecular orbitals study of the conformational preference in alpha-cyano-alpha-fluorophenylacetic acid ester
Journal of Organic Chemistry, (72): 7923-7929 2007.
- Salzner, U.
Theoretical investigation of excited states of oligothiophenes and of their monocations
Journal of Chemical Theory and Computation, (3): 1143-1157 2007.
- Sanchez, A.; Mondragon, F.
Role of the epoxy group in the heterogeneous CO₂ evolution in carbon oxidation reactions
Journal of Physical Chemistry C, (111): 612-617 2007.
- Sanz, P.; Mo, O.; Yanez, M.; Elguero, J.

Non-resonance-assisted hydrogen bonding in hydroxymethylene and aminomethylene cyclobutanones and cyclobutenones and their nitrogen counterparts
Chemphyschem, (8): 1950-1958 2007.

Sarangi, R.; George, S. D.; Rudd, D. J.; Szilagy, R. K.; Ribas, X.; Rovira, C.; Almeida, M.; Hodgson, K. O.; Hedman, B.; Solomon, E. I.

Sulfur K-edge X-ray absorption spectroscopy as a probe of ligand-metal bond covalency: Metal vs ligand oxidation in copper and nickel dithiolene complexes
Journal of the American Chemical Society, (129): 2316-2326 2007.

Sarkar, M.; Samanta, A.

Photophysical and density functional studies of the interaction of a flavone derivative with the halides
Journal of Physical Chemistry B, (111): 7027-7033 2007.

Sateesh, B.; Soujanya, Y.; Sastry, G. N.

Metal ion binding with dehydroannulenes - Plausible two-dimensional molecular sieves
Journal of Chemical Sciences, (119): 509-515 2007.

Sathyabama, V.; Karthika, M.; Senthilkumar, K.; Anandan, K.; Kanakaraju, R.

Post Hartree-Fock and density functional theory studies on Di-Protonated Allopurinol(2+)
Journal of Molecular Structure-Theochem, (810): 25-30 2007.

Sato, H.; Sakaki, S.

Reply to "Comment on 'Analysis on solvated molecules with a new energy partitioning scheme for intra- and intermolecular interactions'"
Journal of Physical Chemistry B, (111): 672-674 2007.

Sawwan, N.; Greer, A.

Rather exotic types of cyclic peroxides: Heteroatom dioxiranes
Chemical Reviews, (107): 3247-3285 2007.

Sawwan, N.; Greer, A.

Rather exotic types of cyclic peroxides: Heteroatom dioxiranes
Chemical Reviews, (107): 3247-3285 2007.

Schafman, B. S.; Wenthold, P. G.

Regioselectivity of pyridine deprotonation in the gas phase
Journal of Organic Chemistry, (72): 1645-1651 2007.

Scheiner, S.; Kar, T.

Underlying source of the relation between polypeptide conformation and strength of NH center dot center dot center dot O hydrogen bonds
Journal of Molecular Structure, (844): 166-172 2007.

Schulz, A.; Mayer, P.; Villinger, A.

An unusual reaction: a GaCl₃-Assisted Methyl/Chlorine exchange in silylated hydrazinodichloroarsane

Inorganic Chemistry, (46): 8316-8322 2007.

Sekharan, S.; Sugihara, M.; Buss, V.

Origin of spectral tuning in rhodopsin - It is not the binding pocket

Angewandte Chemie-International Edition, (46): 269-271 2007.

Semenov, S. N.; Rogachev, A. Y.; Eliseeva, S. V.; Belousov, Y. A.; Drozdov, A. A.; Troyanov, S. I.

5-Nitroaminotetrazole as a building block for extended network structures: Syntheses and crystal structures of a number of heavy metal derivatives

Polyhedron, (26): 4899-4907 2007.

Shaik, S.

Is my chemical universe localized or delocalized? Is there a future for chemical concepts?

New Journal of Chemistry, (31): 2015-2028 2007.

Shainyan, B. A.; Ushakov, I. A.; Meshcheryakov, V. I.; Schilde, U.; Koch, A.; Kleinpeter, E.

The stereodynamics of 3,5-bis(trifluoromethylsulfonyl)-1,3,5-oxadiazinane and 1,3,5-tris(trifluoromethylsulfonyl)-1,3,5-triazinane - an experimental and theoretical study

Tetrahedron, (63): 11828-11837 2007.

Shankar, R.; Kolandaivel, P.

Reaction mechanism of O-acylhydroxamate with cysteine proteases

Journal of Chemical Sciences, (119): 533-544 2007.

Shankar, R.; Kolandaivel, P.; Nirmala, V.; Narayandass, S. K.

Molecular interaction of H-2, N-2, and HF molecules with the silicon carbide (SiC)(n=5-9) clusters: A theoretical study

Journal of Computational and Theoretical Nanoscience, (4): 787-796 2007.

Sharma, P.; Singh, H.; Sharma, S.

Binding of gold nanoclusters with size-expanded DNA bases: A computational study of structural and electronic properties

Journal of Chemical Theory and Computation, (3): 2301-2311 2007.

Shchavlev, A. E.; Pankratov, A. N.; Enchev, V.

Intramolecular hydrogen-bonding interactions in 2-nitrosophenol and nitrosonaphthols: Ab initio, density functional, and nuclear magnetic resonance theoretical study

Journal of Physical Chemistry A, (111): 7112-7123 2007.

Shen, W.; Li, M.; He, R. X.; Zhang, J. S.; Lei, W.

The electronic and structural properties of nonclassical bicyclic thiophene: Monomer, oligomer and polymer

Polymer, (48): 3912-3918 2007.

Shen, W.; Li, M.; Li, Y.; Wang, S. L.

Theoretical study of borazine and its derivatives

Inorganica Chimica Acta, (360): 619-624 2007.

- Sheng, L.; Gerber, R. B.
Predicted stability and structure of (HXeCCH)(n) (n=2 or 4) clusters and of crystalline HXeCCH
Journal of Chemical Physics, (126) 2007.
- Shevtsov, A. V.; Ananikov, V. P.; Makhova, N. N.
Quantum-chemical investigation of the mechanism of reaction between 1,2-dialkyldiaziridines and heterocumulenes
Russian Journal of Organic Chemistry, (43): 1101-1105 2007.
- Shi, F. Q.; Li, X.; Xia, Y.; Zhang, L.; Yu, Z. X.
DFT study of the mechanisms of in water Au(I)-catalyzed tandem [3,3]-rearrangement/Nazarov reaction/[1,2]-hydrogen shift of enynyl acetates: A proton-transport catalysis strategy in the water-catalyzed [1,2]-hydrogen shift
Journal of the American Chemical Society, (129): 15503-15512 2007.
- Shi, F.-Q.; Li, X.; Xia, Y.; Zhang, L.; Yu, Z.-X.
DFT study of the mechanisms of in water Au(I)-catalyzed tandem [3,3]-rearrangement/Nazarov reaction/[1,2]-hydrogen shift of enynyl acetates: A proton-transport catalysis strategy in the water-catalyzed [1,2]-hydrogen shift
Journal of the American Chemical Society, (129): 15503-15512 2007.
- Shieh, M.; Ho, L. F.; Chen, P. C.; Hsu, M. H.; Chen, H. L.; Guo, Y. W.; Pan, Y. W.; Lin, Y. C.
Reaction of [Et4N](2)[Te{Cr(CO)(5)}(n)] (n=2, 3) toward electrophiles: Reactivity comparison and theoretical calculations
Organometallics, (26): 6184-6196 2007.
- Shieh, M.; Hsu, M. H.; Sheu, W. S.; Jang, L. F.; Lin, S. F.; Chu, Y. Y.; Miu, C. Y.; Lai, Y. W.; Liu, H. L.; Her, J. L.
Copper halide-bridged ruthenium telluride carbonyl complexes: Discovery of the semiconducting cluster chain polymer {[PPh4](2)[Te2Ru4(CO)(10)Cu4Br2Cl2]center dot THF}(infinity)
Chemistry-a European Journal, (13): 6605-6616 2007.
- Shirtcliff, L. D.; Haley, M. M.; Herges, R.
CuCl-induced formation and migration of isoindazolyl carbenoids
Journal of Organic Chemistry, (72): 2411-2418 2007.
- Sibert, J. W.; Forshee, P. B.; Hundt, G. R.; Sargent, A. L.; Bott, S. G.; Lynch, V.
Wurster's crowns: A comparative study of ortho- and para-phenylenediamine-containing macrocyclic receptors
Inorganic Chemistry, (46): 10913-10925 2007.
- Sidorkin, V. F.; Belogolova, E. F.; Gordon, M. S.; Lazarevich, M. I.; Lazareva, N. F.
Hypercoordinated carbon in 2,8,9-sila- and thia-substituted carbatranes
Organometallics, (26): 4568-4574 2007.
- Silva, V. D.; Dos Santos, E. N.; Gusevskaya, E. V.; Rocha, W. R.
On the origin of diastereofacial selectivity in the interaction of beta-pinene with rhodium carbonyl: A density functional study
Journal of Molecular Structure-Theochem, (816): 109-117 2007.

