

NBO 2005 – 686 references

- Abbati, G. L.; Aragoni, M. C.; Arca, M.; Carrea, M. B.; Devillanova, F. A.; Garau, A.; Isaia, F.; Lippolis, V.; Marcelli, M.; Silvestru, C.; Verani, G.
Gold(0) and gold(III) reactivity towards the tetraphenyldithioimidodiphosphinic acid, [Ph₂P(S)NHP(S)Ph-2]
European Journal of Inorganic Chemistry: 589-596 2005.
- Abirami, S.; Xing, Y. M.; Tsang, C. W.; Ma, N. L.
Theoretical study of alpha/beta-alanine and their protonated/alkali metal cationized complexes
Journal of Physical Chemistry A, (109): 500-506 2005.
- Adcock, W.; Graton, J.; Laurence, C.; Lucon, M.; Trout, N.
Three-centre hydrogen bonding in the complexes of syn-2,4-difluoroadamantane with 4-fluorophenol and hydrogen fluoride
Journal of Physical Organic Chemistry, (18): 227-234 2005.
- Afanas'yev, D. Y.; Prosyannik, A. V.
Why N-methyleneformamide, CH₂=N-CHO, prefers gauche-conformation? A DFT/NBO study
Journal of Molecular Structure-Theochem, (130): 45-49 2005.
- Agou, T.; Kobayashi, J.; Kawashima, T.
Dibenzophosphaborin: A hetero-pi-conjugated molecule with fluorescent properties based on intramolecular charge transfer between phosphorus and boron atoms
Organic Letters, (7): 4373-4376 2005.
- Ahlquist, M.; Fabrizi, G.; Cacchi, S.; Norrby, P. O.
Palladium(0) alkyne complexes as active species: a DFT investigation
Chemical Communications: 4196-4198 2005.
- Alajarin, M.; Ortín, M. M.; Sanchez-Andrade, P.; Vidal, A.; Bautista, D.
From ketenimines to ketenes to quinolones: Two consecutive pseudopericyclic events
Organic Letters, (7): 5281-5284 2005.
- Alajarin, M.; Sanchez-Andrade, P.; Lopez-Leonardo, C.; Alvarez, A.
On the mechanism of phthalimidine formation via o-phthalaldehyde monoimines. New [1,5]-H sigmatropic rearrangements in molecules with the 5-aza-2,4-pentadienal
Journal of Organic Chemistry, (70): 7617-7623 2005.
- Alajarin, M.; Sanchez-Andrade, P.; Vidal, A.; Tovar, F.
Mode selectivity in the intramolecular cyclization of ketenimines bearing N-acylimino units: A computational and experimental study
Journal of Organic Chemistry, (70): 1340-1349 2005.

Alavi, S.; Thompson, D. L.

Simulations of the solid, liquid, and melting of 1-n-butyl-4-amino-1,2,4-triazolium bromide

Journal of Physical Chemistry B, (109): 18127-18134 2005.

Albers, T.; Grobe, J.; Le Van, D.; Maulitz, A. H.; Wurthwein, E. U.

Reactive E=C(p-p)pi-systems 53 [1]: Reactivity studies on perfluoro-2-arsapropene: [2+2]-cycloaddition reactions and quantum chemical calculations

Heteroatom Chemistry, (16): 406-419 2005.

Alcoba, D. R.; Lain, L.; Torre, A.; Bochicchio, R. C.

A study of the partitioning of the first-order reduced density matrix according to the theory of atoms in molecules

Journal of Chemical Physics, (123) 2005.

Alcoba, D. R.; Lain, L.; Torre, A.; Bochicchio, R. C.

Treatments of non-nuclear attractors within the theory of atoms in molecules

Chemical Physics Letters, (407): 379-383 2005.

Ali, M. M.; Kaliannan, P.; Venuvanalingam, P.

Ab initio computational modeling of glyphosate analogs: Conformational perspective
Structural Chemistry, (16): 491-506 2005.

Alia, J. M.; Edwards, H. G. M.

Vibrational spectroscopic properties of hydrogen bonded acetonitrile studied by DFT
Journal of Physical Chemistry A, (109): 7977-7987 2005.

Alkorta, I.; Picazo, O.; Elguero, J.

Chiral recognition in cyclic alpha-hydroxy carbonyl compounds: A theoretical study
Journal of Physical Chemistry A, (109): 3262-3266 2005.

Alkorta, M.; Picazo, O.; Elguero, J.

Chiral discrimination in lithium complexes of bis(5H-pyrroles) and bis(oxazolines)
Journal of Physical Chemistry A, (109): 9573-9577 2005.

Ammal, S. C.; Yamataka, H.

Linear free energy relationship and kinetic isotope effects as measures for the transition-state variation - A case of the neophyl system

Canadian Journal of Chemistry-Revue Canadienne De Chimie, (83): 1606-1614 2005.

Ammal, S. C.; Yoshikai, N.; Inada, Y.; Nishibayashi, Y.; Nakamura, E.

Synergistic dimetallic effects in propargylic substitution reaction catalyzed by thiolate-bridged diruthenium complex

Journal of the American Chemical Society, (127): 9428-9438 2005.

Anandan, K.; Kolandaivel, P.; Kumaresan, R.

Quantum chemical studies on molecular structural conformations and hydrated forms of salicylamide and O-hydroxybenzoyl cyanide
International Journal of Quantum Chemistry, (104): 286-298 2005.

Anandan, K.; Kolandaivel, P.; Kumaresan, R.
Molecular structural conformations and hydration of internally hydrogen-bonded salicylic acid: Ab initio and DFT studies
International Journal of Quantum Chemistry, (103): 127-139 2005.

Angurell, I.; Rossell, O.; Seco, M.; Ruiz, E.
Dendrimers containing two metallic layers. Chloride migration from peripheral gold, palladium, or rhodium metals to internal ruthenium atoms
Organometallics, (24): 6365-6373 2005.

Anisimov, V. M.; Lamoureux, G.; Vorobyov, I. V.; Huang, N.; Roux, B.; MacKerell, A. D.
Determination of electrostatic parameters for a polarizable force field based on the classical Drude oscillator
Journal of Chemical Theory and Computation, (1): 153-168 2005.

Aquilanti, V.; Cornicchi, E.; Teixidor, M. M.; Saendig, N.; Pirani, F.; Cappelletti, D.
Glory-scattering measurement of water-noble-gas interactions: The birth of the hydrogen bond
Angewandte Chemie-International Edition, (44): 2356-2360 2005.

Ara, I.; Chaouche, N.; Fornies, J.; Fortuno, C.; Kribii, A.; Tsipis, A. C.; Tsipis, C. A.
From a 44-electron to a 48-electron trinuclear phosphido platinum complex: density functional study of [{(CF₃)(PH₃)Pt(mu-PH₂)(mu-H)}₂Pt] and [{(CF₃)(PH₃)Pt(mu-PH₂)(mu-I)}₂Pt] model compounds
Inorganica Chimica Acta, (358): 1377-1385 2005.

Aragoni, M. C.; Arca, M.; Champness, N. R.; De Pasquale, M.; Devillanova, F. A.; Isaia, F.; Lippolis, V.; Oxtoby, N. S.; Wilson, C.
Synthesis and structural characterisation of coordination polymers designed using discrete phosphonodithioato Ni-II complexes and dipyridyl donor ligands
Crystengcomm, (7): 363-369 2005.

Aragoni, M. C.; Arca, M.; Demartin, F.; Devillanova, F. A.; Garau, A.; Isaia, F.; Lippolis, V.; Verani, G.
DFT calculations, structural and spectroscopic studies on the products formed between IBr and N,N'-dimethylbenzimidazole-2(3H)-thione and-2(3H)-selone
Dalton Transactions: 2252-2258 2005.

Ardura, D.; Sordo, T. L.
Three-carbon Dowd-Beckwith ring expansion reaction versus intramolecular 1,5-hydrogen transfer reaction: A theoretical study
Journal of Organic Chemistry, (70): 9417-9423 2005.

Ariafard, A.; Amini, M. M.

Theoretical study on interaction of different coordination modes of BH₄ ligand with transition metal in [TM(BH₄)(CO)(4)](-) (TM = Cr, Mo)

Journal of Organometallic Chemistry, (690): 84-95 2005.

Ariafard, A.; Amini, M. M.; Azadmehr, A.

Density functional theory study on structural isomers and bonding of model complexes M(CO)(5)(BH₃ center dot PH₃) (M = Cr, Mo, W) and W(CO)(5)(BH₃ center dot AH₃) (A = N, P, As, Sb)

Journal of Organometallic Chemistry, (690): 1147-1156 2005.

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

Lewis acid induced [2+2] cycloadditions of silyl enol ethers with alpha,beta-unsaturated esters: A DFT analysis

European Journal of Organic Chemistry: 3973-3979 2005.

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

Density functional theory study of the 5-pyrrolidin-2-yltetrazole-catalyzed aldol reaction

Tetrahedron-Asymmetry, (16): 2764-2770 2005.

Arroyo, P.; Picher, M. T.; Domingo, L. R.; Terrier, F.

A DFT study of the polar Diels-Alder reaction between 4-aza-6-nitrobenzofuroxan and cyclopentadiene

Tetrahedron, (61): 7359-7365 2005.

Asensio, X.; Gonzalez-Lafont, A.; Marquet, J.; Lluch, J. M.

A theoretical study of the competitive homolytic/heterolytic aniomesolytic cleavages of C-O alkyl ether bonds

Journal of Organic Chemistry, (70): 540-548 2005.

Asseily, G. A.; Davies, R. P.; Rzepa, H. S.; White, A. J. P.

A solid-state structural and theoretical study on the 1 : 1 addition compounds of thioethers with dihalogens and interhalogens I-X (X = I, Br, Cl)

New Journal of Chemistry, (29): 315-319 2005.

Auer, D.; Kaupp, M.; Strohmann, C.

Understanding substituent effects on Si-29 chemical shifts and bonding in disilynes. A quantum-chemical analysis

Organometallics, (24): 6331-6337 2005.

Avakyan, V. E.; Kletskii, M. E.; Minyaev, R. M.

Mechanisms of [1,3]-sigmatropic migrations of the nitroso group in the ON-X-CH=X systems (X = O, S, Se, NH, CH₂)

Russian Journal of Organic Chemistry, (41): 1467-1472 2005.

Baba, E.; Cundari, T. R.; Firkin, I.
N-heterocyclic carbenes of the late transition metals: a computational and structural database study
Inorganica Chimica Acta, (358): 2867-2875 2005.

Bachler, V.
The behavior of transition metal nitrido bonds towards protonation rationalized by means of localized bonding schemes and their weights
Journal of Computational Chemistry, (26): 532-551 2005.

Bakalova, S. M.; Frutos, L. M.; Kaneti, J.; Castano, O.
Correlated MO study of the low-barrier intramolecular motions in donor-acceptor ethenes
Journal of Physical Chemistry A, (109): 10388-10395 2005.

Baker, J.; Fowler, P. W.; Soncini, A.; Lillington, M.
Rare-gas insertion compounds of perfluorobenzene: Aromaticity of some unstable species
Journal of Chemical Physics, (123) 2005.

Bako, I.; Megyes, T.; Palinkas, G.
Structural investigation of water-acetonitrile mixtures: An ab initio, molecular dynamics and X-ray diffraction study
Chemical Physics, (316): 235-244 2005.

Balazs, G.; Sierka, M.; Scheer, M.
Antimony-tungsten triple bond: A stable complex with a terminal antimony ligand
Angewandte Chemie-International Edition, (44): 4920-4924 2005.

Ball, D. W.
High-level calculations of the enthalpy of formation of diazomethane
Journal of Molecular Structure-Theochem, (722): 213-215 2005.

Bansal, R. K.; Karaghiosoff, K.; Gupta, N.; Gandhi, N.; Kumawat, S. K.
Diastereo- and regioselectivity in Diels-Alder reaction of [1,4,2]diazaphospholo[4,5-a]pyridines
Tetrahedron, (61): 10521-10528 2005.

Baranovski, V. I.; Korol'kov, D. V.
Free electron model in cluster structure theory. Electronic structures of [Mo₆S₈(CN)(6)](6-), [Mo₆Se₈(CN)(6)](6-), [Re₆S₈(CN)(6)](4-), and Rh-6(CO)(16) clusters
Russian Chemical Bulletin, (54): 2705-2713 2005.

Basumallick, L.; Sarangi, R.; George, S. D.; Elmore, B.; Hooper, A. B.; Hedman, B.; Hodgson, K. O.; Solomon, E. I.

Spectroscopic and density functional studies of the red copper site in nitrosocyanin: Role of the protein in determining active site geometric and electronic structure
Journal of the American Chemical Society, (127): 3531-3544 2005.

Bayse, C. A.; Baker, R. A.; Ortwin, K. N.
Relative strengths of Se center dot center dot center dot N,O interactions: Implications for glutathione peroxidase activity
Inorganica Chimica Acta, (358): 3849-3854 2005.

Bazzicalupi, C.; Bencini, A.; Berni, E.; Di Vaira, M.
Reaction pathways for Zn(II)-catalyzed carboxylic acid esters hydrolysis
Inorganica Chimica Acta, (358): 77-92 2005.

Bendjaballah, S.; Boucekkine, A.; Saillard, J. Y.
The electronic structure of the electron-reservoir complex CpFe(hexamethylbenzene) revisited: a regular metal-centered SOMO
Inorganica Chimica Acta, (358): 1305-1308 2005.

Benidar, A.; Guillemin, J. C.; Mo, O.; Yanez, M.
Infrared spectra of a species of astrochemical interest: Aminoacrylonitrile (3-amino-2-propenenitrile)
Journal of Physical Chemistry A, (109): 4705-4712 2005.

Bertoldo, M.; Cappelli, C.; Catanorchi, S.; Liuzzo, V.; Bronco, S.
Understanding the accelerating effect of epsilon-caprolactam on the formation of urethane linkages
Macromolecules, (38): 1385-1394 2005.

Bharatam, P. V.; Patel, D. S.; Iqbal, P.
Pharmacophoric features of biguanide derivatives: An electronic and structural analysis
Journal of Medicinal Chemistry, (48): 7615-7622 2005.

Bhat, K. L.; Howard, N. J.; Rostami, H.; Lai, J. H.; Bock, C. W.
Intramolecular dative bonds involving boron with oxygen and nitrogen in boronic acids and esters: a computational study
Journal of Molecular Structure-Theochem, (723): 147-157 2005.

Bhattacharya, S.; Vemula, P. K.
Effect of heteroatom insertion at the side chain of 5-Alkyl-1H-tetrazoles on their properties as catalysts for ester hydrolysis at neutral pH
Journal of Organic Chemistry, (70): 9677-9685 2005.

Bitzer, R. S.; Barbosa, A. G. H.; da Silva, C. O.; Nascimento, M. A. C.
On the generalized valence bond description of the anomeric and exo-anomeric effects: an ab initio conformational study of 2-methoxytetrahydropyran
Carbohydrate Research, (340): 2171-2184 2005.

Blaive, B.; Julg, A.; Pellegatti, A.
Quantum microscopic vs. classical macroscopic calculations on the phenomenon of electrostatic influence
European Physical Journal B, (47): 177-184 2005.

Blanco, M. A.; Pendas, A. M.; Francisco, E.
Interacting quantum atoms: A correlated energy decomposition scheme based on the Quantum Theory of Atoms in Molecules
Journal of Chemical Theory and Computation, (1): 1096-1109 2005.

Blitz, J. P.; Diebel, R. E.; Deakyne, C. A.; Christensen, J. M.; Gun'ko, V. M.
Experimental and computational studies of trialkylaluminum and alkylaluminum chloride reactions with silica
Journal of Physical Chemistry B, (109): 5667-5677 2005.

Blomquist, T.; Kirczenow, G.
Poisson-Schrodinger and ab initio modeling of doped Si nanocrystals: Reversal of the charge transfer between host and dopant atoms
Physical Review B, (71) 2005.

Bobadova-Parvanova, P.; Wang, Q. F.; Morokuma, K.; Musaev, D. G.
How many methyl groups in [{(eta(5)-C₅H₅)n}(2)Zr](2)(mu(2),eta(2),eta(2)-N-2)] are needed for dinitrogen hydrogenation? A theoretical study
Angewandte Chemie-International Edition, (44): 7101-7103 2005.

Boxford, W. E.; Dessent, C. E. H.
On the stability of IrCl₆³⁻- and other triply charged anions: Solvent stabilization versus ionic fragmentation and electron detachment for the IrCl₆³⁻-center dot(H₂O)_n n=0-10 microsolvated clusters
Journal of Physical Chemistry A, (109): 5836-5845 2005.

Brand, H.; Mayer, P.; Polborn, K.; Schulz, A.; Weigand, J. J.
Blue alkali dinitrosomethanides: Synthesis, structure, and bonding
Journal of the American Chemical Society, (127): 1360-1361 2005.

Brand, H.; Mayer, P.; Schulz, A.; Weigand, J. J.
Nitro(nitroso)cyanomethanides
Angewandte Chemie-International Edition, (44): 3929-3932 2005.

Bruschi, M.; Giuffreda, M. G.; Luthi, H. P.
'Measuring' electron delocalization in pi-conjugated systems
Chimia, (59): 539-544 2005.

Buda, C.; Kazi, A. B.; Dinescu, A.; Cundari, T. R.

*Stability studies of transition-metal linkage isomers using quantum mechanical methods.
Groups 11 and 12 transition metals*
Journal of Chemical Information and Modeling, (45): 965-970 2005.

Buemi, G.; Zuccarello, F.
Theoretical study of malonamide and nitromalonamide in vacuum and in water solution
Journal of Molecular Structure-Theochem, (719): 137-148 2005.

Buhl, M.
Molecular dynamics of a vanadate-dipeptide complex in aqueous solution
Inorganic Chemistry, (44): 6277-6283 2005.

Buhl, M.; Chaumont, A.; Schurhammer, R.; Wipff, G.
Ab initio molecular dynamics of liquid 1,3-dimethylimidazolium chloride
Journal of Physical Chemistry B, (109): 18591-18599 2005.

Buhl, M.; Hnyk, D.; Machacek, J.
Computational study of structures and properties of metallaboranes: Cobalt bis(dicarbollide)
Chemistry-a European Journal, (11): 4109-4120 2005.

Burck, S.; Gudat, D.; Lissner, F.; Nattinen, K.; Nieger, M.; Schleid, T.
2-Amino-substituted 1,3,2-diazaphospholenes
Zeitschrift Fur Anorganische Und Allgemeine Chemie, (631): 2738-2745 2005.

Burda, J. V.; Shukla, M. K.; Leszczynski, J.
Theoretical model of the aqua-copper [Cu(H₂O)(5)](+) cation interactions with guanine
Journal of Molecular Modeling, (11): 362-369 2005.

Burda, J. V.; Zeizinger, M.; Leszczynski, J.
Hydration process as an activation of trans- and cisplatin complexes in anticancer treatment. DFT and ab initio computational study of thermodynamic and kinetic parameters
Journal of Computational Chemistry, (26): 907-914 2005.

Busico, V.; Talarico, G.; Cipullo, R.
Living Ziegler-Natta polymerizations: True or false?
Macromolecular Symposia, (226): 1-16 2005.

Bzhezovskii, V. M.; Il'chenko, N. N.; Chura, M. B.; Gorb, L. G.; Yagupol'skii, L. M.
An ab initio quantum-chemical study of C₆H₅S(O)CH₃ and C₆H₅S(O)CF₃
Russian Journal of General Chemistry, (75): 86-93 2005.

Cabaleiro-Lago, E. M.; Rodriguez-Otero, J.; Garcia-Lopez, R. M.; Pena-Gallego, A.; Hermida-Ramon, J. M.

A density functional theory study on the electrocyclization of 1,2,4,6-heptatetraene analogues: Converting a pericyclic to a pseudopericyclic reaction
Chemistry-a European Journal, (11): 5966-5974 2005.

Cabaleiro-Lago, E. M.; Rodriguez-Otero, J.; Gonzalez-Lopez, I.; Pena-Gallego, A.; Hermida-Ramon, J. M.
A DFT study of the pericyclic/pseudopericyclic character of cycloaddition reactions of ethylene and formaldehyde to buta-1,3-dien-1-one and derivatives
Journal of Physical Chemistry A, (109): 5636-5644 2005.

Cabaleiro-Lago, E. M.; Rodriguez-Otero, J.; Varela-Varela, S. M.; Pena-Gallego, A.; Hermida-Ramon, J. M.
Are electrocyclization reactions of (3Z)-1,3,5-hexatrienone and nitrogen derivatives pseudopericyclic? A DFT study
Journal of Organic Chemistry, (70): 3921-3928 2005.

Cacelli, I.; Campanile, S.; Giolitti, A.; Molin, D.
Theoretical prediction of the Abraham hydrogen bond acidity and basicity factors from a reaction field method
Journal of Chemical Information and Modeling, (45): 327-333 2005.

Calhorda, M. J.; Costa, P. J.; Hartl, F.; Vergeer, F. W.
A new interpretation of the bonding properties and UV-vis spectra of [M-3(CO)(12)] clusters (M = Ru, Os): a TD-DFT study
Comptes Rendus Chimie, (8): 1477-1486 2005.

Campomanes, P.; Menendez, M. I.; Carderias-Jiron, G. I.; Sordo, T. L.
Synthesis of beta-lactams by Ag⁺-induced ring expansion of 1-hydroxycyclopropylamines: A theoretical analysis
Journal of Physical Chemistry A, (109): 7822-7831 2005.

Campomanes, P.; Menendez, M. I.; Lopez, R.; Sordo, T. L.
A theoretical analysis of the coordination modes of Cu-II with penicillins: Activation of the beta-lactam C-N bond
Chemphyschem, (6): 344-351 2005.

Campomanes, P.; Menendez, M. I.; Lopez, R.; Sordo, T. L.
Stereodynamics of bond rotation in tertiary 1-naphthoic acid amides: a computational study
Journal of Computational Chemistry, (26): 365-373 2005.

Campomanes, P.; Menendez, M. I.; Sordo, T. L.
Mechanism of cycloaddition reactions between ketene and N-silyl-, N-germyl-, and N-stannyliamines: A theoretical investigation
Journal of Physical Chemistry A, (109): 11022-11026 2005.

