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Abbate, S.; Bazzini, C.; Caronna, T.; Fontana, F.; Gambarotti, C.; Gangemi, F.; Longhi, G.; Mele, A.; Natali Sora, I.; Panzeri, W.

Monoaza 5 helicenes. Part 2: Synthesis, characterisation and theoretical calculations
Tetrahedron, (62): 139-148 2006.

Acerbis, S.; Bertin, D.; Boutevin, B.; Gigmes, D.; Lacroix-Desmazes, P.; Le Mercier, C.; Lutz, J. F.; Marque, S. R. A.; Siri, D.; Tordo, P.

Intramolecular hydrogen bonding: The case of beta-phosphorylated nitroxide (= aminoxy radical)
Helvetica Chimica Acta, (89): 2119-2132 2006.

Agapito, L. A.; Maffei, M. G.; Salazar, P. F.; Seminario, J. M.

Performance of multiplicity-based energy correctors for molecules containing second-row elements

Journal of Physical Chemistry A, (110): 4260-4265 2006.

Alajarin, M.; Cabrera, J.; Pastor, A.; Sanchez-Andrada, P.; Bautista, D.

On the 2+2 cycloaddition of 2-aminothiazoles and dimethyl acetylenedicarboxylate. Experimental and computational evidence of a thermal disrotatory ring opening of fused cyclobutenes
Journal of Organic Chemistry, (71): 5328-5339 2006.

Alajarin, M.; Ortín, M. M.; Sanchez-Andrada, P.; Vidal, A.

Tandem pseudopericyclic reactions: 1,5 -X sigmatropic shift/6 pi-electrocyclic ring closure converting N-(2-X-carbonyl)phenyl ketenimines into 2-X-quinolin-4(3H)-ones
Journal of Organic Chemistry, (71): 8126-8139 2006.

Alex, A.; Hansele, E.; Clark, T.

The ethylene/metal(0) and ethylene/metal(I) redox system: model ab initio calculations
Journal of Molecular Modeling, (12): 621-629 2006.

Alexandrova, A. N.; Boldyrev, A. I.; Zhai, H. J.; Wang, L. S.

All-boron aromatic clusters as potential new inorganic ligands and building blocks in chemistry
Coordination Chemistry Reviews, (250): 2811-2866 2006.

Alexandrova, A. N.; Koyle, E.; Boldyrev, A. I.

Theoretical study of hydrogenation of the doubly aromatic B-7(-)
Journal of Molecular Modeling, (12): 569-576 2006.

Aljarilla, A.; Cordoba, R.; Csaky, A. G.; Fernandez, I.; Ortiz, F. L.; Plumet, J.; Gomez, G. R.

Stereochemistry of the tetrabutylammonium cyanide-catalyzed cyanosilylation of cyclic alpha,beta-epoxyketones - Dependence of the diastereoselectivity on the ring size
European Journal of Organic Chemistry: 3969-3976 2006.

Allouti, F.; Manceron, L.; Alikhani, M. E.

The Ni-2+O-2 reaction: the IR spectrum and structure of Ni2O2. A combined IR matrix isolation and theoretical study
Physical Chemistry Chemical Physics, (8): 3715-3725 2006.

Alonso, I.; Alcami, M.; Mauleon, P.; Carretero, J. C.
Understanding sulfone behavior in palladium-catalyzed domino reactions with aryl iodides
Chemistry-a European Journal, (12): 4576-4583 2006.

Alves, C. N.; Carneiro, A. S.; Andres, J.; Domingo, L. R.
A DFT study of the Diels-Alder reaction between methyl acrolein derivatives and cyclopentadiene. Understanding the effects of Lewis acids catalysts based on sulfur containing boron heterocycles
Tetrahedron, (62): 5502-5509 2006.

Amriou, S.; Wang, C. S.; Batsanov, A. S.; Bryce, M. R.; Perepichka, D. F.; Ortí, E.; Viruela, R.; Vidal-Gancedo, J.; Rovira, C.
The interplay of inverted redox potentials and aromaticity in the oxidized states of new pi-electron donors: 9-(1,3-dithiol-2-ylidene)fluorene and 9-(1,3-dithiol-2-ylidene)thioxanthene derivatives
Chemistry-a European Journal, (12): 3389-3400 2006.

Ando, K.
Semiquantal analysis of hydrogen bond
Journal of Chemical Physics, (125) 2006.

Andrews, L.; Cho, H. G.
Matrix preparation and spectroscopic and theoretical investigations of simple methylidene and methylidyne complexes of group 4-6 transition metals
Organometallics, (25): 4040-4053 2006.

Anez, R.; Herize, A.; Sierraalta, A.; Cordova, T.; Chuchani, G.
DFT study of substituent effects of 2-substituted alkyl ethyl methylcarbonates in homogeneous, unimolecular gas phase elimination kinetics
International Journal of Chemical Kinetics, (38): 184-193 2006.

Anez, R.; Izquierdo, R.; Vidal, A.; Cordova, T.; Sierraalta, A.; Chuchani, G.
Theoretical study of the mechanisms for the homogenous gas-phase elimination kinetics of some 2-hydroxynitroalkanes
Journal of Physical Organic Chemistry, (19): 836-840 2006.

Ara, I.; Chaouche, N.; Fornies, J.; Fortuno, C.; Kribii, A.; Tsipis, A. C.
Formation of PPh₂C₆F₅ through phosphido platinum and/or palladium(III) intermediates
Organometallics, (25): 1084-1091 2006.

Aragoni, M. C.; Arca, M.; Devillanova, F. A.; Grimaldi, P.; Isaia, F.; Lelj, F.; Lippolis, V.
Kinetic and thermodynamic aspects of the CT and T-shaped adduct formation between 1,3-dimethylimidazoline-2-thione (or-2-selone) and halogens
European Journal of Inorganic Chemistry: 2166-2174 2006.

- Ardura, D.; Sordo, T. L.
Radical ring expansion reactions of methylenecyclopropane derivatives: A theoretical study
Journal of Organic Chemistry, (71): 4803-4809 2006.
- Atanasov, M.; Comba, P.; Martin, B.; Muller, V.; Rajaraman, G.; Rohwer, H.; Wunderlich, S.
DFT models for copper(II) bispidine complexes: Structures, stabilities, isomerism, spin distribution, and spectroscopy
Journal of Computational Chemistry, (27): 1263-1277 2006.
- Atesin, T. A.; Oster, S. S.; Skugrud, K.; Jones, W. D.
The synthesis and structural properties of M(dippe)(eta(2)-C4H4S) complexes of Pd and Pt and comparison with their Ni analog
Inorganica Chimica Acta, (359): 2798-2805 2006.
- Baba, T.; Takeuchi, M.; Nakai, H.
Natural atomic orbital based energy density analysis: Implementation and applications
Chemical Physics Letters, (424): 193-198 2006.
- Bahrami, H.; Zahedi, M.; Safari, N.
Theoretical investigations of the reactivity of verdoheme analogues: Opening of the planar macrocycle by amide, dimethyl amide, and hydroxide nucleophiles to form helical biliverdin type complexes
Journal of Inorganic Biochemistry, (100): 1449-1461 2006.
- Baig, S.; Richard, B.; Serp, P.; Mijoule, C.; Hussein, K.; Guihery, N.; Barthelat, J. C.; Kalck, P.
Synthesis and theoretical study of a series of dipalladium(I) complexes containing the Pd-2(mu-CO)(2) core
Inorganic Chemistry, (45): 1935-1944 2006.
- Bako, I.; Hutter, J.; Palinkas, G.
Car-parrinello molecular dynamics simulation of liquid formic acid
Journal of Physical Chemistry A, (110): 2188-2194 2006.
- Balazs, G.; Green, J. C.; Scheer, M.
Terminally coordinated AsS and PS ligands
Chemistry-a European Journal, (12): 8603-8608 2006.
- Balta, B.; Monard, G.; Ruiz-Lopez, M. F.; Antoine, M.; Gand, A.; Boschi-Muller, S.; Branlant, G.
Theoretical study of the reduction mechanism of sulfoxides by thiols
Journal of Physical Chemistry A, (110): 7628-7636 2006.
- Bandyopadhyay, D.; Bhattacharyya, D.
Estimation of strength in different extra Watson-Crick hydrogen bonds in DNA double helices through quantum chemical studies
Biopolymers, (83): 313-325 2006.
- Bansal, R. K.; Gupta, N.; Kumawat, S. K.

Origin of the stereo- and regioselectivities in the Diels-Alder reactions of azaphospholes: a DFT investigation
Tetrahedron, (62): 1548-1556 2006.

Bansal, R. K.; Gupta, N.; Kumawat, S. K.; Gupta, R.
Diels-Alder reactions of 5,6-dihydrothiazolo 3,2-d 1,4,2 diazaphospholes: A DFT investigation
Heteroatom Chemistry, (17): 402-410 2006.

Bao, P.; Yu, Z. H.
Theoretical studies on the role of pi-electron delocalization in determining the conformation of N-benzylideneaniline with three types of LMO basis sets
Journal of Computational Chemistry, (27): 809-824 2006.

Barros, N.; Eisenstein, O.; Maron, L.
DFT studies of the methyl exchange reaction between Cp2M-CH3 or Cp M-2-CH3 (Cp = C5H5, Cp*=C5Me5, M = Y, Sc, Ln) and CH4. Does M ionic radius control the reaction?*
Dalton Transactions: 3052-3057 2006.

Barros, N.; Eisenstein, O.; Maron, L.; Tilley, T. D.
DFT investigation of the catalytic hydromethylation of alpha-olefins by metallocenes. 1. Differences between scandium and lutetium in propene hydromethylation
Organometallics, (25): 5699-5708 2006.

Barroso-Flores, J.; Cogordan, J. A.
Influence of intramolecular Sn-chalcogen interactions on the conformational preferences for three diorganotin(IV) xanthates
Journal of Organometallic Chemistry, (691): 4937-4944 2006.

Beaudoin, E.; Bertin, D.; Gigmes, D.; Marque, S. R. A.; Siri, D.; Tordo, P.
Alkoxyamine C-ON bond homolysis: Stereoelectronic effects
European Journal of Organic Chemistry: 1755-1768 2006.

Ben-Ari, E.; Cohen, R.; Gandelman, M.; Shimon, L. J. W.; Martin, J. M. L.; Milstein, D.
ortho C-H activation of haloarenes and anisole by an electron-rich iridium(I) complex: Mechanism and origin of regio- and chemoselectivity. An experimental and theoretical study
Organometallics, (25): 3190-3210 2006.

Berkessel, A.; Adrio, J. A.; Huettenhain, D.; Neudorfl, J. M.
Unveiling the "booster effect" of fluorinated alcohol solvents: Aggregation-induced conformational changes and cooperatively enhanced H-bonding
Journal of the American Chemical Society, (128): 8421-8426 2006.

Bernasconi, C. F.; Bhattacharya, S.; Wenzel, P. J.; Olmstead, M. M.
Kinetic and thermodynamic acidity of Cp(NO(PPh₃)Re(2,5-dimethyl-3-thienyl)carbene (+). Transition state imbalance and intrinsic barriers
Organometallics, (25): 4322-4330 2006.

Bernshtein, V.; Oref, I.

Energy transfer between azulene and krypton: Comparison between experiment and computation
Journal of Chemical Physics, (125) 2006.

Berthier, G.; Savinelli, R.; Adamo, C.; Ciofini, I.
Theoretical study of sticking processes on molecular models of silica surfaces
Theoretical Chemistry Accounts, (115): 379-384 2006.

Besora, M.; Maseras, F.; Lledos, A.; Eisenstein, O.
Silyl, hydrido silylene or alternative bonding modes: The many possible structures of (C5H5)(PH3)IrX (+) (X = SiHR2 and SiR3; R = H, CH3, SiH3, and Cl)
Organometallics, (25): 4748-4755 2006.

Bessac, F.; Frenking, G.
Chemical bonding in phosphane and amine complexes of main group elements and transition metals
Inorganic Chemistry, (45): 6956-6964 2006.

Bharatam, P. V.; Amita; Kaur, D.; Kumar, P. S.
Potential energy surface of thionylimide
International Journal of Quantum Chemistry, (106): 1237-1249 2006.

Bharatam, P. V.; Iqbal, P.
Theoretical studies on electron delocalization in diaminoguanidine
Journal of Computational Chemistry, (27): 334-343 2006.

Bhat, K. L.; Lai, J. H.; Markham, G. D.; DiJulio, A. M.; Bock, C. W.
Amine-catalyzed B-O-C bond formation: Mechanistic insights from density functional theory and second-order Moller-Plesset perturbation theory
Organometallics, (25): 2427-2436 2006.

Bickelhaupt, F. M.; Sola, M.; Guerra, C. F.
Covalency in highly polar bonds. Structure and bonding of methylalkalimetal oligomers (CH3M)_n (M = Li-Rb; n=1, 4)
Journal of Chemical Theory and Computation, (2): 965-980 2006.

Bleiholder, C.; Werz, D. B.; Koppel, H.; Gleiter, R.
Theoretical investigations on chalcogen-chalcogen interactions: What makes these nonbonded interactions bonding?
Journal of the American Chemical Society, (128): 2666-2674 2006.

Bobadova-Parvanova, P.; Quinonero-Santiago, D.; Morokuma, K.; Musaev, D. G.
Theoretical study of the structure and properties of (eta(5)-C5Me4H)(2)Zr(2)(mu(2),eta(2),eta(2)-N-2)
Journal of Chemical Theory and Computation, (2): 336-341 2006.

Bocca, C. C.; Basso, E. A.; Fiorin, B. C.; Tormena, C. F.; dos Santos, F. P.

Conformational behavior of cis-2-methoxy, cis-2-methylthio, and cis-2-methylselenocyclohexanol: A theoretical and experimental investigation
Journal of Physical Chemistry A, (110): 9438-9442 2006.

Bock, C. W.; Markham, G. D.; Katz, A. K.; Glusker, J. P.
The arrangement of first- and second-shell water molecules around metal ions: effects of charge and size
Theoretical Chemistry Accounts, (115): 100-112 2006.

Bogdanov, B.; McMahon, T. B.
Gas phase S(N)2 reactions of halide ions with trifluoromethyl halides: Front- and back-side attack vs. complex formation
Journal of Physical Chemistry A, (110): 1350-1363 2006.

Bohme, U.
Hydrosilylation vs. 2+2 -cycloaddition: A theoretical study with iron and ruthenium complexes
Journal of Organometallic Chemistry, (691): 4400-4410 2006.

Bolton, P. D.; Clot, E.; Adams, N.; Dubberley, S. R.; Cowley, A. R.; Mountford, P.
Experimental and DFT studies of cationic imido titanium alkyls: Agostic interactions and C-H bond and solvent activation reactions of isolobal analogues of group 4 metallocenium cations
Organometallics, (25): 2806-2825 2006.

Bolton, P. D.; Clot, E.; Cowley, A. R.; Mountford, P.
AlMe3 and ZnMe2 adducts of a titanium imido methyl cation: A combined crystallographic, spectroscopic, and DFT study
Journal of the American Chemical Society, (128): 15005-15018 2006.

Bongini, A.; Panunzio, M.
A hetero Diels-Alder concerted vs. aldol stepwise mechanism in the cyclization of silyloxyazadienes with aldehydes: A theoretical study
European Journal of Organic Chemistry: 972-977 2006.

Brand, H.; Liebman, J. F.; Schulz, A.; Mayer, P.; Villinger, A.
Nonlinear, resonance-stabilized pseudohalides: From alkali methanides to ionic liquids of methanides
European Journal of Inorganic Chemistry: 4294-4308 2006.