- Simon, L.; Goodman, J. A.
The mechanism of TBD-catalyzed ring-opening polymerization of cyclic esters
Journal of Organic Chemistry, (72): 9656-9662 2007.
- Simon, L.; Goodman, J. M.
The mechanism of TBD-catalyzed ring-opening polymerization of cyclic esters
Journal of Organic Chemistry, (72): 9656-9662 2007.
- Singh, A.; Ganguly, B.
Probing the influence of solvent effects on the conformational behavior of 1,3-diazacyclohexane systems
Journal of Physical Chemistry A, (111): 9884-9889 2007.
- Singh, R. K.; Sharma, P. D.; Singh, P. P.
Molecular mechanics based study of molecular orbitals of cobalt(II) halides
Asian Journal of Chemistry, (19): 121-142 2007.
- Sizova, O. V.; Skripnikov, L. V.; Sokolov, A. Y.; Ivanova, N. V.
Rhodium and ruthenium tetracarboxylate nitrosyl complexes: Electronic structure and metal-metal bond
Russian Journal of Coordination Chemistry, (33): 588-593 2007.
- Sizova, O. V.; Skripnikov, L. V.; Sokolov, A. Y.; Lyubimova, O. O.
Features of the electronic structure of ruthenium tetracarboxylates with axially coordinated nitric oxide (II)
Journal of Structural Chemistry, (48): 28-36 2007.
- Sizova, O. V.; Sokolov, A. Y.; Skripnikov, L. V.
Quantum-chemical study of donor-acceptor interactions in chelate dicarbonyl complexes of rhodium(I)
Russian Journal of Coordination Chemistry, (33): 800-808 2007.
- Sizova, O. V.; Sokolov, A. Y.; Skripnikov, L. V.; Baranovski, V. I.
Quantum chemical study of the bond orders in the ruthenium, diruthenium and dirhodium nitrosyl complexes
Polyhedron, (26): 4680-4690 2007.
- Sizova, O. V.; Varshavskii, Y. S.; Skripnikov, L. V.
Quantum-chemical study of donor-acceptor interactions in rhodium(I) carbonyl carboxylate complexes with phosphine ligands
Russian Journal of Coordination Chemistry, (33): 313-322 2007.
- Smith, G. L.; Mercier, H. P. A.; Schrobilgen, G. J.
Synthesis of [F3S XeF][AsF6] and structural study by multi-NMR and Raman spectroscopy, electronic structure calculations, and X-ray crystallography
Inorganic Chemistry, (46): 1369-1378 2007.

- Smrcok, L.; Jorik, V.; Scholtzova, E.; Milata, V.
Ab initio structure determination of 5-anilinomethylene-2,2-dimethyl-1,3-dioxane-4,6-dione from laboratory powder data - a combined use of X-ray, molecular and solid-state DFT study
Acta Crystallographica Section B-Structural Science, (63): 477-484 2007.
- So, C. W.; Roesky, H. W.; Gurubasavaraj, P. M.; Oswald, R. B.; Gamer, M. T.; Jones, P. G.; Blaurock, S.
Synthesis and structures of heteroleptic silylenes
Journal of the American Chemical Society, (129): 12049-12054 2007.
- So, C. W.; Roesky, H. W.; Oswald, R. B.; Pal, A.; Jones, P. G.
Synthesis and characterization of [PhC(NBut)(2)]Si(S)SBut]: a silicon thioester analogue with the Si(= S)-S-skeleton
Dalton Transactions: 5241-5244 2007.
- Soderhjelm, P.; Krogh, J. W.; Karlstrom, G.; Ryde, U.; Lindh, R.
Accuracy of distributed multipoles and polarizabilities: Comparison between the LoProp and MpProp models
Journal of Computational Chemistry, (28): 1083-1090 2007.
- Sohar, P.; Csampai, A.; Sillanpaa, R.; Fulop, F.; Stajer, G.
Preparation and structure of bicycloalkane-condensed aryldiaziridines accompanied by pyrimidines
Heterocycles, (71): 1315-+ 2007.
- Soriano, E.; Marco-Contelles, J.
DFT-based mechanism for the unexpected formation of dienes in the PtCl2 isomerization of propargylic acetates: Examples of inhibition of the Rautenstrauch process
Journal of Organic Chemistry, (72): 1443-1448 2007.
- Sparta, M.; Blrve, K. J.; Jensen, V. R.
Activity of rhodium-catalyzed hydroformylation: Added insight and predictions from theory
Journal of the American Chemical Society, (129): 8487-8499 2007.
- Sparta, M.; Borge, K. J.; Jensen, V. R.
Activity of rhodium-catalyzed hydroformylation: Added insight and predictions from theory
Journal of the American Chemical Society, (129): 8487-8499 2007.
- Sporea, C.; Rabilloud, F.
Stability of alkali-encapsulating silicon cage clusters
Journal of Chemical Physics, (127) 2007.
- Sporea, C.; Rabilloud, F.; Aubert-Frecon, M.
Charge transfers in mixed silicon-alkali clusters and dipole moments
Journal of Molecular Structure-Theochem, (802): 85-90 2007.
- Standard, J. M.; Gregory, B. W.; Clark, B. K.
Computational studies of copper, silver, and gold alkanethiolates and alkaneselenates
Journal of Molecular Structure-Theochem, (803): 103-113 2007.