- Campomanes, P.; Menendez, M. I.; Sordo, T. L.
Resonance assisted hydrogen bonding and dynamic mechanism for crystal disorder in the enolic form of acetylacetone: a theoretical analysis
Journal of Molecular Structure-Theochem, (713): 59-63 2005.
- Caramori, G. F.; Galembeek, S. E.; Laali, K. K.
A computational study of [2.2]cyclophanes
Journal of Organic Chemistry, (70): 3242-3250 2005.
- Carrasco, R.; Cano, J.; Ottenwaelder, X.; Aukauloo, A.; Journaux, Y.; Ruiz-Garcia, R.
High-valent nickel oxamides. Part 2. Molecular and electronic structure of square-planar nickel(II), nickel(III) and nickel(III) pi-cation radical complexes with a tetradentate o-phenylenedioxamide redox-active ligand
Dalton Transactions: 2527-2538 2005.
- Castillo, N.; Matta, C. F.; Boyd, R. J.
Fluorine-fluorine spin-spin coupling constants in aromatic compounds: Correlations with the delocalization index and with the internuclear separation
Journal of Chemical Information and Modeling, (45): 354-359 2005.
- Castillo, R.; Andres, J.; Domingo, L. R.
Lewis acid mediated domino reaction between 2-cyclohexenone and methyl azide - A DFT study
European Journal of Organic Chemistry: 4705-4709 2005.
- Chai, J. F.; Zhu, H. P.; Stuckl, A. C.; Roesky, H. W.; Magull, J.; Bencini, A.; Caneschi, A.; Gatteschi, D.
Synthesis and reaction of [{HC(CMeNAr)(2)}Mn](2) (Ar=2,6-iPr(2)C(6)H(3)): The complex containing three-coordinate manganese(I) with a Mn-Mn bond exhibiting unusual magnetic properties and electronic structure
Journal of the American Chemical Society, (127): 9201-9206 2005.
- Chan, G. K. L.; Van Voorhis, T.
Density-matrix renormalization-group algorithms with nonorthogonal orbitals and non-Hermitian operators, and applications to polyenes
Journal of Chemical Physics, (122) 2005.
- Chandra, A. K.; Zeegers-Huyskens, T.
Theoretical study of ((CHC)-C-center dot center dot center dot)(-) hydrogen bonds in CH4-nXn (X = F, Cl; n=0, 1, 2) systems cpmplexed with their homoconjugate and heteroconjugate carbanions
Journal of Physical Chemistry A, (109): 12006-12013 2005.
- Chang, C. H.; Richards, N. G. J.
Intrinsic carbon-carbon bond reactivity at the manganese center of oxalate decarboxylase from density functional theory

Journal of Chemical Theory and Computation, (1): 994-1007 2005.

Chang, Y. C.; Lee, J. C.; Hong, F. E.

Design, synthesis, application, and DFT investigation of Suzuki-Miyaura reactions of a dicobalt carbonyl-containing phosphine ligand
Organometallics, (24): 5686-5695 2005.

Chaplin, A. B.; Harrison, J. A.; Dyson, P. J.

Revisiting the electronic structure of phosphazenes
Inorganic Chemistry, (44): 8407-8417 2005.

Chelli, R.; Pagliai, M.; Procacci, P.; Cardini, G.; Schettino, V.

Polarization response of water and methanol investigated by a polarizable force field and density functional theory calculations: Implications for charge transfer
Journal of Chemical Physics, (122) 2005.

Chen, J. C.; Li, J.; Qian, L.; Zheng, K. C.

Electronic structures and SARs of the isomeric complexes alpha-, beta-, gamma-[Ru(mazpy)(2)Cl₂] with different antitumor activities
Journal of Molecular Structure-Theochem, (728): 93-101 2005.

Chen, J. C.; Qian, L.; Wu, W. J.; Chen, L. M.; Zheng, K. C.

A QSAR study of substituted benzo[a]phenazines as potential anticancer agents
Journal of Molecular Structure-Theochem, (756): 167-172 2005.

Chen, T.; Zhang, X. H.; Wang, C. S.; Chen, S. J.; Wu, Z. Z.; Li, L. T.; Sorasaenee, K. R.;

Diminnie, J. B.; Pan, H. J.; Guzei, I. A.; Rheingold, A. L.; Wu, Y. D.; Xue, Z. L.
A tungsten silyl alkylidyne complex and its bis(alkylidene) tautomer. Their interconversion and an unusual silyl migration in their reaction with dioxygen
Organometallics, (24): 1214-1224 2005.

Chen, W.; Li, Z. R.; Wu, D.; Li, Y.; Sun, C. C.

Li-3-O-Li-3 molecule: A metal-nonmetal-metal sandwichlike compound with a distending electron cloud
Journal of Chemical Physics, (123) 2005.

Chen, X. D.; Wiehle, S.; Chi, L. F.; Muck-Lichtenfeld, C.; Rudert, R.; Vollhardt, D.; Fuchs, H.; Haufe, G.

Phase behavior of 2,3-disubstituted methyl octadecanoate monolayers at the air-water interface
Langmuir, (21): 3376-3383 2005.

Cheng, H. Y.; Chang, S. Y.

Study of the [Cr(H₂O)(5)NO]²⁺ complex via density functional theory
Journal of the Chinese Chemical Society, (52): 415-420 2005.

- Cheng, L. P.; Li, Q. S.
N-4 ring as a square planar ligand in novel MN4 species
Journal of Physical Chemistry A, (109): 3182-3186 2005.
- Cheng, M. J.; Chu, S. Y.
Bonding pattern continuum from covalent to dative carbon-silicon bonds for substituted silenes: A theoretical study
Organometallics, (24): 3746-3752 2005.
- Chien, S. H.; Cheng, M. F.; Lau, K. C.; Li, W. K.
Theoretical study of the Diels-Alder reactions between singlet ((1)Delta(g)) oxygen and acenes
Journal of Physical Chemistry A, (109): 7509-7518 2005.
- Cho, H. G.; Wang, X. F.; Andrews, L.
Reactions of methane with hafnium atoms: CH2=HfH2, agostic bonding, and (CH3)(2)HfH2
Organometallics, (24): 2854-2861 2005.
- Chojnowski, J.; Rubinsztajn, S.; Cella, J. A.; Fortuniak, W.; Cypryk, M.; Kurjata, J.; Kazmierski, K.
Mechanism of the B(C6F5)(3)-catalyzed reaction of silyl hydrides with alkoxysilanes. Kinetic and spectroscopic studies
Organometallics, (24): 6077-6084 2005.
- Chong, D. S.; Nafady, A.; Costa, P. J.; Calhorda, M. J.; Geiger, W. E.
Anodic preparation of [Re2Cp2(CO)(6)](2+): A dimeric dication that provides the powerful one-electron oxidant [ReCp(CO)(3)](+)
Journal of the American Chemical Society, (127): 15676-15677 2005.
- Chung, L. W.; Chan, T. H.; Wu, Y. D.
Theoretical study of the intrinsic reactivities of various allylmetals toward carbonyls and water
Organometallics, (24): 1598-1607 2005.
- Cimpoesu, F.; Hirao, K.; Ferbinteanu, M.; Fukuda, Y.; Linert, W.
New keys for old keywords. Case studies within the updated paradigms of the hybridization and aromaticity
Monatshefte Fur Chemie, (136): 1071-1085 2005.
- Clark, D. L.; Gordon, J. C.; Hay, P. J.; Poli, R.
Existence and stability of lanthanide-main group element multiple bonds. New paradigms in the bonding of the 4f elements. A DFT study of CP(2)CeZ (Z = F+, O, NH, CH-, CH2 and the ligand adduct CP2Ce(CH2)(NH3)
Organometallics, (24): 5747-5758 2005.

- Constantino, E.; Rimola, A.; Rodriguez-Santiago, L.; Sodupe, M.
Coordination properties of glycylglycine to Cu⁺, Ni⁺ and Co⁺. Influence of metal cation electronic configuration
New Journal of Chemistry, (29): 1585-1593 2005.
- Constantino, E.; Rodriguez-Santiago, L.; Sodupe, M.; Tortajada, J.
Interaction of Co⁺ and Co²⁺ with glycine. A theoretical study
Journal of Physical Chemistry A, (109): 224-230 2005.
- Contreras, R.; Andres, J.; Domingo, L. R.; Castillo, R.; Perez, P.
Effect of electron-withdrawing substituents on the electrophilicity of carbonyl carbons
Tetrahedron, (61): 417-422 2005.
- Cornard, J. P.; Rasmussen; Merlin, J. C.
Molecular structure and spectroscopic properties of 4-nitrocatechol at different pH: UV-visible, Raman, DFT and TD-DFT calculations
Chemical Physics, (309): 239-249 2005.
- Corts-Guzman, F.; Bader, R. F. W.
Complementarity of QTAIM and MO theory in the study of bonding in donor-acceptor complexes
Coordination Chemistry Reviews, (249): 633-662 2005.
- Cross, J. B.; Vreven, T.; Meroueh, S. O.; Mobashery, S.; Schlegel, H. B.
Computational investigation of irreversible inactivation of the zinc-dependent protease carboxypeptidase A
Journal of Physical Chemistry B, (109): 4761-4769 2005.
- Cuevas, G.; Martinez-Mayorga, K.; Fernandez-Alonso, M. D.; Jimenez-Barbero, J.; Perrin, C. L.; Juaristi, E.; Lopez-Mora, N. S.
The origin of one-bond C-H coupling constants in OCH fragments: Not primarily n(o)->sigma(CH) delocalization*
Angewandte Chemie-International Edition, (44): 2360-2364 2005.
- De Proft, F.; Fias, S.; Van Alsenoy, C.; Geerlings, P.
Spin-polarized conceptual density functional theory study of the regioselectivity in the [2+2] photocycloaddition of enones to substituted alkenes
Journal of Physical Chemistry A, (109): 6335-6343 2005.
- Deleuze, M. S.; Francois, J. P.; Kryachko, E. S.
The fate of dicationic states in molecular clusters of benzene and related compounds
Journal of the American Chemical Society, (127): 16824-16834 2005.
- DeMatteo, M. P.; Poole, J. S.; Shi, X. F.; Sachdeva, R.; Hatcher, P. G.; Hadad, C. M.; Platz, M. S.

On the electrophilicity of hydroxyl radical: A laser flash photolysis and computational study

Journal of the American Chemical Society, (127): 7094-7109 2005.

Di Vaira, M.; Stoppioni, P.

Pathways for proton migration over the surface of a metal-cyclotriphosphorus cluster

Comptes Rendus Chimie, (8): 1535-1542 2005.

Dias, A. R.; Ferreira, A. P.; Veiros, L. F.

Bonding and fluxionality in group-4 metal complexes with pyrrolyl ligands

Comptes Rendus Chimie, (8): 1444-1452 2005.

Dias, A. R.; Veiros, L. F.

Are cyclopentadienyl complexes more stable than their pyrrolyl analogues?

Journal of Organometallic Chemistry, (690): 1840-1844 2005.

Diaz, C. C.; Kaplan, I. G.; Roszak, S.

Theoretical study of the electron affinities of the alkaline-earth tetramers possessing T-d symmetry: Be-4 and Mg-4

Journal of Molecular Modeling, (11): 330-334 2005.

Diaz, J.; Silva, M. A.; Goodman, J. M.; Pellegrinet, S. C.

Computer-assisted design of asymmetric 1,3-dipolar cycloadditions between dimethylvinylborane and chiral nitrones

Tetrahedron, (61): 10886-10893 2005.

Diefenbach, M.; Schwarz, H.

High-electron-density C6H6 units: Stable ten-pi-electron benzene complexes

Chemistry-a European Journal, (11): 3058-3063 2005.

Dobrogorskaia-Mereau, II; Nemukhin, A. V.

Quantum chemical modeling of the reduction of cis-diammineplatinum(IV) tetrachloride [Pt(NH3)(2)Cl-4] by methyl thiolate anion

Journal of Computational Chemistry, (26): 865-870 2005.

Dobrogorskaya, Y.; Maseetti, J.; Papai, I.; Hannachi, Y.

Theoretical investigation of the reactivity of copper atoms with OCS: Comparison with CS2 and CO2

Journal of Physical Chemistry A, (109): 7932-7937 2005.

Domingo, L. R.; Perez, P.; Contreras, R.

A DFT analysis of the strain-induced regioselective[2+2]cycloaddition of benzyne possessing fused four-membered ring

Letters in Organic Chemistry, (2): 68-73 2005.

Donald, K. J.; Bohm, M. C.; Lindner, H. J.

Analysis of competing bonding parameters. Part 2. The structure of halosilanes and halogermanes (MH_{4-n}X_n, n=1-4; M = Si, Ge; X = F, Cl, Br)
Journal of Molecular Structure-Theochem, (713): 215-226 2005.

Duan, X. M.; Li, Z. H.; Hu, H. R.; Song, G. L.; Wang, W. N.; Chen, G. H.; Fan, K. N.
Linear regression correction to first principle theoretical calculations - Improved descriptors and enlarged training set
Chemical Physics Letters, (409): 315-321 2005.

Duan, X. M.; Li, Z. H.; Song, G. L.; Wang, W. N.; Chen, G. H.; Fan, K. N.
Neural network correction for heats of formation with a larger experimental training set and new descriptors
Chemical Physics Letters, (410): 125-130 2005.

Dudev, T.; Chang, L. Y.; Lim, C.
Factors governing the substitution of La³⁺ for Ca²⁺ and Mg²⁺ in metalloproteins: A DFT/CDM study
Journal of the American Chemical Society, (127): 4091-4103 2005.

DuPre, D. B.
Bonding patterns in a strong 3c2e C-H center dot center dot center dot C hydrogen bond
Journal of Physical Chemistry A, (109): 622-628 2005.

East, A. L. L.; Grittner, K. L.; Afzal, A. I.; Simpson, A. G.; Liebman, J. F.
Length and substituent-scrambling energies of parent and halogen-substituted conjugated polyynes
Journal of Physical Chemistry A, (109): 11424-11428 2005.

Eckert-Maksic, M.; Glasovac, Z.
Ab initio study of the effect of alpha-substituents on the acidity of cyclopropabenzene
Journal of Physical Organic Chemistry, (18): 763-772 2005.

El Firdoussi, A.; Esseffar, M.; Bouab, W.; Abboud, J. L. M.; Mo, O.; Yanez, M.; Ruasse, M. F.
Density functional theory study of the hydrogen bond interaction between lactones, lactams, and methanol
Journal of Physical Chemistry A, (109): 9141-9148 2005.

Erben, M. F.; Diez, R. P.; Della Vedova, C. O.
Theoretical investigation on the conformational space of perfluorohydroxylamine, F2NOF
Chemical Physics, (308): 193-198 2005.

Ernd, M.; Heuschmann, M.; Zippe, H.
Cycloadditions of aryl-substituted 1,2,4-triazines with 2-cyclopropylidene-1,3-dimethylimidazolidine - Zwitterions as discrete intermediates
Helvetica Chimica Acta, (88): 1491-1518 2005.

- Esteves, P. M.; Ferreira, N. B. P.; Corroa, R. J.
Neutral structures with a planar tetracoordinated carbon based on spiropentadiene analogues
Journal of the American Chemical Society, (127): 8680-8685 2005.
- Fang, G. Y.; Xu, L. N.; Hu, X. G.; Li, X. H.
Density functional theory study of the interaction between 3-nitro-1,2,4-triazole-5-one and ammonia
International Journal of Quantum Chemistry, (105): 148-153 2005.
- Fang, G. Y.; Xu, L. N.; Hu, X. G.; Li, X. H.; Xiao, H. M.; Ju, X. H.; Gong, X. D.
Density functional theory study of the interaction between 3-nitro-1,2,4-triazole-5-one and water
Journal of Theoretical & Computational Chemistry, (4): 849-856 2005.
- Fang, G. Y.; Xu, L. N.; Xiao, H. M.; Ju, X. H.
Theoretical study on intermolecular interactions of 3-nitro-1,2,4-triazole-5-one with NH₃ and H₂O
Acta Chimica Sinica, (63): 1055-1061 2005.
- Fernandez, I.; Sierra, M. A.; Gomez-Gallego, M.; Mancheno, M. J.; Cossio, F. P.
Computational and experimental studies on the mechanism of the photochemical carbonylation of Group 6 Fischer carbene complexes
Chemistry-a European Journal, (11): 5988-5996 2005.
- Fernandez, L. E.; Marigliano, A. C. G.; Varetti, E. L.
The vibrational properties of formic acid as monomer and dimer: a DFT study
Vibrational Spectroscopy, (37): 179-187 2005.
- Fernandez, L. E.; Varetti, E. L.
A scaled quantum mechanical force field for the sulfonyl halides II. The SO₂X_F (X = Cl, Br) halides
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (62): 221-225 2005.
- Ferrer, S.; Ruiz-Pernia, J. J.; Tunon, I.; Moliner, V.; Garcia-Viloca, M.; Gonzalez-Lafont, A.; Lluch, J. M.
A QM/MM exploration of the potential energy surface of pyruvate to lactate transformation catalyzed by LDH. Improving the accuracy of semiempirical descriptions
Journal of Chemical Theory and Computation, (1): 750-761 2005.
- Ferullo, R. M.; Castellani, N. J.
A quantum-chemical study of CO adsorption on small Cu particles supported on reduced SiO₂
Journal of Molecular Catalysis a-Chemical, (234): 121-127 2005.

- Filippou, A. C.; Schnakenburg, G.; Philippopoulos, A. I.; Weidemann, N.
Ge-2 trapped by triple bonds between two metal centers: The germylidyne complexes trans,trans-[Cl(depe)(2)M Ge-Ge M(depe)(2)Cl] (M = Mo, W) and bonding analyses of the M Ge-Ge M chain
Angewandte Chemie-International Edition, (44): 5979-5985 2005.
- Fischer, G.; Herler, S.; Mayer, P.; Schulz, A.; Villinger, A.; Weigand, J. J.
Mono-, Di-, and tricoordinated phosphorus attached to a N-N unit: An experimental and theoretical study
Inorganic Chemistry, (44): 1740-1751 2005.
- Fleischer, H.
Kinetics and mechanism of the nucleophilic substitution of Tellurium(II) dialkanethiolates, Te(SR₁)₂ with thiols, HSR₂
Phosphorus Sulfur and Silicon and the Related Elements, (180): 815-825 2005.
- Fleischer, H.; Dienes, Y.; Mathiasch, B.; Schmitt, V.; Schollmeyer, D.
Cysteamine and its homoleptic complexes with group 12 metal ions. Differences in the coordination chemistry of Zn-II, Cd-II, and Hg-II with a small N,S-donor ligand
Inorganic Chemistry, (44): 8087-8096 2005.
- Fleischer, H.; Schollmeyer, D.
Formation of meso-1,2-bis(dimethylamino)-1,2-diphenylethane by oxidative C-C coupling reaction
Zeitschrift Fur Naturforschung Section B-a Journal of Chemical Sciences, (60): 1083-1087 2005.
- Fleischer, H.; Wann, D. A.; Hinchley, S. L.; Borisenko, K. B.; Lewis, J. R.; Mawhorter, R. J.; Robertson, H. E.; Rankin, D. W. H.
Molecular structures of Se(SCH₃)₂ and Te(SCH₃)₂ using gas-phase electron diffraction and ab initio and DFT geometry optimisations
Dalton Transactions: 3221-3228 2005.
- Flores, J. R.; Perez-Juste, I.; Carballeira, L.
A theoretical study of the SiCNH isomers
Chemical Physics, (313): 1-15 2005.
- Flores-Sandoval, C. A.; Zaragoza, I. P.; Maranon-Ruiz, V. F.; Correa-Basurto, J.; Trujillo-Ferrara, J.
Theoretical study of aryl succinic and maleic acid derivatives
Journal of Molecular Structure-Theochem, (713): 127-134 2005.
- Fornies, J.; Martin, A.; Martin, L. F.; Menjon, B.
All-organometallic analogues of Zeise's salt for the three group 10 metals
Organometallics, (24): 3539-3546 2005.

- Frackiewicz, K.; Czerwinski, M.; Siekierski, S.
Secondary periodicity in the tetrahalogeno complexes of the group 13 elements
European Journal of Inorganic Chemistry: 3850-3856 2005.
- Frank, P.; Benfatto, M.; Szilagyi, R. K.; D'Angelo, P.; Della Longa, S.; Hodgson, K. O.
The solution structure of $[Cu(aq)](2+)$ and its implications for rack-induced bonding in blue copper protein active
Inorganic Chemistry, (44): 1922-1933 2005.
- Freitas, M. P.; Rittner, R.; Tormena, C. F.; Abraham, R. J.
Conformational analysis and stereoelectronic effects in trans-1,2-dihalocyclohexanes: H-1 NMR and theoretical investigation
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (61): 1771-1776 2005.
- Frenking, G.; Sola, M.; Vyboishchikov, S. F.
Chemical bonding in transition metal carbene complexes
Journal of Organometallic Chemistry, (690): 6178-6204 2005.
- Froeyen, M.; Herdewijn, P.
Correct bond order assignment in a molecular framework using integer linear programming with application to molecules where only non-hydrogen atom coordinates are available
Journal of Chemical Information and Modeling, (45): 1267-1274 2005.
- Fu, Y.; Liu, L.; Guo, Q. X.
Extraordinary beta-silyl effects on C-H, N-H, and O-H bond dissociation energies
Journal of Molecular Structure-Theochem, (725): 1-4 2005.
- Fukushima, K.; Iwahashi, H.
Natural bond orbital analysis of pericyclic and pseudopericyclic 1,5-electrocyclizations of conjugated azides
Heterocycles, (65): 2605-2618 2005.
- Gahungu, G.; Zhang, J. P.
Molecular geometry, electronic structure and optical properties study of meridional tris(8-hydroxyquinolinato)gallium(III) with ab initio and DFT methods
Journal of Molecular Structure-Theochem, (755): 19-30 2005.
- Gahungu, G.; Zhang, J. P.
"CH"/N substituted mer-Gaq3 and mer-Alq3 derivatives: An effective approach for the tuning of emitting color
Journal of Physical Chemistry B, (109): 17762-17767 2005.
- Gais, H. J.; Bruns, P. R.; Raabe, G.; Hainz, R.; Schleusner, M.; Rumsink, J.; Babu, G. S.

Dynamic behavior of chiral sulfonimidoyl-substituted allyl and alkyl (dimethylamino)titanium(IV) complexes: Metallotropic shift, reversible beta-hydride elimination/reinsertion, and ab initio calculations of allyl and alkyl aminosulfoxonium ylides

Journal of the American Chemical Society, (127): 6617-6631 2005.