Brauer, C. S.; Craddock, M. B.; Kilian, J.; Grumstrup, E. M.; Orilall, M. C.; Mo, Y. R.; Gao, J. L.; Leopold, K. R.
Amine-hydrogen halide complexes: Experimental electric dipole moments and a theoretical decomposition of dipole moments and binding energies
Journal of Physical Chemistry A, (110): 10025-10034 2006.

Britovsek, G. J. P.; Ugolotti, J.; Hunt, P.; White, A. J. P.
Lewis and Bronsted multifunctionality: an unusual heterocycle from the reaction of bis(pentafluorophenyl)borinic acid with nitriles
Chemical Communications: 1295-1297 2006.

Britton, D.; Cramer, C. J.
2-formylbenzonitrile
Acta Crystallographica Section C-Crystal Structure Communications, (62): O307-O309 2006.

Bucher, D.; Raugei, S.; Guidoni, L.; Dal Peraro, M.; Rothlisberger, U.; Carloni, P.; Klein, M. L.
Polarization effects and charge transfer in the KcsA potassium channel
Biophysical Chemistry, (124): 292-301 2006.

Buhl, M.; Holub, J.; Hnyk, D.; Machacek, J.
Computational studies of structures and properties of metallaboranes. 2. Transition-metal dicarbollide complexes
Organometallics, (25): 2173-2181 2006.

Buhl, M.; Kabrede, H.; Diss, R.; Wipff, G.
Effect of hydration on coordination properties of uranyl(VI) complexes. A first-principles molecular dynamics study
Journal of the American Chemical Society, (128): 6357-6368 2006.

Bunuel, E.; Marco-Martinez, J.; Diaz-Tendero, S.; Martin, F.; Alcami, M.; Cardenas, D. J.
Computational studies on the cyclization of polycyclic aromatic hydrocarbons in the synthesis of curved aromatic derivatives
Chemphyschem, (7): 475-481 2006.

Burnette, R. R.; Weinhold, F.
Determination of the conformation of 2-hydroxy- and 2-aminobenzoic acid dimers using C-13 NMR and density functional theory/natural bond order analysis: The central importance of the carboxylic acid carbon
Journal of Physical Chemistry A, (110): 8832-8839 2006.

Bylikin, S. Y.; Shipov, A. G.; Negrebetsky, V. V.; Baukov, Y. I.; Ovchinnikov, Y. E.; Pogozhikh, S. A.; Pestunovich, S. V.; Belousova, L. I.; Belogolova, E. F.; Sidorkin, V. F.; Voronkov, M. G.; Pestunovich, V. A.; Kalikhman, I.; Kost, D.
Reaction of N-trimethylsilyl derivatives of amides and lactams with chloro(chloromethyl)dimethylstannane: Crystal and molecular structure of 1-(chlorodimethylstannylmethyl)-2-piperidone
Journal of Organometallic Chemistry, (691): 779-786 2006.

Bzhezovskii, V. M.; Chura, M. B.; Il'chenko, N. N.
Methyl and trifluoromethyl vinyl sulfones: Steric and electronic structure
Russian Journal of General Chemistry, (76): 366-375 2006.

Bzhezovskii, V. M.; Chura, M. B.; Il'chenko, N. N.
Methyl and trifluoromethyl vinyl sulfoxides. Steric and electronic structure
Russian Journal of General Chemistry, (76): 359-365 2006.

Cai, X.; Zhang, Y. X.; Zhang, X. X.; Jiang, J. Z.

Structures and properties of 2,3,9,10,16,17,23,24-octasubstituted phthalocyaninato-lead complexes: The substitutional effect study on the basis of density functional theory calculations
Journal of Molecular Structure-Theochem, (801): 71-80 2006.

Cai, X. C.; Cygon, P.; Goldfuss, B.; Griesbeck, A. G.; Heckroth, H.; Fujitsuka, M.; Majima, T.
alpha-carbonyl substituent effect on the lifetimes of triplet 1,4-biradicals from Norrish-Type-II reactions
Chemistry-a European Journal, (12): 4662-4667 2006.

Cantat, T.; Ricard, L.; Mezailles, N.; Le Floch, P.
Synthesis, reactivity, and DFT studies of S-C-S zirconium(IV) complexes
Organometallics, (25): 6030-6038 2006.

Cardenas, D. J.; Martin-Matute, B.; Echavarren, A. M.
Aryl transfer between Pd(II) centers or Pd(IV) intermediates in Pd-catalyzed domino reactions
Journal of the American Chemical Society, (128): 5033-5040 2006.

Cardenas-Jiron, G. I.; Paredes-Garcia, V.; Venegas-Yazigi, D.; Zagal, J. H.; Paez, M.; Costamagna, J.
Theoretical modeling of the oxidation of hydrazine by iron(II) phthalocyanine in the gas phase. Influence of the metal character
Journal of Physical Chemistry A, (110): 11870-11875 2006.

Cargnoni, F.; Molteni, G.; Cooper, D. L.; Raimondi, M.; Ponti, A.
The electronic structure of nitrilimine: absence of the carbenic form
Chemical Communications: 1030-1032 2006.

Castillo, N.; Boyd, R. J.
Theoretical study of the thermolysis of beta-hydroxyl aldehydes
Journal of Physical Chemistry A, (110): 8710-8718 2006.

Cauchy, T.; Ruiz, E.; Alvarez, S.
Exchange coupling interactions in a Fe-6 complex: A theoretical study using density functional theory
Physica B-Condensed Matter, (384): 116-119 2006.

Cauchy, T.; Ruiz, E.; Alvarez, S.
Magnetostructural correlations in polynuclear complexes: The Fe-4 butterflies
Journal of the American Chemical Society, (128): 15722-15727 2006.

Cee, V. J.; Cramer, C. J.; Evans, D. A.
Theoretical investigation of enolborane addition to alpha-heteroatom-substituted aldehydes. Relevance of the cornforth and polar Felkin-Anh models for asymmetric induction
Journal of the American Chemical Society, (128): 2920-2930 2006.

Chakraborty, A.; De, R.; Guchhait, N.
Dissection of methyl internal rotational barrier in thioacetone
Chemical Physics Letters, (432): 616-622 2006.

- Chalmet, S.; Ruiz-Lopez, M. F.
Structure of the HO₂O radical in liquid water: A theoretical study
Chemphyschem, (7): 463-467 2006.
- Chang, G. R.; Zhou, L. X.; Chen, D.
How can the cross-link adducts formed by novel trans platinum drug be influenced by hydrogen bond
Chinese Journal of Chemistry, (24): 1514-1522 2006.
- Chang, G. R.; Zhou, L. X.; Chen, D.
Theoretical study of nonclassical platinum complexes bonding to purine bases: How the long-lived monofunctional adducts can be in existence?
Chinese Journal of Structural Chemistry, (25): 407-416 2006.
- Chemouri, H.; Benchouk, W.; Mekelleche, S. M.
Regioselectivity of hetero Diels-Alder reactions between 1-aza-1,3-butadiene derivatives and dimethylvinylamine: A theoretical investigation
Journal of Theoretical & Computational Chemistry, (5): 707-718 2006.
- Chemouri, H.; Mekelleche, S. M.
An analysis of the regioselectivity in hetero Diels-Alder reactions using DFT-based reactivity indexes
Journal of Theoretical & Computational Chemistry, (5): 197-206 2006.
- Chen, D. L.; Tian, W. Q.; Lu, W. C.; Sun, C. C.
Special stability of cationic MPb₁₂₊ clusters and superalkali character of neutral MPb₁₂ clusters (M=B, Al, Ga, In, and Tl)
Journal of Chemical Physics, (124) 2006.
- Chen, X.; Wu, W. P.; Zhang, J. L.; Cao, Z. X.
Theoretical studies on the interactions of cations with diazine
Chinese Journal of Structural Chemistry, (25): 1321-1330 2006.
- Chen, X. F.; Guo, W. Y.; Zhao, L. M.; Fu, Q. T.
Theoretical survey of the potential energy surface of Ni⁺ plus acetone reaction
Chemical Physics Letters, (432): 27-32 2006.
- Chen, X. H.; Turecek, F.
The arginine anomaly: Arginine radicals are poor hydrogen atom donors in electron transfer induced dissociations
Journal of the American Chemical Society, (128): 12520-12530 2006.
- Cheng, H. Y.; Chang, S.; Liao, W. C.
Studies of the Cr(CN)(5)NO (3-) and Cr(NH₃)(5)NO (2+) complex ions via density functional theory
Journal of Molecular Structure-Theochem, (776): 77-82 2006.
- Cheng, L. P.; Li, X. Q.
Theoretical study of XN₅ (-) (X=O, S, Se, Te) systems

Journal of Molecular Modeling, (12): 805-811 2006.

Cheng, L. P.; Liu, Y.

Theoretical study of XN₆ (2-) (X = O, S, Se, Te) systems

Chemical Physics Letters, (418): 272-280 2006.

Cho, H. G.; Kim, T. H.; Andrews, L.

Periodic trends in the agostic interaction in zirconium and hafnium methylidene hydride halide complexes

Chemistry-an Asian Journal, (1): 404-416 2006.

Cid, M. B.; Alonso, I.; Alfonso, F.; Bonilla, J. B.; Lopez-Prados, J.; Martin-Lomas, M.

Simultaneous regio- and enantiodifferentiation in carbohydrate coupling

European Journal of Organic Chemistry: 3947-3959 2006.

Cimino, P.; Bifulco, G.; Riccio, R.; Gomez-Paloma, L.; Barone, V.

On the role of stereo-electronic effects in tuning the selectivity and rate of DNA alkylation by duocarmycins

Organic & Biomolecular Chemistry, (4): 1242-1251 2006.

Cinelli, M. A.; Minghetti, G.; Cocco, F.; Stoccoro, S.; Zucca, A.; Manassero, M.; Arca, M.

Synthesis and properties of gold alkene complexes. Crystal structure of Au(bipy(oXyl))(eta(2)-CH₂=CHPh) (PF₆) and DFT calculations on the model cation Au(bipy)(eta(2)-CH₂=CH₂)

Dalton Transactions: 5703-5716 2006.

Clennan, E. L.; Hightower, S. E.

Natural bond orbital analyses of persulfoxide stabilization by remote functional groups. The conformationally induced electrostatic stabilization sulfide photooxygenation mechanism

Journal of Organic Chemistry, (71): 1247-1250 2006.

Contreras, R. H.; Esteban, A. L.; Diez, E.; Della, E. W.; Lochert, I. J.; dos Santos, F. P.; Tormena, C. F.

Experimental and theoretical study of hyperconjugative interaction effects on NMR (1)J(CH) scalar couplings

Journal of Physical Chemistry A, (110): 4266-4275 2006.

Contreras, R. H.; Esteban, A. L.; Diez, E.; Head, N. J.; Della, E. W.

Transmission mechanisms of NMR long-range J(C-13, F-19) scalar couplings in 1-F,4-X-cubanes: a DFT and experimental study

Molecular Physics, (104): 485-492 2006.

Cornard, J. P.; Lapouge, C.

Absorption spectra of caffeic acid, caffeoate and their 1 : 1 complex with Al(III): Density functional theory and time-dependent density functional theory investigations

Journal of Physical Chemistry A, (110): 7159-7166 2006.

Corral, I.; Mo, O.; Yanez, M.

Analysis of the bonding in XH₃-Cu⁺ (X=B, Al, Ga) complexes

International Journal of Quantum Chemistry, (106): 659-663 2006.

- Corral, I.; Mo, O.; Yanez, M.
Cu⁺ association to some Ph-X (X = OH, NH₂, CHO, COOH, CF₃) phenyl derivatives. A comparison with Li⁺ complexes
International Journal of Mass Spectrometry, (255): 20-27 2006.
- Corral, I.; Mo, O.; Yanez, M.
On the stability of non-conventional pi-complexes between Ni⁺ and toluene, phenyl-silane and phenyl-germane
Journal of Physical Organic Chemistry, (19): 495-502 2006.
- Cossio, F. P.; Alonso, C.; Lecea, B.; Ayerbe, M.; Rubiales, G.; Palacios, F.
Mechanism and stereoselectivity of the aza-Wittig reaction between phosphazenes and aldehydes
Journal of Organic Chemistry, (71): 2839-2847 2006.
- Cysewski, P.; Shyichuk, A.
A first principle characterization of polyethylene, poly(propylene) and polystyrene macroradicals properties
Macromolecular Theory and Simulations, (15): 331-338 2006.
- Czarnik-Matusewicz, B.; Michalska, D.; Sandorfy, C.; Zeegers-Huyskens, T.
Experimental and theoretical study of the vibrational spectra of halothane
Chemical Physics, (322): 331-342 2006.
- de la Lande, A.; Gerard, H.; Moliner, V.; Izzet, G.; Reinaud, O.; Parisel, O.
Theoretical modelling of tripodal CuN₃ and CuN₄ cuprous complexes interacting with O₂, CO or CH₃CN
Journal of Biological Inorganic Chemistry, (11): 593-608 2006.
- de Oliveira, P. R.; Tasic, L.; Rocco, S. A.; Rittner, R.
Stereoelectronic and inductive effects on H-1 and C-13 NMR chemical shifts of some cis-1,3-disubstituted cyclohexanes
Magnetic Resonance in Chemistry, (44): 790-796 2006.
- de Visser, S. P.
Can the replacement of a single atom in the enzyme horseradish peroxidase convert it into a monooxygenase? A density functional study
Journal of Physical Chemistry B, (110): 20759-20761 2006.
- Deakyne, C. A.; Corum, A. K.; Thomas, H. M.; Liebman, J. F.
The structure and energetics of singlet, closed-shell B, C, F, H(2) : Simplicity resulting in diversity
Journal of Fluorine Chemistry, (127): 1355-1367 2006.
- Del Piero, S.; Di Bernardo, P.; Fedele, R.; Melchior, A.; Polese, P.; Tolazzi, M.
Affinity of polypyridines towards Cd-II and Co-II ions: a thermodynamic and DFT study
European Journal of Inorganic Chemistry: 3738-3745 2006.

- Delgado, F. S.; Kerbellec, N.; Ruiz-Perez, C.; Cano, J.; Lloret, F.; Julve, M.
Malonate-containing manganese(III) complexes: Synthesis, crystal structure, and magnetic properties of AsPh₄Mn(mal)(2)(H₂O)(2)
Inorganic Chemistry, (45): 1012-1020 2006.
- Demange, M.; Boubeker, L.; Auffrant, A.; Mezailles, N.; Ricard, L.; Le Goff, X.; Le Floch, P.
A new and convenient approach towards bis(iminophosphoranyl)methane ligands and their dicationic, cationic, anionic and dianionic derivatives
New Journal of Chemistry, (30): 1745-1754 2006.
- Demirhan, F.; Cagatay, B.; Demir, D.; Baya, M.; Daran, J. C.; Poli, R.
*Reduction of Cp*²Mo2O5 in aqueous medium: Structure and properties of a triangular mixed oxo-hydroxo-bridged product, Cp*Mo-3(3)(μ-O)(2)(μ-OH)(4)(X)(2) (X = CF₃CO₂ or CF₃SO₃)*
European Journal of Inorganic Chemistry: 757-764 2006.
- Dem'yanov, P. I.; Gschwind, R. M.
Formation of hydrogen bonds in complexes between dimethylcuprate(I) anion and methane, propane, or dimethyl ether. A theoretical study
Organometallics, (25): 5709-5723 2006.
- Deng, W. Y.; Qiu, W. Y.
Theoretical studies on the structure and stability of C-30 carbyne trefoil knot
Acta Chimica Sinica, (64): 2322-2326 2006.
- Derat, E.; Shaik, S.
Two-state reactivity, electromerism, tautomerism, and "surprise" isomers in the formation of Compound II of the enzyme horseradish peroxidase from the principal species, Compound I
Journal of the American Chemical Society, (128): 8185-8198 2006.
- Dhumal, N. R.; Gejji, S. P.
Theoretical studies on blue versus red shifts in diglyme-M+-X- (M = Li, Na, and K and X = CF₃SO₃, PF₆, and (CF₃SO₂)(2)N)
Journal of Physical Chemistry A, (110): 219-227 2006.
- Dhumal, N. R.; Gejji, S. P.
Theoretical studies on blue versus red shifts in diglyme-M+-X-(M=Li, Na, K and X=BF₄, ClO₄, SCN)
Journal of Molecular Structure-Theochem, (758): 233-240 2006.
- Diaz, M. C.; Illescas, B. M.; Martin, N.; Perepichka, I. F.; Bryce, M. R.; Levillain, E.; Viruela, R.; Orti, E.
Electronic interactions in a new pi-extended tetrathiafulvalene dimer
Chemistry-a European Journal, (12): 2709-2721 2006.
- Dillen, J.; Woldu, M. G.; Koch, K. R.
N,N-di-n-butyl-N'-pivaloylthiourea
Acta Crystallographica Section E-Structure Reports Online, (62): O4819-O4820 2006.
- Dilman, A. D.; Levin, V. V.; Karni, M.; Apeloig, Y.
Activation of pentafluorophenylsilanes by weak Lewis bases in reaction with iminium cations

Journal of Organic Chemistry, (71): 7214-7223 2006.