- Stanger, A.
A simple and intuitive description of C-H bond energies
European Journal of Organic Chemistry: 5717-5725 2007.
- Steudel, R.; Steudel, Y.
Charge-transfer complexes between the sulfur molecules SO₂, S₂O, S-3, SONH, and SOCl₂ and the amine donors NH₃ and NMe₃ - A theoretical study
European Journal of Inorganic Chemistry: 4385-4392 2007.
- Suarez-Varela, J.; Sakiyama, H.; Cano, J.; Colacio, E.
Interplay between covalent and aurophilic interactions in a series of isostructural 3D Hoffman-like frameworks containing bipyrimidine and dicyanoaurate bridges. X-Ray structure and magnetic properties of $\{(\mu\text{-Au}(\text{CN})_2)_2\}[(\text{M}(\text{NH}_3)_2)_2(\mu\text{-bpym})]\{\text{Au}(\text{CN})_2\}_2$ (M = Ni(II), Co(II) and Cu(II))
Dalton Transactions: 249-256 2007.
- Subbotina, J. O.; Sadchikova, E. V.; Bakulev, V. A.; Fabian, W. M. F.; Herges, R.
DFT study of cycloaddition reaction of isothiocyanates with diazoazoles to 4-imino-4H-pyrazolo[5,1-d] [1,2,3,5]thiatriazines
International Journal of Quantum Chemistry, (107): 2479-2488 2007.
- Sugimoto, H.; Nakamura, S.; Ohwada, T.
Retro-Diels-Alder reaction of 4H-1,2-benzoxazines to generate o-quinone methides: Involvement of highly polarized transition states
Journal of Organic Chemistry, (72): 10088-10095 2007.
- Sui, Y. Q.; Glaser, R.; Sarkar, U.; Gates, K.
Stabilities and spin distributions of benzannulated benzyl radicals
Journal of Chemical Theory and Computation, (3): 1091-1099 2007.
- Sumpter, B. G.; Huang, J.; Meunier, V.; Romo-Herrera, J. M.; Cruz-Silva, E.; Terrones, H.; Terrones, M.
A Theoretical and Experimental Study On Manipulating the Structure and Properties of Carbon Nanotubes Using Substitutional Dopants: 97-118 2007.
- Sumpter, B. G.; Meunier, V.; Valeev, E. F.; Lampkins, A. J.; Li, H.; Castellano, R. K.
A new class of supramolecular wires
Journal of Physical Chemistry C, (111): 18912-18916 2007.
- Sumpter, B. G.; Meunier, V.; Vazquez-Mayagoitia, A.; Castellano, R. K.
Investigation of the nanoscale self-assembly of donor-sigma-acceptor molecules
International Journal of Quantum Chemistry, (107): 2233-2242 2007.
- Sun, D. F.; Ke, Y. X.; Collins, D. J.; Lorigan, G. A.; Zhou, H. C.
Construction of robust open metal-organic frameworks with chiral channels and permanent porosity
Inorganic Chemistry, (46): 2725-2734 2007.

- Sun, G. Y.; Nicklaus, M. C.
Natural resonance structures and aromaticity of the nucleobases
Theoretical Chemistry Accounts, (117): 323-332 2007.
- Sun, H.; Zhang, D. J.
Density functional theory study on the cycloaddition of carbon dioxide with propylene oxide catalyzed by alkylmethylimidazolium chloride ionic liquids
Journal of Physical Chemistry A, (111): 8036-8043 2007.
- Sun, H.; Zhang, D. J.; Ma, C.; Liu, C. B.
Theoretical study on the Diels-Alder reaction of cyclopentadiene with methacrolein catalyzed by diethylimidazolium cation
International Journal of Quantum Chemistry, (107): 1875-1885 2007.
- Sun, H.; Zhang, D. J.; Wang, F.; Liu, C. B.
Theoretical study of the mechanism for the Markovnikov addition of imidazole to vinyl acetate catalyzed by the ionic liquid [bmIm]OH
Journal of Physical Chemistry A, (111): 4535-4541 2007.
- Sun, X.-Q.; Ju, X.-H.; Xu, X.-J.; Fan, X.-W.
Theoretical study on the intermolecular interactions between 1,1-diamino-2,2-dinitroethylene and H₂O
Journal of the Chinese Chemical Society, (54): 1451-1456 2007.
- Sun, X. Y.; Li, Z. R.; Wu, D.; Sun, C. C.
Extraordinary superatom containing double shell nucleus: Li(HF)(3)Li connected mainly by intermolecular interactions
International Journal of Quantum Chemistry, (107): 1215-1222 2007.
- Sun, Y. X.; Zhang, R.; Zhang, L. F.; Xie, X. H.; Xu, L. X.
Experimental and ab initio calculational studies on nitrato[2,4-dichloro-6-((pyridin-2-ylmethylimino)methyl)phenolato]copper (II)
Journal of Coordination Chemistry, (60): 2607-2619 2007.
- Sundberg, M. R.; Sanchez-Gonzalez, A.
Hydrogen storage in ammonia triborane: Properties and behavior of the chemical bonds
Inorganic Chemistry Communications, (10): 1229-1232 2007.
- Sydora, O. L.; Kilyanek, S. M.; Jordan, R. F.
Cationic zirconocene and hafnocene aryl complexes
Organometallics, (26): 4746-4755 2007.
- Szatylowicz, H.; Krygowski, T. M.; Hobza, P.
How the shape of the NH₂ group depends on the substituent effect and H-bond formation in derivatives of aniline
Journal of Physical Chemistry A, (111): 170-175 2007.
- Tabacchi, G.; Vanon, M. A.; Gamba, A.; Fois, E.

Does negative hyperconjugation assist enzymatic dehydrogenations?
Chemphyschem, (8): 1283-1288 2007.

Takahashi, O.; Yamasaki, K.; Kohno, Y.; Ueda, K.; Suezawa, H.; Nishio, M.
Origin of the gauche preference of n-propyl halides and related molecules investigated by ab initio MO calculations: Importance of the CH/n hydrogen bond
Chemical Physics Letters, (440): 64-69 2007.

Tamm, M.; Petrovic, D.; Randoll, S.; Beer, S.; Bannenberg, T.; Jones, P. G.; Grunenberg, O.
Structural and theoretical investigation of 2-iminoimidazolines - carbene analogues of iminophosphoranes
Organic & Biomolecular Chemistry, (5): 523-530 2007.

Tamulis, A.; Tsifrinovich, V. I.; Tretiak, S.; Berman, G. P.; Allara, D. L.
Neutral radical molecules ordered in self-assembled monolayer systems for quantum information processing
Chemical Physics Letters, (436): 144-149 2007.

Tang, D. Y.; Qin, S.; Su, Z. S.; Hu, C. W.
Comprehensive theoretical study on the mechanism of regioselective hydroformylation of phosphinobutene catalyzed by a heterobinuclear rhodium(I)-chromium complex
Organometallics, (26): 33-47 2007.

Tang, D. Y.; Zhu, L. F.; Qin, S.; Su, Z. S.; Hu, C. W.
A theoretical study on the mechanism of the oxidation of hydroxylamine by VO₂⁺
Journal of Molecular Structure-Theochem, (805): 143-152 2007.

Tayyari, S. F.; Rahemi, H.; Nekoei, A. R.; Zahedi-Tabrizi, M.; Wang, Y. A.
Vibrational assignment and structure of dibenzoylmethane - A density functional theoretical study
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (66): 394-404 2007.

Tayyari, S. F.; Vakili, M.; Nekoei, A. R.; Rahemi, H.; Wang, Y. A.
Vibrational assignment and structure of trifluorobenzoylacetone - A density functional theoretical study
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (66): 626-636 2007.

Tayyari, S. F.; Zahedi-Tabrizi, M.; Laleh, S.; Moosavi-Tekyeh, Z.; Rahemi, H.; Wang, Y. A.
Structure and vibrational assignment of 3,4-diacetyl-2,5-hexanedione. A density functional theoretical study
Journal of Molecular Structure, (827): 176-187 2007.

Thakur, T. S.; Desiraju, G. R.
Theoretical investigation of C-H center dot center dot center dot M interactions in organometallic complexes: A natural bond orbital (NBO) study
Journal of Molecular Structure-Theochem, (810): 143-154 2007.