Garberoglio, G.; Skouidas, A. I.; Johnson, J. K.

Adsorption of gases in metal organic materials: Comparison of simulations and experiments

Journal of Physical Chemistry B, (109): 13094-13103 2005.

Garcia-Cruz, I.; Martinez-Magadan, J. M.; Salcedo, R.; Illas, F.

Electronic structure properties of dibenzofurane and dibenzothiophene derivatives:

Implications on asphaltene formation

Energy & Fuels, (19): 998-1002 2005.

Ge, Q. Y.; Wang, H. J.; Chen, J. H.

Theoretical chemistry study of the hydrogen-bonded interaction between acylamine and chloromethane compounds

Chinese Journal of Structural Chemistry, (24): 1416-1424 2005.

Georgieva, I.; Trendafilova, N.; Rodriguez-Santiago, L.; Sodupe, M.

Coordination properties of the oxime analogue of glycine to Cu(II)

Journal of Physical Chemistry A, (109): 5668-5676 2005.

Ghiasi, R.

A computational study of the arsabenzenes: Structure, properties and aromaticity

Journal of Organometallic Chemistry, (690): 4761-4767 2005.

Ghiasi, R.

The mono- and di-silanaphthalene: structure, properties, and aromaticity

Journal of Molecular Structure-Theochem, (718): 225-233 2005.

Ghosh, D. C.; Bhattacharyya, S.

Computation of quantum mechanical hybridization and dipole correlation of the electronic structure of the F3B-NH₃ supermolecule

International Journal of Quantum Chemistry, (105): 270-279 2005.

Giannakopoulos, E.; Christoforidis, K. C.; Tsipis, A.; Jerzykiewicz, M.; Deligiannakis, Y.

Influence of Pb(II) on the radical properties of humic substances and model compounds

Journal of Physical Chemistry A, (109): 2223-2232 2005.

Gilbert, T. M.

Computational prediction of regiospecificity in the [4+2] Diels-Alder cyclizations between the iminoborane (F3C)(3)C-B=N-(t-Bu) and substituted cis-butadienes

Organometallics, (24): 6445-6449 2005.

- Glaser, R.; Wu, H.; Lewis, M.
Cytosine catalysis of nitrosative guanine deamination and interstrand cross-link formation
Journal of the American Chemical Society, (127): 7346-7358 2005.
- Glatzel, P.; Bergmann, U.
High resolution 1s core hole X-ray spectroscopy in 3d transition metal complexes - electronic and structural information
Coordination Chemistry Reviews, (249): 65-95 2005.
- Glendening, E. D.
Natural energy decomposition analysis: Extension to density functional methods and analysis of cooperative effects in water clusters
Journal of Physical Chemistry A, (109): 11936-11940 2005.
- Glendening, E. D.; Halpern, A. M.
Ab initio study of cyclobutane: Molecular structure, ring-puckering potential, and origin of the inversion barrier
Journal of Physical Chemistry A, (109): 635-642 2005.
- Glendening, E. D.; Shrout, A. L.
Influence of resonance on the acidity of sulfides, sulfoxides, sulfones, and their group 16 congeners
Journal of Physical Chemistry A, (109): 4966-4972 2005.
- Godinho, S.; do Couto, P. C.; Cabral, B. J. C.
Polarization effects and charge separation in AgCl-water clusters
Journal of Chemical Physics, (122) 2005.
- Goebbert, D. J.; Hernandez, H.; Francisco, J. S.; Wenthold, P. G.
The binding energy and bonding in dialane
Journal of the American Chemical Society, (127): 11684-11689 2005.
- Goettmann, F.; Boissiere, C.; Grosso, D.; Mercier, F.; Le Floch, P.; Sanchez, C.
New hybrid bidentate ligands as precursors for smart catalysts
Chemistry-a European Journal, (11): 7416-7426 2005.
- Gomes, J. R. B.; Gomes, P.
Gas-phase acidity of sulfonamides: implications for reactivity and prodrug design
Tetrahedron, (61): 2705-2712 2005.
- Gomez-Balderas, R.; Raffa, D. F.; Rickard, G. A.; Brunelle, P.; Rauk, A.
Computational studies of Cu(II)/Met and Cu(I)/met binding motifs relevant for the chemistry of Alzheimer's disease
Journal of Physical Chemistry A, (109): 5498-5508 2005.

- Gonzalez, J. A. R.; Lorono, M.; Cordova, T.; Chuchani, G.
MP2 study of substituent effects of 2-substituted alkyl ethyl methylcarbamates in homogeneous, unimolecular gas phase elimination reaction
Journal of Molecular Structure-Theochem, (732): 55-61 2005.
- Goodman, L.; Gu, H. B.; Pophristic, V.
Gauche effect in 1,2-difluoroethane. Hyperconjugation, bent bonds, steric repulsion
Journal of Physical Chemistry A, (109): 1223-1229 2005.
- Goodman, L.; Sauers, R. R.
1-fluoropropane. Torsional potential surface
Journal of Chemical Theory and Computation, (1): 1185-1192 2005.
- Goodman, L.; Sauers, R. R.
Ethyl anion preferred conformation
International Journal of Quantum Chemistry, (102): 829-837 2005.
- Goossen, L. J.; Koley, D.; Hermann, H. L.; Thiel, W.
The palladium-catalyzed cross-coupling reaction of carboxylic anhydrides with arylboronic acids: A DFT study
Journal of the American Chemical Society, (127): 11102-11114 2005.
- Goossen, L. J.; Koley, D.; Hermann, H. L.; Thiel, W.
Mechanistic pathways for oxidative addition of aryl halides to palladium(0) complexes: A DFT study
Organometallics, (24): 2398-2410 2005.
- Gordon, A. J.; Palmer, M. H.
The molecular structures and electron distributions of the 1,8-bis-(dimethylamino)-naphthalenes, studied by density functional and ab initio MP2 calculations
Molecular Physics, (103): 2773-2787 2005.
- Gorelsky, S. I.; Basumallick, L.; Vura-Weis, J.; Sarangi, R.; Hodgson, K. O.; Hedman, B.; Fujisawa, K.; Solomon, E. I.
Spectroscopic and DFT investigation of [M{HB(3,5-(i)Pr(2)pz)(3)}(SC₆F₅)] (M = Mn, Fe, Co, Ni, Cu, and Zn) model complexes: Periodic trends in metal-thiolate bonding
Inorganic Chemistry, (44): 4947-4960 2005.
- Gosavi, T.; Wagner, C.; Merzweiler, K.; Schmidt, H.; Steinborn, D.
Reactions of platina-beta-diketones with 2-aminopyridines: Synthesis and characterization of aminocarbene complexes of platinum(II)
Organometallics, (24): 533-538 2005.
- Gosavi, T.; Wagner, C.; Schmidt, H.; Steinborn, D.

Reactivity of the dinuclear platina-beta-diketone [Pt-2{(COMe)(2)H}(2)(mu-Cl)(2)] towards chelating ligands - Bridge cleavage versus formation of acetyl(chloro)platinum(II) complexes
Journal of Organometallic Chemistry, (690): 3229-3236 2005.

Grabowski, S. J.; Sokalski, W. A.; Leszczynski, J.

How short can the H center dot center dot center dot H intermolecular contact be? New findings that reveal the covalent nature of extremely strong interactions
Journal of Physical Chemistry A, (109): 4331-4341 2005.

Gracon, A. S. A.; Pernecky, S. J.; Milletti, M. C.; Park, J. A.; Yuan, Y.; Kim, H.

Computational characterization of a series of eicosanoids
Letters in Drug Design & Discovery, (2): 322-328 2005.

Graterol, M.; Rotinov, A.; Cordova, T.; Chuchani, G.

Experimental and theoretical studies of the elimination kinetics of 3-hydroxy-3-methyl-2-butanone in the gas phase
Journal of Physical Organic Chemistry, (18): 595-601 2005.

Gribanova, T. N.; Dubonosov, A. D.; Tolpygin, I. E.; Rybalkin, V. P.; Bren, V. A.; Minyaev, R. M.; Minkin, V. I.

Structure and stability of complexes of N,N'-di(9-anthrylmethyl)-1,2-diaminoethane with cations of metals from IIB group: Quantum-chemical study
Russian Journal of Organic Chemistry, (41): 1175-1182 2005.

Gu, J. D.; Xie, Y. M.; Schaefer, H. F.

Structural and energetic characterization of a DNA nucleoside pair and its anion: Deoxyriboadenosine (dA) - Deoxyribothymidine (dT)
Journal of Physical Chemistry B, (109): 13067-13075 2005.

Guest, M. F.; Bush, I. J.; Van Dam, H. J. J.; Sherwood, P.; Thomas, J. M. H.; Van Lenthe, J. H.; Havenith, R. W. A.; Kendrick, J.

The GAMESS-UK electronic structure package: algorithms, developments and applications
Molecular Physics, (103): 719-747 2005.

Guillemin, J. C.; Riague, E. H.; Gal, J. F.; Maria, P. C.; Mo, O.; Yanez, M.

Acidity trends in alpha,beta-unsaturated sulfur, selenium, and tellurium derivatives: Comparison with C-, Si-, Ge-, Sn-, N-, P-, As-, and Sb-containing analogues
Chemistry-a European Journal, (11): 2145-2153 2005.

Gutsev, G. L.; Mochena, M. D.; Bauschlicher, C. W.

Interaction of water with small Fe-n clusters
Chemical Physics, (314): 291-298 2005.

Gutsev, G. L.; Mochena, M. D.; Bauschlicher, C. W.

Dissociative and associative attachment of OH to iron clusters
Chemical Physics Letters, (407): 180-185 2005.

- Gutta, P.; Tantillo, D. J.
Proton sandwiches: Nonclassical carbocations with tetracoordinate protons
Angewandte Chemie-International Edition, (44): 2719-2723 2005.
- Guzei, I. A.; Li, K. L.; Darkwa, J.
Conformational studies of 1-4-bis(3,5-di-tert-butylpyrazolyl-1-carbonyl)benzene
Journal of Chemical Crystallography, (35): 197-202 2005.
- Haas, J.; Bissmire, S.; Wirth, T.
Iodine monochloride-amine complexes: An experimental and computational approach to new chiral electrophiles
Chemistry-a European Journal, (11): 5777-5785 2005.
- Hackett, J. C.; Brueggemeier, R. W.; Hadad, C. M.
The final catalytic step of cytochrome P450 aromatase: A density functional theory study
Journal of the American Chemical Society, (127): 5224-5237 2005.
- Han, J.; Lee, H.; Tao, F. M.
Molecular structures and properties of the complete series of bromophenols: Density functional theory calculations
Journal of Physical Chemistry A, (109): 5186-5192 2005.
- Han, Y. K.; Jung, J.
Does the Al-13(-) core exist in the Al-13 polyhalide Al₁₃In-(n=1-12) clusters?
Journal of Chemical Physics, (123) 2005.
- Handzlik, J.
Metathesis activity and properties of Mo-alkylidene sites differently located on silica. A density functional theory study
Journal of Physical Chemistry B, (109): 20794-20804 2005.
- Handzlik, J.; Ogonowski, J.; Tokarz-Sobieraj, R.
Dependence of metathesis activity of Mo-methylidene sites on their location on (100) gamma-Al₂O₃ - a theoretical study
Catalysis Today, (101): 163-173 2005.
- Hassan, S. A.; Mehler, E. L.
From quantum chemistry and the classical theory of polar liquids to continuum approximations in molecular mechanics calculations
International Journal of Quantum Chemistry, (102): 986-1001 2005.
- Hasson, A. S.; Kuwata, K. T.; Arroyo, M. C.; Petersen, E. B.

Theoretical studies of the reaction of hydroperoxy radicals (HO_2 center dot) with ethyl peroxy ($\text{CH}_3\text{CH}_2\text{O}_2$ center dot), acetyl peroxy ($\text{CH}_3\text{C}(\text{O})\text{O}-2$ (center dot)) and acetonyl peroxy ($\text{CH}_3\text{C}(\text{O})\text{CH}_2\text{O}_2$ center dot) radicals
Journal of Photochemistry and Photobiology a-Chemistry, (176): 218-230 2005.

Hazebroutcq, S.; Picard, G. S.; Adamo, C.

A theoretical investigation of gadolinium (III) solvation in molten salts
Journal of Chemical Physics, (122) 2005.

He, Q.; Zhou, L. X.

Theoretical study on the interaction of platinum compounds with DNA base pairs
Acta Physico-Chimica Sinica, (21): 846-851 2005.

He, Q.; Zhou, L. X.; Zhang, Z. Q.

Theoretical study on the protonation of platinated adenine
Chinese Journal of Chemistry, (23): 1355-1360 2005.

He, R. X.; Li, M.; Li, X. Y.

On the regioselective mechanism of novel rearrangements of 1,6-enynes catalyzed by PtCl_2 : a DFT study
Journal of Molecular Structure-Theochem, (717): 21-32 2005.

He, W. D.; Zhou, G.; Wong, N. B.; Tian, A. M.; Long, X. P.

Intramolecular H-bonds in LLM-105 and its derivatives: a DFT study
Journal of Molecular Structure-Theochem, (723): 217-222 2005.

Held, I.; Villinger, A.; Zipse, H.

The stability of acylpyridinium cations and their relation to the catalytic activity of pyridine bases
Synthesis-Stuttgart: 1425-1430 2005.

Herges, R.; Papaffilippopoulos, A.; Hess, K.; Chiappe, C.; Lenoir, D.; Detert, H.

cis-bromination of alkynes without cationic intermediates
Angewandte Chemie-International Edition, (44): 1412-1416 2005.

Herler, S.; Mayer, P.; auf der Gunne, J. S.; Schulz, A.; Villinger, A.; Weigand, J. J.

A triazadiphosphole
Angewandte Chemie-International Edition, (44): 7790-7793 2005.

Herrmann, C.; Reiher, M.; Hess, B. A.

Comparative analysis of local spin definitions - 034102
Journal of Chemical Physics, (122) 2005.

Herzog, A.; Jalasatgi, S. S.; Knobler, C. B.; Wedge, T. J.; Hawthorne, M. F.

Camouflaged carborarods derived from B-permethyl-1,12-diethynyl-para-and B-octamethyl-1,7-diethynyl-meta-carborane modules

Chemistry-a European Journal, (11): 7155-7174 2005.

Heyl, D. L.; Fernandes, S.; Khullar, L.; Stephens, J.; Blaney, E.; Opang-Owusu, H.; Stahelin, B.; Pasko, T.; Jacobs, J.; Bailey, D.; Brown, D.; Milletti, M. C.
Correlation of LUMO localization with the alpha-amylase inhibition constant in a Tendamistat-based series of linear and cyclic peptides
Bioorganic & Medicinal Chemistry, (13): 4262-4268 2005.

Ho, H. O.; Li, W. K.
A G3(MP2) study on the concerted cycloaddition reactions between ethylene and azines as well as other related heterocyclic systems
Journal of Molecular Structure-Theochem, (723): 195-204 2005.

Hoffmann, M.; Plutecka, A.; Rychlewska, U.; Kucybala, Z.; Paczkowski, J.; Pyszka, I.
New type of bonding formed from an overlap between pi aromatic and pi C=O molecular orbitals stabilizes the coexistence in one molecule of the ionic and neutral meso-ionic forms of imidazopyridine*
Journal of Physical Chemistry A, (109): 4568-4574 2005.

Holm, A. H.; Brinck, T.; Daasbjerg, K.
Elucidation of the thermochemical properties of triphenyl- or tributyl-substituted Si-, Ge-, and Sn-centered radicals by means of electrochemical approaches and computations
Journal of the American Chemical Society, (127): 2677-2685 2005.

Horn, K. H.; Bores, N.; Lehnert, N.; Mersmann, K.; Nather, C.; Peters, G.; Tuczek, F.
Reduction pathway of end-on terminally coordinated dinitrogen. IV. Geometric, electronic, and vibrational structure of a W(IV) dialkylhydrazido complex and its two-electron-reduced derivative undergoing N-N cleavage upon protonation
Inorganic Chemistry, (44): 3016-3030 2005.

Hou, R. B.; Gu, J. D.; Xie, Y. M.; Yi, X. H.; Schaefer, H. F.
The 2'-deoxyadenosine-5-phosphate anion, the analogous radical, and the different hydrogen-abstracted radical anions: Molecular structures and effects on DNA damage
Journal of Physical Chemistry B, (109): 22053-22060 2005.

Hou, S. M.; Li, R.; Qian, Z. K.; Zhang, J. X.; Shen, Z. Y.; Zhao, X. Y.; Xue, Z. Q.
Evaluation of basis sets with 11-electron analytic effective core potentials of gold for modeling molecular electronic devices
Journal of Physical Chemistry A, (109): 8356-8360 2005.

Hugas, D.; Simon, S.; Duran, M.
MH center dot center dot center dot HX dihydrogen bond with M=Li, Na and X=F, Cl, Br: A CP-corrected PES calculation and an AIM analysis
Structural Chemistry, (16): 257-263 2005.

Hughes, S. R.; Nguyen, T. N.; Capobianco, J. A.; Peslherbe, G. H.

A theoretical study of trivalent lanthanide ion microsolvation in water clusters from first principles

International Journal of Mass Spectrometry, (241): 283-294 2005.

Huntley, D. R.; Markopoulos, G.; Donovan, P. M.; Scott, L. T.; Hoffmann, R.

Squeezing C-C bonds

Angewandte Chemie-International Edition, (44): 7549-7553 2005.

Hush, N. S.; Schamberger, J.; Bacska, G. B.

A quantum chemical computational study of the relative stabilities of cis- and trans-platinum dichloride in aqueous solution

Coordination Chemistry Reviews, (249): 299-311 2005.

Iftimie, R.; Tuckerman, M. E.

Decomposing total IR spectra of aqueous systems into solute and solvent contributions: A computational approach using maximally localized Wannier orbitals

Journal of Chemical Physics, (122) 2005.

Ignat'ev, I. S.; Kochina, T. A.

Proton migration in benzene complexes of methyl and silyl cations

Russian Journal of General Chemistry, (75): 1221-1224 2005.

Ignat'ev, I. S.; Kochina, T. A.

Energies of association of carbenium and silylium cations with oxygen-containing molecules

Russian Journal of General Chemistry, (75): 711-713 2005.

Ignatyev, I. S.; Montejo, M.; Urena, F. P.; Gonzalez, J. J. L.

Structure and vibrational spectra of dimethylsilanediol and methylsilanetriol dimers

Chemical Physics Letters, (412): 359-364 2005.

Ilkhechi, A. H.; Mercero, J. M.; Silanes, I.; Bolte, M.; Scheibitz, M.; Lerner, H. W.; Ugalde, J. M.; Wagner, M.

A joint experimental and theoretical study of cation-pi interactions: Multiple-decker sandwich complexes of ferrocene with alkali metal ions (Li^+ , Na^+ , K^+ , Rb^+ , Cs^+)

Journal of the American Chemical Society, (127): 10656-10666 2005.

Impronta, R.; Santoro, F.

Excited-state behavior of trans and cis isomers of stilbene and stiff stilbene: A TD-DFT study

Journal of Physical Chemistry A, (109): 10058-10067 2005.

Impronta, R.; Santoro, F.

A theoretical study on the factors influencing cyanine photo isomerization: The case of thiacyanine in gas phase and in methanol

Journal of Chemical Theory and Computation, (1): 215-229 2005.

- In, S.; Cho, S. J.; Kang, J. M.
Anion receptor with xylene bridged two imidazolium rings
Supramolecular Chemistry, (17): 443-446 2005.
- In, S.; Cho, S. J.; Lee, K. H.; Kang, J.
Participation of benzene hydrogen bonding upon anion binding
Organic Letters, (7): 3993-3996 2005.
- Ivanova, E. V.; Muchall, H. M.
Influence of the number of water molecules on the mechanism of N-sulfinylaniline hydrolysis
Canadian Journal of Chemistry-Revue Canadienne De Chimie, (83): 1588-1596 2005.
- Iwaoka, M.; Katsuda, T.; Komatsu, H.; Tomoda, S.
Experimental and theoretical studies on the nature of weak nonbonded interactions between divalent selenium and halogen atoms
Journal of Organic Chemistry, (70): 321-327 2005.
- Iwaoka, M.; Tomoda, S.
Studies on the nonbonded interactions of divalent organic selenium
Journal of Synthetic Organic Chemistry Japan, (63): 911-920 2005.
- Iwaoka, M.; Tomoda, S.
Physical- and bio-organic chemistry of nonbonded selenium center dot center dot center dot oxygen interactions
Phosphorus Sulfur and Silicon and the Related Elements, (180): 755-766 2005.
- Izquierdo, M. A.; Domingo, L. R.; Miranda, M. A.
Theoretical calculations on the cycloreversion of oxetane radical cations
Journal of Physical Chemistry A, (109): 2602-2607 2005.
- Jasien, P. G.; Cross, R.
Calculation of sequential hydrogen atom binding energies on a model lithium cluster
Journal of Molecular Structure-Theochem, (756): 11-17 2005.
- Jena, N. R.; Mishra, P. C.
An ab initio and density functional study of microsolvation of carbon dioxide in water clusters and formation of carbonic acid
Theoretical Chemistry Accounts, (114): 189-199 2005.
- Jena, N. R.; Mishra, P. C.
Study of relationship of atomic orbital hybridization with bonding using hybridization displacement charge: optimal hybridization principle
Journal of Molecular Structure-Theochem, (719): 75-84 2005.