Ding, Y. Q.; Feng, D. C.; Feng, S. Y.; Zhang, J.; Xie, J.

The DFT study on the electronic structures of polytitasilanes: Several new classes of narrow band gap polymers

Polymer, (47): 3681-3688 2006.

Domingo, L. R.; Arno, M.; Merino, P.; Tejero, T.

A DFT study of the molecular mechanisms of the nucleophilic addition of ester-derived lithium enolates and silyl ketene acetals to nitrones: Effects of the Lewis acid catalyst

European Journal of Organic Chemistry: 3464-3472 2006.

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

pi-Strain-induced electrophilicity in small cycloalkynes: A DFT analysis of the polar cycloaddition of cyclopentyne towards enol ethers

European Journal of Organic Chemistry: 498-506 2006.

Domingo, L. R.; Perez-Prieto, J.

Exploring two-state reaction pathways in the photodimerization of cyclohexadiene

Chemphyschem, (7): 614-618 2006.

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

Towards an understanding of the polar Diels-Alder reactions of nitrosoalkenes with enamines: A theoretical study

European Journal of Organic Chemistry: 2570-2580 2006.

Domingo, L. R.; Picher, M. T.; Arroyo, P.; Saez, J. A.

1,3-dipolar cycloadditions of electrophilically activated benzonitrile N-oxides. Polar cycloaddition versus oxime formation

Journal of Organic Chemistry, (71): 9319-9330 2006.

Domingo, L. R.; Saez, J. A.; Palmucci, C.; Sepulveda-Arques, J.; Gonzalez-Rosende, M. E.

A DFT study for the formation of imidazo 1,2-c pyrimidines through an intramolecular Michael addition

Tetrahedron, (62): 10408-10416 2006.

dos Santos, F. P.; Tormena, C. F.

Orbital interactions and their effects on the conformational stability in six-membered rings containing nitrogen atoms

Journal of Molecular Structure-Theochem, (763): 145-148 2006.

Doskocz, J.; Doskocz, M.; Roszak, S.; Soloducho, J.; Leszczynski, J.

Theoretical studies of symmetric five-membered heterocycle derivatives of carbazole and fluorene: Precursors of conducting polymers

Journal of Physical Chemistry A, (110): 13989-13994 2006.

Duan, H. X.; Gong, Z.; Cheng, J. G.; Zhu, W. L.; Chen, K. X.; Jiang, H. L.

Induction of an aromatic six-membered nitrogen ring via cation-pi interaction

Journal of Physical Chemistry A, (110): 12236-12240 2006.

Dubillard, S.; Rota, J. B.; Saue, T.; Faegri, K.

Bonding analysis using localized relativistic orbitals: Water, the ultrarelativistic case and the heavy homologues H₂X (X=Te, Po, eka-Po)
Journal of Chemical Physics, (124) 2006.

Ducati, L. C.; Freitas, M. P.; Tormena, C. F.; Rittner, R.

Conformational and stereoelectronic investigation of chloromethyl methyl sulfide and its sulfinyl and sulfonyl analogs
Journal of Molecular Structure, (800): 45-50 2006.

Dudev, T.; Lim, C.

A DFT/CDM study of metal-carboxylate interactions in metalloproteins: Factors governing the maximum number of metal-bound carboxylates
Journal of the American Chemical Society, (128): 1553-1561 2006.

Ebrahimi, A.; Roohi, H.; Habibi, M.; Karimian, T.; Vaziri, R.

Topological and natural population analyses of gas-phase identity S(N)2 reactions of some methyl halides: Backside attack
Chemical Physics Letters, (419): 179-183 2006.

Ebrahimi, A.; Roohi, H.; Habibi, M.; Mohammadi, M.; Vaziri, R.

Characterization of conformers of non-ionized proline on the basis of topological and NBO analyses: Can nitrogen be a donor of hydrogen bond?
Chemical Physics, (322): 289-297 2006.

Ellis, B. D.; Macdonald, C. L. B.

Phosphorus(I) iodide: A versatile metathesis reagent for the synthesis of low oxidation state phosphorus compounds
Inorganic Chemistry, (45): 6864-6874 2006.

El-Nahas, A. M.; Uchimaru, T.; Sugie, M.; Tokuhashi, K.; Sekiya, A.

Relative reactivity and regioselectivity of halogen-substituted ethenes and propene toward addition of an OH radical or O (P-3) atom: An ab initio study
Journal of Molecular Structure-Theochem, (770): 59-65 2006.

Enescu, M.; Cardey, B.

Mechanism of cysteine oxidation by a hydroxyl radical: A theoretical study
Chemphyschem, (7): 912-919 2006.

Erben, M. F.; Boese, R.; Della Vedova, C. O.; Oberhammer, H.; Willner, H.

Toward an intimate understanding of the structural properties and conformational preference of oxoesters and thioesters: Gas and crystal structure and conformational analysis of dimethyl monothiocarbonate, CH₃OC(O)SCH₃
Journal of Organic Chemistry, (71): 616-622 2006.

Escoubet, S.; Gastaldi, S.; Vanthuyne, N.; Gil, G.; Siri, D.; Bertrand, M. P.

Thiyl radical mediated racemization of benzylic amines
European Journal of Organic Chemistry: 3242-3250 2006.

Esteban-Gomez, D.; Platas-Iglesias, C.; Enriquez-Perez, T.; Avecilla, F.; de Blas, A.; Rodriguez-Blas, T.
Lone-pair activity in lead(II) complexes with unsymmetrical lariat ethers
Inorganic Chemistry, (45): 5407-5416 2006.

Evangelista, F. A.; Schaefer, H. F.
Hydrogen atom and hydride anion addition to adenine: Structures and energetics
Chemphyschem, (7): 1471-1480 2006.

Fabian, J.; Komiha, N.; Linguerri, R.; Rosmus, P.
The absorption wavelengths of sulfur chromophors of ultramarines calculated by time-dependent density functional theory
Journal of Molecular Structure-Theochem, (801): 63-69 2006.

Fanfrlik, J.; Lepsik, M.; Horinek, D.; Havlas, Z.; Hobza, P.
Interaction of carboranes with biomolecules: Formation of dihydrogen bonds
Chemphyschem, (7): 1100-1105 2006.

Farras, P.; Teixidor, F.; Branchadell, V.
Prediction of pK(a) values of nido-carboranes by density functional theory methods
Inorganic Chemistry, (45): 7947-7954 2006.

Fedorova, I. V.; Krishtal, S. P.; Kiselev, M. G.; Safonova, L. P.
Structure of orthophosphoric Acid-N,N-Dimethylformamide complexes
Russian Journal of Physical Chemistry, (80): S7-S13 2006.

Fernandez, I.; Frenking, G.
Correlation between Hammett substituent constants and directly calculated pi-conjugation strength
Journal of Organic Chemistry, (71): 2251-2256 2006.

Fernandez, I.; Sierra, M. A.; Cossio, F. P.
Effect of the metal fragment in the thermal cycloaddition between alkynyl metal(0) Fischer carbene complexes and nitrones
Journal of Organic Chemistry, (71): 6178-6184 2006.

Fernandez, I.; Sierra, M. A.; Cossio, F. P.
Stereoelectronic effects on type I 1,2-dyotropic rearrangements in vicinal dibromides
Chemistry-a European Journal, (12): 6323-6330 2006.

Fernandez, L. E.; Varetti, E. L.
Scaled quantum mechanical force fields for trifluoromethyl selenium derivatives. I. The CF₃SeCN and CF₃SeCH₃ molecules
Canadian Journal of Chemistry-Revue Canadienne De Chimie, (84): 1626-1631 2006.

Fernandez, M. I.; Oliva, J. M.; Armesto, X. L.; Canle, M.; Santaballa, J. A.

Extended planarity and pi delocalization in triazine-based derivatives
Chemical Physics Letters, (426): 290-295 2006.

Ferullo, R. M.; Garda, G. R.; Belletti, P. G.; Branda, M. M.; Castellani, N. J.
Deposition of small Cu, Ag and Au particles on reduced SiO₂
Journal of Molecular Structure-Theochem, (769): 217-223 2006.

Fesun, I. M.; Rozhenko, A. B.; Timoshenko, V. M.
Reduction of 4-fluoro-5-(1,1,2,2-tetrafluoroethyl)-3H-1,2-dithiole-3-thione with sodium sulfide: Synthesis of fluoro-containing sulfur-rich heterocycles
Journal of Fluorine Chemistry, (127): 774-779 2006.

Filatov, A. S.; Rogachev, A. Y.; Petrukhina, M. A.
Gas-phase assembling of dirhodium units into a novel organometallic ladder: Structural and DFT study
Crystal Growth & Design, (6): 1479-1484 2006.

Filippov, O. A.; Filin, A. M.; Tsupreva, V. N.; Belkova, N. V.; Lledos, A.; Ujaque, G.; Epstein, L. M.; Shubina, E. S.
Proton-transfer and H-2-elimination reactions of main-group hydrides EH4- (E = B, Al, Ga) with alcohols
Inorganic Chemistry, (45): 3086-3096 2006.

Fir, B.; Whalen, J. M.; Mercier, H. P. A.; Dixon, D. A.; Schrobilgen, G. J.
Syntheses of F5TeNH3 AsF₆, F5TeN(H)Xe AsF₆, and F5TeNF2 and characterization by multi-NMR and Raman spectroscopy and by electronic structure calculations: The X-ray crystal structures of alpha- and beta-F5TeNH2, F5TeNH3 AsF₆, and F5TeN(H)Xe AsF₆
Inorganic Chemistry, (45): 1978-1996 2006.

Fischer, J.; Schurmann, M.; Mehring, M.; Zachwieja, U.; Jurkschat, K.
The first O,C,S-coordinating pincer-type ligand and its application to the synthesis of a triorganotin cation stabilized by two different donor atoms
Organometallics, (25): 2886-2893 2006.

Fischer, J. T.; Wehner, S. G.; Reinscheid, U. M.
Interpretation of cytidine proton chemical shifts and J coupling constants calculated by DFT
Journal of Molecular Structure-Theochem, (767): 81-85 2006.

Fish, C.; Green, M.; Jeffery, J. C.; Kilby, R. J.; Lynam, J. M.; McGrady, J. E.; Pantazis, D. A.; Russell, C. A.; Willans, C. E.
A main-group analogue of housene: The subtle influence of the inert-pair effect in group 15 clusters
Angewandte Chemie-International Edition, (45): 6685-6689 2006.

Fornili, A.; Moreau, Y.; Sironi, M.; Assfeld, X.
On the suitability of strictly localized orbitals for hybrid QM/MM calculations
Journal of Computational Chemistry, (27): 515-523 2006.

- Francisco, E.; Pendas, A. M.; Blanco, M. A.
A molecular energy decomposition scheme for atoms in molecules
Journal of Chemical Theory and Computation, (2): 90-102 2006.
- Francisco, J. S.
Ab initio study of the structure, bonding, vibrational spectra, and energetics of XBS+ (where X=H, F, and Cl)
Journal of Chemical Physics, (124) 2006.
- Freeman, F.; Po, H. N.
Dimers of and tautomerism between 2-pyrimidinethiol and 2(1H)-pyrimidinethione: A density functional theory (DFT) study
Journal of Physical Chemistry A, (110): 7904-7912 2006.
- Freitas, R. F.; Galembeck, S. E.
Computational study of the interaction between TIBO inhibitors and Y181 (C181), K101, and Y188 amino acids
Journal of Physical Chemistry B, (110): 21287-21298 2006.
- Freitas, R. F.; Galembeck, S. E.
Effect of C-H center dot center dot center dot S and C-H center dot center dot center dot Cl interactions on the conformational preference of inhibitors of TIBO family
Chemical Physics Letters, (423): 131-137 2006.
- Freund, C.; Barros, N.; Gornitzka, H.; Martin-Vaca, B.; Maron, L.; Bourissou, D.
Enforced eta(1)-fluorenyl coordination to rhodium(I) with the FluPPh(2)NPh (-) ligand
Organometallics, (25): 4927-4930 2006.
- Frey, J. A.; Leist, R.; Leutwyler, S.
Hydrogen bonding of the nucleobase mimic 2-pyridone to fluorobenzenes: An ab initio investigation
Journal of Physical Chemistry A, (110): 4188-4195 2006.
- Fu, A. P.; Li, H. L.; Du, D. M.
Thiol-thione tautomerism in 2-pyridinethione: Effect of hydration
Journal of Molecular Structure-Theochem, (767): 51-60 2006.
- Fu, A. P.; List, B.; Thiel, W.
Density functional study of enantioselectivity in the 2-methylproline-catalyzed alpha-alkylation of aldehydes
Journal of Organic Chemistry, (71): 320-326 2006.
- Fu, A. P.; Thiel, W.
Density functional study of noncovalent catalysis of the Diels-Alder reaction by the neutral hydrogen bond donors thiourea and urea
Journal of Molecular Structure-Theochem, (765): 45-52 2006.
- Fueno, H.; Hayashi, M.; Nin, K.; Kubo, A.; Misaki, Y.; Tanaka, K.

Orbital analysis of TTF molecules adsorbed on the Au surface
Current Applied Physics, (6): 939-942 2006.

Fukuzawa, K.; Mochizuki, Y.; Tanaka, S.; Kitaura, K.; Nakano, T.
Molecular interactions between estrogen receptor and its ligand studied by the ab initio fragment molecular orbital method
Journal of Physical Chemistry B, (110): 16102-16110 2006.

Furuya, A.; Misaizu, F.; Ohno, K.
Photodissociation of Mg+-XCH₃ (X=F, Cl, Br, and I) complexes. I. Electronic spectra and dissociation pathways
Journal of Chemical Physics, (125) 2006.

Furuya, A.; Misaizu, F.; Ohno, K.
Photodissociation of Mg+-XCH₃ (X=F, Cl, Br, and I) complexes. II. Fragment angular and energy distributions
Journal of Chemical Physics, (125) 2006.

Gabriel, C. J.; DeMatteo, M. P.; Paul, N. M.; Takaya, T.; Gustafson, T. L.; Hadad, C. M.; Parquette, J. R.
A new class of intramolecularly hydrogen-bonded dendrons based on a 2-methoxyisophthalamide repeat unit
Journal of Organic Chemistry, (71): 9035-9044 2006.

Gagliardi, L.; Cramer, C. J.
Quantum chemical characterization of the bonding of N-heterocyclic carbenes to Cp₂MI compounds M = Ce(III), U(III)
Inorganic Chemistry, (45): 9442-9447 2006.