Thompson, D.

In silico engineering of tailored ink-binding ability at molecular printboards
Chemphyschem, (8): 1684-1693 2007.

Thompson, D.; Lazennec, C.; Plateau, P.; Simonson, T.
Ammonium scanning in an enzyme active site - The chiral specificity of aspartyl-tRNA synthetase
Journal of Biological Chemistry, (282): 30856-30868 2007.

Tian, S. X.; Yang, J. L.
Driving energies of hydrogen scrambling motions in CH5+
Journal of Physical Chemistry A, (111): 415-418 2007.

Tian, S. X.; Yang, J. L.
Driving energies of hydrogen scrambling motions in CH5+
Journal of Physical Chemistry A, (111): 415-418 2007.

Toner, A.; Matthes, J.; Grundemann, S.; Limbach, H. H.; Chaudret, B.; Clot, E.; Sabo-Etienne, S.
Agostic interaction and intramolecular proton transfer from the protonation of dihydrogen ortho metalated ruthenium complexes
Proceedings of the National Academy of Sciences of the United States of America, (104): 6945-6950 2007.

Tong, H.; Eklof, A. M.; Steel, P. G.; Ottosson, H.
A computational investigation of the retrocyclization reaction of silacyclo-but-2-enes to 1-silabuta-1,3-dienes: Focus on the effect of the substituents
Journal of Molecular Structure-Theochem, (811): 153-160 2007.

Tormena, C. F.; dos Santos, F. P.; Neto, A. C.; Rittner, R.; Yoshinaga, F.; Temistocles, J. C. T.
Electronic interactions and their influence on the conformational stability of trans-2-halocyclopentanol
Journal of Physical Chemistry A, (111): 295-298 2007.

Toth, G.; Bowers, S. G.; Truong, A. P.; Probst, G.
The role and significance of unconventional hydrogen bonds in small molecule recognition by biological receptors of pharmaceutical relevance
Current Pharmaceutical Design, (13): 3476-3493 2007.

Tricamo, A. J.; Knaus, K. J.; Ball, D. W.
G2, G3, and complete basis set calculations of the thermodynamic properties of two isomers of diazadiboretidine, cyclo-B2N2H4
Journal of Molecular Structure-Theochem, (807): 67-72 2007.

Trujillo, C.; Mo, O.; Yanez, M.
A theoretical study of hydration effects on the prototropic tautomerism of selenouracils
Organic & Biomolecular Chemistry, (5): 3092-3099 2007.

Tsipis, A. C.; Kefalidis, C. E.; Tsipis, C. A.
Unraveling the origin of the peculiar reaction field of triruthenium ring core structures
Journal of the American Chemical Society, (129): 13905-13922 2007.

- Tsipis, C. A.; Depastas, I. G.; Kefalidis, C. E.
Growth format, electronic architecture, magnetic, and optical properties of aromatic cyclo-Cu₃Au₃ homotops
Journal of Computational Chemistry, (28): 1893-1908 2007.
- Tsipis, C. A.; Kefalidis, C. E.
Hydrosilylation, hydrocyanation, and hydroamination of ethene catalyzed by bis(hydrido-bridged)diplatinum complexes: Added insight and predictions from theory
Journal of Organometallic Chemistry, (692): 5245-5255 2007.
- Tsuda, M.; Kasai, H.
Imidazole ligand effect on O₂ interaction with metalloporphyrins
Surface Science, (601): 5200-5206 2007.
- Tsuda, M.; Kasai, H.
Proton transfer to oxygen adsorbed on Pt: How to initiate oxygen reduction reaction
Journal of the Physical Society of Japan, (76) 2007.
- Tuononen, H. M.; Roesler, R.; Duffon, J. L.; Ragogna, P. J.
Electronic structures of main-group carbene analogues
Inorganic Chemistry, (46): 10693-10706 2007.
- Tuttolomondo, M. E.; Navarro, A.; Ruiz, T. P.; Varetto, E. L.; Hayes, S. A.; Wann, D. A.; Robertson, H. E.; Rankin, D. W. H.; Altabef, A. B.
Gas-phase structure, rotational barrier, and vibrational properties of methyl methanethiosulfonate, CH₃SO₂SCH₃: An experimental and computational study
Journal of Physical Chemistry A, (111): 9952-9960 2007.
- Tuzun, N. S.; Aviyente, V.
Modeling the cyclopolymerization of diallyl ether and methyl alpha-[(allyloxy)methyl]acrylate
International Journal of Quantum Chemistry, (107): 894-906 2007.
- Tzavellas, L. C.; Pachini, S.; Tsiamis, C.; Hatzidimitriou, A. G.
Conformation and coordination of beta-diketonates in mixed-ligand copper(II) chelates of 1,2-diamines. Theoretical approach and experimental verification. Crystal structure of [bis(N,N'-dimethyl-1,2-diaminoethane) bis(3-cyano-2,4-pentanedionate)copper(II)]dihydrate
Polyhedron, (26): 1404-1416 2007.
- Uhl, W.; Vinogradov, A.; Grimme, S.
C-H bond activation by hyperconjugation with Al-C bonds and by chelating coordination of the hydride ion
Journal of the American Chemical Society, (129): 11259-11264 2007.
- Urakawa, A.; Iannuzzi, M.; Hutter, J.; Baiker, A.
Towards a rational design of ruthenium CO₂ hydrogenation catalysts by ab initio metadynamics
Chemistry-a European Journal, (13): 6828-6840 2007.

- Urakawa, A.; Iannuzzi, M.; Hutter, J.; Baiker, A.
Towards a rational design of ruthenium CO₂ hydrogenation catalysts by ab initio metadynamics
Chemistry-a European Journal, (13): 6828-6840 2007.
- Urakawa, A.; Jutz, F.; Laurency, G.; Baiker, A.
Carbon dioxide hydrogenation catalyzed by a ruthenium dihydride: A DFT and high-pressure spectroscopic investigation
Chemistry-a European Journal, (13): 3886-3899 2007.
- Urakawa, A.; Jutz, F.; Laurency, G.; Baiker, A.
Carbon dioxide hydrogenation catalyzed by a ruthenium dihydride: A DFT and high-pressure spectroscopic investigation
Chemistry-a European Journal, (13): 3886-3899 2007.
- van Mourik, T.; Dingley, A. J.
Characterizing the cooperativity in h-bonded amino structures
Journal of Physical Chemistry A, (111): 11350-11358 2007.
- van Mourik, T.; Dingley, A. J.
Geometry dependence of spin-spin couplings in cyanamide by DFT analysis
Chemphyschem, (8): 288-296 2007.
- van Walree, C. A.; van der Wiel, B. C.; Jenneskens, L. W.; Lutz, M.; Spek, A. L.; Havenith, R. W. A.; van Lenthe, J. H.
On the structure of cross-conjugated 2,3-diphenylbutadiene
European Journal of Organic Chemistry: 4746-4751 2007.
- Vandermeeren, L.; Leysens, T.; Peeters, D.
Theoretical study of the properties of sulfone and sulfoxide functional groups
Journal of Molecular Structure-Theochem, (804): 1-8 2007.
- Velazquez, A.; Fernandez, I.; Frenking, G.; Merino, G.
Multimetalloenes. A theoretical study
Organometallics, (26): 4731-4736 2007.
- Velkov, Z.; Velkov, Y.; Balabanova, E.; Tadjer, A.
First principle study of the structure of conjugated amides and thioamides
International Journal of Quantum Chemistry, (107): 1765-1771 2007.
- Venter, G. A.; Raubenheimer, H. G.; Dillen, J.
On the structure and bonding of first row transition metal ozone carbonyl hydrides
Journal of Physical Chemistry A, (111): 8193-8201 2007.
- Vignolle, J.; Gornitzka, H.; Maron, L.; Schoeller, W. W.; Bourissou, D.; Bertrand, G.
Transient palladadiphosphenylcarbenes: Singlet carbenes with an "inverse" electronic configuration ($p(\pi)^2$ instead of σ^2) and unusual transannular metal-carbene interactions ($\pi(C \rightarrow Pd)$ donation and $\sigma(Pd \rightarrow C)$ back-donation)
Journal of the American Chemical Society, (129): 978-985 2007.