- Jian, F. F.; Zhao, P. S.; Bai, Z. S.; Zhang, L.
Quantum chemical calculation studies on 4-phenyl-1-(propan-2-ylidene)thiosemicarbazide
Structural Chemistry, (16): 635-639 2005.
- Jian, F. F.; Zhao, P. S.; Hou, Y. X.
Experimental and theoretical studies on (p-methoxyphenyl)thiosemicarbazide
Structural Chemistry, (16): 361-367 2005.
- Jian, F. F.; Zhao, P. S.; Hou, Y. X.; Bei, F. L.
Experimental and density functional theory calculational studies on 2,3-diaryl-tetrazole-5-thione
Chinese Journal of Chemistry, (23): 548-556 2005.
- Jian, F. F.; Zhao, P. S.; Wang, Q. X.
Density functional calculations on a double hydrogen-bonded dimer
Chinese Journal of Structural Chemistry, (24): 184-190 2005.
- Jian, F. F.; Zhao, P. S.; Zhang, L.; Hou, Y. X.
Synthesis of 2,3-diaryltetrazole-5-thiones and theoretical studies on atomic charge distributions of 2,3-diphenyltetrazole-5-thione
Journal of Organic Chemistry, (70): 8322-8326 2005.
- Jiang, L. Y.; Liu, Y. M.
Quantum chemistry calculation of quercetin-silver complex
Chinese Journal of Structural Chemistry, (24): 1340-1346 2005.
- Jin, Q.; Biao, J.; Xu, W. G.; Zhu, W.
Aromaticity of planar P-5(-) anion in the P5M ($M = Li, Na, and K$) clusters
Journal of Molecular Structure-Theochem, (713): 113-117 2005.
- Joo, H.; Biswas, M. A. S.; Hill, W. E.; McKee, M. L.
An experimental and theoretical evaluation of the reactions of silver hyponitrite with phosphorus halides. In search of the elusive phosphorus-containing hyponitrites
Journal of Physical Chemistry A, (109): 1420-1429 2005.
- Joo, H.; McKee, M. L.
Computational study of the "stable" bis(amino)silylene reaction with halomethanes. A radical or concerted mechanism?
Journal of Physical Chemistry A, (109): 3728-3738 2005.
- Joshi, A. M.; Delgass, W. N.; Thomson, K. T.
Comparison of the catalytic activity of Au-3, Au-4(+), Au-5, and Au-5(-) in the gas-phase reaction of H-2 and O-2 to form hydrogen peroxide: A density functional theory investigation
Journal of Physical Chemistry B, (109): 22392-22406 2005.

- Ju, X. H.; Xiao, H. M.; Chen, L. T.
Periodic DFT approach to benzotrifuroxan crystal
International Journal of Quantum Chemistry, (102): 224-229 2005.
- Ju, X. H.; Xu, X. J.; Xiao, H. M.
Computational study of picric acid and potassium picrate
Journal of Energetic Materials, (23): 121-130 2005.
- Jung, J. H.; Kim, J. C.; Han, Y. K.
Structure and electronic properties of Al13X (X=F, Cl, Br, and I) clusters
Physical Review B, (72) 2005.
- Justicia, J.; Oller-Lopez, J. L.; Campana, A. G.; Oltra, J. E.; Cuerva, J. M.; Bunuel, E.; Cardenas, D. J.
7-endo Radical cyclizations catalyzed by titanocene(III). Straightforward synthesis of terpenoids with seven-membered carbocycles
Journal of the American Chemical Society, (127): 14911-14921 2005.
- Kakkar, R.; Pathak, M.; Chadha, P.
Theoretical study of unimolecular rearrangements of vinylidenes to acetylenes
International Journal of Quantum Chemistry, (102): 189-199 2005.
- Kalaiselvan, A.; Venuvanalingam, P.
Oxaphosphetane versus betaine formation in epoxide ring opening by PPh₃: a mechanistic probe by ab initio and DFT modeling
Tetrahedron Letters, (46): 4087-4090 2005.
- Kalaiselvan, A.; Venuvanalingam, P.; Poater, J.; Sola, M.
Ab initio and DFT modeling of stereoselective deamination of aziridines by nitrosyl chloride
International Journal of Quantum Chemistry, (102): 139-146 2005.
- Kamachi, T.; Kouno, T.; Yoshizawa, K.
Participation of multioxidants in the pH dependence of the reactivity of ferrate(VI)
Journal of Organic Chemistry, (70): 4380-4388 2005.
- Kan, Y. H.; Zhu, Y. L.; Hou, L. M.; Su, Z. M.
Electronic structure and optical spectra of tris(8-hydroxyquinolinato)aluminum derivative with mixed ligand containing chlorine: A TDDFT study
Acta Chimica Sinica, (63): 1263-1268 2005.
- Kang, H. S.
Magnetic couplings in vanadium aromatic sandwich complexes and their crystals by using DFT methods
Journal of Physical Chemistry A, (109): 9292-9298 2005.

- Kang, H. S.
Theoretical study of complexes of extended cyclopentadienyl ligands with zinc and cadmium
Journal of Physical Chemistry A, (109): 4342-4351 2005.
- Kang, H. S.
Theoretical study of main-group metal - Borazine sandwich complexes
Journal of Physical Chemistry A, (109): 1458-1467 2005.
- Kaplan, I. G.; Diaz, C. C.
Comparative study of the electron affinities of beryllium and magnesium dimers and trimers
International Journal of Quantum Chemistry, (104): 468-474 2005.
- Karafiloglou, P.; Harcourt, R. D.
Aspects of three-electron two-centre, four-electron three-centre and six-electron five-centre bonding in cycloimmonium ylides
Journal of Molecular Structure-Theochem, (729): 155-161 2005.
- Kassaee, M. Z.; Ghambanian, M.; Musavi, S. M.
In search of triplet ground state GeCNX germylenes ($X = H, F, Cl, and Br$): An ab initio and DFT study
Journal of Organometallic Chemistry, (690): 4692-4703 2005.
- Kassaee, M. Z.; Musavi, S. M.; Buazar, F.
An ab initio and DFT comparative study of electronic effects on spin multiplicities and structures of $X\text{-C}_2\text{N}$ carbenes
Journal of Molecular Structure-Theochem, (728): 15-24 2005.
- Kassaee, M. Z.; Musavi, S. M.; Ghambanian, M.
Divalent propargylenic $\text{C}_2\text{H}_2\text{M}$ group 14 elements: Structures and singlet-triplet energy splittings ($M = C, Si, Ge, Sn$ and Pb)
Journal of Molecular Structure-Theochem, (731): 225-231 2005.
- Kassaee, M. Z.; Musavi, S. M.; Ghambanian, M.; Buazar, F.
Multiplicity vs. stability in C_2HP carbenes and their halogenated analogues: an ab initio and DFT study
Journal of Molecular Structure-Theochem, (726): 171-181 2005.
- Kassaee, M. Z.; Musavi, S. M.; Hamadi, H.; Ghambanian, M.; Hosseini, S. E.
Ab initio and DFT energetics of silylenic $X\text{-CNSi}$ ($X = H, F, Cl, and Br$)
Journal of Molecular Structure-Theochem, (130): 33-44 2005.
- Kaur, D.; Kaur, R. P.

Evaluation of N-H bond dissociation energies in some amides using ab initio and density functional methods

Journal of Molecular Structure-Theochem, (757): 53-59 2005.

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

Amide resonance in thio- and seleno- carbamates: A theoretical study

Journal of Molecular Structure-Theochem, (757): 149-153 2005.

Kawahara, S.; Tsuzuki, S.; Uchimaru, T.

Lewis acidity/basicity of pi-electron systems: theoretical study of a molecular interaction between a pi system and a Lewis acid/base

Chemistry-a European Journal, (11): 4458-4464 2005.

Kazansky, V. B.; Pidko, E. A.

A new insight in the unusual adsorption properties of Cu⁺ cations in Cu-ZSM-5 zeolite

Catalysis Today, (110): 281-293 2005.

Kelly, C. P.; Cramer, C. J.; Truhlar, D. G.

Accurate partial atomic charges for high-energy molecules using class IV charge models with the MIDI! basis set

Theoretical Chemistry Accounts, (113): 133-151 2005.

Kim, C. K.; Lee, K. A.; Sohn, C. K.; Sung, D. D.; Oh, H. K.; Lee, I.

DFT-PCM studies of solvent effects on the cross-interaction constants in benzhydryl cation and anion formation

Journal of Physical Chemistry A, (109): 2978-2983 2005.

Kimura, T.; Murai, T.

P-chiral phosphinoselenoic chlorides and phosphinochalcogenoselenoic acid esters:

Synthesis, characterization, and conformational studies

Journal of Organic Chemistry, (70): 952-959 2005.

Kleinpeter, E.; Schulenburg, A.; Zug, I.; Hartmann, H.

The interplay of thio(seleno)amide/vinylogous thio(seleno)amide "Resonance" and the

anisotropic effect of thiocarbonyl and selenocarbonyl functional groups

Journal of Organic Chemistry, (70): 6592-6602 2005.

Klinker, E. J.; Kaizer, J.; Brennessel, W. W.; Woodrum, N. L.; Cramer, C. J.; Que, L.

Structures of nonheme oxoiron(IV) complexes from x-ray crystallography, NMR spectroscopy, and DFT calculations

Angewandte Chemie-International Edition, (44): 3690-3694 2005.

Kluge, S.; Weston, J.

Can a hydroxide ligand trigger a change in the coordination number of magnesium ions in biological systems?

Biochemistry (Mosc), (44): 4877-4885 2005.

- Kobrsi, I.; Knox, J. E.; Heeg, M. J.; Schlegel, H. B.; Winter, C. H.
Weak carbon-hydrogen-nitrogen interactions affect the heterocyclic ligand bonding modes in barium complexes containing eta(2)-tetrazolato and eta(2)-pentazolato ligands
Inorganic Chemistry, (44): 4894-4896 2005.
- Koch, R.; Bruhn, T.; Weidenbruch, M.
Theoretical group 14 chemistry. 4. Cyclotriplumbanes: Relativistic and substituents effects
Journal of Chemical Theory and Computation, (1): 1298-1303 2005.
- Kochina, T. A.; Ignat'ev, I. S.; Vrazhnov, D. V.
Effect of the electronic structure of carbenium and silylum ions on their chemical behavior
Russian Journal of General Chemistry, (75): 1225-1229 2005.
- Kolandaivel, P.; Praveena, G.; Selvarengan, P.
Study of atomic and condensed atomic indices for reactive sites of molecules
Journal of Chemical Sciences, (117): 591-598 2005.
- Korchowiec, J.
Role of charge-transfer effects in regioselectivity
International Journal of Quantum Chemistry, (101): 714-721 2005.
- Kostova, I.; Trendafilova, N.; Mihaylov, T.
Theoretical and spectroscopic studies of pyridyl substituted bis-coumarins and their new neodymium(III) complexes
Chemical Physics, (314): 73-84 2005.
- Krivdin, L. B.; Scherbina, N. A.; Istomina, N. V.
Non-empirical calculations of NMR indirect carbon-carbon coupling constants. Part 12 - Aliphatic and alicyclic oximes
Magnetic Resonance in Chemistry, (43): 435-443 2005.
- Kumar, P. S.; Bharatam, P. V.
Theoretical studies on the S-N interactions in sulfoximine
Tetrahedron, (61): 5633-5639 2005.
- Kumar, P. S.; Singh, P.; Uppal, P.; Bharatam, P. V.
Electronic structure of sulfimides: A theoretical study
Bulletin of the Chemical Society of Japan, (78): 1417-1424 2005.
- Kuramshina, G. M.; Takahashi, H.
Ab initio and DFT theoretical studies of pyridoxal-5'-phosphate methylamine Schiff base isomers
Journal of Molecular Structure, (735-36): 39-51 2005.

- Kusama, H.; Sugihara, H.
Theoretical study of quinolines-I-2 intermolecular interaction and implications on dye-sensitized solar cell performance
Journal of Computational Chemistry, (26): 1372-1382 2005.
- Kutateladze, A. G.; McHale, W. A.
Toward parameterization of spin-orbit coupling in triplet organic diradicals separated by a partially conjugated spacer
Arkivoc: 88-101 2005.
- Kuwata, K. T.; Valin, L. C.; Converse, A. D.
Quantum chemical and master equation studies of the methyl vinyl carbonyl oxides formed in isoprene ozonolysis
Journal of Physical Chemistry A, (109): 10710-10725 2005.
- Kuznetsov, M. L.; Dement'ev, A. I.; Nazarov, A. A.
Theoretical analysis of the vibrational spectra and the nature of the coordination bond of platinum nitrile complexes
Russian Journal of Inorganic Chemistry, (50): 731-739 2005.
- Kuznetsov, M. L.; Nazarov, A. A.; Pombeiro, A. J. L.
Protic conversion of nitrile into azavinylidene complexes of rhenium, a mechanistic theoretical study
Journal of Physical Chemistry A, (109): 8187-8198 2005.
- Kwon, O.; Barlow, S.; Odom, S. A.; Beverina, L.; Thompson, N. J.; Zojer, E.; Bredas, J. L.; Marder, S. R.
Aromatic amines: A comparison of electron-donor strengths
Journal of Physical Chemistry A, (109): 9346-9352 2005.
- Laali, K. K.; Hupertz, S.; Temu, A. G.; Galembeck, S. E.
Electrospray mass spectrometric and DFT study of substituent effects in Ag⁺ complexation to polycyclic aromatic hydrocarbons (PAHs)
Organic & Biomolecular Chemistry, (3): 2319-2326 2005.
- Ladinig, M.; Leupin, W.; Meuwly, M.; Respondek, M.; Wirz, J.; Zoete, V.
Protonation equilibria of Hoechst 33258 in aqueous solution
Helvetica Chimica Acta, (88): 53-67 2005.
- Laitar, D. S.; Muller, P.; Gray, T. G.; Sadighi, J. P.
A carbene-stabilized gold(I) fluoride: Synthesis and theory
Organometallics, (24): 4503-4505 2005.
- Lam, C. S.; Li, W. K.; Chiu, S. W.

G3(MP2) study of the C₃H₆O+center dot isomers fragmented from 1,4-dioxane(+center dot)

Journal of Physical Chemistry A, (109): 7296-7308 2005.

Lamsabhi, A. M.; Escobar, C. A.; Perez, P.

Do substituents make any contribution to the formation of systems where the electronic effects seem to be neutralized? The case of the indigo dye formation

Journal of Physical Organic Chemistry, (18): 1161-1168 2005.

Latosinska, J. N.

Structure-activity study of thiazides by magnetic resonance methods (NQR, NMR, EPR) and DFT calculations

J Mol Graph Model, (23): 329-337 2005.

Lau, K. C.; Deshpande, M.; Pandey, R.

A theoretical study of vibrational properties of neutral and cationic B-12 clusters

International Journal of Quantum Chemistry, (102): 656-664 2005.

Laurence, C.; Berthelot, M.; Evain, K.; Illien, B.

pK(HB) scales and hydrogen bond acceptor strength enthalpies of thioethers, thiols et disulfides

Canadian Journal of Chemistry-Revue Canadienne De Chimie, (83): 138-145 2005.

Lecea, B.; Arrieta, A.; Cossio, F. P.

Substituent effects in eight-electron electrocyclic reactions

Journal of Organic Chemistry, (70): 1035-1041 2005.

Lee, E. C.; Hong, B. H.; Lee, J. Y.; Kim, J. C.; Kim, D.; Kim, Y.; Tarakeshwar, P.; Kim, K. S.

Substituent effects on the edge-to-face aromatic interactions

Journal of the American Chemical Society, (127): 4530-4537 2005.

Lev, D. A.; Grotjahn, D. B.; Amouri, H.

Reversal of reactivity in diene-complexed o-quinone methide complexes: Insights and explanations from ab initio density functional theory calculations

Organometallics, (24): 4232-4240 2005.

Leyssens, T.; Geerlings, P.; Peeters, D.

The importance of the external potential on group electronegativity

Journal of Physical Chemistry A, (109): 9882-9889 2005.

Li, J. S.; Huang, Y. G.; Dong, H. S.

A theoretical study of polynitropyridines and their N-oxides

Journal of Energetic Materials, (23): 133-149 2005.

Li, M.; Tang, D. Y.; Luo, X. L.; Shen, W.

Mechanism of asymmetric hydrogenation of enamides with [Rh(BisP)](+) catalyst: Model DFT study*
International Journal of Quantum Chemistry, (102): 53-63 2005.

Li, Q. S.; Duan, H. X.
A theoretical study of the structures and stabilities of N4O2 isomers
Molecular Physics, (103): 249-256 2005.

Li, Q. S.; Zhao, Y.; Xu, W. G.; Li, N.
Structure and stability of B-8 clusters
International Journal of Quantum Chemistry, (101): 219-229 2005.

Li, S. D.; Guo, J. C.; Miao, C. Q.; Ren, G. M.
[(eta(6)-B6X)(2)M] (X = C, N; M = Mn, Fe, Co, Ni): A new class of transition-metal sandwich-type complexes
Angewandte Chemie-International Edition, (44): 2158-2161 2005.

Li, W. Q.; Tian, W. Q.; Feng, J. K.; Liu, Z. Z.; Ren, A. M.; Zhang, G.
Theoretical studies on the structure and aromaticity of Ti2P6+
Journal of Physical Chemistry A, (109): 8391-8397 2005.

Li, Y.; Li, Z. R.; Wu, D.; Chen, W.; Sun, C. C.
The trigonal bipyramidal MN3M species: A new kind of aromatic complex containing a multiple-fold aromatic N-3 subunit
Chemphyschem, (6): 2562-2569 2005.

Liang, J.; Li, H. Y.; Liu, Y.; Cheng, S.
Complexes of alkali metal cations with trifluoromethyl: A computational investigation on the structure and stability of M+-(CF3) (M = Li, Na, K) isomers
Journal of Molecular Structure-Theochem, (725): 151-155 2005.

Lilly, M. J.; Miller, N. A.; Edwards, A. J.; Willis, A. C.; Turner, P.; Paddon-Row, M. N.;
Sherburn, M. S.
Allylic stereocontrol of the intramolecular Diels-Alder reaction
Chemistry-a European Journal, (11): 2525-2536 2005.

Lin, Y. L.; Lee, Y. M.; Lim, C.
Differential effects of the Zn-His-Bkb vs Zn-His-[Asp/Glu] triad on Zn-core stability and reactivity
Journal of the American Chemical Society, (127): 11336-11347 2005.

Liu, F. L.; Wang, J. S.; Peng, L.
DFT study on two C4N12O4 isomers with pagodane- and isopagodane-like structures
Chinese Journal of Structural Chemistry, (24): 1264-1270 2005.

Liu, J.; Hadad, C. M.; Platz, M. S.

The reaction of triplet nitrenes with oxygen: A computational study
Organic Letters, (7): 549-552 2005.

Liu, J. N.; Chen, Z. R.; Yuan, S. F.
Prediction of visible absorption of pyridone azo compounds
Acta Physico-Chimica Sinica, (21): 402-407 2005.

Liu, K. H.; Pu, M.; Chen, B. H.
DFT study on the structure of ionic liquid 1-ethyl-3-methylimidazolium hexafluorophosphate
Chinese Journal of Structural Chemistry, (24): 576-580 2005.

Liu, K. H.; Pu, M.; Li, H. Y.; Chen, B. H.
Quantum chemistry study of the ionic liquid 1-ethyl-3-methylimidazolium tetrafluoroborate
Chinese Journal of Chemical Physics, (18): 331-335 2005.

Liu, X. W.; Bao, P.; Ma, Y. P.; Yu, Z. H.
The difference in the degree of localization between the LFMO and NBO basis sets, and its effects on the energy partitions
Journal of Molecular Structure-Theochem, (729): 185-191 2005.

Liu, X. W.; Bao, P.; Xuan, Z. Q.; Yu, Z. H.
Analysis of molecular distortion over the NBO and LFMO basis sets with the automatic d(SH) program
Acta Chimica Sinica, (63): 2229-2237 2005.

Liu, Y.; Lopez, X.; York, D. M.
Kinetic isotope effects on thio-substituted biological phosphoryl transfer reactions from density-functional theory
Chemical Communications: 3909-3911 2005.

Liu, Y.; Nekvasil, H.; Tossell, J.
Explaining the effects of T-O-T bond angles on NMR chemical shifts in aluminosilicates: A natural bonding orbital (NBO) and natural chemical shielding (NCS) analysis
Journal of Physical Chemistry A, (109): 3060-3066 2005.

Ljubic, I.; Sabljic, A.
Fluorocarbonyl oxide: CASSCF/CASPT2 study of structure, cis effect and unimolecular decomposition paths
Chemical Physics, (309): 157-165 2005.

Loncke, P. G.; Peslherbe, G. H.
Substituent effects and the role of negative hyperconjugation in siloxycarbene rearrangements
Organic & Biomolecular Chemistry, (3): 2191-2201 2005.

- Lopez, C. S.; Faza, A. N.; Cossio, F. P.; York, D. M.; de Lera, A. R.
Ellipticity: A convenient tool to characterize electrocyclic reactions
Chemistry-a European Journal, (11): 1734-1738 2005.
- Lord, R. L.; Wheeler, S. E.; Schaefer, H. F.
The pentacyanocyclopentadienyl system: Structures and energetics
Journal of Physical Chemistry A, (109): 10084-10091 2005.
- Lorenz, I. P.; Maier, M.; Schulz, A.
On the electronic structure and bonding of the intriguing mixed Fe²⁺/Fe³⁺ [{Cp(CO)(2)Fe}(Bu₂Po₂FeCl₂)-Bu-t](2)-complex
Heteroatom Chemistry, (16): 398-405 2005.
- Luo, X. L.; Tang, D. Y.; Li, M.
Quantum investigation on the mechanism of isomerization of 1-butylene catalyzed by Rh-complex
Journal of Molecular Structure-Theochem, (731): 139-147 2005.
- Luo, X. L.; Tang, D. Y.; Li, M.
Computational investigation of enantio- and regioselectivity of rhodium-catalyzed asymmetric hydroformylation of vinyl formate with CHIRAPHOS-type ligand
International Journal of Quantum Chemistry, (105): 108-123 2005.
- Luo, X. L.; Tang, D. Y.; Li, M.
Computational experiment on hydroformylation and hydrogenation of ethyne catalyzed by Rh complex: a competitive study
Journal of Molecular Structure-Theochem, (714): 179-188 2005.
- Luo, X. L.; Tang, D. Y.; Li, M.
Computational experiment on hydroformylation and hydrogenation of propenal catalyzed by Rh complex: a competitive study
Journal of Molecular Structure-Theochem, (714): 61-72 2005.
- Luo, Y.; Baldamus, J.; Tardif, O.; Hou, Z. M.
DFT study of the tetrานuclear lutetium and yttrium polyhydride cluster complexes [(C₅Me₄SiMe₃)(4)Ln(4)Hs(8)] (Ln = Lu, Y) that contain a four-coordinate hydrogen atom
Organometallics, (24): 4362-4366 2005.
- Machura, B.; Jaworska, M.; Kruszynski, R.
The synthesis, spectroscopic characterisation, crystal and molecular structure of the [ReCl₃(NO)(OPPh₃)(pyz)] complex. DFT calculations for [ReCl₃(NO)(OPPh₃)(pyz)] and [ReCl₃(NO)(OPPh₃) (PPh₃)]
Polyhedron, (24): 267-279 2005.