Gagliardo, M.; Havenith, R. W. A.; van Klink, G.; van Koten, G.
(P-Bis(pentafluorophenyl) substituted) PCP-pincer Ru(II) complexes: A theoretical study of the molecular structure and electronic properties
Journal of Organometallic Chemistry, (691): 4411-4418 2006.

Gaina, L.; Csampai, A.; Turos, G.; Lovasz, T.; Zsoldos-Mady, V.; Silberg, I. A.; Sohar, P.
(E)-3-(2-Alkyl-10H-phenothiazin-3-yl)-1-arylprop-2-en-1-ones: preparative, IR, NMR and DFT study on their substituent-dependent reactivity in hydrazinolysis and sonication-assisted oxidation with copper(II) nitrate
Organic & Biomolecular Chemistry, (4): 4375-4386 2006.

Galabov, B.; Ilieva, S.; Schaefer, H. F.
An efficient computational approach for the evaluation of substituent constants
Journal of Organic Chemistry, (71): 6382-6387 2006.

Galano, A.; Cruz-Torres, A.; Alvarez-Idaboy, J. R.
Isopropylcyclopropane plus OH gas phase reaction: A quantum chemistry plus CVT/SCT approach
Journal of Physical Chemistry A, (110): 1917-1924 2006.

Galvez, O.; Zoermer, A.; Grothe, H.

Theoretical study on the structure of the BrO hydrates
Journal of Physical Chemistry A, (110): 8818-8825 2006.

Gandon, V.; Agenet, N.; Vollhardt, K. P. C.; Malacria, M.; Aubert, C.
Cobalt-mediated cyclic and linear 2 : 1 cooligomerization of alkynes with alkenes: A DFT study
Journal of the American Chemical Society, (128): 8509-8520 2006.

Gao, P.
Structures and properties of the isomers of hexanitrosobenzene: A DFT study
Journal of Molecular Structure-Theochem, (767): 119-130 2006.

Garcia-Iglesias, M.; Bunuel, E.; Cardenas, D. J.
Cationic (η (1-allyl)-palladium complexes as feasible intermediates in catalyzed reactions
Organometallics, (25): 3611-3618 2006.

Gaudel-Siri, A.; Siri, D.; Tordo, P.
Homolysis of N-alkoxyamines: A computational study
Chemphyschem, (7): 430-438 2006.

Gauze, G. F.; Tormena, R.; Basso, E. A.; Tormena, C. F.
Stereoelectronic interactions and their effects on conformational preference for 1,3-dithiane-1-oxide and 1,4-dithiane-1-oxide. A theoretical and experimental study
Chemical Physics Letters, (426): 176-179 2006.

Geerlings, P.; Vos, A. M.; Schoonheydt, R. A.
A computational and conceptual DFT approach to the kinetics of acid zeolite catalyzed electrophilic aromatic substitution reactions
Journal of Molecular Structure-Theochem, (762): 69-78 2006.

Georgieva, I.; Trendafilova, N.
Comprehensive DFT and MO studies on glyoxilic acid oxime and related ions in gas phase and solution: Conformations, basicities and acidities
Chemical Physics, (321): 311-324 2006.

Ghaderi, A. R.; Sabzyan, H.; Hadipour, N. L.
Correlation between NQR parameters and residue size of aliphatic amino acids and their dimers
Biophysical Chemistry, (120): 62-70 2006.

Gheorghiu, M. D.; Racoveanu, A.; Zakin, M. R.
Electronic and molecular structure of aminimides (1-acyl-2,2,2-trimethyldiazan-2-iium-1-ide). 1. Formaminimide ($HCON-N+Me_3$)
Journal of Physical Chemistry A, (110): 3977-3985 2006.

Ghosh, D. C.; Chakraborty, A.
Dipole correlation of the electronic structures of the conformations of water molecule evolving through the normal modes of vibrations between angular (C_{2v}) to linear (D -proportional to h) shapes
International Journal of Molecular Sciences, (7): 71-96 2006.

- Ghosh, S.; Chaitanya, G. K.; Bhanuprakash, K.; Nazeeruddin, M. K.; Gratzel, M.; Reddy, P. Y.
Electronic structures and absorption spectra of linkage isomers of trithiocyanato (4,4',4''-tricarboxy-2,2':6,2''-terpyridine) ruthenium(II) complexes: A DFT study
Inorganic Chemistry, (45): 7600-7611 2006.
- Giese, T. J.; Gregersen, B. A.; Liu, Y.; Nam, K.; Mayaan, E.; Moser, A.; Range, K.; Faza, A. N.; Lopez, C. S.; de Lera, A. R.; Schaftenaar, G.; Lopez, X.; Lee, T. S.; Karypis, G.; York, D. M.
QCRNA 1.0: A database of quantum calculations for RNA catalysis
Journal of Molecular Graphics and Modelling, (25): 423-433 2006.
- Gil, A.; Bertran, J.; Sodupe, M.
Effects of ionization on N-glycylglycine peptide: Influence of intramolecular hydrogen bonds
Journal of Chemical Physics, (124) 2006.
- Gilbert, A. T. B.; Gill, P. M. W.
A point-charge model for electrostatic potentials based on a local projection of multipole moments
Molecular Simulation, (32): 1249-1253 2006.
- Girichev, G. V.; Giricheva, N. I.; Haaland, A.; Kuzmina, N. P.; Samdal, S.; Strenalyuk, T. N.; Tverdova, N. V.; Zaitseva, I. G.
Molecular structures of tris(dipivaloylmethanato) complexes of the lanthanide metals, Ln(dpm)(3), studied by gas electron diffraction and density functional theory calculations: A comparison of the Ln-O bond distances and enthalpies in Ln(dpm)(3) complexes and the cubic sesquioxides, Ln₂O₃
Inorganic Chemistry, (45): 5179-5186 2006.
- Glaser, R.; Knotts, N.
Coordinate covalent C → B bonding in phenylborates and latent formation of phenyl anions from phenylboronic acid
Journal of Physical Chemistry A, (110): 1295-1304 2006.
- Glaser, R.; Wu, H.; von Saint Paul, F.
Chemical carcinogens in non-enzymatic cytosine deamination: 3-isocyanatoacrylonitrile
Journal of Molecular Modeling, (12): 731-737 2006.
- Glasnov, T. N.; Vugts, D. J.; Koningstein, M. M.; Desai, B.; Fabian, W. M. F.; Orru, R. V. A.; Kappe, C. O.
Microwave-assisted Dimroth rearrangement of thiazines to dihydropyrimidinethiones: Synthetic and mechanistic aspects
Qsar & Combinatorial Science, (25): 509-518 2006.
- Glassey, W. V.
Energy partitioning studies of adsorbate repulsion: Chemisorption and coadsorption of CO and NO on the Pd(111) surface
Surface Science, (600): 173-194 2006.
- Glendening, E. D.

Extension of natural energy decomposition analysis (NEDA) to density functional methods
Abstracts of Papers of the American Chemical Society, (231) 2006.

Gong, L. F.; Guo, W. L.; Wu, X. M.; Li, Q. S.

B-7(-) as a novel ligand: Theoretical investigations on structures and chemical bonding of LiB7 and BeB7+

Chemical Physics Letters, (429): 326-334 2006.

Gong, L. F.; Guo, W. L.; Xiong, J. M.; Li, R. X.; Wu, X. M.; Li, W.

Structures and stability of ionic liquid model with imidazole and hydrogen fluorides chains: Density functional theory study

Chemical Physics Letters, (425): 167-178 2006.

Gonzalez-Bejar, M.; Stiriba, S. E.; Domingo, L. R.; Perez-Prieto, J.; Miranda, M. A.

Mechanism of triplet photosensitized Diels-Alder reaction between indoles and cyclohexadienes: Theoretical support for an adiabatic pathway

Journal of Organic Chemistry, (71): 6932-6941 2006.

Gonzalez-Montiel, S.; Andrade-Lopez, N.; Garcia-Montalvo, V.; Cogordan, J. A.; Alvarado-Rodriguez, J. G.

Pentacoordination at germanium by transannular bonding of sulfur or oxygen in an eight-membered ring: An experimental and theoretical study

European Journal of Inorganic Chemistry: 4752-4760 2006.

Goossen, L. J.; Koley, D.; Hermann, H. L.; Thiel, W.

Palladium monophosphine intermediates in catalytic cross-coupling reactions: A DFT study

Organometallics, (25): 54-67 2006.

Gorelsky, S. I.; Ghosh, S.; Solomon, E. I.

Mechanism of N2O reduction by the mu(4)-S tetranuclear Cu-z cluster of nitrous oxide reductase

Journal of the American Chemical Society, (128): 278-290 2006.

Gotz, N.; Herler, S.; Mayer, P.; Schulz, A.; Villinger, A.; Weigand, J. J.

On the staudinger reaction of SP(N-3)(3) with PPh3 and (Me3Si)(2)N-(Me3Si)N-PPh2

European Journal of Inorganic Chemistry: 2051-2057 2006.

Gourlaouen, C.; Piquemal, J. P.; Parisel, O.

Pb(H2O) (2+) and Pb(OH) (+): Four-component density functional theory calculations, correlated scalar relativistic constrained-space orbital variation energy decompositions, and topological analysis

Journal of Chemical Physics, (124) 2006.

Gourlaouen, C.; Piquemal, J. P.; Saue, T.; Parisel, O.

Revisiting the geometry of nd(10) (n+1)s(0) M(H2O) (P+) complexes using four-component relativistic DFT calculations and scalar relativistic correlated CSOV energy decompositions (MP+=Cu+, Zn2+, Ag+, Cd2+, Au+, Hg2+)

Journal of Computational Chemistry, (27): 142-156 2006.

Grabarkiewicz, T.; Hoffmann, M.

Syn- and anti-conformations of 5'-deoxy- and 5'-O-methyl-uridine 2',3'-cyclic monophosphate
Journal of Molecular Modeling, (12): 205-212 2006.

Gracia, L.; Andres, J.; Beltran, A.; Sambrano, J. R.
DFT study on the water-assisted mechanism for the reaction between VO⁺ and NH₃ to yield VNH⁺ and H₂O
Chemical Physics Letters, (427): 265-270 2006.

Gracia, L.; Sambrano, J. R.; Andres, J.; Beltran, A.
Mechanistic insights into the reaction between VO₂⁺ and propene based on a DFT study
Organometallics, (25): 1643-1653 2006.

Graham, D. C.; Cavell, K. J.; Yates, B. F.
The influence of N-substitution on the reductive elimination behaviour of hydrocarbyl-palladium-carbene complexes - a DFT study
Dalton Transactions: 1768-1775 2006.

Graterol, M.; Cordova, T.; Chuchani, G.
Theoretical study of the gas-phase elimination kinetics of several heterocyclic carbamates
Journal of Physical Organic Chemistry, (19): 700-705 2006.

Green, S. P.; Jones, C.; Lippert, K. A.; Mills, D. P.; Stasch, A.
Complexes of an anionic gallium(I) N-heterocyclic carbene analogue with group 14 element(II) fragments: Synthetic, structural and theoretical studies
Inorganic Chemistry, (45): 7242-7251 2006.

Greene, S. N.; Richards, N. G. J.
Electronic structure, bonding, spectroscopy and energetics of Fe-dependent nitrile hydratase active-site models
Inorganic Chemistry, (45): 17-36 2006.

Gribanova, T. N.; Minyaev, R. M.; Minkin, V. I.
Sandwich compounds of second-row elements: a quantum chemical study
Russian Chemical Bulletin, (55): 1893-1903 2006.

Grobe, J.; Lutke-Brochtrup, K.; Krebs, B.; Lage, M.; Niemeyer, H. H.; Wurthwein, E. U.
Alternative ligands, XXXVII. Phosphane ligands with boron as Lewis-acidic centre: Synthesis and coordinating properties
Zeitschrift Fur Naturforschung Section B-a Journal of Chemical Sciences, (61): 882-895 2006.

Gronowski, M.; Kolos, R.
Isomers of cyanodiacylene: Theoretical structures and IR spectra
Chemical Physics Letters, (428): 245-248 2006.

Grubisic, S.; Milicic, M. K.; Radanovic, D. D.; Niketic, S. R.
Conformational analysis of edta-type rhodium(III) complexes with mixed five- and six-membered chelate rings. Structural analysis of conformational flexibility in rhodium(III) complexes containing 1,3-propanediamine-N,N'-diacetate-N,N'-di-3-propionate ligand

Journal of Molecular Structure, (794): 125-132 2006.

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

Electron attachment to Nucleotides in aqueous solution
Chemphyschem, (7): 1885-1887 2006.

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

Understanding electron attachment to the DNA double helix: The thymidine monophosphate-adenine pair in the gas phase and aqueous solution
Journal of Physical Chemistry B, (110): 19696-19703 2006.

Gu, J. D.; Wang, J.; Leszczynski, J.

Molecular basis of the recognition process: Hydrogen-bonding patterns in the guanine primary recognition site of ribonuclease T1
Journal of Physical Chemistry B, (110): 13590-13596 2006.

Gupta, N.; Shah, K. K.; Garg, R.

Substituent-dependent anomeric effects as a source of conformational preference in pyridinium methylides
Journal of Organic Chemistry, (71): 1344-1350 2006.

Gutowski, K. E.; Dixon, D. A.

Predicting the energy of the water exchange reaction and free energy of solvation for the uranyl ion in aqueous solution
Journal of Physical Chemistry A, (110): 8840-8856 2006.

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

All-electron DFT modeling of SWCNT growth on iron catalysts from carbon monoxide feedstock
Journal of Nanoscience and Nanotechnology, (6): 1281-1289 2006.

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

Structure and Properties of Mn-n, Mn-n(-), and Mn-n(+) clusters (n= 3-10)
Journal of Physical Chemistry A, (110): 9758-9766 2006.

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

Dissociative and associative attachment of NO to iron clusters
Journal of Chemical Physics, (125) 2006.

Guvench, O.; MacKerell, A. D.

Quantum mechanical analysis of 1,2-ethanediol conformational energetics and hydrogen bonding
Journal of Physical Chemistry A, (110): 9934-9939 2006.

Guzei, I. A.; Timokhin, V. I.; West, R.

Bis(trimethylsilyl)amido-kappa N {tert-butyl (E)-2-(tert-butylimino)ethyl amido-kappa N-2,N'-tin(II), a key intermediate in synthesis of 1,3-di-tert-butyl-2,3-dihydro-1H-1,3,2-diazastannole
Acta Crystallographica Section C-Crystal Structure Communications, (62): M90-M92 2006.

Hansen, D. F.; Gorelsky, S. I.; Sarangi, R.; Hodgson, K. O.; Hedman, B.; Christensen, H. E. M.; Solomon, E. I.; Led, J. J.

Reinvestigation of the method used to map the electronic structure of blue copper proteins by NMR relaxation

Journal of Biological Inorganic Chemistry, (11): 277-285 2006.

Hansen, D. F.; Led, J. J.

Determination of the geometric structure of the metal site in a blue copper protein by paramagnetic NMR

Proceedings of the National Academy of Sciences of the United States of America, (103): 1738-1743 2006.

Hargittai, M.; Reffy, B.; Kolonits, M.

An intricate molecule: Aluminum triiodide. Molecular structure of AlI₃ and Al₂I₆ from electron diffraction and computation

Journal of Physical Chemistry A, (110): 3770-3777 2006.

Havenith, R. W. A.; van Lenthe, J. H.; van Walree, C. A.; Jenneskens, L. W.

Orbital interactions expressed in resonance structures: An approach to compute stabilisation of cyclobutanediyl diradicals

Journal of Molecular Structure-Theochem, (763): 43-50 2006.

He, W. D.; Xue, Y.; Zhang, H.; Tian, A. M.; Wong, N. B.