- Villamena, F. A.; Locigno, E. J.; Rockenbauer, A.; Hadad, C. M.; Zweier, J. L.
Theoretical and experimental studies of the spin trapping of inorganic radicals by 5,5-dimethyl-1-pyrroline N-oxide (DMPO). 2. Carbonate radical anion
Journal of Physical Chemistry A, (111): 384-391 2007.
- Villamena, F. A.; Merle, J. K.; Hadad, C. M.; Zweier, J. L.
Rate constants of hydroperoxyl radical addition to cyclic nitrones: A DFT study
Journal of Physical Chemistry A, (111): 9995-10001 2007.
- Vitorge, P.; Phrommavanh, V.; Siboulet, B.; You, D.; Vercouter, T.; Descostes, M.; Marsden, C. J.; Beaucaire, C.; Gaudet, J. P.
Estimating the stabilities of actinide aqueous species. Influence of sulfoxy-anions on uranium(IV) geochemistry and discussion of Pa(V) first hydrolysis
Comptes Rendus Chimie, (10): 978-993 2007.
- Wang, F.; Yang, H. M.; Yang, Z. Y.; Zhang, J. C.; Cao, W. L.
Geometries and properties of bimetallic phosphido-bridged complex Cp(CO)(2)W(mu-PPh2)W(CO)(5) and Cp(CO)(3)W(mu-PPh2)W(CO)(5)
Chemical Physics, (332): 33-38 2007.
- Wang, F. F.; Hou, J. H.; Li, Z. R.; Wu, D.; Li, Y.; Lu, Z. Y.; Cao, W. L.
Unusual halogen-bonded complex FBr delta+center dot center dot center dot delta+BrF and hydrogen-bonded complex FBr delta+center dot center dot center dot delta+HF formed by interactions between two positively charged atoms of different polar molecules
Journal of Chemical Physics, (126) 2007.
- Wang, H. J.; Dong, W. B.; Ren, X. H.; Shan, Y. Y.
DFT and MP2 investigations on the interaction of furan homologues C4H4Y (Y = O, S) with BX3 (X = H, F, Cl)
Journal of Molecular Structure-Theochem, (814): 85-90 2007.
- Wang, J.; Gu, J. D.; Leszczynski, J.; Feliks, M.; Sokalski, W. A.
Oxime-induced reactivation of sarin-inhibited AChE: A theoretical mechanisms study
Journal of Physical Chemistry B, (111): 2404-2408 2007.
- Wang, N.; Li, P.; Hu, Y.; Bu, Y.; Wang, W.; Xie, X.
Association of uracil with zn(2+) and the hydrated zn(2+) : A DFT investigation
Journal of Theoretical & Computational Chemistry, (6): 197-212 2007.
- Wang, N. X.; Yu, A. G.; Wang, G. X.; Zhang, X. H.; Li, Q. S.; Li, Z.
Synthesis of (S,R,R,R,)-alpha,alpha'-iminobis(methylene)bis(6-fluoro-3H,4H-dihydro-2H-1-benzopyran-2-methanol)
Synthesis-Stuttgart: 1154-1158 2007.
- Wang, S. W.; Li, A. Y.; Tan, H. W.
Theoretical study on red and blue shifting hydrogen bonding between pyridine and HCl, CHCl3
Chemical Journal of Chinese Universities-Chinese, (28): 1962-1967 2007.

- Wang, X. F.; Andrews, L.
Infrared spectra and theoretical calculations of KH and (KH)₂ in solid hydrogen
Journal of Physical Chemistry A, (111): 12260-12265 2007.
- Wang, X. F.; Andrews, L.
Sodium hydride clusters in solid hydrogen and neon: Infrared spectra and theoretical calculations
Journal of Physical Chemistry A, (111): 7098-7104 2007.
- Wang, X. F.; Andrews, L.; Marsden, C. J.
Infrared spectrum and structure of thorumine (HN=ThH₂)
Chemistry-a European Journal, (13): 5601-5606 2007.
- Wang, Y. H.; Li, L.; Lu, Y. X.; Zou, J. W.
Halogen bonds in adenine-5-bromouracil complexes
Chinese Journal of Chemical Physics, (20): 531-536 2007.
- Wang, Y. P.; Leu, H. L.; Wang, Y.; Cheng, H. Y.; Lin, T. S.
Cyclopentadienyl chromium complexes with halide, methyl, isothiocyanate and isoselenocyanate ligands: Structures of [eta(5)-(C₅H₄-COOCH₃)]Cr(NO)(2)(Br) and [eta(5)-(C₅H₄-COOCH₃)]Cr(NO)(2)(N=C=S)
Journal of Organometallic Chemistry, (692): 3340-3350 2007.
- Wang, Y. W.; Hu, Q. S.; Li, L. C.; Wang, X.; Tian, A. M.
Theoretical study of the reaction mechanism of hydroxyl ZnO catalyzing methanol decomposition
Acta Chimica Sinica, (65): 1951-1955 2007.
- Wang, Y. X.; Bu, Y. X.
Noncovalent interactions between cytosine and SWCNT: Curvature dependence of complexes via pi center dot center dot center dot pi stacking and cooperative CH center dot center dot center dot pi/NH center dot center dot center dot pi
Journal of Physical Chemistry B, (111): 6520-6526 2007.
- Wang, Y. X.; Paulus, B.
A comparative electron correlation treatment in H₂S-benzene dimer with DFT and wavefunction-based ab initio methods
Chemical Physics Letters, (441): 187-193 2007.
- Wang, Z. X.; Zhang, J. C.; Cao, W. L.
Theoretical study on intermolecular interactions between HCN (HNC) and NH₃, H₂O, HF
Chemical Journal of Chinese Universities-Chinese, (28): 320-324 2007.
- Wang, Z. X.; Zhang, J. C.; Wu, J. Y.; Cao, W. L.
Theoretical investigation on intermolecular interactions between HCN and HNC: The nature and thermodynamic properties
Journal of Molecular Structure-Theochem, (806): 239-246 2007.
- Wang, Z. X.; Zhang, J. C.; Wu, J. Y.; Cao, W. L.