Machura, B.; Kruszynski, R.; Jaworska, M.

Synthesis, crystal, molecular and electronic structure of rhenium nitrosyl with pyrazole in the coordination sphere

Inorganic Chemistry Communications, (8): 960-965 2005.

Machura, B.; Kruszynski, R.; Jaworska, M.

Reactivity of [ReOX₃(PPh₃)₂] complexes towards 1,4-diaminobenzene: X-ray structure and DFT calculations of the [Re(4-NC₆H₄NH₂)Cl-3(PPh₃)₂]center dot PPh₃ complex

Polyhedron, (24): 1454-1460 2005.

Machura, B.; Kruszynski, R.; Jaworska, M.; Lodowski, P.

Synthesis, spectroscopic characterization, crystal, molecular and electronic structure of the [{ReOBr₂(pyz)(2)}(2)(mu-O)] and [{ReOBr₂

Polyhedron, (24): 1893-1906 2005.

Maire, P.; Buttner, T.; Breher, F.; Le Floch, P.; Grutzmacher, H.

Heterolytic splitting of hydrogen with rhodium(I) amides

Angewandte Chemie-International Edition, (44): 6318-6323 2005.

Malar, E. J. P.

Density functional theory analysis of some triple-decker sandwich complexes of iron containing cyclo-P-5 and cyclo-As-5 ligands

Theoretical Chemistry Accounts, (114): 213-221 2005.

Malde, A.; Khedkar, S.; Coutinho, E.; Saran, A.

Geometry, transition states, and vibrational spectra of boron isostere of N-methylacetamide by ab initio calculations

International Journal of Quantum Chemistry, (102): 734-742 2005.

Manard, M. J.; Kemper, P. R.; Bowers, M. T.

Probing the structure of gas-phase metallic clusters via ligation energetics: Sequential addition of C₂H₄ to Ag-m(+) (m=3-7)

Journal of the American Chemical Society, (127): 9994-9995 2005.

Manard, M. J.; Kemper, P. R.; Bowers, M. T.

Binding interactions of mono- and diatomic silver cations with small alkenes: experiment and theory

International Journal of Mass Spectrometry, (241): 109-117 2005.

Manz, T. A.; Fenwick, A. E.; Phomphrai, K.; Rothwell, I. P.; Thomson, K. T.

The nature of aryloxide and arylsulfide ligand bonding in dimethyltitanium complexes containing cyclopentadienyl ligation

Dalton Transactions: 668-674 2005.

Marincean, S.; Custelcean, R.; Stein, R. S.; Jackson, J. E.

Structural reinvestigation of ammonium hypophosphite: Was dihydrogen bonding observed long ago?

Inorganic Chemistry, (44): 45-48 2005.

Martin, F.; Zipse, H.

Charge distribution in the water molecule - A comparison of methods

Journal of Computational Chemistry, (26): 97-105 2005.

Martinez, M.; Michelin, M. D.; Rivalta, I.; Russo, N.; Sicilia, E.

Acetylene cyclotrimerization by early second-row transition metals in the gas phase. A theoretical study

Inorganic Chemistry, (44): 9807-9816 2005.

Martins, J. B. L.; Fialho, T. A. S.

Interaction of pyridine on Nb₂O₅

Journal of Molecular Structure-Theochem, (732): 1-5 2005.

Matito, E.; Poater, J.; Sola, M.; Duran, M.; Salvador, P.

Comparison of the AIM delocalization index and the Mayer and Fuzzy atom bond orders

Journal of Physical Chemistry A, (109): 9904-9910 2005.

Matos, M. A. R.; Morais, V. M. F.; da Silva, M.; Marques, M. C. F.; Sousa, E. A.; Castineiras, J. P.; Santos, C. P.; Acree, W. E.

Thermochemical and theoretical studies of dimethylpyridine-2,6-dicarboxylate and pyridine-2,3-, pyridine-2,5-, and pyridine-2,6-dicarboxylic acids

Journal of Chemical and Engineering Data, (50): 1184-1191 2005.

Matsumoto, K.; Arai, S.; Ochiai, M.; Chen, W. Z.; Nakata, A.; Nakai, H.; Kinoshita, S.

Synthesis of the pivalamidate-bridged pentanuclear platinum(II,III) linear complexes with Pt center dot center dot center dot Pt interactions

Inorganic Chemistry, (44): 8552-8560 2005.

Matyjaszewski, K.; Poli, R.

Comparison of bond dissociation energies of dormant species relevant to degenerative transfer and atom transfer radical polymerization

Macromolecules, (38): 8093-8100 2005.

Mawhinney, R. C.; Muchall, H. M.; Peslherbe, G. H.

A computational study of the 1,3-dipolar cycloaddition reaction mechanism for nitrilimines

Canadian Journal of Chemistry-Revue Canadienne De Chimie, (83): 1615-1625 2005.

McDowell, S. A. C.

Redshift and blueshift of the Ar-H vibrational stretching frequency in complexes of FArH and acetylene

Journal of Chemical Physics, (122) 2005.

- McDowell, S. A. C.
A computational study of the hydrogen-bonded complexes FArH center dot center dot center OCO and FKrH center dot center dot center OCO
Chemical Physics Letters, (406): 228-231 2005.
- McDowell, S. A. C.; Buckingham, A. D.
A theory of vibrational frequency shifts revisited: application to dimers of LiH with the inert gases He, Ne, Ar and Kr
Molecular Physics, (103): 257-262 2005.
- McGrady, G. S.; Haaland, A.; Verne, H. P.; Volden, H. V.; Downs, A. J.; Shorokhov, D.; Eickerling, G.; Scherer, W.
Valence shell charge concentrations at pentacoordinate d(0) transition-metal centers: Non-VSEPR structures of Me(2)NhCl(3) and Me3NbCl2
Chemistry-a European Journal, (11): 4921-4934 2005.
- Meek, T. L.; Garner, L. D.
Electronegativity and the bond triangle
Journal of Chemical Education, (82): 325-333 2005.
- Mendizabal, F.; Zapata-Torres, G.; Olea-Azar, C.
Theoretical study of the interaction d(10)-s(2) between Pt(0) and Tl(I) on the [Pt(PH3)(3)Tl](+) complex
Chemical Physics Letters, (412): 477-481 2005.
- Mendoza-Wilson, A. M.; Glossman-Mitnik, D.
CHIH-DFT study of the electronic properties and chemical reactivity of quercetin
Journal of Molecular Structure-Theochem, (716): 67-72 2005.
- Meng, F. C.; Wang, H. J.; Xu, W. R.; Liu, C. B.
Substituent effect of large conjugate groups on the DNA base pair derivatives: Density functional study
International Journal of Quantum Chemistry, (104): 79-86 2005.
- Meng, F. C.; Wang, H. J.; Xu, W. R.; Liu, C. B.
Theoretical study of GC(+)/GC base pair derivatives
Chemical Physics, (308): 117-123 2005.
- Meng, Q. X.; Li, M.; Zhang, J. S.
The computational study on the mechanism of rhodium(I)-catalyzed asymmetric carbonylative [4+1] cycloaddition with (R,R)-Me-DuPHOS-type ligand. A DFT study
Journal of Molecular Structure-Theochem, (726): 47-54 2005.
- Mercier, H. P. A.; Moran, M. D.; Sanders, J. C. P.; Schrobilgen, G. J.; Suontamo, R. J.

Synthesis, structural characterization, and computational study of the strong oxidant salt [XeOTeF5][Sb(OTeF5)(6)]center dot SO2CIF
Inorganic Chemistry, (44): 49-60 2005.

Merino, G.; Vela, A.; Heine, T.

Description of electron delocalization via the analysis of molecular fields
Chemical Reviews, (105): 3812-3841 2005.

Mikosch, H.; Uzunova, E. L.; St Nikolov, G.

Interaction of molecular nitrogen and oxygen with extraframework cations in zeolites with double six-membered rings of oxygen-bridged silicon and aluminum atoms: A DFT study
Journal of Physical Chemistry B, (109): 11119-11125 2005.

Misaizu, F.; Tsuruta, M.; Tsunoyama, H.; Furuya, A.; Ohno, K.; Lintuluoto, M.

Size-dependent structures of NanIn-1+ cluster ions with a methanol adsorbate: A combined study by photodissociation spectroscopy and density-functional theory calculation

Journal of Chemical Physics, (123) 2005.

Mitrasinovic, P. M.

Cross-linking between thymine and indolyl radical: Possible mechanisms for cross-linking of DNA and tryptophan-containing peptides
Bioconjugate Chemistry, (16): 588-597 2005.

Mitzel, N. W.; Vojinovic, K.; Foerster, T.; Robertson, H. E.; Borisenko, K. B.; Rankin, D. W. H.
(Dimethylaminomethyl)trifluorosilane, Me₂NCH₂SiF₃ - A model for the alpha-effect in aminomethylsilanes
Chemistry-a European Journal, (11): 5114-5125 2005.

Mitzel, N. W.; Vojinovic, K.; Frohlich, R.; Foerster, T.; Robertson, H. E.; Borisenko, K. B.; Rankin, D. W. H.
Three-membered ring or open chain molecule - (F₃C)F₂SiONMe₂ a model for the alpha-effect in silicon chemistry
Journal of the American Chemical Society, (127): 13705-13713 2005.

Mo, O.; Yanez, M.; Del Bene, J. E.; Alkorta, L.; Elguero, J.

Cooperativity and proton transfer in hydrogen-bonded triads
Chempyschem, (6): 1411-1418 2005.

Mo, O.; Yanez, M.; Eckert-Maksic, M.; Maksic, Z. B.; Alkorta, I.; Elguero, J.
Periodic trends in bond dissociation energies. A theoretical study
Journal of Physical Chemistry A, (109): 4359-4365 2005.

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

A theoretical study on the dimers of aminoacrylonitrile (3-amino-2-propenenitrile), a compound of astrochemical interest
Arkivoc: 239-252 2005.

Mochizuki, Y.; Fukuzawa, K.; Kato, A.; Tanaka, S.; Kitaura, K.; Nakano, T.
1A configuration analysis for fragment interaction
Chemical Physics Letters, (410): 247-253 2005.

Monajjemi, M.; Chahkandi, B.
Theoretical investigation of hydrogen bonding in Watson-Crick, Hoogesteijn and their reversed and other models: comparison and analysis for configurations of adenine-thymine base pairs in 9 models
Journal of Molecular Structure-Theochem, (714): 43-60 2005.

Monajjemi, M.; Ghiasi, R.; Abedi, A.
Theoretical investigation of the interaction of cytosine and its tautomers with alkali metals
Russian Journal of Inorganic Chemistry, (50): 382-388 2005.

Monajjemi, M.; Sajadi, M. A. S.; Sayadia, R.; Kia, M.; Ghasemi, G.
Structural studies and investigation of NMR shielding tensors in coordination of magnesium hydrate to purine nucleotide 5'-monophosphates (AMP, GMP, IMP)
Main Group Metal Chemistry, (28): 71-84 2005.

Monajjemi, M.; Sayyadia, R.; Ghasemi, G.; Lalateh, K.; Nouria, A.; Naderi, F.
Bond energies and phosphate-coordination of magnesium hydrate to pyrimidine nucleotide 5'-monophosphates (CMP, UMP, dTMP) and NMR shielding tensors
Main Group Metal Chemistry, (28): 247-263 2005.

Monev, V.; Spassova, M.; Champagne, B.
Charge distributions in polyacetylene chains containing a positively charged defect
International Journal of Quantum Chemistry, (104): 354-366 2005.

Moore, D. T.; Oomens, J.; Eyler, J. R.; von Helden, G.; Meijer, G.; Dunbar, R. C.
Infrared spectroscopy of gas-phase Cr⁺ coordination complexes: Determination of binding sites and electronic states
Journal of the American Chemical Society, (127): 7243-7254 2005.

Morales, J.; Espinos, J. P.; Caballero, A.; Gonzalez-Elipe, A. R.; Mejias, J. A.
XPS study of interface and ligand effects in supported Cu₂O and CuO nanometric particles
Journal of Physical Chemistry B, (109): 7758-7765 2005.

Morgan, K. M.; Rawlins, M. L.; Montgomery, M. N.
Influence of methyl substituents on the stability of 1-aza-2-adamantanone, Kirby's most twisted amide

Journal of Physical Organic Chemistry, (18): 310-314 2005.

Moskaleva, L. V.; Rosch, N.

Lewis base interaction with gallium hydrides: a computational study
Inorganica Chimica Acta, (358): 4163-4171 2005.

Mothana, B.; Ban, F.; Boyd, R. J.; Thompson, A.; Hadden, C. E.

The effect of electron-withdrawing groups on N-15 and C-13 chemical shifts: a density functional study on a series of pyrroles
Molecular Physics, (103): 1113-1129 2005.

Mrazkova, E.; Hobza, P.; Bohl, M.; Gauger, D. R.; Pohle, W.

Hydration-induced changes of structure and vibrational frequencies of methylphosphocholine studied as a model of biomembrane lipids
Journal of Physical Chemistry B, (109): 15126-15134 2005.

Mucsi, Z.; Szabo, A.; Hermecz, I.; Kucsman, A.; Csizmadia, I. G.

Modeling rate-controlling solvent effects. The pericyclic meisenheimer rearrangement of N-propargylmorpholine N-oxide
Journal of the American Chemical Society, (127): 7615-7631 2005.

Mudring, A. V.; Babai, A.; Arenz, S.; Giernoth, R.

The "Noncoordinating" anion Tf₂N- coordinates to Yb²⁺: A structurally characterized Tf₂N- complex from the ionic liquid [mppyr][Tf₂N]
Angewandte Chemie-International Edition, (44): 5485-5488 2005.

Muller-Rosing, H. C.; Schulz, A.; Hargittai, M.

Structure and bonding in silver halides. A quantum chemical study of the monomers: Ag₂X, AgX, AgX₂, and AgX₃ (X = F, Cl, Br, I)
Journal of the American Chemical Society, (127): 8133-8145 2005.

Mutoh, Y.; Murai, T.

Chalcogenoiminium salts: Systematic synthesis and applications to carbon-carbon bond forming reactions
Journal of Synthetic Organic Chemistry Japan, (63): 815-824 2005.

Nakanishi, W.; Yamanaka, M.; Nakamura, E.

Reactivity and stability of organocopper(I), silver(I), and gold(I) ate compounds and their trivalent derivatives
Journal of the American Chemical Society, (127): 1446-1453 2005.

Nam, K.; Gao, J. L.; York, D. M.

An efficient linear-scaling Ewald method for long-range electrostatic interactions in combined QM/MM calculations
Journal of Chemical Theory and Computation, (1): 2-13 2005.

Navarro-Vazquez, A.; Schreiner, P. R.

1,2-didehydro[10]annulenes: Structures, aromaticity, and cyclizations

Journal of the American Chemical Society, (127): 8150-8159 2005.

Nazmutdinov, R. R.; Zinkicheva, T. T.

Adsorption of the fluoride ion on the surface of various faces of a single crystal of silver: A quantum-chemical study

Russian Journal of Electrochemistry, (41): 206-212 2005.

Nazmutdinov, R. R.; Zinkicheva, T. T.; Probst, M.; Lust, K.; Lust, E.

Adsorption of halide ions from aqueous solutions at a Cd(0001) electrode surface: quantum chemical modelling and experimental study

Surface Science, (577): 112-126 2005.

Nechaev, M. S.; Ustyynyuk, Y. A.

Molecular geometry and electronic structures of stable organic derivatives of divalent germanium and tin [(Me₃Si)(2)N-M-OCH₂CH₂ Me-2]n (M = Ge, n=1; M = Sn, n=2): a theoretical study

Russian Chemical Bulletin, (54): 108-116 2005.

Nemes, G. C.; Ranaivonjatovo, H.; Escudie, J.; Silaghi-Dumitrescu, I.; Silaghi-Dumitrescu, L.; Gornitzka, H.

A surprisingly stable 1-(chlorosilyl)-2-phosphaethenyllithium compound, RCl₂SiC(Li)=PMes

European Journal of Inorganic Chemistry: 1109-1113 2005.

Nemukhin, A. V.; Rogachev, A. Y.; Konyukhov, S. V.; Bochenkova, A. V.; Granovsky, A. A.

QM/MM modeling of the structures and properties of the beta-diketonate-based lanthanide complexes

International Journal of Quantum Chemistry, (104): 203-213 2005.

Nguyen, T.; Sutton, A. D.; Brynda, S.; Fettinger, J. C.; Long, G. J.; Power, P. P.

Synthesis of a stable compound with fivefold bonding between two chromium(I) centers

Science, (310): 844-847 2005.

Ni, Z. P.; Ren, X. M.; Ma, J.; Xie, J. L.; Ni, C. L.; Chen, Z. D.; Meng, Q. J.

Theoretical studies on the magnetic switching controlled by stacking patterns of bis(maleonitriledithiolato) nickelate(III) dimers

Journal of the American Chemical Society, (127): 14330-14338 2005.

Niemeyer, M.

An unusual biphenylsubstituted lithiumchlorotriarylsamarate

Zeitschrift Fur Anorganische Und Allgemeine Chemie, (631): 1413-1418 2005.

Nikolai, J.; Maas, G.; Taubmann, G.

Boron trifluoride activated enaminocarbonyl compounds: the influence of intermolecular interactions on the ab initio determination of structures and vibrational spectra
Journal of Physical Organic Chemistry, (18): 217-226 2005.

Nilsson, A.; Ogasawara, H.; Cavalleri, M.; Nordlund, D.; Nyberg, M.; Wernet, P.; Pettersson, L. G. M.
The hydrogen bond in ice probed by soft x-ray spectroscopy and density functional theory
Journal of Chemical Physics, (122) 2005.

Nirmala, V.; Kolandaivel, P.
Density functional studies on hydrogen-bonded clusters of hydrogen halides and the interaction on halide anions
International Journal of Quantum Chemistry, (103): 322-331 2005.

Notario, R.; Quijano, J.; Sanchez, C.; Velez, E.
Theoretical study of the mechanism of thermal decomposition of carbonate esters in the gas phase
Journal of Physical Organic Chemistry, (18): 134-141 2005.

Nyerges, B.; Kovacs, A.
Density functional study of the conformational space of C-4(1) D-glucuronic acid
Journal of Physical Chemistry A, (109): 892-897 2005.

Oh, H. K.; Jin, Y. C.; Sung, D. D.; Lee, I.
Kinetics and mechanism of the aminolysis of aryl thiocarbamates: effects of the non-leaving group
Organic & Biomolecular Chemistry, (3): 1240-1244 2005.

Oh, H. K.; Lee, J. M.; Sung, D. D.; Lee, I.
Kinetics and mechanism of the addition of benzylamines to benzylidene-3,5-heptadione in acetonitrile
Journal of Organic Chemistry, (70): 3089-3093 2005.

Ohno, K.; Okimura, M.; Akai, N.; Katsumoto, Y.
The effect of cooperative hydrogen bonding on the OH stretching-band shift for water clusters studied by matrix-isolation infrared spectroscopy and density functional theory
Physical Chemistry Chemical Physics, (7): 3005-3014 2005.

Okamoto, K.; Fukuzumi, S.
Hydrogen bonds not only provide a structural scaffold to assemble donor and acceptor moieties of zinc porphyrin-quinone dyads but also control the photoinduced electron transfer to afford the long-lived charge-separated states
Journal of Physical Chemistry B, (109): 7713-7723 2005.

Olah, J.; De Proft, F.; Vespremi, T.; Geerlings, P.
Hard-soft acid-base interactions of silylenes and germylenes

Journal of Physical Chemistry A, (109): 1608-1615 2005.

Olson, E. W.; Standard, J. M.

Structure and bonding in hexamethyldisilazane and a series of analogues, (XH₃)(2)YH (X = CSi, Ge and Y=N, P, As), by ab initio and density functional methods

Journal of Molecular Structure-Theochem, (719): 17-30 2005.

Orian, L.; Ganis, P.; Santi, S.; Ceccon, A.

Molecular conformations and pi-hydrogen bonds in anti- and syn-binuclear Rh(I) complexes of as-indacene-diide: a computational study

Journal of Organometallic Chemistry, (690): 482-492 2005.

Orimoto, Y.; Naka, K.; Aoki, Y.

N130-based CI/MP through-space/bond interaction analysis and its application to stereoelectronic effects in S(N)2 reactions

International Journal of Quantum Chemistry, (104): 911-918 2005.

Orti, E.; Viruela, P. M.; Viruela, R.; Effenberger, F.; Hernandez, V.; Navarrete, J. T. L.

Raman and theoretical study of the solvent effects on the sizable intramolecular charge transfer in the push-pull 5-(dimethylamino)-5'-nitro-2,2'-bithiophene

Journal of Physical Chemistry A, (109): 8724-8731 2005.

Ozturk, C.; Aviyente, V.; Houk, K. N.

Modeling the stereoselectivity of the Johnson-Claisen rearrangements in the Danishefsky synthesis of gelsemine

Journal of Organic Chemistry, (70): 7028-7034 2005.

Pacios, L. F.; Galvez, O.; Gomez, P. C.

Variation of geometries and electron properties along proton transfer in strong hydrogen-bond complexes

Journal of Chemical Physics, (122) 2005.

Pakiari, A. H.; Nazari, F.

The study of relationship between chemical geometry and electronic configuration, non-Walsh type B Part II

Journal of Molecular Structure-Theochem, (717): 189-197 2005.

Paredes-Garcia, V.; Cardenas-Jiron, G. I.; Venegas-Yazigi, D.; Zagal, J. H.; Paez, M.;

Costamagna, J.

Through-space and through-bond mixed charge transfer mechanisms on the hydrazine oxidation by cobalt(II) phthalocyanine in the gas phase

Journal of Physical Chemistry A, (109): 1196-1204 2005.

Park, S. S.

Structural and bonding trends among the B7C11-, B6C2, and B5C3I+

Bulletin of the Korean Chemical Society, (26): 63-71 2005.