Modeling of hydrogen bonds in monohydrated 2,4-dithiothymine: An ab initio and AIM study

Journal of Physical Chemistry B, (110): 1416-1422 2006.

Heppner, D. E.; Gherman, B. F.; Tolman, W. B.; Cramer, C. J.

Can an ancillary ligand lead to a thermodynamically stable end-on 1 : 1 Cu-O-2 adduct supported by a beta-diketiminate ligand?

Dalton Transactions: 4773-4782 2006.

Herbert, J. M.; Head-Gordon, M.

Accuracy and limitations of second-order many-body perturbation theory for predicting vertical detachment energies of solvated-electron clusters

Physical Chemistry Chemical Physics, (8): 68-78 2006.

Herbert, J. M.; Head-Gordon, M.

Charge penetration and the origin of large O-H vibrational red-shifts in hydrated-electron clusters, (H₂O)(n)(-)

Journal of the American Chemical Society, (128): 13932-13939 2006.

Heredia, M. M.; Lorono, M.; Cordova, T.; Chuchani, G.

Theoretical study of the elimination kinetics of several 2-substituted ethyl N,N-dimethylcarbamates in the gas phase, (CH₃)₂NCOOCH(2)CH(2)Z, Z = CH₂Cl, C CH, C N

Journal of Molecular Structure-Theochem, (770): 131-137 2006.

Hnyk, D.; Buhl, M.; Holub, J.; Hayes, S. A.; Wann, D. A.; Mackie, I. D.; Borisenko, K. B.; Robertson, H. E.; Rankin, D. W. H.

Molecular structures of arachno-decaborane derivatives 6,9-X₂B₈H₁₀ (X = CH₂, NH, Se) including a gas-phase electron-diffraction study of 6,9-C₂B₈H₁₄
Inorganic Chemistry, (45): 6014-6019 2006.

Hnyk, D.; Holub, J.
Handles for the dicarbadodecaborane basket based on arachno-5,10-C₂B₈H₁₃ (-): Oxygen
Dalton Transactions: 2620-2622 2006.

Hnyk, D.; Holub, J.; Hayes, S. A.; Robinson, M. F.; Wann, D. A.; Robertson, H. E.; Rankin, D. W. H.
Molecular structures of Arachno-heteroboranes with decaborane frameworks: Two C-symmetrical azacarba- and carbathiaboranes
Inorganic Chemistry, (45): 8442-8446 2006.

Hobza, P.; Zahradník, R.; Muller-Dethlefs, K.
The world of non-covalent interactions: 2006
Collection of Czechoslovak Chemical Communications, (71): 443-531 2006.

Holland, J. P.; Green, J. C.; Dilworth, J. R.
Probing the mechanism of hypoxia selectivity of copper bis(thiosemicarbazone) complexes: DFT calculation of redox potentials and absolute acidities in solution
Dalton Transactions: 783-794 2006.

Hostetler, K. J.; Crabtree, K. N.; Poole, J. S.
The photochemistry of 4-azidopyridine-1-oxide
Journal of Organic Chemistry, (71): 9023-9029 2006.

Hou, J. Q.; Kang, H. S.
Density functional study of chemical stability and nitrogen encapsulation of C₄₈N₁₂ and C₅₈N₁₂
Journal of Physical Chemistry A, (110): 12241-12248 2006.

Hou, X. J.; Janssens, E.; Lievens, P.; Nguyen, M. T.
Theoretical study of the geometric and electronic structure of neutral and anionic doped silver clusters, Ag₅X₀-, with X = Sc, Ti, V, Cr, Mn, Fe, Co, and Ni
Chemical Physics, (330): 365-379 2006.

Houston, J. R.; Richens, D. T.; Casey, W. H.
Distinct water-exchange mechanisms for trinuclear transition-metal clusters
Inorganic Chemistry, (45): 7962-7967 2006.

Hrobarik, P.; Straka, M.; Pyykko, P.
Computational study of bonding trends in the metalloactinyl series ET_nM and MThM' (E = N-, O, F-; M, M' = Ir-, Pt, Au+)
Chemical Physics Letters, (431): 6-12 2006.

Hsu, M. H.; Chen, R. T.; Sheu, W. S.; Shieh, M.
Carbon dioxide fixation by an unprecedented hydroxo lead-chromium carbonyl complex: Synthesis, reactivity, and theoretical calculations
Inorganic Chemistry, (45): 6740-6747 2006.

- Huang, B.; Zhang, J. X.; Li, R.; Shen, Z. Y.; Hou, S. M.; Zhao, X. Y.; Xue, Z. Q.; Wu, Q. D.
First-principles calculation of the conductance of the Al-C-60-Al junction
Acta Physico-Chimica Sinica, (22): 161-166 2006.
- Huang, J.; Song, J. R.; Ren, T. H.; Ma, H. X.; Wang, H. L.; Hu, H. M.; Wen, Z. Y.
Preparation, crystal structure and theoretical calculation of 4,6-dimethoxy-2-(methoxycarbamidothiocarbamido)pyrimidine
Acta Chimica Sinica, (64): 9-16 2006.
- Huang, M. Q.; Zhang, W. J.; Yang, Y.; Wang, Z. Y.; Hao, L. Q.; Zhao, W. W.; Zhao, W. X.; Li, J. S.; Gao, X. M.
Theoretical study of the intramolecular hydrogen bonds of aromatic peroxy radicals from OH-toluene reactions
Journal of Molecular Structure-Theochem, (774): 1-6 2006.
- Huetz, P.; Boiteux, C.; Compoint, M.; Ramseyer, C.; Girardet, C.
Incidence of partial charges on ion selectivity in potassium channels
Journal of Chemical Physics, (124) 2006.
- Hunt, P. A.; Kirchner, B.; Welton, T.
Characterising the electronic structure of ionic liquids: An examination of the 1-butyl-3-methylimidazolium chloride ion pair
Chemistry-a European Journal, (12): 6762-6775 2006.
- Hyla-Kryspin, I.; Nie, Y.; Pritzkow, H.; Siebert, W.
Molecular and electronic structure of (η (5)-pentaalkyl-2,3-dihydro-1,3-diborolyl) (η (5)-pentamethylcyclopentadienyl)metal complexes, M = Fe, Ru
Journal of Organometallic Chemistry, (691): 4565-4572 2006.
- Ida, B. N.; Fudacz, P. S.; Pulsifer, D. H.; Standard, J. M.
A gas- and condensed-phase density functional study of donor-acceptor complexes of sulfur trioxide
Journal of Physical Chemistry A, (110): 5831-5838 2006.
- Ikeda, A.; Nakao, Y.; Sato, H.; Sakaki, S.
A new analysis of molecular orbital wave functions based on resonance theory
Journal of Physical Chemistry A, (110): 9028-9030 2006.
- Ikeda, A.; Yokogawa, D.; Sato, H.; Sakaki, S.
Solvation effect on resonance structure: Extracting valence bond-like character from molecular orbitals
Chemical Physics Letters, (424): 449-452 2006.
- Illia, O.; Bagan, X.; Cazorla, A. M.; Lyon, C.; Baceiredo, A.; Branchadell, V.; Ortuno, R. M.
Reaction of C-silylated alpha-diazophosphines as nucleophiles toward carbonyl compounds: A mechanistic study and application to the synthesis of alkynes and alpha-hydroxyphosphonamides
Journal of Organic Chemistry, (71): 5320-5327 2006.

- Inerbaev, T. M.; Belosludov, R. V.; Mizuseki, H.; Takahashi, M.; Kawazoe, Y.
First excited state properties and static hyperpolarizability of ruthenium(II) ammine complexes
Journal of Chemical Theory and Computation, (2): 1325-1334 2006.
- Inerbaev, T. M.; Saito, S.; Belosludov, R. V.; Mizuseki, H.; Takahashi, M.; Kawazoe, Y.
Excited state properties and quadratic optical nonlinearities in charged organic chromophores: Theoretical analysis
Journal of Chemical Physics, (125) 2006.
- Ionescu, A.; Wang, L. J.; Whitfield, M.
Two unexpected effects found with 2,3,4,6-tetra-O-methyl-D-glucosid- and mannosidopyranosyl oxacarbenium ions - An O-2 pseudoequatorial preference and a large H-2-C-2--O-2-CHO3 syn preference
Nmr Spectroscopy and Computer Modeling of Carbohydrates: Recent Advances, (930): 302-319 2006.
- Iriarte, A. G.; Cutin, E. H.; Della Vedova, C. O.
Infrared and Raman spectra of 2-chloro-2,2-difluoroacetamide (ClF₂CC(O)NH₂)
Journal of Molecular Structure, (800): 154-157 2006.
- Ishida, T.; Morita, A.
Extended treatment of charge response kernel comprising the density functional theory and charge regulation procedures
Journal of Chemical Physics, (125) 2006.
- Ishikawa, T.; Mochizuki, Y.; Nakano, T.; Amari, S.; Mori, H.; Honda, H.; Fujita, T.; Tokiwa, H.; Tanaka, S.; Komeiji, Y.; Fukuzawa, K.; Tanaka, K.; Miyoshi, E.
Fragment molecular orbital calculations on large scale systems containing heavy metal atom
Chemical Physics Letters, (427): 159-165 2006.
- Itoh, K.; Kitoh, K.; Kishimoto, S.
Concerted and stepwise mechanisms in the Diels-Alder and Michael reactions of furans with methyl 3-nitroacrylate - Experimental and theoretical studies
Canadian Journal of Chemistry-Revue Canadienne De Chimie, (84): 392-406 2006.
- Itoh, Y.; Houk, K. N.; Mikami, K.
Experimental and theoretical studies on radical trifluoromethylation of titanium ate and lithium enolates
Journal of Organic Chemistry, (71): 8918-8925 2006.
- Izadyar, M.; Gholmi, M. R.
Substituent effects on the gas phase reactivity of alkyl allyl sulfides, a theoretical study
Journal of Molecular Structure-Theochem, (759): 11-15 2006.
- Izadyar, M.; Zamani, N.; Gholami, M. R.
Kinetics and mechanism of 2-pyridylacetic acid pyrolysis in the gas phase: A joint experimental and theoretical study

Chemical Physics, (330): 394-400 2006.

Izod, K.; McFarlane, W.; Tyson, B. V.; Carr, I.; Clegg, W.; Harrington, R. W.
Stabilization of a dialkylstannylene by unusual B-H center dot center dot center dot Sn gamma-agostic-type interactions. A structural, spectroscopic, and DFT study
Organometallics, (25): 1135-1143 2006.

Jaime, E.; Weston, J.
Mechanism of the MeOH/H₂O substitution in a series of biomimetic bimetallo zinc-based H₃O²⁺ complexes
European Journal of Inorganic Chemistry: 793-801 2006.

Janczyk, A.; Lichtenberger, D. L.; Ziurys, L. M.
Competition between metal-amido and metal-imido chemistries in the alkaline earth series: An experimental and theoretical study of BaNH
Journal of the American Chemical Society, (128): 1109-1118 2006.

Janssens, E.; Hou, X. J.; Nguyen, M. T.; Lievens, P.
The geometric, electronic, and magnetic properties of Ag₅X⁺ (X=Sc, Ti, V, Cr, Mn, Fe, Co, and Ni) clusters
Journal of Chemical Physics, (124) 2006.

Jaworska, M.
DFT calculations for model diimine-iron complexes with nitric oxide and water ligands
Inorganic Chemistry Communications, (9): 284-289 2006.

Jaworska, M.; Stasicka, Z.
Structure and UV-vis spectroscopy of Roussin black salt Fe₄S₃(NO)(7) (-)
Journal of Molecular Structure, (785): 68-75 2006.

Jemmis, E. D.; Pathak, B.; King, R. B.; Schaefer, H. F.
Bond length and bond multiplicity: sigma-bond prevents short pi-bonds
Chemical Communications: 2164-2166 2006.

Jensen, W. B.
The origin of the term "hypervalent"
Journal of Chemical Education, (83): 1751-1752 2006.

Jian, F. F.; Zhang, K. J.; Zhao, P. S.; Zheng, J.
Ab initio and experimental studies on dibenzothiazyl-disulfide
Bulletin of the Korean Chemical Society, (27): 1048-1052 2006.

Jian, F. F.; Zhao, P. S.; Bai, Z. S.; Cai, Z. J.
Experimental and theoretical study on 4-phenyl-3-(1,2,4-triazol-1-yl)methyl -triazole-5-thione
Polish Journal of chemistry, (80): 325-333 2006.

Jian, F. F.; Zhao, P. S.; Zhang, L.; Zheng, J.

Synthesis, structure and quantum chemical calculations on p-trifluoromethylphenyl thioacid amide

Journal of Fluorine Chemistry, (127): 63-67 2006.

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

Electrostatic field-adapted molecular fractionation with conjugated caps for energy calculations of charged biomolecules

Journal of Chemical Physics, (124) 2006.

Jiang, Z. Y.; Lee, K. H.; Li, S. T.; Chu, S. Y.

Structures and charge distributions of cationic and neutral C_n-1Ag clusters (n=2-8)

Physical Review B, (73) 2006.

Jiang, Z. Y.; Lee, K. H.; Li, S. T.; Chu, S. Y.

Structures and charge distributions of cationic and neutral L_nX_m (X = Na and K)

International Journal of Mass Spectrometry, (253): 104-111 2006.

Jimenez-Oses, G.; Corzana, F.; Bustos, J. H.; Perez-Fernandez, M.; Peregrina, J. M.; Avenoza, A.

Conformational analysis of 2-substituted cyclobutane-alpha-amino acid derivatives. A synergistic experimental and computational study

Journal of Organic Chemistry, (71): 1869-1878 2006.

Jones, R. M.; Goldcamp, M. J.; Krause, J. A.; Baldwin, M. J.

Theoretical, structural, and spectroscopic studies of a series of Ni-II(TrisoxH₃)X-2 complexes

Polyhedron, (25): 3145-3158 2006.

Joshi, A. M.; Delgass, W. N.; Thomson, K. T.

Analysis of O₂ adsorption on binary-alloy clusters of gold: Energetics and correlations

Journal of Physical Chemistry B, (110): 23373-23387 2006.

Joubert, L.; Pavone, M.; Barone, V.; Adamo, C.

Comparative static and dynamic study of a prototype S(N)2 reaction

Journal of Chemical Theory and Computation, (2): 1220-1227 2006.

Ju, X. H.; Qiu, L.; Xiao, H. M.

Computational investigation on 2,4,6-trinitrochlorobenzene crystal

Propellants Explosives Pyrotechnics, (31): 38-41 2006.

Kalaiselvan, A.; Venuvanalingam, P.

Ab initio and DFT investigations on the stereochemistry of ring opening of episulfides

Journal of Molecular Structure-Theochem, (763): 1-5 2006.

Kamachi, T.; Kouno, T.; Nam, W.; Yoshizawa, K.

How axial ligands control the reactivity of high-valent iron(IV)-oxo porphyrin pi-cation radicals in alkane hydroxylation: A computational study

Journal of Inorganic Biochemistry, (100): 751-754 2006.

Kandt, C.; Xu, Z. T.; Tielemans, D. P.

Opening and closing motions in the periplasmic vitamin B-12 binding protein BtuF
Biochemistry, (45): 13284-13292 2006.

Kang, H. S.

Theoretical study of endohedral C-36 and its dimers
Journal of Physical Chemistry A, (110): 4780-4786 2006.

Kar, T.; Panja, N.; Nandi, P. K.

Electronic structure and spectroscopic properties of the two structural isomers of donor-acceptor substituted sesquifulvalene in the gas and solution phases - A case study of sudden polarization
Journal of Physical Chemistry A, (110): 12684-12692 2006.

Karafiloglou, P.

Control of delocalization and structural changes by means of an electric field
Journal of Computational Chemistry, (27): 1883-1891 2006.