- Theoretical study on intermolecular interactions between furan and dihalogen molecules XY(X,Y=F,Cl, Br)*
Journal of Chemical Physics, (126) 2007.
- Wannere, C. S.; Paul, A.; Herges, R.; Houk, K. N.; Schaefer, H. F.; Schleyer, P. V.
The existence of secondary orbital interactions
Journal of Computational Chemistry, (28): 344-361 2007.
- Weigand, J. J.; Burford, N.; Decken, A.; Schulz, A.
Preparation and characterization of a ligand-stabilized trimethylphosphane dication
European Journal of Inorganic Chemistry: 4868-4872 2007.
- Weinberg, J.; Cimpoesu, F.; Teanu, M.; Lerner, D. A.
Computational study of the molecular complexes between cholesterol and two isomers of the pralidoxime (PAM)
Journal of Molecular Structure-Theochem, (813): 3-8 2007.
- Weinhold, F.; Landis, C. R.
High bond orders in metal-metal bonding
Science, (316): 61-63 2007.
- Werkema, E. L.; Maron, L.; Eisenstein, O.; Andersen, R. A.
Reactions of monomeric [1,2,4-(Me3C)(3)C5H2](2)CeH and CO with or without H-2: An experimental and computational study
Journal of the American Chemical Society, (129): 2529-2541 2007.
- Wijeratne, N. R.; Wenthold, P. G.
Structure and reactivity of benzoynitrene radical anion in the gas phase
Journal of Organic Chemistry, (72): 9518-9522 2007.
- Wild, D. A.; Lenzer, T.
Structures, energetics, and infrared spectra of the Cl--(H2S)(n) and Br--(H2S)(n) anion clusters from ab initio calculations
Physical Chemistry Chemical Physics, (9): 5776-5784 2007.
- Williams, A. C.; Ramsden, D. B.
Hydrogen symbioses in evolution and disease
Qjm-an International Journal of Medicine, (100): 451-459 2007.
- Williams, A. C.; Ramsden, D. B.
Hydrogen symbioses in evolution and disease
Qjm-an International Journal of Medicine, (100): 451-459 2007.
- Wojciechowski, P. M.; Michalska, D.
Computational note on the molecular and electronic structures of para-halogenoanilines: DFT study
Journal of Molecular Structure-Theochem, (805): 71-71 2007.

- Wong, M. W.; Steudel, Y.; Steudel, R.
Structures and vibrational spectra of the sulfur-rich oxides SnO (n=4-9): The importance of pi-pi* interactions*
Chemistry-a European Journal, (13): 502-514 2007.
- Wong-Ekkabut, J.; Xu, Z. T.; Triampo, W.; Tang, I. M.; Tieleman, D. P.; Monticelli, L.
Effect of lipid peroxidation on the properties of lipid bilayers: A molecular dynamics study
Biophysical Journal, (93): 4225-4236 2007.
- Wu, C. W.; Chen, H. L.; Ho, J. J.
The calculated effects of substitution on intramolecular cyclization of 2,5-hexadienyl radicals
Journal of Molecular Structure-Theochem, (815): 11-20 2007.
- Wu, D. L.; Liu, L.; Liu, G. F.; Jia, D. Z.
Ab initio/DFT and AIM studies on dual hydrogen-bonded complexes of 2-hydroxypyridine/2-pyridone tautomerism
Journal of Physical Chemistry A, (111): 5244-5252 2007.
- Wu, J. Y.; Zhang, J. C.; Wang, Z. X.; Cao, W. L.
Study on the nature of interaction of BrCl with HF, H2O, and NH3
International Journal of Quantum Chemistry, (107): 1897-1906 2007.
- Wu, J. Y.; Zhang, J. C.; Wang, Z. X.; Cao, W. L.
Study on the nature of interaction of furan with various hydrides
Journal of Chemical Physics, (127) 2007.
- Wu, J. Y.; Zhang, J. C.; Wang, Z. X.; Cao, W. L.
Theoretical investigations of the nature of interaction of ClF with HF, H2O, and NH3
Journal of Chemical Theory and Computation, (3): 95-102 2007.
- Wu, J. Y.; Zhang, J. C.; Wang, Z. X.; Cao, W. L.
Theoretical study on intermolecular interactions in BrF/HnX adducts
Chemical Physics, (338): 69-74 2007.
- Wu, W. J.; Chen, J. C.; Qian, L.; Zheng, K. C.
QSAR and molecular design of benzo[b] acronycine derivatives as antitumor agents
Journal of Theoretical & Computational Chemistry, (6): 223-231 2007.
- Wu, X. H.; Quan, J. M.; Wu, Y. D.
Theoretical study of the catalytic mechanism and metal-ion dependence of peptide deformylase
Journal of Physical Chemistry B, (111): 6236-6244 2007.
- Wu, Y. B.; Yuan, C. X.; Gao, F.; Lu, H. G.; Guo, J. C.; Li, S. D.; Wang, Y. K.; Yang, P.
Hydrometal complexes with more than one planar and quasi-planar tetracoordinate carbon atom: From hydrogen-surrounded pieces to the rudiment of hydrogen-sealed nanotubes
Organometallics, (26): 4395-4401 2007.
- Wysokinski, R.; Hernik, K.; Szostak, R.; Michalska, D.

- Electronic structure and vibrational spectra of cis-diammine-(orotato)platinum(II), a potential cisplatin analogue: DFT and experimental study*
Chemical Physics, (333): 37-48 2007.
- Xi, S.; Li, H. B.
A theoretical study of the photodetachment and intramolecular hydrogen-bonding energies of hydrogen maleate anions
Journal of Physical Chemistry A, (111): 4404-4410 2007.
- Xie, H. J.; Cao, Z. X.
Electron attachment to the DNA bases adenine and guanine and dehydrogenation of their anionic derivatives: Density functional study
International Journal of Quantum Chemistry, (107): 1261-1269 2007.
- Xie, H. J.; Xia, F.; Cao, Z. X.
Density functional study toward understanding dehydrogenation of the adenine-thymine base pair and its anion
Journal of Physical Chemistry A, (111): 4384-4390 2007.
- Xing, D. X.; Chena, X. H.; Bu, Y. X.
Pairing strength and proton characters of the N7, N9-dimethylated GC and AT base pairs: a density functional theory investigation
New Journal of Chemistry, (31): 1514-1524 2007.
- Xiong, J. M.; Gong, L. F.; Li, Q. S.
Stability and aromaticity of B₆X- (X = N, P, As, Sb, Bi) clusters
Chemical Journal of Chinese Universities-Chinese, (28): 1968-1971 2007.
- Xu, Z. T.; Luo, H. H.; Tieleman, D. P.
Modifying the OPLS-AA force field to improve hydration free energies for several amino acid side chains using new atomic charges and an off-plane charge model for aromatic residues
Journal of Computational Chemistry, (28): 689-697 2007.
- Xue, Z. M.; Ding, Y. Z.; Chen, C. H.
A DFT study of electronic structures, energies, and molecular properties of lithium bis[croconato]borate and its derivatives
Electrochimica Acta, (53): 990-997 2007.
- Yan, S.; Lee, S. J.; Kang, S.; Choi, K. H.; Rhee, S. K.; Lee, J. Y.
Attractive sulfur center dot center dot center dot pi interaction between fluorinated dimethyl sulfur (FDMS) and benzene
Bulletin of the Korean Chemical Society, (28): 959-964 2007.
- Yang, G. C.; Fang, L.; Tan, K.; Shi, S. Q.; Su, Z. M.; Wang, R. S.
Quantum chemical study of structures, electronic spectrum, and nonlinear optical properties of gold-pentacene complexes
Organometallics, (26): 2082-2087 2007.