- Park, S. S.; Liu, D.; Hagelberg, F.
Comparative investigation on non-IPR C-68 and IPR C-78 fullerenes encaging Sc₃N molecules
Journal of Physical Chemistry A, (109): 8865-8873 2005.
- Parra, R. D.; Bulusu, S.; Zeng, X. C.
Cooperative effects in two-dimensional ring-like networks of three-center hydrogen bonding interactions
Journal of Chemical Physics, (122) 2005.
- Pavel, I.; Cota, S.; Cinta-Pinzaru, S.; Kiefer, W.
Raman, surface enhanced Raman spectroscopy, and DFT calculations: A powerful approach for the identification and characterization of 5-fluorouracil anticarcinogenic drug species
Journal of Physical Chemistry A, (109): 9945-9952 2005.
- Peralta, J. E.; Batista, E. R.; Scuseria, G. E.; Martin, R. L.
All-electron hybrid density functional calculations on UF_n and UCl_n (n=1-6)
Journal of Chemical Theory and Computation, (1): 612-616 2005.
- Petit, L.; Adamo, C.; Russo, N.
Absorption spectra of first-row transition metal complexes of bacteriochlorins: A theoretical analysis
Journal of Physical Chemistry B, (109): 12214-12221 2005.
- Petz, W.; Kutschera, C.; Heitbaum, M.; Frenking, G.; Tonner, R.; Neumuller, B.
Experimental and theoretical studies of carbodiphosphorane-CX₂ adducts with unusual bonding situations: Preparation, crystal structures, and bonding analyses of S₂CC(PPh₃)₂, O₂CC(PPh₃)₂, and [(CO)(4)MS₂CC(PPh₃)₂] (M = Cr, Mo, W)
Inorganic Chemistry, (44): 1263-1274 2005.
- Pichierri, F.; Kumar, V.; Kawazoe, Y.
Encapsulation of halide anions in perhydrogenated silicon fullerene: X-@Si₂₀H₂₀ (X = F, Cl, Br, I)
Chemical Physics Letters, (406): 341-344 2005.
- Pidko, E.; Kazansky, V.
sigma-Type ethane adsorption complexes with Cu⁺ ions in Cu(I)-ZSM-5 zeolite. Combined DRIFTS and DFT study
Physical Chemistry Chemical Physics, (7): 1939-1944 2005.
- Pinter, B.; De Proft, F.; Vespremi, T.; Geerlings, P.
Regioselectivity in the [2+2] cyclo-addition reaction of triplet carbonyl compounds to substituted alkenes (Paterno-Buchi reaction): A spin-polarized conceptual DFT approach

Journal of Chemical Sciences, (117): 561-571 2005.

Pirani, A. M.; Mercier, H. P. A.; Suontamo, R. J.; Schrobilgen, G. J.; Santry, D. P.; Borrmann, H.

Syntheses; Se-77, (Tl)-T-203, and (Tl)-T-205 NMR; and theoretical studies of the Tl₂Se_{6,6-}, Tl₃Se₆₅₋, and Tl₃Se₇₅₋ anions and the X-ray crystal structures of [2,2,2-crypt-Na](4)[Tl₄Se₈]center dot en and [2,2,2-crypt-Na](2)[Tl₂Se₄](infinity)(1)center dot en

Inorganic Chemistry, (44): 8770-8785 2005.

Planas, J. G.; Vinas, C.; Teixidor, F.; Comas-Vives, A.; Ujaque, G.; Lledos, A.; Light, M. E.; Hursthouse, M. B.

Self-assembly of mercaptane-metallacarborane complexes by an unconventional cooperative effect: A C-H center dot center dot center dot S-H center dot center dot center dot H-B hydrogen/dihydrogen bond interaction

Journal of the American Chemical Society, (127): 15976-15982 2005.

Platas-Iglesias, C.; Esteban-Gomez, D.; Enriquez-Perez, T.; Avecilla, F.; de Blas, A.; Rodriguez-Blas, T.

Lead(II) thiocyanate complexes with bibrachial lariat ethers: An X-ray and DFT study
Inorganic Chemistry, (44): 2224-2233 2005.

Poater, J.; Duran, M.; Sola, M.; Silvi, B.

Theoretical evaluation of electron delocalization in aromatic molecules by means of atoms in molecules (AIM) and electron localization function (ELF) topological approaches

Chemical Reviews, (105): 3911-3947 2005.

Poater, J.; Sodupe, M.; Bertran, J.; Sola, M.

Hydrogen bonding and aromaticity in the guanine-cytosine base pair interacting with metal cations (M = Cu⁺, Ca²⁺ and Cu²⁺)

Molecular Physics, (103): 163-173 2005.

Poli, R.; Stoffelbach, F.; Maria, S.; Mata, J.

*An experimental and computational study on the effect of Al(O*i*Pr)₃ on atom-transfer radical polymerization and on the catalyst-dormant-chain halogen exchange*
Chemistry-a European Journal, (11): 2537-2548 2005.

Polo, V.; Domingo, L. R.; Andres, J.

Toward an understanding of the catalytic role of hydrogen-bond donor solvents in the hetero-Diels-Alder reaction between acetone and butadiene derivative

Journal of Physical Chemistry A, (109): 10438-10444 2005.

Pongor, G.; Kolos, Z.; Szalay, R.; Knausz, D.

Pseudo-pentacoordination in silylcarbamates: structure-based prediction of silylating power

Journal of Molecular Structure-Theochem, (714): 87-97 2005.

Prabhakar, C.; Yesudas, K.; Chaitanya, G. K.; Sitha, S.; Bhanuprakash, K.; Rao, V. J.

Near-infrared absorption in symmetric squarylium and croconate dyes: A comparative study using symmetry-adapted cluster-configuration interaction methods

Journal of Physical Chemistry A, (109): 8604-8616 2005.

Pradhan, B.; Singh, B. P.; Nandi, C. K.; Chakraborty, T.; Kundu, T.

Origin of methyl torsional barrier in 1-methyl-2-(1H)-pyridone

Journal of Chemical Physics, (122) 2005.

Profatilova, I. A.; Bumber, A. A.; Tolpygin, I. E.; Rybalkin, V. P.; Gribanova, T. N.; Mikhailov, I. E.; Bren, V. A.

A voltammetric study of the chemosensor activity of aminoanthracene derivatives

Russian Journal of General Chemistry, (75): 1774-1781 2005.

Pu, X. M.; Wong, N. B.; Zhou, G.; Gu, J. D.; Tian, A. M.

Substituent effects on the trans/cis isomerization and stability of diazenes

Chemical Physics Letters, (408): 101-106 2005.

Puchta, R.; Hommes, N. V.; van Eldik, R.

Evidence for interchange ligand-exchange processes on solvated beryllium cations

Helvetica Chimica Acta, (88): 911-922 2005.

Puskar, L.; Tomlins, K.; Duncombe, B.; Cox, H.; Stace, A. J.

What is required to stabilize Al³⁺? a gas-phase perspective

Journal of the American Chemical Society, (127): 7559-7569 2005.

Puzzarini, C.; Peterson, K. A.

Multiple bonds to gold: a theoretical investigation of XAuC (X = F, Cl, Br, I) molecules

Chemical Physics, (311): 177-186 2005.

Qiao, Q. A.; Jin, Y. Q.; Yang, C. L.; Zhang, Z. H.; Wang, M. S.

A quantum chemical study on the mechanism of glycinamide ribonucleotide

transformylase inhibitor: 10-Formyl-5,8,10-trideazafolic acid

Biophysical Chemistry, (118): 78-83 2005.

Qin, S.; Hu, C. W.; Yang, H. Q.

Theoretical study on the mechanism of the reaction of Ni(d(10 1)S)+H-2+CO2 ->

NiCO+H2O

Journal of Theoretical & Computational Chemistry, (4): 449-459 2005.

Qu, Y. H.; Bian, X. F.

Electronic structure and stability of Al_nPn (n=2-4) clusters

Journal of Computational Chemistry, (26): 226-234 2005.

- Qu, Y. H.; Ma, W. Y.; Bian, X. F.; Tang, H. W.; Tian, W. X.
Theoretical study of aluminum arsenide clusters: Equilibrium geometries and electronic structures of Al_nAs_n (n=1-4)
J Mol Graph Model, (24): 167-174 2005.
- Quinonero, D.; Frontera, A.; Garau, C.; Costa, A.; Ballester, P.; Deya, P. M.
Ab initio investigations of lithium insertion in boron and nitrogen-doped single-walled carbon nanotubes
Chemical Physics Letters, (411): 256-261 2005.
- Raghunath, P.; Bhanuprakash, K.; Srinivas, R.
Theoretical study on the potential energy surface of [HNCS2]
Journal of Molecular Structure-Theochem, (722): 217-232 2005.
- Rapacioli, M.; Calvo, F.; Spiegelman, F.; Joblin, C.; Wales, D. J.
Stacked clusters of polycyclic aromatic hydrocarbon molecules
Journal of Physical Chemistry A, (109): 2487-2497 2005.
- Rasul, G.; Prakash, G. K. S.; Olah, G. A.
Comparative ab initio study of the structures and stabilities of the ethane dication C₂H₆²⁺ and its silicon analogues Si₂H₆²⁺ and CSiH₆²⁺
Journal of Physical Chemistry A, (109): 798-801 2005.
- Ratajczyk, T.; Czerski, I.; Kamienska-Trela, K.; Szymanski, S.; Wojcik, J.
(1)J(C,H) couplings to the individual protons in a methyl group: Evidence of the methyl protons' engagement in hydrogen bonds
Angewandte Chemie-International Edition, (44): 1230-1232 2005.
- Ray, K.; Begum, A.; Weyhermuller, T.; Piligkos, S.; van Slageren, J.; Neese, F.; Wieghardt, K.
The electronic structure of the isoelectronic, square-planar complexes [Fe-II(L)(2)](2-) and [Co-III(L-Bu)(2)](-) (L²⁻ and (L-Bu)²⁻ = benzene-1,2-dithiolates): An experimental and density functional theoretical study
Journal of the American Chemical Society, (127): 4403-4415 2005.
- Ray, K.; Weyhermuller, T.; Neese, F.; Wieghardt, K.
Electronic structure of square planar bis(benzene-1,2-dithiolato)metal complexes [M(L)(2)](z) (z = 2-, 1-, 0; M = Ni, Pd, Pt, Cu, Au): An experimental, density functional, and correlated ab initio study
Inorganic Chemistry, (44): 5345-5360 2005.
- Remenyi, C.; Kaupp, M.
Where is the spin? Understanding electronic structure and g-tensors for ruthenium complexes with redox-active quinonoid Ligands
Journal of the American Chemical Society, (127): 11399-11413 2005.
- Ren, Y.; Li, M.; Wong, N. B.

Prototropic tautomerism of imidazolone in aqueous solution: a density functional approach using the combined discrete/self-consistent reaction field (SCRF) models
Journal of Molecular Modeling, (11): 167-173 2005.

Reyes, L.; Castro, M.; Cruz, J.; Rubio, M.
Substituent effects in the migration step of the Baeyer-Villiger rearrangement. A theoretical study
Journal of Physical Chemistry A, (109): 3383-3390 2005.

Rincon, L.; Alvarellos, J. E.; Almeida, R.
Electron density, exchange-correlation density, and bond characterization from the perspective of the valence-bond theory. I. Two simple analytical cases
Journal of Chemical Physics, (122) 2005.

Rodriguez-Borges, J. E.; Garcia-Mera, X.; Fernandez, F.; Lopes, V. H. C.; Magalhaes, A. L.; Cordeiro, M.
Experimental and DFT study of the aza-Diels-Alder reaction between cyclopentadiene and protonated benzylimine derivated from glyoxylates
Tetrahedron, (61): 10951-10957 2005.

Rodriguez-Valdez, L. M.; Martinez-Villafane, A.; Glossman-Mitnik, D.
CHIH-DFT theoretical study of isomeric thiatriazoles and their potential activity as corrosion inhibitors
Journal of Molecular Structure-Theochem, (716): 61-65 2005.

Rodziewicz, P.; Rutkowski, K. S.; Melikova, S. M.; Koll, A.
Ab initio studies of electron acceptor-donor interactions with blue- and red-shifted hydrogen bonds
Chemphyschem, (6): 1282-1292 2005.

Rogachev, A. Y.; Nemukhin, A. V.; Granovskii, A. A.; Kuz'mina, N. P.
Theoretical modeling of the structures and properties of copper(II) and Nickel(II) complexes with Schiff bases
Russian Journal of Inorganic Chemistry, (50): 1036-1043 2005.

Romanenko, E. A.
Specific interactions and the nature of the chemical nonequivalence of chlorine atoms in the ECl₃ group (E = C, P) of trichlorophosphonium ylides and isomeric dichloro(trichloromethyl)phosphine
Russian Journal of General Chemistry, (75): 1085-1090 2005.

Roohi, H.; Deyhimi, F.; Ebrahimi, A.; Khanmohammady, A.
Restricted rotation in six-membered cyclic nitrosamine compounds: an ab initio and DFT study and NBO analysis
Journal of Molecular Structure-Theochem, (718): 123-132 2005.

- Roohi, H.; Ebrahimi, A.
Anomeric effect and rotational barrier in fluoromethanol: A theoretical study
Journal of Molecular Structure-Theochem, (726): 141-148 2005.
- Roohi, H.; Ebrahimi, A.; Alirezapoor, F.; Hajalirezahi, M.
AIM and NBO analyses of N-N rotational barrier in monocyclic nitrosamine compounds
Chemical Physics Letters, (409): 212-218 2005.
- Rotinov, A.; Dominguez, R. M.; Cordova, T.; Chuchani, G.
Kinetics and mechanisms of the elimination of ethyl and tert-butyl esters of carbazic acid in the gas phase: experimental and theoretical studies
Journal of Physical Organic Chemistry, (18): 616-624 2005.
- Rowley, C. N.; DiLabio, G. A.; Barry, S. T.
Theoretical and synthetic investigations of carbodlimide insertions into Al-CH₃ and Al-N(CH₃)₂ bonds
Inorganic Chemistry, (44): 1983-1991 2005.
- Roy, D. R.; Parthasarathi, R.; Maiti, B.; Subramanian, V.; Chattaraj, P. K.
Electrophilicity as a possible descriptor for toxicity prediction
Bioorganic & Medicinal Chemistry, (13): 3405-3412 2005.
- Rozas, I.; Alkorta, I.; Elguero, J.
Modelling protein RNA interactions: an electron density study of the guanidinium and formate complexes with RNA bases
Organic & Biomolecular Chemistry, (3): 366-371 2005.
- Rozas, I.; Kruger, P. E.
Theoretical study of the interaction between the guanidinium cation and chloride and sulfate anions
Journal of Chemical Theory and Computation, (1): 1055-1062 2005.
- Ruben, E. A.; Chapman, M. S.; Evanseck, J. D.
Generalized anomeric interpretation of the "high-energy" N-P bond in N-methyl-N'-phosphorylguanidine: Importance of reinforcing stereoelectronic effects in "high-energy" phosphoester bonds
Journal of the American Chemical Society, (127): 17789-17798 2005.
- Rubin, M.; Trofimov, A.; Gevorgyan, V.
Can polarization of triple bond in tolanes be deduced from C-13 NMR shifts? Re-evaluation of factors affecting regiochemistry of the palladium-catalyzed hydrostannation of alkynes
Journal of the American Chemical Society, (127): 10243-10249 2005.
- Rudner, M. S.; Jeremic, S.; Petterson, K. A.; Kent, D. R.; Brown, K. A.; Drake, M. D.; Goddard, W. A.; Roberts, J. D.

Intramolecular hydrogen bonding in disubstituted ethanes. A comparison of NH...O- and OH...O- hydrogen bonding through conformational analysis of 4-amino-4-oxobutanoate (succinamate) and monohydrogen 1,4-butanoate (monohydrogen succinate) anions
Journal of Physical Chemistry A, (109): 9076-9082 2005.

Ruiz, E.; Cano, J.; Alvarez, S.

Density functional study of exchange coupling constants in single-molecule magnets: The Fe-8 complex
Chemistry-a European Journal, (11): 4767-4771 2005.

Ruiz, E.; Cirera, J.; Alvarez, S.

Spin density distribution in transition metal complexes
Coordination Chemistry Reviews, (249): 2649-2660 2005.

Ruiz, T. P.; Navarro, A.; Kearley, G. J.; Gomez, M. F.

Hydrogen bonds in 1-indanone: Charge density analysis and simulation of the inelastic neutron scattering spectrum in solid phase
Chemical Physics, (317): 159-170 2005.

Rulisek, L.; Sebek, P.; Havlas, Z.; Hrabal, R.; Capek, P.; Svatos, A.

An experimental and theoretical study of stereoselectivity of furan-maleic anhydride and furan-maleimide Diels-Alder reactions
Journal of Organic Chemistry, (70): 6295-6302 2005.

Sadekov, I. D.; Minkin, V. I.; Zakharov, A. V.; Starikov, A. G.; Borodkin, G. S.; Aldoshin, S. M.; Tkachev, V. V.; Shilov, G. V.; Berry, F. J.

Synthesis and structure of N-arylimines of beta-tellurocyclohexenals with the intramolecular coordination N -> Te bonds

Journal of Organometallic Chemistry, (690): 103-116 2005.

Saez, J. A.; Arno, M.; Domingo, L. R.

Lewis acid induced [4+3] cycloadditions of 2-silyloxyacroleins. Insights on the mechanism from a DFT analysis
Tetrahedron, (61): 7538-7545 2005.

Safi, B.; Mertens, J.; De Proft, F.; Alberto, R.; Geerlings, P.

Relative stability of mixed [3+1] Tc and Re complexes: a computational and conceptual DFT study
Journal of Physical Chemistry A, (109): 1944-1951 2005.

Sahin, Y.; Prasang, C.; Hofmann, M.; Geiseler, G.; Massa, W.; Berndt, A.

Derivatives of the simplest polyhedral carborane anion: Structures at the borderline between two-and three-dimensional aromatic compounds
Angewandte Chemie-International Edition, (44): 1643-1646 2005.

Saitoh, T.; Naoe, T.; Ikuta, S.

Ab initio molecular-orbital study of structures and energetics of Si₃H₃ neutral and anion
Journal of Chemical Physics, (122) 2005.

Sangthong, W.; Probst, M.; Limtrakul, J.

Computational study of the carbonyl-ene reaction of encapsulated formaldehyde in Na-FAU zeolite
Journal of Molecular Structure, (748): 119-127 2005.

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

Theoretical and experimental evidence for a new kind of spin-coupled singlet species: Isomeric mixed-valent complexes bridged by a radical anion ligand
Angewandte Chemie-International Edition, (44): 5655-5658 2005.

Sarkar, U.; Roy, D. R.; Chattaraj, P. K.; Parthasarathi, R.; Padmanabhan, J.; Subramanian, V.
A conceptual DFT approach towards analysing toxicity
Journal of Chemical Sciences, (117): 599-612 2005.

Sarma, B. K.; Mugesh, G.

Glutathione peroxidase (GPx)-like antioxidant activity of the organoselenium drug ebselen: Unexpected complications with thiol exchange reactions
Journal of the American Chemical Society, (127): 11477-11485 2005.

Saur, I.; Alonso, S. G.; Gornitzka, H.; Lemierre, V.; Chrostowska, A.; Barrau, J.

In search of cationic germanium(II)-transition metal complexes (LGe)-Ge-2+W(CO)(5) and (LGe)-Ge-2+W(CO)(4)Ge+L-2
Organometallics, (24): 2988-2996 2005.

Scheibitz, M.; Bolte, M.; Bats, J. W.; Lerner, H. W.; Nowik, I.; Herber, R. H.; Krapp, A.; Lein, M.; Holthausen, M. C.; Wagner, M.
C₅H₄-BR₂ bending in ferrocenylboranes: A delocalized through-space interaction between iron and boron
Chemistry-a European Journal, (11): 584-603 2005.

Schenk, S.; Weston, J.; Anders, E.

Density functional investigation of the Mitsunobu reaction
Journal of the American Chemical Society, (127): 12566-12576 2005.

Schott, D.; Pregosin, P. S.; Veiros, L. F.; Calhorda, M. J.

PGSE NMR diffusion, overhauser, and DFT studies on the salts [Pd(eta(3)-CH₃CHCHCHPh) (dppe)] (anion)
Organometallics, (24): 5710-5717 2005.

Schultz, N. E.; Zhao, Y.; Truhlar, D. G.

Databases for transition element bonding: Metal-metal bond energies and bond lengths and their use to test hybrid, hybrid meta, and meta density functionals and generalized gradient approximations

Journal of Physical Chemistry A, (109): 4388-4403 2005.

Schweiger, S.; Hartke, B.; Rauhut, G.

Double proton transfer reactions at the transition from a concerted to a stepwise mechanism: a comparative ab initio study

Physical Chemistry Chemical Physics, (7): 493-500 2005.

Schwieger, S.; Wagner, C.; Bruhn, C.; Schmidt, H.; Steinborn, D.

Synthesis and structures of Zeise-type complexes with vinylsilane ligands and quantum chemical analysis of the platinum-vinylsilane bonding

Zeitschrift Fur Anorganische Und Allgemeine Chemie, (631): 2696-2704 2005.

Schyman, P.; Danielsson, J.; Pinak, M.; Laaksonen, A.

Theoretical study of the human DNA repair protein HOGG1 activity

Journal of Physical Chemistry A, (109): 1713-1719 2005.

Scott, N. M.; Dorta, R.; Stevens, E. D.; Correa, A.; Cavallo, L.; Nolan, S. P.

Interaction of a bulky N-heterocyclic carbene ligand with Rh(I) and Ir(I). Double C-H activation and isolation of bare 14-electron Rh(III) and Ir(III) complexes

Journal of the American Chemical Society, (127): 3516-3526 2005.

Seidl, P. R.; Carneiro, J. W. D.; Tostes, J. G. R.; Koch, A.; Kleinpeter, E.

Interpretation of conformational effects on 2-endo-norborneol by natural chemical shielding analysis

Journal of Physical Chemistry A, (109): 802-806 2005.

Semenov, S. G.; Ionin, B. I.; Sigolaev, Y. F.

Quantum-chemical investigation of pentafluorophenylxenonium and (heptafluorocyclohexa-1,4-dien-1-yl)xenonium cations and related molecules

Russian Journal of General Chemistry, (75): 1706-1711 2005.

Semenov, S. G.; Sigolaeva, I. Y.

p-Hydroxyphenyldiazonium cation and conjugated base: A quantum chemical study

Russian Journal of General Chemistry, (75): 764-769 2005.