Karaghiosoff, K.; Klapotke, T. M.; Mayer, P.; Piotrowski, H.; Polborn, K.; Willer, R. L.; Weigand, J. J.

N-nitroso- and N-nitraminotetrazoles

Journal of Organic Chemistry, (71): 1295-1305 2006.

Karamat, S.; Fabian, W. M. F.

Computational study of the conformational space of methyl 2,4-diacetyl-beta-D-xylopyranoside: C-4(1) and C-1(4) chairs, skew-boats ((SO)-S-2, S-1(3)), and B-3,B-o boat forms
Journal of Physical Chemistry A, (110): 7477-7484 2006.

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

Novel triplet ground state silylenes: H-N = C = Si, CN-N = C = Si, and MeO-N = C = Si at DFT levels
Monatshefte fur Chemie, (137): 1385-1400 2006.

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

From halo-azasilylenes to halo-phosphasilylenes (X-CNSi vs. X-CPSi) at ab initio and DFT levels
Journal of Organometallic Chemistry, (691): 2666-2678 2006.

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

A quest for triplet silylenes XHSi3 at ab initio and DFT levels (X = H, F, Cl and Br)
Journal of Organometallic Chemistry, (691): 1845-1856 2006.

Kassaee, M. Z.; Musavi, S. M.; Ghambarian, M.; Zanjani, M. R. K.

Switching of global minima of novel germylenic reactive intermediates via halogens (X): C2GeH2 vs. C2GeHX at ab initio and DFT levels
Journal of Organometallic Chemistry, (691): 2933-2944 2006.

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

A theoretical study on phosphasilylenes CPSi-X (X = H, CN, NH2 and OMe)
Journal of Molecular Structure-Theochem, (761): 7-16 2006.

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

Steric effects on the dialkyl substituted X2C2Si silylenes: A theoretical study

Heteroatom Chemistry, (17): 619-633 2006.

Katsumoto, Y.; Komatsu, H.; Ohno, K.

Origin of the blue shift of the CH stretching band for 2-butoxyethanol in water

Journal of the American Chemical Society, (128): 9278-9279 2006.

Kaulgud, T. V.; Dhumal, N. R.; Gejji, S. P.

Electronic structure and normal vibrations of $CH_3(OCH_2CH_2)(n)OCH_3\text{-}M\text{+}\text{-}CF_3SO_3$ - ($n=2\text{-}4$, $M = Li, Na, K$)

Journal of Physical Chemistry A, (110): 9231-9239 2006.

Kaur, D.; Kaur, R. P.; Kaur, P.

Geometrical isomerism and stability of mono- and dichalcogenide analogs of carbamic acid $H_2NC(=X)YH$ ($X, Y=O, S, Se$)

Bulletin of the Chemical Society of Japan, (79): 1869-1875 2006.

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

Substituent and solvent effects on the rotational barriers in selenoamides: A theoretical study

Journal of Molecular Structure-Theochem, (759): 41-49 2006.

Keese, R.

Carbon flatland: Planar tetracoordinate carbon and fenestrane

Chemical Reviews, (106): 4787-4808 2006.

Kim, C. K.; Han, I. S.; Ryu, W. S.; Lee, H. W.; Lee, B. S.; Kim, C. K.

Unusual pi-donating effects of pi-accepting substituents on the stabilities of benzylic cations: A theoretical study

Journal of Physical Chemistry A, (110): 2500-2504 2006.

Kimura, M.; Iwata, A.; Itoh, M.; Yamada, K.; Kimura, T.; Sugiura, N.; Ishida, M.; Kato, S.

Synthesis, structures, and some reactions of (thioacyl)thio - and (acylseleno)antimony and - bismuth derivatives ((RCSS)(x)MR_{3-x}1 (RCOSe)(x)MR_{3-x}1 with $M=Sb, Bi$ and $x=1\text{-}3$)

Helvetica Chimica Acta, (89): 747-783 2006.

Kishimoto, N.; Matsumoto, M.; Matsumura, E.; Ohno, K.

Collision-energy-resolved Penning ionization electron spectroscopy of toluene and chlorotoluenes

European Physical Journal D, (38): 75-84 2006.

Klanicova, A.; Travnicek, Z.; Popa, I.; Cajan, M.; Dolezal, K.

Synthesis, characterization and in vitro cytotoxicity of Co(II) complexes with N6-substituted adenine derivatives: X-ray structures of 6-(4-chlorobenzylamino)purin-di-ium diperchlorate dihydrate and Co-6(mu-L-6)(4)Cl-8(DMSO)(10) center dot 4DMSO

Polyhedron, (25): 1421-1432 2006.

Klein, R. A.

Lack of intramolecular hydrogen bonding in glucopyranose: Vicinal hydroxyl groups exhibit negative cooperativity

Chemical Physics Letters, (433): 165-169 2006.

- Kleinpeter, E.
Push-pull alkenes: structure and pi-electron distribution
Journal of the Serbian Chemical Society, (71): 1-17 2006.
- Knize, M. G.; Hatch, F. T.; Tanga, M. J.; Lau, E. Y.; Colvin, M. E.
A QSAR for the mutagenic potencies of twelve 2-amino-trimethylimidazopyridine isomers: Structural, quantum chemical, and hydropathic factors
Environmental and Molecular Mutagenesis, (47): 132-146 2006.
- Kobrsi, I.; Zheng, W. J.; Knox, J. E.; Heeg, M. J.; Schlegel, H. B.; Winter, C. H.
Experimental and theoretical study of the coordination of 1,2,4-triazolato, tetrazolato, and pentazolato ligands to the K(18-crown-6) (+) fragment
Inorganic Chemistry, (45): 8700-8710 2006.
- Koch, R.; Bolter, E.; Stroot, J.; Beckhaus, R.
Theoretical studies on titanium pentafulvene complexes
Journal of Organometallic Chemistry, (691): 4539-4544 2006.
- Kochina, T. A.; Vrazhnov, D. V.; Ignat'ev, I. S.; Voronkov, M. G.
Reactions of silylum ions with nucleophiles
Russian Journal of General Chemistry, (76): 1774-1777 2006.
- Koltunov, K. Y.; Prakash, G. K. S.; Rasul, G.; Olah, G. A.
Superacidic activation of maleimide and phthalimide and their reactions with cyclohexane and arenes
European Journal of Organic Chemistry: 4861-4866 2006.
- Krawczyk, H.; Sliwinski, M.; Kedzia, J.; Wojciechowski, J.; Wolf, W. M.
Highly enantioselective synthesis of alpha-methylene-delta-valerolactones by an asymmetric Michael reaction
Tetrahedron-Asymmetry, (17): 908-915 2006.
- Krishtal, A.; Senet, P.; Yang, M.; Van Alsenoy, C.
A Hirshfeld partitioning of polarizabilities of water clusters
Journal of Chemical Physics, (125) 2006.
- Krivdin, L. B.; Larina, L. I.; Chernyshev, K. A.; Rulev, A. Y.
Nonempirical calculations of NMR indirect spin-spin coupling constants Part 14: Azomethines of the alpha,beta-unsaturated aldehydes
Magnetic Resonance in Chemistry, (44): 178-187 2006.
- Krugler, M. C.; Legouin, B.; Gargadennec, S.; Mouret, L.; Burgot, J. L.
The 3-thioxo-1,2-dithiol-4-yl group: A versatile one endowed also with a -R electronic effect
Phosphorus Sulfur and Silicon and the Related Elements, (181): 2307-2320 2006.
- Kruszynski, R.; Siwy, M.; Porwolik-Czomperlik, I.; Trzesowska, A.
A new regioselective method of macrobicyclic Schiff bases synthesis

Inorganica Chimica Acta, (359): 649-658 2006.

Kunze, A.; Gleiter, R.; Bethke, S.; Rominger, F.

Complexes of pi-prisms with gallium(I)

Organometallics, (25): 4787-4791 2006.

Kusama, H.; Sugihara, H.

Theoretical studies of 1 : 1 charge-transfer complexes between nitrogen-containing heterocycles and I-2 molecules, and implications on the performance of dye-sensitized solar cell

Journal of Photochemistry and Photobiology a-Chemistry, (181): 268-273 2006.

Kuznetsov, M. L.; Kozlova, L. V.; Dement'ev, A. I.

Theoretical study of 1,3-dipolar cycloaddition of nitrones to doubly activated nitriles

Russian Journal of Inorganic Chemistry, (51): 1602-1612 2006.

Kuznetsov, M. L.; Kukushkin, V. Y.

Theoretical study of reactant activation in 1,3-dipolar cycloadditions of cyclic nitrones to free and Pt-bound nitriles

Journal of Organic Chemistry, (71): 582-592 2006.

Kwon, K. D.; Vadillo-Rodriguez, V.; Logan, B. E.; Kubicki, J. D.

Interactions of biopolymers with silica surfaces: Force measurements and electronic structure calculation studies

Geochimica et Cosmochimica Acta, (70): 3803-3819 2006.

Lam, W. H.; Cheng, E. C. C.; Yam, V. W. W.

Computational studies on the photophysical properties and NMR fluxionality of the tetranuclear copper(I) complexes Cu-4(mu-dppm)(4)(mu(4)-E) (2+) (E = PPh and S)

Inorganic Chemistry, (45): 9434-9441 2006.

Lamsabhi, A. M.; Alcami, M.; Mo, O.; Yanez, M.; Tortajada, J.

Gas-phase deprotonation of uracil-Cu2+ and thiouracil-Cu2+ complexes

Journal of Physical Chemistry A, (110): 1943-1950 2006.

Landis, C. R.; Weinhold, F.

Origin of trans-bent geometries in maximally bonded transition metal and main group molecules

Journal of the American Chemical Society, (128): 7335-7345 2006.

Langer, V.; Scholtzova, E.; Mach, P.; Solcan, T.; Smrcok, L.

2-Anilinomethylene-3-oxobutane-nitrile: an X-ray and density functional theory study

Acta Crystallographica Section C-Crystal Structure Communications, (62): O544-O546 2006.

Larabi, L.; Benali, O.; Mekelleche, S. M.; Harek, Y.

2-mercapto-1-methylimidazole as corrosion inhibitor for copper in hydrochloric acid

Applied Surface Science, (253): 1371-1378 2006.

Laromaine, A.; Teixidor, F.; Kivekas, R.; Sillanpaa, R.; Arca, M.; Lippolis, V.; Crespo, E.; Vinas, C.

Synthesis, reactivity and structural studies of selenide bridged carboranyl compounds

Dalton Transactions: 5240-5247 2006.

Layfield, R. A.; Buhl, M.; Rawson, J. M.

Structure, bonding, and paramagnetism in the manganese(II) tris-allyl anions Mn{eta(x)-(C(3)H(3)R(2))(3)} (-) (R = H, SiMe(3); x = 1 or 3): Insight from theory
Organometallics, (25): 3570-3575 2006.

Leblanc, M.; Siri, D.; Marque, S. R. A.; Grimaldi, S.; Bertin, D.; Tordo, P.

beta-fragmentation of alkoxy radicals: Natural bond orbital analysis
International Journal of Quantum Chemistry, (106): 676-685 2006.

Leclerc, F.; Karplus, M.

Two-metal-ion mechanism for hammerhead-ribozyme catalysis
Journal of Physical Chemistry B, (110): 3395-3409 2006.

Leo, E. A.; Domingo, L. R.; Miranda, M. A.; Tormos, R.

Photogeneration and reactivity of 1,n-diphenyl-1,n-azabiradicals
Journal of Organic Chemistry, (71): 4439-4444 2006.

Leopoldini, M.; Russo, N.; Toscano, M.

Gas and liquid phase acidity of natural antioxidants
Journal of Agricultural and Food Chemistry, (54): 3078-3085 2006.

Lerner, D. A.; Weinberg, J.; Cimpoesu, F.; Balaceanu-Stolnici, C.

Theoretical study of DHEA: comparative HF and DFT calculations of the electronic properties of a complex between DHEA and serotonin
Journal of Molecular Modeling, (12): 146-151 2006.

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

A group electronegativity equalization scheme including external potential effects
Journal of Physical Chemistry A, (110): 8872-8879 2006.

Li, A. Y.

Theoretical investigation of hydrogen bonds between CO and HNF2, H2NF, and HNO
Journal of Physical Chemistry A, (110): 10805-10816 2006.

Li, H.; Gordon, M. S.; Jensen, J. H.

Charge transfer interaction in the effective fragment potential method
Journal of Chemical Physics, (124) 2006.

Li, H.; Ma, J.; Evans, D. G.; Zhou, T.; Li, F.; Duan, X.

Molecular dynamics modeling of the structures and binding energies of alpha-nickel hydroxides and nickel-aluminum layered double hydroxides containing various interlayer guest anions
Chemistry of Materials, (18): 4405-4414 2006.

Li, H. F.; Bu, Y. X.; Yan, S. H.; Li, P.; Cukier, R. I.

Proton character of the peptide unit in the Ca2+-binding sites of calcium pump
Journal of Physical Chemistry B, (110): 11005-11013 2006.

- Li, Q. S.; Xu, Y.
A DFT study on dinuclear metallocenes RMMR R= (BCO)(5), (BNN)(5); M = Be, Mg, Ca, Zn, Cd
Journal of Physical Chemistry A, (110): 11898-11902 2006.
- Li, Q. Z.; Wu, G. S.; Yu, Z. W.
The role of methyl groups in the formation of hydrogen bond in DMSO-methanol mixtures
Journal of the American Chemical Society, (128): 1438-1439 2006.
- Li, S. D.; Miao, C. Q.; Ren, G. M.; Guo, J. C.
Triple-decker transition-metal complexes (C_nH_n)M(B₆C)M(C_nH_n) (M = Fe, Ru, Mn, Re; n=5, 6) containing planar hexacoordinate carbon atoms
European Journal of Inorganic Chemistry: 2567-2571 2006.
- Li, S. G.; Dixon, D. A.
Molecular and electronic structures, Bronsted basicities, and Lewis acidities of group VIB transition metal oxide clusters
Journal of Physical Chemistry A, (110): 6231-6244 2006.
- Li, Y.; Li, Z. R.; Wu, D.; Chen, W.; Sun, C. C.
Cyclobutadiene complexed with Li atom and the effects of substituting by F atom in LiC₄H₄
Journal of Molecular Structure-Theochem, (758): 21-28 2006.
- Li, Y.; Wu, D.; Li, Z. R.; Chen, W.; Sun, C. C.
Do single-electron lithium bonds exist? Prediction and characterization of the H₃C center dot center dot center dot Li-Y (Y = H, F, OH, CN, NC, and CCH) complexes
Journal of Chemical Physics, (125) 2006.
- Li, Z. R.; Wang, F. F.; Wu, D.; Li, Y.; Chen, W.; Sun, X. Y.; Gu, F. L.; Aoki, Y.
Royal crown-shaped electride Li-3-N-3-Be containing two superatoms: New knowledge on aromaticity
Journal of Computational Chemistry, (27): 986-993 2006.
- Liang, X. Q.; Pu, X. M.; Shu, Y. J.; Tian, A. M.
Theoretical studies on structures and properties of benzene and its nitrogen isoelectronic equivalents
Acta Chimica Sinica, (64): 2057-2064 2006.
- Linares, M.; Braida, B.; Humbel, S.
Lewis-based valence bond scheme: Application to the allyl cation
Journal of Physical Chemistry A, (110): 2505-2509 2006.
- Ling, S. L.; Yu, W. B.; Huang, Z. J.; Lin, Z. J.; Haranczyk, M.; Gutowski, M.
Gaseous arginine conformers and their unique intramolecular interactions
Journal of Physical Chemistry A, (110): 12282-12291 2006.
- Lisowskaya, N. A.; Alajarin, M.; Sanchez-Andrade, P.