- Yang, J. B.; Chen, T. P.; Tan, S. S.; Ng, C. M.; Chan, L.
Modeling and characterization of nitrogen-enhanced negative-bias temperature instability in p-channel MOSFETs
Journal of the Electrochemical Society, (154): G255-G261 2007.
- Yang, Y.; Cui, Q.
Interactions between phosphate and water in solution: A natural bond orbital based analysis in a QM/MM framework
Journal of Physical Chemistry B, (111): 3999-4002 2007.
- Yang, Y.; Yu, H.; York, D.; Cui, Q.; Elstner, M.
Extension of the self-consistent-charge density-functional tight-binding method: Third-order expansion of the density functional theory total energy and introduction of a modified effective coulomb interaction
Journal of Physical Chemistry A, (111): 10861-10873 2007.
- Yang, Y.; Zhang, W. J.
Theoretical study of N-H center dot center dot center dot H-B blue-shifted dihydrogen bond
Journal of Molecular Structure-Theochem, (814): 113-117 2007.
- Yang, Y.; Zhang, W. J.; Pei, S. X.; Shao, J.; Huang, W.; Gao, X. M.
Theoretical study of the N-H center dot center dot center dot O red-shifted and blue-shifted hydrogen bonds
Science in China Series B-Chemistry, (50): 32-40 2007.
- Yano, T.; Wasada-Tsutsui, Y.; Arii, H.; Yamaguchi, S.; Funahashi, Y.; Ozawa, T.; Masuda, H.
Co(III) complexes with N-2(SO)(2)-type equatorial planar ligands similar to the active center of nitrile hydratase: Role of the sulfenate group in the enzymatic reaction
Inorganic Chemistry, (46): 10345-10353 2007.
- Yao, C. X.; Syrstad, E. A.; Turecek, F.
Electron transfer to protonated beta-alanine N-methylamide in the gas phase: An experimental and computational study of dissociation energetics and mechanisms
Journal of Physical Chemistry A, (111): 4167-4180 2007.
- Yao, L.; Du, L.; Ge, M. F.; Ma, C. P.; Wang, D. X.
Experimental and theoretical study of substituent effects of Iodonitrobenzenes
Journal of Physical Chemistry A, (111): 10105-10110 2007.
- Ye, A.; Patchkovskii, S.; Autschbach, J.
Static and dynamic second hyperpolarizability calculated by time-dependent density functional cubic response theory with local contribution and natural bond orbital analysis
Journal of Chemical Physics, (127) 2007.
- Yeguas, V.; Campomanes, P.; Menendez, M. I.; Sordo, T. L.
A theoretical study of the cleavage of the amide bond of formamide by attack of the hydroxyl ligand in [Mo(OH)(eta(3)-C3H5(CO)(2)(N2C2H4))] and [Re(OH)(CO)(3)(N2C2H4)] complexes
Journal of Molecular Structure-Theochem, (811): 241-247 2007.

- Yerushalmi, R.; van der Boom, M. E.; Cohen, H.
Chemical site capacitance: Submolecular measurements and a model
Journal of Physical Chemistry C, (111): 13652-13654 2007.
- Yeung, C. S.; Liu, L. V.; Wang, Y. A.
Novel nanotube-coordinated platinum complexes
Journal of Computational and Theoretical Nanoscience, (4): 1108-1119 2007.
- Yokogawa, D.; Sato, H.; Sakaki, S.
New generation of the reference interaction site model self-consistent field method: Introduction of spatial electron density distribution to the solvation theory
Journal of Chemical Physics, (126) 2007.
- Yoshioka, Y.; Satoh, H.; Mitani, M.
Theoretical study on electronic structures of FeOO, FeOOH, FeO(H₂O), and FeO in hemes: As intermediate models of dioxygen reduction in cytochrome c oxidase
Journal of Inorganic Biochemistry, (101): 1410-1427 2007.
- Yu, W. B.; Lina, Z. J.; Ding, C. F.
Electronic structures and electron detachment energies of halogen substituted acetate anions, XCH₂COO⁻ (X=F, Cl, Br)
Journal of Chemical Physics, (126) 2007.
- Zarzycki, P.
Comparison of the Monte Carlo estimation of surface electrostatic potential at the hematite (0001)/electrolyte interface with the experiment
Applied Surface Science, (253): 7604-7612 2007.
- Zarzycki, P.
Computational study of proton binding at the rutile/electrolyte solution interface
Journal of Physical Chemistry C, (111): 7692-7703 2007.
- Zeng, T.; Jamshidi, Z.; Mori, H.; Miyoshi, E.; Klobukowski, M.
Electron affinities of heavier phosphoryl and thiophosphoryl halides APX(3) (A = O, S and X = Br, I)
Journal of Computational Chemistry, (28): 2027-2033 2007.
- Zhang, C. R.; Chen, H. S.; Song, Y.; Xu, G. J.
DFT study on the structure and spectra of Ga₅P₅ cluster
Chinese Physics, (16): 2394-2399 2007.
- Zhang, C. Y.; Wu, H. S.
Spherical double electric layer structure of C₂₀F₂₀ and its endohedral complexes X@C₂₀F₂₀ (X = O²⁻, S²⁻, Se²⁻)
Journal of Molecular Structure-Theochem, (815): 71-74 2007.
- Zhang, C. Y.; Wu, H. S.; Jiao, H.
Aromatic C₂₀F₂₀ cage and its endohedral complexes X@C₂₀F₂₀ (X = H⁻, F⁻, Cl⁻, Br⁻, H, He)

- Journal of Molecular Modeling, (13): 499-503 2007.
- Zhang, G. L.; Ma, J.; Wen, J.
Interchain impacts on electronic structures of Heterocyclic oligomers and polymers containing group 14, 15, and 16 heteroatoms: Quantum chemical calculations in combination with molecular dynamics Simulations
Journal of Physical Chemistry B, (111): 11670-11679 2007.
- Zhang, G. L.; Zhang, H.; Sun, M.; Liu, Y. H.; Pang, X. H.; Yu, X. Y.; Liu, B.; Li, Z. S.
Substitution effect on the geometry and electronic structure of the ferrocene
Journal of Computational Chemistry, (28): 2260-2274 2007.
- Zhang, J. D.; Schaefer, H. F.
Molecular structures and energetics associated with hydrogen atom addition to the guanine-cytosine base pair
Journal of Chemical Theory and Computation, (3): 115-126 2007.
- Zhang, J. S.; Shen, W.; Li, M.
DFT study on the SnII-catalyzed diastereoselective synthesis of tetrahydrofuran from D-A cyclopropane and benzaldehyde
European Journal of Organic Chemistry: 4855-4866 2007.
- Zhang, R. B.; Eriksson, L. A.
Effects of OH radical addition on proton transfer in the guanine-cytosine base pair
Journal of Physical Chemistry B, (111): 6571-6576 2007.
- Zhang, R. B.; Gao, F. X.; Eriksson, L. A.
Radical-induced damage in 3' dTMP - Insights into a mechanism for DNA strand cleavage
Journal of Chemical Theory and Computation, (3): 803-810 2007.
- Zhang, S. G.; Li, H.; Yang, P.
Theoretical investigation on the geometries and properties of guanine-BX₃ (X = F, Cl) complex
Chinese Journal of Structural Chemistry, (26): 783-792 2007.
- Zhang, Y.; Huang, K. X.
The influence of the hydrated metal cations binding to adenine-N7 or adenine-N3 on the hydrogen bonding in adenine-thymine base pair: A comparative study
Journal of Molecular Structure-Theochem, (822): 57-64 2007.
- Zhang, Y.; Huang, K. X.
On the interactions of hydrated metal cations (Mg²⁺, Mn²⁺, Ni²⁺, Zn²⁺) with guanine-cytosine Watson-Crick and guanine-guanine reverse-Hoogsteen DNA base pairs
Journal of Molecular Structure-Theochem, (812): 51-62 2007.
- Zhang, Y.; Xu, Y.; Li, Q. S.
The correlation between aromaticity and stability in planar N₂X₂ (X = O, S, SE, and TE) species
Molecular Physics, (105): 1883-1889 2007.