Sensato, F. R.; Custodio, R.; Longo, E.; Safont, V. S.; Andres, J.

Why do peroxomolybdenum complexes chemoselectively oxidize the sulfur centers of unsaturated sulfides and sulfoxides? A DFT analysis

European Journal of Organic Chemistry: 2406-2415 2005.

Senthilkumar, L.; Kolandaivel, P.

Study of effective hardness and condensed Fukui functions using AIM, ab initio, and DFT methods

Molecular Physics, (103): 547-556 2005.

Shchavlev, A. E.; Pankratov, A. N.; Borodulin, V. B.; Chaplygina, O. A.

DFT study of the monomers and dimers of 2-pyrrolidone: Equilibrium structures, vibrational, orbital, topological, and NBO analysis of hydrogen-bonded interactions
Journal of Physical Chemistry A, (109): 10982-10996 2005.

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

Theoretical studies on the intramolecular hydrogen bond and tautomerism of 8-mercaptopquinoline in the gaseous phase and in solution using modern DFT methods
Journal of Physical Chemistry A, (109): 4137-4148 2005.

Shi, F. Q.; An, J. Y.; Ju, J. Y.

Theoretical study on measure of hydrogen bonding strength: R-C=N center dot center dot center dot pyrrole complexes
Chinese Journal of Chemistry, (23): 400-403 2005.

Shi, T.; He, S. Y.; Wang, X. F.; Wang, Y. B.; Tang, Z. X.; Wen, Z. Y.

Electronic structure calculations of copper (II) complexes of [Cu(C₁₀H₈N₂O₄)(H₂O)(2)] and [Cu(C₁₀H₈N₂O₄)(CH₃OH)(H₂O)]
Journal of Molecular Structure-Theochem, (732): 201-209 2005.

Shi, T. J.; Zhao, J. F.; Shek, P. Y. I.; Hopkinson, A. C.; Siu, K. W. M.

Carbonate, carbamate, urea, and guanidine as model species for functional groups in biological molecules - A combined density functional theory and mass spectrometry examination of polysodiation and gas-phase dissociation
Canadian Journal of Chemistry-Revue Canadienne De Chimie, (83): 1941-1952 2005.

Shindo, M.; Yoshikawa, T.; Itou, Y.; Mori, S.; Nishii, T.; Shishido, K.

Heteroatom-guided torque-selective olefination of alpha-oxy and alpha-amino ketones via ynolates
Chemistry-a European Journal, (12): 524-536 2005.

Shor, E. A.; Shor, A. M.; Nasluzov, V. A.; Rubaylo, A. I.

Correlation between structure and spectral characteristics of rhodium(I) chelate dicarbonyl complexes and their electron
Journal of Structural Chemistry, (46): 220-229 2005.

Shuku, T.; Sugimori, K.; Sugiyama, A.; Nagao, H.; Sakurai, T.; Nishikawa, K.

Molecular orbital analysis of active site of oxidized azurin: Dependency of electronic properties on molecular structure
Polyhedron, (24): 2665-2670 2005.

Sibert, J. W.; Hundt, G. R.; Sargent, A. L.; Lynch, V.

Wurster's crownophanes: an alternate topology for para-phenylenediamine-based macrocycles

Tetrahedron, (61): 12350-12357 2005.

Sierraalta, A.; Bermudez, A.; Rosa-Brussin, M.

Density functional study of the interaction of Cu⁺ ion-exchanged zeolites with H₂O and SO₂ molecules

Journal of Molecular Catalysis a-Chemical, (228): 203-210 2005.

Silva, G. R.; Borges, I.; Figueroa-Villar, J. D.

DFT conformational studies of the HI-6 molecule

International Journal of Quantum Chemistry, (105): 260-269 2005.

Simaan, A. J.; Boillot, M. L.; Carrasco, R.; Cano, J.; Girerd, J. J.; Mattioli, T. A.; Ensling, J.; Spiering, H.; Gutlich, P.

Electronic, vibrational, and structural properties of a spin-crossover catecholato-iron system in the solid state: Theoretical study of the electronic nature of the doublet and sextet states

Chemistry-a European Journal, (11): 1779-1793 2005.

Simmonett, A. C.; Gilbert, A. T. B.; Gill, P. M. W.

An optimal point-charge model for molecular electrostatic potentials

Molecular Physics, (103): 2789-2793 2005.

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

Structure and fragmentation of glycine, alanine, serine and cysteine radical cations. A theoretical study

Journal of Molecular Structure-Theochem, (727): 191-197 2005.

Singh, V.; Lee, J. E.; Nunez, S.; Howell, P. L.; Schramm, V. L.

Transition state structure of 5'-methylthioadenosine/S-adenosylhomocysteine

nucleosidase from Escherichia coli and its similarity to transition state analogues

Biochemistry (Mosc), (44): 11647-11659 2005.

Sivasankar, C.; Bores, N.; Peters, G.; Habeck, C. M.; Studt, F.; Tuczek, F.

Dismutation of a molybdenum(IV) acetonitrile-NNH₂ complex to a molybdenum(IV) ethylimido complex plus N-2: Mechanistic implications on the protonation of coordinated nitriles at the beta-carbon atom

Organometallics, (24): 5393-5406 2005.

Sizova, O. V.; Varshavskii, Y. S.; Nikol'skii, A. B.

Binuclear rhodium(I) carbonyl carboxylate complexes: DFT study of structural and spectral properties

Russian Journal of Coordination Chemistry, (31): 875-883 2005.

Smurnyy, Y.; Bibal, C.; Pink, M.; Caulton, K. G.

New features of bis(phosphinimine)-"carbene" binding to Ru-II

Organometallics, (24): 3849-3855 2005.

- Solans-Monfort, X.; Clot, E.; Coperet, C.; Eisenstein, O.
d(0) Re-based olefin metathesis catalysts, Re(=CR)(=CHR)(X)(Y): The key role of X and Y ligands for efficient active sites
Journal of the American Chemical Society, (127): 14015-14025 2005.
- Solans-Monfort, X.; Clot, E.; Coperet, C.; Eisenstein, O.
Understanding structural and dynamic properties of well-defined rhenium-based olefin metathesis catalysts, Re(=CR)(=CHR)(X)(Y), from DFT and QAVMM calculations
Organometallics, (24): 1586-1597 2005.
- Solimannejad, M.; Haratian, M.; Boutalib, A.
*Ab initio molecular orbital investigation of SiOH+-XH, SiOH+-X-2 and SiOH+-XY(YX)
(X = Y=F, Cl and Br) proton-bond complexes*
International Journal of Mass Spectrometry, (240): 1-5 2005.
- Solomon, E. I.; Hedman, B.; Hodgson, K. O.; Dey, A.; Szilagyi, R. K.
Ligand K-edge X-ray absorption spectroscopy: covalency of ligand-metal bonds
Coordination Chemistry Reviews, (249): 97-129 2005.
- Song, L. C.; Lin, Y. C.; Wu, W.; Zhang, Q. N.; Mo, Y. R.
Steric strain versus hyperconjugative stabilization in ethane congeners
Journal of Physical Chemistry A, (109): 2310-2316 2005.
- Song, L. C.; Liu, M. H.; Wu, W.; Zhang, Q.; Mo, Y. R.
Origins of rotational barriers in hydrogen peroxide and hydrazine
Journal of Chemical Theory and Computation, (1): 394-402 2005.
- Soriano, E.; Ballesteros, P.; Marco-Contelles, J.
Theoretical investigation on the mechanisms of the PtCl₂-mediated cycloisomerization of polyfunctionalized 1,6-enynes. 1. Role of the propargylic substituents
Organometallics, (24): 3172-3181 2005.
- Soriano, E.; Ballesteros, P.; Marco-Contelles, J.
Theoretical investigation on the mechanisms of the PtCl₂-mediated cycloisomerization of polyfunctionalized 1,6-enynes. 2. Propargylic carboxylates
Organometallics, (24): 3182-3191 2005.
- Soriano, E.; Marco-Contelles, J.
Theoretical analysis of the high versatility in PtCl₂-mediated cycloisomerization of enynes on a common mechanistic basis
Journal of Organic Chemistry, (70): 9345-9353 2005.
- Soriano, E.; Marco-Contelles, J.
A DFT-based theoretical investigation of the mechanism of the PtCl₂-mediated cycloisomerization of allenynes

Chemistry-a European Journal, (11): 521-533 2005.

Spangler, K. A.; Milletti, M. C.

Theoretical modeling of the isopropylum cation: Exploring nonclassical carbonyl behavior

Journal of Coordination Chemistry, (58): 595-603 2005.

Steinke, T.; Cokoja, M.; Gemel, C.; Kempfer, A.; Krapp, A.; Frenking, G.; Zenneck, U.; Fischer, R. A.

C-H activated isomers of [M(AlCp)(5)] (M=Fe, Ru)*

Angewandte Chemie-International Edition, (44): 2943-2946 2005.

Stephan, G. C.; Peters, G.; Lehnert, N.; Habeck, C. M.; Nather, C.; Tuczak, F.

Bonding, activation, and protonation of dinitrogen on a molybdenum pentaphosphine complex - Comparison to trans-bis(dinitrogen) and -nitrile - dinitrogen complexes with tetraphosphine coordination

Canadian Journal of Chemistry-Revue Canadienne De Chimie, (83): 385-402 2005.

Steudel, Y.; Wong, M. W.; Steudel, R.

Electrophilic attack on sulfur-sulfur bonds: Coordination of lithium cations to sulfur-rich molecules studied by ab initio MO methods

Chemistry-a European Journal, (11): 1281-1293 2005.

Straka, M.; Hrobarik, P.; Kaupp, M.

Understanding structure and bonding in early actinide 6d(0)5f(0) MX₆q (M = Th-Np; X = H, F) complexes in comparison with their transition metal 5d(0) analogues

Journal of the American Chemical Society, (127): 2591-2599 2005.

Straka, M.; Kaupp, M.

Calculation of F-19 NMR chemical shifts in uranium complexes using density functional theory and pseudopotentials

Chemical Physics, (311): 45-56 2005.

Straka, M.; Kaupp, M.; Roduner, E.

Understanding solvent effects on hyperfine coupling constants of cyclohexadienyl radicals

Theoretical Chemistry Accounts, (114): 318-326 2005.

Straka, M.; Pyykko, P.

Linear HThThH: A candidate for a Th-Th triple bond

Journal of the American Chemical Society, (127): 13090-13091 2005.

Streitwieser, A.; Jayasree, E. G.; Leung, S. S. H.; Choy, G. S. C.

A theoretical study of substituent effects on allylic ion and ion pair S(N)2 reactions

Journal of Organic Chemistry, (70): 8486-8491 2005.

- Studt, F.; MacKay, B. A.; Johnson, S. A.; Patrick, B. O.; Fryzuk, M. D.; Tuczek, F.
Lewis adducts of the side-on end-on dinitrogen-bridged complex [{(NPN)Ta}(2)(mu-H)(2)(mu-eta(1):eta(2)-N-2)] with AlMe₃, GaMe₃, and B(C₆F₅)₃: Synthesis, structure, and spectroscopic properties
Chemistry-a European Journal, (11): 604-618 2005.
- Subotnik, J. E.; Dutoi, A. D.; Head-Gordon, M.
Fast localized orthonormal virtual orbitals which depend smoothly on nuclear coordinates
Journal of Chemical Physics, (123) 2005.
- Sugimori, K.; Shuku, T.; Sugiyama, A.; Nagao, H.; Sakurai, T.; Nishikawa, K.
Solvent effects on electronic structure of active site of azurin by polarizable continuum model
Polyhedron, (24): 2671-2675 2005.
- Sun, Q.; Bu, Y. X.; Sun, L. X.; Yan, S. H.; Cheng, X. L.
Electron transfer reactivity of methyl-substituted amine NH_n(CH₃)_(3-n)/NH_n(CH₃)₍₊₎(3-n) (n=0-3) self-exchange systems: a theoretical investigation
Journal of Physical Organic Chemistry, (18): 69-82 2005.
- Sun, Q.; Li, Z.; Zeng, X. Q.; Ge, M. F.; Wang, D. X.
Studies on the structural properties of iodine-containing complexes: DFT calculations for IO-H₂O and HOI-H₂O systems
Journal of Molecular Structure-Theochem, (724): 155-161 2005.
- Sun, Q.; Li, Z.; Zeng, X. Q.; Ge, M. F.; Wang, D. X.
Structures and properties of the hydrogen-bond complexes: Theoretical studies for the coupling modes of the pyrazole-imidazole system
Journal of Molecular Structure-Theochem, (724): 167-172 2005.
- Sun, Q.; Li, Z.; Zeng, X. Q.; Ge, M. F.; Wang, D. X.
Theoretical study on the coupling mode of BrO-H₂O and HOBr-H₂O complexes
Chinese Journal of Chemistry, (23): 483-490 2005.
- Sundaraganesan, N.; Ilakiamani, S.; Saleem, H.; Wojciechowski, P. M.; Michalska, D.
FT Raman and FT IR spectra, vibrational assignments and density functional studies of 5-bromo-2-nitropyridine
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (61): 2995-3001 2005.
- Sushko, P. V.; Mukhopadhyay, S.; Mysovsky, A. S.; Sulimov, V. B.; Taga, A.; Shluger, A. L.
Structure and properties of defects in amorphous silica: new insights from embedded cluster calculations
Journal of Physics-Condensed Matter, (17): S2115-S2140 2005.

- Syrstad, E. A.; Turecek, F.
Toward a general mechanism of electron capture dissociation
Journal of the American Society for Mass Spectrometry, (16): 208-224 2005.
- Szafran, M.; Koput, J.; Dega-Szafran, Z.
B3LYP study of the conformers and rotamers of isostructural N-methylpiperidine betaine hydrochloride and (1-methylcyclohexyl)-acetic acid. The effect of electrostatic attraction on rotation barriers
Journal of Molecular Structure, (749): 114-121 2005.
- Szalay, R.; Pongor, G.; Harmat, V.; Bocskei, Z.; Knausz, D.
Surprisingly great difference in reactivity depending upon the ring size: solvolysis and molecular structure study of some N-trimethylsilylated cyclic ureas
Journal of Organometallic Chemistry, (690): 1498-1506 2005.
- Szilagyi, R. K.; Schwab, D. E.
Sulfur K-edge X-ray absorption spectroscopy as an experimental probe for S-nitroso proteins
Biochemical and Biophysical Research Communications, (330): 60-64 2005.
- Tabaka, K.; Jezierska, J.
Positional and angular dependence of hyperfine interactions in cyclic and bicyclic iminoxy radicals with C=O or CH₂ group - DFT and EPR studies
Chemical Physics Letters, (410): 391-399 2005.
- Takahashi, M.; Kawazoe, Y.
Theoretical study on planar anionic polysilicon chains and cyclic Si-6 anions with D-6h symmetry
Organometallics, (24): 2433-2440 2005.
- Tan, H.; Wong, L. K.; Lai, M. Y.; Kiruba, G. S. M.; Leong, W. K.; Wong, M. W.; Fan, W. Y.
Preparation and characterization of Cr(CO)(4)dpp (Chromium tetracarbonyl 2,3-bis(2'-pyridyl)pyrazine) adsorbed on silver nanoparticles
Journal of Physical Chemistry B, (109): 19657-19663 2005.
- Tanaka, N.; Sisk, W. N.
Theoretical study on the (O-2-HF)(+) complex
Journal of Fluorine Chemistry, (126): 313-317 2005.
- Tang, D. Y.; Luo, X. L.; Shen, W.; Li, M.
The mechanism of enantioselective palladium(0)-catalyzed allylic alkylation with chiral oxazolinylpyridines: a DFT study
Journal of Molecular Structure-Theochem, (716): 79-87 2005.
- Taurian, O. E.; De Kowalewski, D. G.; Perez, J. E.; Contreras, R. H.

*NMR J(C-13, C-13) spin-spin coupling constants in pyridine-carboxaldehydes.
Experimental and DFT-B3LYP studies*
Journal of Molecular Structure, (754): 1-9 2005.

Tian, S. X.
Electron propagator theory study of N/O-methylglycine conformers
Journal of Chemical Physics, (123) 2005.

Tian, S. X.
Theoretical study of isoelectronic molecules: B6H10, 2-CB5H9, 2,3-C2B4H8, 2,3,4-C3B3H7, and 2,3,4,5-C4B2H6
Journal of Physical Chemistry A, (109): 6580-6586 2005.

Tian, S. X.
Marked influences on the adenine-cytosine base pairs by electron attachment and ionization
Journal of Physical Chemistry A, (109): 5153-5159 2005.

Tian, S. X.
Dialane anion: Three-center two-electron or two-center one-electron bonded
Journal of Physical Chemistry A, (109): 4428-4430 2005.

Tian, W. Q.; Ge, M. F.; Gu, F. L.; Aoki, Y.
Bimetallic clusters Pt6Au: Geometric and electronic structures within density functional theory
Journal of Physical Chemistry A, (109): 9860-9866 2005.

Tian, W. Q.; Wang, Y. A.
Dynamics of the Staudinger reaction
Journal of Chemical Theory and Computation, (1): 353-362 2005.

Tian, Z. X.; Tang, Z. C.
Experimental and theoretical studies of the interaction of silver cluster cations Ag-n(+) (n=1-4) with ethylene
Rapid Communications in Mass Spectrometry, (19): 2893-2904 2005.

Timoshkin, A. Y.; Schaefer, H. F.
Donor-acceptor sandwiches of main-group elements
Organometallics, (24): 3343-3345 2005.

Toma, L.; Toma, L. M.; Lescouezec, R.; Armentano, D.; De Munno, G.; Andruh, M.; Cano, J.; Lloret, F.; Julve, M.
Synthesis, crystal structures and magnetic properties of cyanide- and phenolate-bridged [(MNiII)-Ni-III](2) tetrานuclear complexes (M = Fe and Cr)
Dalton Transactions: 1357-1364 2005.

- Torre, A.; Alcoba, D. R.; Lain, L.; Bochicchio, R. C.
Determination of three-center bond indices from population analyses: A fuzzy atom treatment
Journal of Physical Chemistry A, (109): 6587-6591 2005.
- Trevisanutto, P. E.; Sushko, P. V.; Shluger, A. L.; Beck, K. M.; Henyk, M.; Joly, A. G.; Hess, W. P.
A mechanism of photo-induced desorption of oxygen atoms from MgO nano-crystals
Surface Science, (593): 210-220 2005.
- Tripathi, S. K.; Patel, U.; Roy, D.; Sunoj, R. B.; Singh, H. B.; Wolmershauser, G.; Butcher, R. J.
o-hydroxymethylphenylchalcogens: Synthesis, intramolecular nonbonded chalcogen center dot center dot center dot OH interactions, and glutathione peroxidase-like activity
Journal of Organic Chemistry, (70): 9237-9247 2005.
- Trzesowska, A.; Kruszynski, R.
The bonds analysis of hexamethylenetetramine
Polish Journal of Chemistry, (79): 1155-1168 2005.
- Trzesowska, A.; Kruszynski, R.
The structure and quantum chemical study of the potassium chloride
Journal of Molecular Structure-Theochem, (714): 175-178 2005.
- Trzesowska, A.; Kruszynski, R.; Bartczak, T. J.
New lanthanide-nitrogen bond-valence parameters
Acta Crystallographica Section B-Structural Science, (61): 429-434 2005.
- Tsipis, A. C.; Tsipis, C. A.
Ligand-stabilized aromatic three-membered gold rings and their sandwichlike complexes
Journal of the American Chemical Society, (127): 10623-10638 2005.
- Tsipis, C. A.; Karipidis, P. A.
Mechanistic insights into the Bazarov synthesis of urea from NH₃ and CO₂ using electronic structure calculation methods
Journal of Physical Chemistry A, (109): 8560-8567 2005.
- Tsuda, M.; Dino, W. A.; Kasai, H.
Behavior of hydrogen atom at Nafion-Pt interface
Solid State Communications, (134): 601-605 2005.
- Tsuda, M.; Dino, W. A.; Kasai, H.
Spin polarization effects on O-2 dissociation from heme-O-2 adduct
Japanese Journal of Applied Physics Part 2-Letters & Express Letters, (44): L57-L59 2005.
- Tsuda, M.; Dino, W. A.; Kasai, H.

Hydrogenase-based nanomaterials as anode electrode catalyst in polymer electrolyte fuel cells

Solid State Communications, (133): 589-591 2005.

Tsuda, M.; Dino, W. A.; Kasai, H.; Nakanishi, H.

Magnetized/charged MgH₂-based hydrogen storage materials

Applied Physics Letters, (86) 2005.

Tsuda, M.; Dino, W. A.; Nakanishi, H.; Kasai, H.

Orientation dependence of O₂ dissociation from heme-O₂ adduct

Chemical Physics Letters, (402): 71-74 2005.

Tsuda, M.; Dy, E. S.; Kasai, H.

Comparative study of O₂ dissociation on various metalloporphyrins

Journal of Chemical Physics, (122) 2005.

Tuononen, H. M.; Armstrong, A. F.

Theoretical investigation of paramagnetic diazabutadiene gallium(III)-pnictogen complexes: Insights into the interpretation and simulation of electron paramagnetic resonance spectra

Inorganic Chemistry, (44): 8277-8284 2005.

Turecek, F.; Chen, X. H.

Protonated adenine: Tautomers, solvated clusters, and dissociation mechanisms

Journal of the American Society for Mass Spectrometry, (16): 1713-1726 2005.

Tuttle, T.; Kraka, E.; Cremer, D.

Docking, triggering, and biological activity of dynemicin A in DNA: A computational study

Journal of the American Chemical Society, (127): 9469-9484 2005.

Tuttolomondo, M. E.; Navarro, A.; Pena, T.; Varetti, E. L.; Ben Altabef, A.

Theoretical structure and vibrational analysis of ethyl methanesulfonate, CH₃SO₂OCH₂CH₃

Journal of Physical Chemistry A, (109): 7946-7956 2005.

Udomvech, A.; Kerdcharoen, T.; Osotchan, T.

First principles study of Li and Li⁺ adsorbed on carbon nanotube: Variation of tubule diameter and length

Chemical Physics Letters, (406): 161-166 2005.

Urban, J. J.

Computational study of stereoelectronic effects in fluorinated alkylamines

Journal of Physical Organic Chemistry, (18): 1061-1071 2005.