New cyclization mode of N-(diarylmethyleneamino)carbonimidoyl ketenes: Synthesis of 9H-pyrazolo 3,2-b 1,3 benzoxazines
European Journal of Organic Chemistry: 1468-1475 2006.

Liu, C. S.; Chen, P. Q.; Yang, E. C.; Tian, J. L.; Bu, X. H.; Li, Z. M.; Sun, H. W.; Lin, Z. Y.
Silver(I) complexes in coordination supramolecular system with bulky acridine-based ligands: Syntheses, crystal structures, and theoretical investigations on C-H center dot center dot center dot Ag close interaction
Inorganic Chemistry, (45): 5812-5821 2006.

Liu, D.; Hagelberg, F.; Park, S. S.
Charge transfer and electron backdonation in metallofullerenes encapsulating NSc3
Chemical Physics, (330): 380-386 2006.

Liu, F. L.; Wang, S.; Peng, L.; Wang, J. S.; Du, A. M.
DFT study on two C₂₄H₂₀ isomers with pagodane-like structure
Journal of Molecular Structure-Theochem, (759): 79-85 2006.

Liu, L. V.; Tian, W. Q.; Wang, Y. A.
Chemical reaction of nitric oxides with the 5-1DB defect of the single-walled carbon nanotube
Journal of Physical Chemistry B, (110): 1999-2005 2006.

Liu, L. V.; Tian, W. Q.; Wang, Y. A.
Ozonization at the vacancy defect site of the single-walled carbon nanotube
Journal of Physical Chemistry B, (110): 13037-13044 2006.

Liu, P.; Jordan, R. W.; Kibbee, S. P.; Goddard, J. D.; Tam, W.
Remote substituent effects in ruthenium-catalyzed 2+2 cycloadditions: An experimental and theoretical study
Journal of Organic Chemistry, (71): 3793-3803 2006.

Liu, X. W.; Bao, P.; Yu, Z. H.
Localization character of LFMO and NBO and interaction energy analysis
Chemical Journal of Chinese Universities-Chinese, (27): 96-99 2006.

Liu, Y.; Gregersen, B. A.; Hengge, A.; York, D. M.
Transesterification thio effects of phosphate diesters: Free energy barriers and kinetic and equilibrium isotope effects from density-functional theory
Biochemistry, (45): 10043-10053 2006.

Liu, Y.; Huang, X. R.; Yu, G. T.; Liu, H. L.; Sun, C. C.
Structure and stability of isomers of the promising interstellar molecule PC₃O
Theoretical Chemistry Accounts, (115): 410-426 2006.

Liu, Y.; Liu, W. Q.; Li, H. Y.; Liu, J. G.; Yang, Y.
Theoretical study of hydrogen bonding interaction in nitroxyl (HNO) dimer: Interrelationship of the two N-H center dot center dot center dot O blue-shifting hydrogen bonds
Journal of Physical Chemistry A, (110): 11760-11764 2006.

- Liu, Y.; Liu, W. Q.; Li, H. Y.; Yang, Y.; Cheng, S.
Computational study of hydrogen bonding interaction between formamide and nitrosyl hydride
Journal of Molecular Structure-Theochem, (778): 49-53 2006.
- Liu, Y.; Liu, W. Q.; Yang, Y.; Liu, J. G.
Theoretical study of the red- and blue-shifted hydrogen bonds of nitroxyl and pacetylene dimers
International Journal of Quantum Chemistry, (106): 2122-2128 2006.
- Lochan, R. C.; Head-Gordon, M.
Computational studies of molecular hydrogen binding affinities: The role of dispersion forces, electrostatics, and orbital interactions
Physical Chemistry Chemical Physics, (8): 1357-1370 2006.
- Lopez, C. S.; Faza, O. N.; Alvarez, R.; de Lera, A. R.
Cycloisomerization of activated (2E,4Z)-heptatrienoate and its relevance to crispatene (bio)synthesis. A case of concerted and stepwise uncertainty
Journal of Organic Chemistry, (71): 4497-4501 2006.
- Loverix, S.; Versees, W.; Steyaert, J.; Geerlings, P.
Quantum chemical study of leaving group activation in T-vivax nucleoside hydrolase
International Journal of Quantum Chemistry, (106): 565-570 2006.
- Lu, H. G.; Dai, D.; Yang, P.; Li, L. M.
Atomic orbitals in molecules: general electronegativity and improvement of Mulliken population analysis
Physical Chemistry Chemical Physics, (8): 340-346 2006.
- Lu, L. L.; Liu, X. W.; Wang, Y. C.; Wang, H. Q.
DFT study of the spin-forbidden reaction between Ti+ and N2O
Journal of Molecular Structure-Theochem, (774): 59-65 2006.
- Lukes, V.; Matuszna, K.
Density functional study of structural and opto-electronical properties of fluoranthenenopyracylene oligomers in their neutral and oxidized forms
Journal of Molecular Structure-Theochem, (776): 69-75 2006.
- Luna, A.; Mo, O.; Yanez, M.; Gal, J. F.; Maria, P. C.; Guillemin, J. C.
Gas-phase protonation and deprotonation of acrylonitrile derivatives N equivalent to C-CH=CH-X (X=CH3, NH2, PH2, SiH3)
Chemistry-a European Journal, (12): 9254-9261 2006.
- Luo, Q.; Li, Q. S.; Zhang, J.; Xie, Y. M.; Schleyer, P. V.; Schaefer, H. F.
Molecular oxygen dianions trapped in lithium cluster cages
Inorganic Chemistry, (45): 6431-6434 2006.
- Luzanov, A. V.; Prezhdo, O. V.
Analysis of multiconfigurational wave functions in terms of hole-particle distributions

Journal of Chemical Physics, (124) 2006.

Lyon, J. T.; Andrews, L.

Electron deficient carbon-titanium triple bonds: Formation of triplet XC divided by TiX₃ methylidyne complexes

Inorganic Chemistry, (45): 9858-9863 2006.

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

An unusual oxo-bridged mixed-valent dinuclear rhenium complex with the Re centers in various different coordination environments

Inorganica Chimica Acta, (359): 1303-1313 2006.

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

Natural bond orbital analysis and density functional study of linear and bent oxo-bridged dimers of rhenium(V)

Journal of Molecular Structure-Theochem, (766): 1-8 2006.

Machura, B.; Kruszynski, R.

Synthesis, crystal, molecular and electronic structure of the Re(NO)Cl₂(PPh₃)(PPh(2)py-P,N) complex

Polyhedron, (25): 1985-1993 2006.

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

Synthesis, crystal, molecular and electronic structure of the ReOCl₂(pzH)(2)(OAsPh₃) (ReO₄) and {ReCl₂(pzH)(2)}(2)(μ-O) complexes

Polyhedron, (25): 1111-1124 2006.

Machura, B.; Kruszynski, R.; Jaworska, M.; Klak, J.; Mrozinski, J.

Synthesis, crystal, molecular and electronic structure of ReOCl₃(phen) and ReCl₂(phen)(PPh₃)(2) (ReO₄) complexes

Polyhedron, (25): 2537-2549 2006.

Maciel, G. S.; Garcia, E.

Study of charges transferability for use in force fields

Chemical Physics Letters, (420): 497-502 2006.

Maganas, D.; Staniland, S. S.; Grigoropoulos, A.; White, F.; Parsons, S.; Robertson, N.; Kyritsis, P.; Pneumatikakis, G.

Structural, spectroscopic and magnetic properties of M R₂P(E)NP(E)R'(2) (2) complexes, M = Co, Mn, E = S, Se and R, R' = Ph or Pr-i. Covalency of M-S bonds from experimental data and theoretical calculations

Dalton Transactions: 2301-2315 2006.

Malde, A. K.; Khedkar, S. A.; Coutinho, E. C.

The omega, phi, and psi space of N-hydroxy-N-methylacetamide and N-acetyl-N'-hydroxy-N'-methylamide of alanine and their boron isosteres

Journal of Chemical Theory and Computation, (2): 312-321 2006.

- Malde, A. K.; Khedkar, S. A.; Coutinho, E. C.
Stationary points on the PES of N-methoxy peptides and their boron isosteres: An ab initio study
Journal of Chemical Theory and Computation, (2): 1664-1674 2006.
- Manard, M. J.; Kemper, P. R.; Bowers, M. T.
An experimental and theoretical investigation into the binding interactions of silver cluster cations with ethene and propene
International Journal of Mass Spectrometry, (249): 252-262 2006.
- Manna, S. C.; Zangrando, E.; Bencini, A.; Benelli, C.; Chaudhuri, N. R.
Syntheses, crystal structures, and magnetic properties of Ln(III)2(succinate) (3)(H₂O)(2) center dot 0.5H(2)O Ln = Pr, Nd, Sm, Eu, Gd, and Dy polymeric networks: Unusual ferromagnetic coupling in Gd derivative
Inorganic Chemistry, (45): 9114-9122 2006.
- Mansfield, N. E.; Grundy, J.; Coles, M. P.; Avent, A. G.; Hitchcock, P. B.
A conformational study of phospha(III)- and phospha(V)-guanidine compounds
Journal of the American Chemical Society, (128): 13879-13893 2006.
- Mao, S.; Pu, X. M.; Li, L. C.; Shu, Y. J.; Tian, A. M.
Theoretical study on the structure and property of N6H₆
Acta Chimica Sinica, (64): 1429-1436 2006.
- Marcano, C. J.; Lorono, M.; Cordova, T.; Chuchani, G.
Ab initio and DFT studies on the elimination kinetics 2-substituted ethyl N,N-dimethylcarbamates (CH₃)₂NCOOCH(2)CH(2)Z, Z=CH₂C₆H₅, C₆H₅, C(CH₃)=CH₂ in the gas phase
Journal of Molecular Structure-Theochem, (764): 201-204 2006.
- Marco-Contelles, J.; Soriano, E.
Computational analysis of the selective cyclopropanation mode for the PtCl₂-catalyzed cycloisomerization of a polyunsaturated precursor
Journal of Molecular Structure-Theochem, (761): 45-51 2006.
- Marcoin, W.; Pasterny, K.; Pasterna, G.; Wrzalik, R.
Quantum-mechanical calculations and spectroscopic characteristics of magnesium glutamate-glycine and magnesium glutamate-arginine
Journal of Molecular Structure, (792): 186-193 2006.
- Markovic, D.; Varela-Alvarez, A.; Sordo, J. A.; Vogel, P.
Mechanism of the diphenyldisulfone-catalyzed isomerization of alkenes. Origin of the chemoselectivity: Experimental and quantum chemistry studies
Journal of the American Chemical Society, (128): 7782-7795 2006.
- Markovic, Z.; Markovic, S.; Begovic, N.
Influence of alkali metal cations upon the Kolbe-Schmitt reaction mechanism
Journal of Chemical Information and Modeling, (46): 1957-1964 2006.
- Marrot, S.; Kato, T.; Cossio, F. P.; Gornitzka, H.; Baceiredo, A.

Cyclic carbodiphosphorane-diphosphinocarbene thermal interconversion
Angewandte Chemie-International Edition, (45): 7447-7450 2006.

Martin, J. M. L.
Heats of formation of perchloric acid, HClO₄, and perchloric anhydride, Cl₂O₇. Probing the limits of W1 and W2 theory
Journal of Molecular Structure-Theochem, (771): 19-26 2006.

Martin, M.; Sola, E.; Tejero, S.; Lopez, J. A.; Oro, L. A.
Mechanistic investigations of imine hydrogenation catalyzed by dinuclear iridium complexes
Chemistry-a European Journal, (12): 4057-4068 2006.

Martinez, A.
Solvation of yttrium with ammonia revisited. Di-amide formation in the reaction of yttrium with ammonia
Journal of Physical Chemistry A, (110): 1978-1981 2006.

Martins, J. B. L.; Politi, J. R. D.; Braga, A. D.; Gargano, R.
Complexes of water with the fluoromethanes
Chemical Physics Letters, (431): 51-55 2006.

McDowell, S. A. C.
Harmonic vibrational blue shifts in FXeH ... Y complexes (Y = N-2, CO, BF and HF) predicted by a perturbative model
Chemical Physics, (328): 69-74 2006.

McDowell, S. A. C.
Studies of neutral rare-gas compounds and their non-covalent interactions with other molecules
Current Organic Chemistry, (10): 791-803 2006.

Meng, Q. X.; Li, M.
Theoretical insights of copper(I) carbenes
Journal of Molecular Structure-Theochem, (765): 13-20 2006.

Merino, G.; Beltran, H. I.; Vela, A.
Donor-acceptor heteroleptic open sandwiches
Inorganic Chemistry, (45): 1091-1095 2006.

Mieusset, J. L.; Brinker, U. H.
Reactions of endo-3-diazotricyclo 3.2.1.0(2,4) oct-6-ene, a potential precursor for the generation of a neutral C₈H₈ molecule with a pyramidal coordinated carbon
Journal of Organic Chemistry, (71): 6975-6982 2006.

Migda, W.; Rys, B.
Conformational analysis of nine-membered cyclic acetals. Stereoelectronic effect in 2,4- and 3,5-benzodioxonine derivatives
Journal of Organic Chemistry, (71): 5498-5506 2006.

- Mihaylov, T.; Georgieva, I.; Bauer, G.; Kostova, I.; Manolov, I.; Trendafilova, N.
Theoretical study of the substituent effect on the intramolecular hydrogen bonds in di(4-hydroxycoumarin) derivatives
International Journal of Quantum Chemistry, (106): 1304-1315 2006.
- Milcic, M. K.; Medakovic, V. B.; Sredojevic, D. N.; Juranic, N. O.; Zaric, S. D.
Electron delocalization mediates the metal-dependent capacity for CH/pi interactions of acetylacetonato chelates
Inorganic Chemistry, (45): 4755-4763 2006.
- Mo, Y. R.
Intramolecular electron transfer: Computational study based on the orbital deletion procedure (ODP)
Current Organic Chemistry, (10): 779-790 2006.
- Mo, Y. R.; Gao, J. L.
Polarization and charge-transfer effects in aqueous solution via ab initio QM/MM simulations
Journal of Physical Chemistry B, (110): 2976-2980 2006.
- Moc, J.; Panek, J.
The hypervalent PF(4)H species dimer: A system with double blue-shifted P-H center dot center dot center dot F hydrogen bonding?
Chemical Physics Letters, (419): 362-368 2006.
- Mohajeri, A.; Abasi, M.
Metal ion-ligand interaction: HSAB principle versus NBO and AIM view points
Journal of Theoretical & Computational Chemistry, (5): 87-98 2006.
- Mohajeri, A.; Karimi, E.
AIM and NBO analyses of cation-pi interaction
Journal of Molecular Structure-Theochem, (774): 71-76 2006.
- Mohareb, M. M.; Ghosh, K. K.; Orlova, G.; Palepu, R. M.
S(N)2 reaction of a sulfonate ester in the presence of alkyltriphenylphosphonium bromides and mixed cationic-cationic systems
Journal of Physical Organic Chemistry, (19): 281-290 2006.
- Molev, G.; Bravo-Zhivotovskii, D.; Karni, M.; Tumanskii, B.; Botoshansky, M.; Apeloig, Y.
Synthesis, molecular structure, and reactivity of the isolable silylenoid with a tricoordinate silicon
Journal of the American Chemical Society, (128): 2784-2785 2006.
- Mora, J. R.; Lorono, M.; Cordova, T.; Chuchani, G.
Ab initio calculations of the gas-phase elimination kinetics of ethyl oxamate, ethyl oxanilate, and ethyl NN-dimethyl oxamate
Journal of Physical Organic Chemistry, (19): 503-511 2006.
- Mori, H.; Ishii, K.; Miyoshi, E.

Electronic structure and photochemistry of inorganic photochromic complex Cu(N,N'-diethylethylenediamine)(2) (2+): planar-tetrahedral geometry change accompanied with d(9)-d(10) electronic transition
Journal of Theoretical & Computational Chemistry, (5): 887-894 2006.