- Zhang, Y.; Xu, Y.; Li, S.; Li, Q. S.; Cui, J.
Potential high-energy compounds: H₂N₅M₁ similar to 2N₅H₂ (M = Be, Mg, Ca, Zn, and Cd)
Molecular Physics, (105): 2951-2959 2007.
- Zhang, Z.; Xu, X.; Zuo, X. X.; Li, W. S.
Stabilizing effect of amine on small molecules in electrolyte of lithium batteries
Acta Physico-Chimica Sinica, (23): 526-530 2007.
- Zhao, P. S.; Cai, Z. J.; Zhang, L. L.; Li, R. Q.
Quantum chemical calculation studies on 4-phenyl-1-(1-phenylethylidene)thiosemicarbazide
Structural Chemistry, (18): 325-330 2007.
- Zhao, P. S.; Li, R. Q.; Xu, J. M.; Zhang, W. G.
Experimental and theoretical study on 3-benzyl-4-phenyl-1,2,4-triazole-5-thione
Polish Journal of chemistry, (81): 1495-1503 2007.
- Zhao, P. S.; Xu, J. M.; Zhang, W. G.; Jian, F. F.; Zhang, L.
Synthesis, characterization, and quantum chemical calculational studies on 3-p-methylphenyl-4-amino-1,2,4-triazole-5-thione
Structural Chemistry, (18): 993-1000 2007.
- Zhao, S.; Li, Z. H.; Liu, Z. P.; Wang, W. N.; Fan, K. N.
Density functional study of the interaction of halogen atom (F, Br, I) with silver clusters
Acta Chimica Sinica, (65): 1294-1298 2007.
- Zhao, S. K.; Sun, X. Y.; Fang, L.; Zhu, Y. L.
Theoretical studies on electronic structures and third-order nonlinear optical properties of di-metalocene complexes Zn-2 (eta(5)-E-5)(2) (E = N, P, As, Sb)
Chemical Journal of Chinese Universities-Chinese, (28): 1731-1734 2007.
- Zhao, Y. M.; Zhou, N. Z.; Slepko, A. D.; Ciulei, S. C.; McDonald, R.; Hegmann, F. A.; Tykwinski, R. R.
Donor/acceptor effects on the linear and nonlinear optical properties of geminal diethynylethenes (g-DEEs)
Helvetica Chimica Acta, (90): 909-927 2007.
- Zhao, Y. Y.; Zhang, M. Y.; Xu, S. H.; Sun, C. C.
Structure and properties of polycordinate planar boron compounds
Journal of Chemical Physics, (126) 2007.
- Zheng, S. L.; Volkov, A.; Nygren, C. L.; Coppens, P.
The nature of the Ag-I center dot center dot center dot Ag-I interaction in different Ag(NH₃)(₂) dimers embedded in supramolecular
Chemistry-a European Journal, (13): 8583-8590 2007.
- Zheng, W. R.; Fu, Y.; Liu, L.; Guo, Q. X.
Hydrogen bonding interaction between ureas or thioureas and carbonyl compounds
Acta Physico-Chimica Sinica, (23): 1018-1024 2007.

- Zheng, W. R.; Fu, Y.; Shen, K.; Liu, L.; Guo, Q. X.
Theoretical study on hydrogen bonding interaction of ureas and thioureas with imines
Journal of Molecular Structure-Theochem, (822): 103-110 2007.
- Zhong, G.; Chan, B.; Radom, L.
Hydrogenation of simple aromatic molecules: A computational study of the mechanism
Journal of the American Chemical Society, (129): 924-933 2007.
- Zhou, D. H.; Zhang, Y.; Zhu, H. Y.; Ma, D.; Bao, X. H.
The structure, stability, and reactivity of mo-oxo species in H-ZSM5 zeolites: Density functional theory study
Journal of Physical Chemistry C, (111): 2081-2091 2007.
- Zhou, H.
Structures and properties of porphyrazine with annulated 1,2,5-thiadiazole and 1,4-diamyloxybenzene and its magnesium complex: Density functional theory calculations
Chinese Journal of Inorganic Chemistry, (23): 778-784 2007.
- Zhou, H.; Wong, N. B.; Lau, K. C.; Tian, A.; Li, W. K.
Discovery of singlet diradicals: Theoretical study on the cage species C14N12-H-6 and its six derivatives
Journal of Physical Chemistry A, (111): 9838-9847 2007.
- Zhou, H. W.; Wong, N. B.; Tian, A. M.; Li, W. K.
Theoretical investigation on carbon-centered tri-s-tetrazine and its 10 derivatives
Journal of Molecular Graphics and Modelling, (26): 788-799 2007.
- Zhou, J.; Xiao, F.; Liu, Z. P.; Fan, K. N.
Coaxial alkaline-earth dimetal units sandwiched between hydrosilver compounds: A DFT Study
Journal of Molecular Structure-Theochem, (808): 163-166 2007.
- Zhou, J.; Xiao, F.; Wang, W. N.; Fan, K. N.
Theoretical study of the interaction of nitric oxide with small neutral and charged silver clusters
Journal of Molecular Structure-Theochem, (818): 51-55 2007.
- Zhou, Y. B.; Cao, F. L.
Mechanistic competition variations due to the substituents in the lithium carbenoid promoted cyclopropanation reactions
Journal of Organometallic Chemistry, (692): 3723-3731 2007.
- Zhou, Z.-J.; Liu, H.-L.; Huang, X.-R.; Sun, C.-C.
Theoretical study on the potential energy surface of Si2NS
Journal of Theoretical & Computational Chemistry, (6): 929-946 2007.
- Zhu, H. Y.; Zhang, Y.; Zhou, D. H.; Guan, J.; Bao, X. H.
Density functional theory study on structure of molybdenum carbide loaded on MCM-22 zeolite and mechanism for methane activation
Chinese Journal of Catalysis, (28): 180-186 2007.

- Zhu, R. X.; Zhang, D. J.; Wu, J.; Liu, C. B.
A DFT study on the mechanism and regio selectivity of the tandem O-nitroso aldol/Michael reaction of nitrosobenzene and cyclohexenone
Journal of Molecular Structure-Theochem, (815): 105-109 2007.
- Zhu, X.-Y.; Zhang, D.-J.; Liu, C.-B.
Theoretical study of the structural characterizations of N-alkylpyridinium cations and their ion-pairs with some anions
Acta Chimica Sinica, (65): 2701-2706 2007.
- Zhu, Y. L.; Zhou, S. Y.; Kan, Y. H.; Yan, L. K.; Su, Z. M.
Theoretical investigation of electronic structures and excitation energies of doubly N-confused porphyrin and its group 11 transition metal (III) complexes
Journal of Chemical Physics, (126) 2007.
- Zhu, Y. Q.; Guo, Y.; Xie, D.
Theoretical investigation on the GaCl₃-Catalyzed ring-closing metathesis reaction of N-2,3-butadienyl-2-propynyl-1-amine: Three-membered ring versus four-membered ring mechanism
Journal of Physical Chemistry A, (111): 9387-9392 2007.
- Zubarev, D. Y.; Boldyrev, A. I.
Comprehensive analysis of chemical bonding in boron clusters
Journal of Computational Chemistry, (28): 251-268 2007.
- Zubatyuk, R. I.; Volovenko, Y. M.; Shishkin, O. V.; Gorb, L.; Leszczynski, J.
Aromaticity-controlled tautomerism and resonance-assisted hydrogen bonding in heterocyclic enaminone-iminoenol systems
Journal of Organic Chemistry, (72): 725-735 2007.