Van Cauter, K.; Hemelsoet, K.; Van Speybroeck, V.; Reyniers, M. F.; Waroquier, M.

Comparative study of kinetics and reactivity indices of free radical polymerization reactions

International Journal of Quantum Chemistry, (102): 454-460 2005.

van Mourik, T.; Dingley, A. J.

Characterization of the monovalent ion position and hydrogen-bond network in guanine quartets by DFT calculations of NMR parameters

Chemistry-a European Journal, (11): 6064-6079 2005.

Varela-Alvarez, A.; Sordo, J. A.; Scuseria, G. E.

Doping of polyaniline by acid-base chemistry: Density functional calculations with periodic boundary conditions

Journal of the American Chemical Society, (127): 11318-11327 2005.

Veirois, L. F.

Zirconium bis(indenyl) sandwich complexes with an unprecedented indenyl coordination mode and their role in the reactivity of the parent bent-metallocenes: A detailed DFT mechanistic study

Chemistry-a European Journal, (11): 2505-2518 2005.

Vijayakumar, S.; Kolandaivel, P.

Red-shifted and improper blue-shifted hydrogen bonds in dimethyl ether (DME)(n) (n=1-4) and hydrated (DME)(n) (n=1-4) clusters. A theoretical study

Journal of Molecular Structure, (734): 157-169 2005.

Vitillo, J. G.; Damin, A.; Zecchina, A.; Ricchiardi, G.

Theoretical characterization of dihydrogen adducts with alkaline cations

Journal of Chemical Physics, (122) 2005.

Vyboishchikov, S. F.; Salvador, P.; Duran, M.

Density functional energy decomposition into one- and two-atom contributions

Journal of Chemical Physics, (122) 2005.

Wandschneider, D.; Michalik, M.; Oehme, H.; Heintz, A.

Ab initio study of some intramolecularly donor-stabilized silenes

European Journal of Inorganic Chemistry: 3331-3336 2005.

Wang, B. W.; Wei, H. Y.; Wang, M. W.; Chen, Z. D.

Ab initio multireference configuration-interaction theoretical study on the low-lying spin states in binuclear transition-metal complex: Magnetic exchange of [(NH₃)₅Cr(mu-OH)Cr(NH₃)₅]⁵⁺ and [Cl₃FeOFeCl₃]²⁻

Journal of Chemical Physics, (122) 2005.

Wang, G. C.; Jiang, L.; Pang, X. Y.; Nakamura, J.

Cluster and periodic DFT calculations: The adsorption of atomic nitrogen on M(111) (M = Cu, Ag, Au) surfaces

Journal of Physical Chemistry B, (109): 17943-17950 2005.

Wang, S. C.; Sahu, P. K.; Lee, S. L.

Intermolecular orbital repulsion effect on the blue-shifted hydrogen bond
Chemical Physics Letters, (406): 143-147 2005.

Wang, W. Z.; Tian, A. M.; Wong, N. B.

Theoretical study on the bromomethane-water 1 : 2 complexes
Journal of Physical Chemistry A, (109): 8035-8040 2005.

Wang, W. Z.; Zhang, Y.; Huang, K. X.

S(N)2-like reaction in hydrogen-bonded complexes: A theoretical study
Journal of Physical Chemistry A, (109): 9353-9355 2005.

Wang, W. Z.; Zhang, Y.; Huang, K. X.

Unconventional interaction in N(P)-related systems
Chemical Physics Letters, (411): 439-444 2005.

Wang, X.; Zhou, G.; Tian, A. M.; Wong, N. B.

An initio investigation on blue shift and red shift of C-H stretching vibrational frequency in NH₃ center dot center dot center dot CH_nX(4--n) (n=1,3, X = F, Cl, Br, I) complexes
Journal of Molecular Structure-Theochem, (718): 1-7 2005.

Wang, X. F.; Andrews, L.

Infrared spectra and structures of the coinage metal dihydroxide molecules
Inorganic Chemistry, (44): 9076-9083 2005.

Wang, Y.; Ma, J.; Inagaki, S.; Pei, Y.

[2+2] cycloaddition reactions of ethylene derivatives with the Si(100)-2x1 surface: A theoretical study
Journal of Physical Chemistry B, (109): 5199-5206 2005.

Wang, Y. C.; Lu, L. L.; Geng, Z. Y.; Dai, G. L.; Wang, D. M.

Theoretical studies on the intermonomer interaction of F- center dot(H₂O)(n) (n=1,2)
Chinese Journal of Structural Chemistry, (24): 561-567 2005.

Wang, Y. C.; Lv, L. L.; Geng, Z. Y.; Dai, G. L.; Wang, D. M.; Wang, H. Q.

Theoretical study of the reactivity of X(P-3) (X = Ge, Sn, Pb) with N₂O(X-1 Sigma)
Journal of Molecular Structure-Theochem, (724): 185-193 2005.

Wang, Y. J.; Ma, J.; Jiang, Y. S.

Tuning of electronic structures of poly(p-phenylenevinylene) analogues of phenyl, thiienyl, furyl, and pyrrolyl by double-bond linkages of group 14 and 15 elements
Journal of Physical Chemistry A, (109): 7197-7206 2005.

Wannere, C. S.; Corminboeuf, C.; Wang, Z. X.; Wodrich, M. D.; King, R. B.; Schleyer, P. V. R.

Evidence for d orbital aromaticity in square planar coinage metal clusters
Journal of the American Chemical Society, (127): 5701-5705 2005.

Ward, B. D.; Orde, G.; Clot, E.; Cowley, A. R.; Gade, L. H.; Mountford, P.
Reactions of neutral and cationic diamide-supported imido complexes with CO₂ and other heterocumulenes: Issues of site selectivity
Organometallics, (24): 2368-2385 2005.

Wartelle, C.; Viruela, P. M.; Viruela, R.; Ortí, E.; Sauvage, F. X.; Levillain, E.; Le Derf, F.; Salle, M.
A study by spectroelectrochemical FTIR and density functional theory calculations of the reversible complexing ability of an electroactive tetrathiafulvalene crown
Journal of Physical Chemistry A, (109): 1188-1195 2005.

Weinhold, F.
Comments on Purser's article: "Lewis structures are models for predicting molecular structure, not electronic structure"
Journal of Chemical Education, (82) 2005.

Werkema, E. L.; Messines, E.; Perrin, L.; Maron, L.; Eisenstein, O.; Andersen, R. A.
Hydrogen for fluorine exchange in CH_{4-x}F_x by monomeric [1,2,4-(Me₃C)(3)C₅H₂](2)CeH: Experimental and computational studies
Journal of the American Chemical Society, (127): 7781-7795 2005.

Westerhausen, M.; Rotter, T.; Pfaller, C.; Kneifel, A. N.; Schulz, A.
NMR spectroscopy and crystal structure of [Me₂GaP(H)SiBu(3)](2) and theoretical investigations of the model compounds [R'₂GaP(H)R"](2)
Inorganica Chimica Acta, (358): 4253-4260 2005.

Wielgus, P.; Roszak, S.; Majumdar, D.; Leszczynski, J.
Thermodynamic properties of germanium/carbon microclusters
Journal of Chemical Physics, (123) 2005.

Wild, D. A.; Lenzer, T.
Structures and infrared spectra of fluoride-hydrogen sulfide clusters from ab initio calculations: F--(H₂S)(n), n=1-5
Physical Chemistry Chemical Physics, (7): 3793-3804 2005.

Wisnioski, P.; Bobrowski, K.; Filipiak, P.; Carmichael, I.; Hug, G. L.
Reactions of hydrogen atoms with alpha-(alkylthio) carbonyl compounds. Time-resolved ESR detection and DFT calculations
Research on Chemical Intermediates, (31): 633-641 2005.

Wong, C. Y.; Che, C. M.; Chan, M. C. W.; Han, J.; Leung, K. H.; Phillips, D. L.; Wong, K. Y.; Zhu, N. Y.

Probing ruthenium-acetylide bonding interactions: Synthesis, electrochemistry, and spectroscopic studies of acetylide-ruthenium complexes supported by tetradentate macrocyclic amine and diphosphine ligands
Journal of the American Chemical Society, (127): 13997-14007 2005.

Wong, M. W.

Roles of C-H center dot center dot center O=S and pi-stacking interactions in the 2-bromoacrolein complex with N-tosyl-(S)-tryptophan-derived oxazaborolidinone catalyst
Journal of Organic Chemistry, (70): 5487-5493 2005.

Wong, M. W.; Steudel, Y.; Steudel, R.

Isomers of cyclo-heptasulfur and their coordination to Li⁺: An ab initio molecular orbital study
Inorganic Chemistry, (44): 8908-8915 2005.

Wu, H. S.; Xu, X. H.; Strout, D. L.; Jiao, H. J.

The structure and stability of B36N36 cages: a computational study
Journal of Molecular Modeling, (12): 1-8 2005.

Wu, H. S.; Zhang, Z. X.

Structure and stability of endohedral complexes X@B12P12
Acta Physico-Chimica Sinica, (21): 479-484 2005.

Wu, H. S.; Zhang, Z. X.

Structure and stability of endohedral complexes X@Al12P12
Acta Chimica Sinica, (63): 973-978 2005.

Wu, W.; Shaik, S.; Saunders, W. H.

Valence bond calculations on the transition state for the E2 reaction of fluoride ion with ethyl fluoride - Implications for the More O'Ferrall-Jencks diagram
Canadian Journal of Chemistry-Revue Canadienne De Chimie, (83): 1649-1653 2005.

Wu, Y.; Xu, K. L.; Xie, D. Q.

A computational study on the mechanism for the GaCl₃-catalyzed [4+1] cycloaddition of alpha,beta-unsaturated ketone and 2,6-dimethylphenyl isocyanide
Tetrahedron, (61): 507-512 2005.

Wysokinski, R.; Bienko, D. C.; Michalska, D.; Zeegers-Huyskens, T.

Theoretical study of the interaction between cytosine and hydrogen peroxide
Chemical Physics, (315): 17-26 2005.

Xiao, X. S.; Antony, S.; Pommier, Y.; Cushman, M.

On the binding of indeno[1,2-c]isoquinolines in the DNA-topoisomerase I cleavage complex
Journal of Medicinal Chemistry, (48): 3231-3238 2005.

- Xie, J.; Feng, D. C.; Feng, S. Y.; Zhang, J.
Theoretical study on insertion of silylenoid H₂SiLiF into X-H bonds (X = CH₃, SiH₃, NH₂, PH₂, OH, SH and F)
Journal of Molecular Structure-Theochem, (755): 55-63 2005.
- Xie, J.; Feng, D. C.; He, M. X.; Feng, S. Y.
Insertion reactions of silylenoid Ph₂SiLi(OBu-t) into X=H bonds (X = F, OH, and NH₂)
Journal of Physical Chemistry A, (109): 10563-10570 2005.
- Xie, Y. M.; Schaefer, H. F.; Jemmis, E. D.
Characteristics of novel sandwiched beryllium, magnesium, and calcium dimers: C₅H₅BeBeC₅H₅, C₅H₅MgMgC₅H₅, and C₅H₅CaCaC₅H₅
Chemical Physics Letters, (402): 414-421 2005.
- Xu, L. N.; Xiao, H. M.; Fang, G. Y.; Ju, X. H.
Theoretical study on intermolecular interactions of 3-nitro-1,2,4-triazol-5-one dimers
Acta Chimica Sinica, (63): 1062-1068 2005.
- Xu, W. G.; Jin, B.
Aromaticity of the S quare As-4(2-) dianion in the MAs₄- (M = Li, Na, K, Rb, and Cs) and MAs₄ (M = Be, Mg, Ca, Sr, and Ba) clusters
Journal of Molecular Structure-Theochem, (731): 61-66 2005.
- Xu, X. J.; Xiao, H. M.; Gong, X. D.; Ju, X. H.; Chen, Z. X.
Theoretical studies on the vibrational spectra, thermodynamic properties, detonation properties, and pyrolysis mechanisms for polynitroadamantanes
Journal of Physical Chemistry A, (109): 11268-11274 2005.
- Xu, Y. C.; Shen, J. H.; Zhu, W. L.; Luo, X. M.; Chen, K. X.; Jiang, H. L.
Influence of the water molecule on cation-pi interaction: Ab initio second order Moller-Plesset perturbation theory (MP2) calculations
Journal of Physical Chemistry B, (109): 5945-5949 2005.
- Xue, Z. M.; Liu, B.; Chen, C. H.
A theoretical study of electrical and electrochemical properties of dicyanomethylene derivatives of squaric acid
Electrochimica Acta, (51): 4554-4561 2005.
- Yadav, V. K.; Singh, L.
Investigation of the diastereoselectivity of tricyclo(5.2.1.0(2,6))decan-10-ones: Controversies and agreements
Journal of Organic Chemistry, (70): 692-695 2005.
- Yamamoto, T.; Kaneno, D.; Tomoda, S.
The importance of lone pair electron delocalization in the cis-trans isomers of 1,2-dibromoethenes

Chemistry Letters, (34): 1190-1191 2005.

Yamamoto, T.; Mahmut, A.; Abe, M.; Kuroda, S. I.; Imase, T.; Sasaki, S.

Alternating copolymer of thiophene and N-(phenylethynyl)pyrrole. New pi-conjugated alternating five-membered ring copolymer and its packing structure

Journal of Polymer Science Part B-Polymer Physics, (43): 2219-2224 2005.

Yamamoto, T.; Yoshizawa, M.; Mahmut, A.; Abe, M.; Kuroda, S.; Imase, T.; Sasaki, S.

Preparation of new pi-conjugated polypyrroles by organometallic polycondensations.

Synthesis of N-BOC (t-butoxycarbonyl) and N-phenylethynyl polymers, thermal deprotection of the BOC group, and packing structure of the N-phenylethynyl polymer

Journal of Polymer Science Part a-Polymer Chemistry, (43): 6223-6232 2005.

Yang, P.; Murthy, P. P. N.; Brown, R. E.

Synergy of intramolecular hydrogen-bonding network in myo-inositol-2-monophosphate:

Theoretical investigations into the electronic structure, proton transfer, and pK(a)

Journal of the American Chemical Society, (127): 15848-15861 2005.

Yang, Y.; Zhang, W. J.; Pei, S. X.; Shao, H.; Huang, W.; Gao, X. M.

Blue-shifted and red-shifted hydrogen bonds: Theoretical study of the CH₃CHO center dot center dot center dot NH₃ complexes

Journal of Molecular Structure-Theochem, (732): 33-37 2005.

Yang, Z.; Ma, X. L.; Oswald, R. B.; Roesky, H. W.; Zhu, H. P.; Schulzke, C.; Starke, K.; Baldus, M.; Schmidt, H. G.; Noltemeyer, M.

Janus-faced aluminum: A demonstration of unique Lewis acid and Lewis base behavior of the aluminum atom in [AlB(C₆F₅)₃]

Angewandte Chemie-International Edition, (44): 7072-7074 2005.

Yap, G. P. A.; Jove, F. A.; Claramunt, R. M.; Sanz, D.; Alkorta, I.; Elguero, J.

The X-ray molecular structure of 1-(2',4'-dinitrophenyl)-1,2,3-triazole and the problem of the orthogonal interaction between a 'pyridine-like' nitrogen and a nitro group

Australian Journal of Chemistry, (58): 817-822 2005.

Yatsenko, A. V.

Structure of organic molecules in the crystals: Modelling using the electrostatic potential

Uspekhi Khimii, (74): 575-584 2005.

Yong, L.; Hoffmann, S. D.; Fassler, T. F.; Riedel, S.; Kaupp, M.

[Pb-5{Mo(CO)(3)}(2)](4-) : A complex containing a planar Pb-5 unit

Angewandte Chemie-International Edition, (44): 2092-2096 2005.

Zampella, G.; Fantucci, P.; Pecoraro, V. L.; De Gioia, L.

Reactivity of peroxy forms of the vanadium haloperoxidase cofactor. A DFT investigation

Journal of the American Chemical Society, (127): 953-960 2005.

- Zaragoza, R. J.; Aurell, M. J.; Domingo, L. R.
The role of the transfer group in the intramolecular [5+2] cycloadditions of substituted beta-hydroxy-gamma-pyrone: a DFT analysis
Journal of Physical Organic Chemistry, (18): 610-615 2005.
- Zeggari, S.; Lapouge, C.; Buntinx, G.; Poizat, O.
Theoretical and experimental resonance Raman study of the fluorene radical cation
Chemical Physics, (313): 113-122 2005.
- Zhang, C. R.; Chen, H. S.; Chen, Y. H.; Feng, W. J.; Li, W. X.; Xu, G. J.; Kou, S. Z.
Density functional theory study on the ring-like structure and properties of Al₈P₈ cluster
Acta Physico-Chimica Sinica, (21): 1368-1372 2005.
- Zhang, C. Y.; Shu, Y. J.; Zhao, X. D.; Dong, H. S.; Wang, X. F.
Computational investigation on HEDM of azoic and azoxy derivatives of DAF, FOX-7, TATB, ANPZ and LLM-105
Journal of Molecular Structure-Theochem, (728): 129-134 2005.
- Zhang, C. Y.; Wu, H. S.
Structure and stability of endohedral complexes X@HAINH(12) (X = He, Ne, Ar, Kr)
Chinese Journal of Structural Chemistry, (24): 684-690 2005.
- Zhang, C. Y.; Wu, H. S.
Structure and stability of X@HAINH(12) and X(HAINH)(12) (X=F-, Cl-, Br-, O2-, S2-, Se2-) complexes
Acta Chimica Sinica, (63): 979-984 2005.
- Zhang, C. Y.; Wu, H. S.; Jiao, H. J.
Structure and stability of endohedral X@Si₂₀H₂₀ complexes (X = LiO⁺, NaO⁺, KO⁺, BeO²⁺, MgO²⁺, CaO²⁺)
Chemical Physics Letters, (410): 457-461 2005.
- Zhang, G. L.; Ma, J.; Jiang, Y. S.
Charge-doped and heteroatom-substituted polysilane, poly(vinylenedisilanylene), and poly(butadienylenedisilanylene): Electronic structures and band gaps
Journal of Physical Chemistry B, (109): 13499-13509 2005.
- Zhang, R. B.; Zeegers-Huyskens, T.; Ceulemans, A.; Nguyen, M. T.
Interaction of triplet uracil and thymine with water
Chemical Physics, (316): 35-44 2005.
- Zhang, S. G.; Pin, Y.
Structures and properties of thymine-BH₃ complex: DFT and MP2 calculation
Chinese Journal of Chemical Physics, (18): 39-44 2005.
- Zhang, S. G.; Yang, P.

Structures and properties of cytosine-BX3 (X = F, Cl) complexes: an investigation with DFT and MP2 methods

Journal of Molecular Structure-Theochem, (757): 77-86 2005.

Zhang, T.; Ng, C. Y.; Qi, F.; Lam, C. S.; Li, W. K.

A 193 nm laser photofragmentation time-of-flight mass spectrometric study of chloroiodomethane

Journal of Chemical Physics, (123) 2005.

Zhang, Z. Q.; Zhou, L. X.; He, Q.; Zhao, Y. Y.

Pt(II), Pd(II) and Ni(II) complexes binding to the N(7) position of guanine: Influence on the guanine and Watson-crick GC base pair

Chinese Journal of Structural Chemistry, (24): 114-120 2005.

Zhao, S.; Li, Z. H.; Wang, W. N.; Fan, K. N.

Density functional study of the interaction of chlorine atom with small neutral and charged silver clusters

Journal of Chemical Physics, (122) 2005.

Zhao, S. W.; Liu, L.; Fu, Y.; Guo, Q. X.

Assessment of the metabolic stability of the methyl groups in heterocyclic compounds using C-H bond dissociation energies: effects of diverse aromatic groups on the stability of methyl radicals

Journal of Physical Organic Chemistry, (18): 353-367 2005.

Zhao, Z. M.; Duesler, E.; Wang, C. H.; Guo, H.; Mariano, P. S.

Photocyclization reactions of cyclohexa- and cyclopenta-fused pyridinium salts. Factors governing regioselectivity

Journal of Organic Chemistry, (70): 8508-8512 2005.

Zheng, W. X.; Wong, N. B.; Tian, A.

Anion-tri-s-triazine bonding: A case for anion recognition

Journal of Physical Chemistry A, (109): 1926-1932 2005.

Zhou, H. W.; Zheng, W. X.; Wang, X.; Ren, Y.; Wong, N. B.; Shu, Y. J.; Tian, A. M.

A Gaussian-3 investigation on the stabilities and bonding of the nine N-10 clusters

Journal of Molecular Structure-Theochem, (732): 139-148 2005.

Zhou, J. X.; Zhang, Y. C.; Guo, X. W.

Effects of anions and cations on pi-complexation between olefin and metal halide

Chemical Research in Chinese Universities, (21): 217-219 2005.

Zhou, S. Q.; Ju, X. H.; Xiao, H. M.

Theoretical study on the intermolecular interactions of tetrazole dimers

Chinese Journal of Structural Chemistry, (24): 1203-1210 2005.

Zhu, H. J.; Ren, Y.; Ren, J.; Chu, S. Y.

DFT explorations of tautomerism of 2-mercaptopimidazole in aqueous solution
Journal of Molecular Structure-Theochem, (130): 199-205 2005.

Zhu, H. J.; Ren, Y.; Ren, J.; Chu, S. Y.

Theoretical investigation of ion pair S(N)2 reactions of alkali isothiocyanates with alkyl halides. Part 1. Reaction of lithium isothiocyanate and methyl fluoride with inversion mechanism
International Journal of Quantum Chemistry, (101): 104-112 2005.

Zhu, M. Q.; Pan, G.

Quantum chemical studies of mononuclear zinc species of hydration and hydrolysis
Journal of Physical Chemistry A, (109): 7648-7652 2005.

Zierkiewicz, W.; Jurecka, P.; Hobza, P.

On differences between hydrogen bonding and improper blue-shifting hydrogen bonding
Chemphyschem, (6): 609-617 2005.

Zimmermann, T.; Zeizinger, M.; Burda, J. V.

Cisplatin interaction with cysteine and methionine, a theoretical DFT study
Journal of Inorganic Biochemistry, (99): 2184-2196 2005.

Znamenskiy, V. S.; Green, M. E.

Calculations of certain properties of hydrogen bonds in clusters, using atoms in molecules (AIM) and natural bond orbitals (NBO)
Biophysical Journal, (88): 515A-515A 2005.