Morzyk-Ociepa, B.; Rozycka-Sokolowska, E.
Structures and spectroscopic studies of indolecarboxylic acids. Part III. Diamminetetrakis-mu-(O,O'-indole-3-carboxylate)dicopper(II)
Journal of Molecular Structure, (784): 69-77 2006.

Muchova, E.; Spirko, V.; Hobza, P.; Nachtigallova, D.
Theoretical study of photoacidity of HCN: the effect of complexation with water
Physical Chemistry Chemical Physics, (8): 4866-4873 2006.

Mukhopadhyay, A.; Pal, S.
Intramolecular apical C-H center dot center dot center dot M interactions in square-planar nickel(II) complexes with dianionic tridentate ligands and 2-phenylimidazole
European Journal of Inorganic Chemistry: 4879-4887 2006.

Munro, O. Q.; du Toit, K.; Drewes, S. E.; Crouch, N. R.; Mulholland, D. A.
Experimental and theoretical studies of a naturally occurring non-oligomeric steroidal supramolecular zipper
New Journal of Chemistry, (30): 197-207 2006.

Murakami, M.; Miyamoto, Y.; Hasegawa, M.; Usui, I.; Matsuda, T.
Torque control by metal-orbital interactions
Pure and Applied Chemistry, (78): 415-423 2006.

Musin, R. N.; Mariam, Y. H.
An integrated approach to the study of intramolecular hydrogen bonds in malonaldehyde enol derivatives and naphthazarin: trend in energetic versus geometrical consequences
Journal of Physical Organic Chemistry, (19): 425-444 2006.

Musio, R.; Sciacovelli, O.
S-33 NMR spectroscopy 3. Substituent effects on S-33 NMR parameters in 2-substituted ethanesulfonates
Magnetic Resonance in Chemistry, (44): 753-760 2006.

Nakamura, T.; Koyama, E.; Shimoi, Y.; Abe, S.; Ishida, T.; Tsukagoshi, K.; Mizutani, W.; Tokuhisa, H.; Kanesato, M.; Nakai, I.; Kondoh, H.; Ohta, T.
Surface potential switching by metal ion complexation/decomplexation using bipyridinethiolate monolayers on gold
Journal of Physical Chemistry B, (110): 9195-9203 2006.

Nama, D.; Schott, D.; Pregosin, P. S.; Veiros, L. F.; Calhorda, M. J.
Diffusion and overhauser NMR studies on dicationic palladium complexes of BINAP
Organometallics, (25): 4596-4604 2006.

- Namuangruk, S.; Tantanak, D.; Limtrakul, J.
Application of ONIOM calculations in the study of the effect of the zeolite framework on the adsorption of alkenes to ZSM-5
Journal of Molecular Catalysis a-Chemical, (256): 113-121 2006.
- Nazari, F.
Stable structures of oxocarbons and pseudooxocarbons of group VI
Journal of Molecular Structure-Theochem, (760): 29-37 2006.
- Nazmutdinov, R. R.; Zhang, J. D.; Zinkicheva, T. T.; Manyurov, I. R.; Ulstrup, J.
Adsorption and in situ scanning tunneling microscopy of cysteine on Au(111): Structure, energy, and tunneling contrasts
Langmuir, (22): 7556-7567 2006.
- Nelyubina, Y. V.; Lyssenko, K. A.; Sigachev, A. S.; Antipin, M. Y.; Kravchenko, A. N.
Nature of weak inter- and intramolecular interactions in crystals - 7. Stability of homochiral supramolecular organization of dications in crystals of 1,3-dialkyl-4,5-bis(3-guanidinoamino)imidazolidin-2-one salts
Russian Chemical Bulletin, (55): 399-407 2006.
- Nemcsok, D.; Kovacs, A.; Szecsenyi, K. M.; Levac, V. M.
Vibrational spectroscopic and theoretical study of 3,5-dimethyl-1-thiocarboxamide pyrazole (L) and the complexes Co₂L₂Cl₄, Cu₂L₂Cl₄ and Cu₂L₂Br₂
Chemical Physics, (328): 85-92 2006.
- Nemeth, B.; Weber, C.; Veszpremi, T.; Gati, T.; Demeter, A.
Carbon protonation of 2,4,6-triaminopyrimidines: Synthesis, NMR studies, and theoretical calculations
Journal of Organic Chemistry, (71): 4910-4918 2006.
- Nemukhin, A. V.; Grigorenko, B. L.; Topol, I. A.; Burt, S. K.
Modeling dioxygen binding to the non-heme iron-containing enzymes
International Journal of Quantum Chemistry, (106): 2184-2190 2006.
- Nemukhin, A. V.; Topol, I. A.; Cachau, R. E.; Burt, S. K.
On the nature of oxoiron (IV) intermediate in dioxygen activation by non-heme enzymes
Theoretical Chemistry Accounts, (115): 348-353 2006.
- Nenu, C. N.; van Lingen, J. N. L.; de Groot, F. M. F.; Koningsberger, D. C.; Weckhuysen, B. M.
Controlled assembly of a heterogeneous single-site ethylene trimerization catalyst as probed by X-ray absorption spectroscopy
Chemistry-a European Journal, (12): 4756-4763 2006.
- Nguyen, H. M. T.; Peeters, J.; Zeegers-Huyskens, T.
Theoretical study of the blue-shifting hydrogen bonds between CH₂X₂ and CHX₃ (X = F, Cl, Br) and hydrogen peroxide
Journal of Molecular Structure, (792): 16-22 2006.

Nirmala, V.; Kolandaivel, P.
Molecular interaction of H-2 and H₂O molecules with the boron nitride (BN)(n=3-5) clusters: A theoretical study
Journal of Molecular Structure-Theochem, (758): 9-15 2006.

Nomura, M.; Cauchy, T.; Geoffroy, M.; Adkine, P.; Fourmigue, M.
CpNi(dithiolene) (and diselenolene) neutral radical complexes
Inorganic Chemistry, (45): 8194-8204 2006.

Norinder, J.; Backvall, J. E.; Yoshikai, N.; Nakamura, E.
Unusual homocoupling in the reaction of diorganocuprates with an allylic halide
Organometallics, (25): 2129-2132 2006.

Nori-Shargh, D.; Abbasi, A.; Jamed-Borzorghi, S.; Deyhimi, F.; Naeem-Abyaneh, R.; Sarkar, F.
Ab initio and NBO studies of the decomposition (2+2 and 2+4 elimination) mechanisms of alkylisothiocyanates (alkyl = ethyl-, iso-propyl- and tert-butyl)
Phosphorus Sulfur and Silicon and the Related Elements, (181): 75-85 2006.

Nori-Shargh, D.; Malekhosseini, M.; Deyhimi, F.
Ab initio study and NBO analysis of the enantiomerization energy profile of tetra-peri-substituted overcrowded naphthalenes
Journal of Molecular Structure-Theochem, (763): 187-198 2006.

Nori-Shargh, D.; Roohi, F.; Deyhimi, F.; Naeem-Abyaneh, R.
DFT study and NBO analysis of the metallotropic shifts in cyclopentadienyl(trimethyl)silane, -germane and -stannane
Journal of Molecular Structure-Theochem, (763): 21-28 2006.

Nori-Shargh, D.; Tahmassebi, D.; Poukalhor, M.; Amini, M. M.; Jameh-Bozorghi, S.; Deyhimi, F.; Khanizadeh, M.; Malekhosseini, M.
An ab initio study and NBO analysis of the stability and conformational properties of hexakis(trimethylelementhyl)benzene (element = C, Si, Ge, and Sn)
Phosphorus Sulfur and Silicon and the Related Elements, (181): 2419-2434 2006.

Norton, J. E.; Briseno, A. L.; Wudl, F.; Houk, K. N.
Lone-pair orbital interactions in polythiaadamantanes
Journal of Physical Chemistry A, (110): 9887-9899 2006.

Notario, R.; Roux, M. V.; Cuevas, G.; Cardenas, J.; Leyva, V.; Juaristi, E.
Computational study of 1,3-dithiane 1,1-dioxide (1,3-dithiane sulfone). Description of the inversion process and manifestation of stereoelectronic effects on (1)J(C-H) coupling constants
Journal of Physical Chemistry A, (110): 7703-7712 2006.

Nowroozi, A.; Raissi, H.
Strong intramolecular hydrogen bond in triformylmethane ab-initio, AIM and NBO study
Journal of Molecular Structure-Theochem, (759): 93-100 2006.

Nozaki, K.

Theoretical studies on photophysical properties and mechanism of phosphorescence in fac-Ir(2-phenylpyridine)(3)

Journal of the Chinese Chemical Society, (53): 101-112 2006.

Nsangou, A.; Jaidane, N.; Ben Lakhdar, Z.

Cooperativity and ground-state proton transfer in 7-hydroxyimidazo 1,2-a pyridine center dot ammonia clusters: DFT study

Journal of Molecular Structure-Theochem, (758): 87-95 2006.

Nsikabaka, S.; Harb, W.; Ruiz-Lopez, M. F.

The role of water on the acid-promoted E/Z isomerization of oximes in aqueous solution

Journal of Molecular Structure-Theochem, (764): 161-166 2006.

Nyulasi, B.; Kovacs, A.

Theoretical study of F--(H-2)(n) and Cl--(H-2)(n) (n=1-8) anion complexes

Chemical Physics Letters, (426): 26-29 2006.

Oberhammer, H.

Anomeric effect in the N-C-F moiety

Mendeleev Communications: 136-137 2006.

O'Hagan, D.; Rzepa, H. S.; Schuler, M.; Slawin, A. M. Z.

The vicinal difluoro motif: The synthesis and conformation of erythro- and threo-diastereoisomers of 1,2-difluorodiphenylethanes, 2,3-difluorosuccinic acids and their derivatives

Beilstein Journal of Organic Chemistry, (2) 2006.

Ohman, K. T.; Sanderud, A.; Hole, E. O.; Sagstuen, E.

Single crystals of L-O-serine phosphate X-irradiated at low temperatures: EPR, ENDOR, EIE, and DFT studies

Journal of Physical Chemistry A, (110): 9585-9596 2006.

Ohta, Y.; Demura, A.; Okamoto, T.; Hitomi, H.; Nagaoka, M.

The body-centered cubic structure of methyl lithium tetramer crystal: Staggered methyl conformation by electrostatic stabilization via intratetramer multipolarization

Journal of Physical Chemistry B, (110): 12640-12644 2006.

Ohtaki, H.; Niwa, Y.; Ozutsumi, K.; Probst, M.; Mroz, B.; Perez, F. R.; Alvarez, J.; Bolado, S.

Anomaly of the basicity of water in mixed solvents

Journal of Molecular Liquids, (129): 49-56 2006.

Olah, J.; Blockhuys, F.; Veszpremi, T.; Van Alsenoy, C.

On the usefulness of bond orders and overlap populations to chalcogen-nitrogen systems

European Journal of Inorganic Chemistry: 69-77 2006.

Oliferenko, A. A.; Pisarev, S. A.; Palyulin, V. A.; Zefirov, N. S.

Atomic charges via electronegativity equalization: Generalizations and perspectives

Advances in Quantum Chemistry, Vol 51, (51): 139-156 2006.

Oliva, M. M.; Casado, J.; Raposo, M. M. M.; Fonseca, A. M. C.; Hartmann, H.; Hernandez, V.; Navarrete, J. T. L.

Structure-property relationships in push-pull amino/cyanovinyl end-capped oligothiophenes: Quantum chemical and experimental studies
Journal of Organic Chemistry, (71): 7509-7520 2006.

Orlova, G.; Blagojevic, V.; Bohme, D. K.

Water-catalyzed hydrolysis of the radical cation of ketene in the gas phase: Theory and experiment
Journal of Physical Chemistry A, (110): 8266-8274 2006.

Ortiz, F. L.

The chemistry of phosphazenes. synthetic applications of C-alpha-lithiated derivatives
Current Organic Synthesis, (3): 187-214 2006.

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

Synthesis, structure, and reactivity of a stabilized calcium carbene: R2CCa
Journal of the American Chemical Society, (128): 14676-14684 2006.

Otero-Calvi, A.; Aullon, G.; Alvarez, S.; Montero, L. A.; Stohrer, W. D.

Bonding and solvation preferences of nickel complexes Ni(S₂PR₂)₂ (R = H, Me, OMe) according a natural bond orbital analysis
Journal of Molecular Structure-Theochem, (767): 37-41 2006.

Pacheco-Torres, J.; Perez-Mayoral, E.; Soriano, E.; Lopez-Larrubia, P.; Ouari, O.; Gonzalez-Cortes, A.; Cerdan, S.; Ballesteros, P.

A convenient and efficient synthesis of the first (nitroimidazolyl)succinic esters and their diacids
Synthesis-Stuttgart: 3859-3864 2006.

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

Variation of atomic charges on proton transfer in strong hydrogen bonds: The case of anionic and neutral imidazole-acetate complexes
Journal of Computational Chemistry, (27): 1650-1661 2006.

Pagliai, M.; Bellucci, L.; Muniz-Miranda, M.; Cardini, G.; Schettino, V.

A combined Raman, DFT and MD study of the solvation dynamics and the adsorption process of pyridine in silver hydrosols
Physical Chemistry Chemical Physics, (8): 171-178 2006.

Pakiari, A. H.; Eskandari, K.

The chemical nature of very strong hydrogen bonds in some categories of compounds
Journal of Molecular Structure-Theochem, (759): 51-60 2006.

Palacios, F.; Herran, E.; Alonso, C.; Rubiales, G.; Lecea, B.; Ayerbe, M.; Cossio, F. P.

Reaction of N-vinylic phosphazenes with alpha,beta-unsaturated aldehydes. Azatriene-mediated synthesis of dihydropyridines and pyridines derived from beta-amino acids
Journal of Organic Chemistry, (71): 6020-6030 2006.

- Palafox, M. A.; Rastogi, V. K.; Vats, J. K.
4-Aminobenzonitrile: ab initio calculations, FTIR and Raman spectra
Journal of Raman Spectroscopy, (37): 85-99 2006.
- Palmer, E. J.; Bursten, B. E.
Theoretical studies of pi-loading and structural diversity in Cp₃MX (M = Zr, Hf; X = H, CH₃, OR, NR₂) compounds
Polyhedron, (25): 575-584 2006.
- Pan, L. X.; Zhang, G. B.; Cao, Z. X.
Density functional calculations on structures and Ni-CO bond dissociation energies of Ni(CO)(n)(n=1-4)
Chemical Journal of Chinese Universities-Chinese, (27): 1327-1331 2006.
- Pan, Q. J.; Zhang, H. X.; Fu, H. G.; Yu, H. T.
Theoretical studies on metal-metal interaction and intrinsic (1,3) sigma(d)sigma(s/p) excited states of dinuclear d(10) complexes with bridging phosphane Ligands*
European Journal of Inorganic Chemistry: 1050-1059 2006.
- Panda, D.; Datta, A.
The role of the ring nitrogen and the amino group in the solvent dependence of the excited-state dynamics of 3-aminoquinoline
Journal of Chemical Physics, (125) 2006.
- Panisch, R.; Bolte, M.; Muller, T.
Hydrogen- and fluorine-bridged disilyl cations and their use in catalytic C-F activation
Journal of the American Chemical Society, (128): 9676-9682 2006.
- Park, Y. H.; Lee, O. S.; Koo, I. S.; Yang, K.; Lee, I.
DFT studies on hydrolyses of dimethylchlorothiophosphate
Bulletin of the Korean Chemical Society, (27): 1865-1868 2006.
- Parkin, G.
Valence, oxidation number, and formal charge: Three related but fundamentally different concepts
Journal of Chemical Education, (83): 791-799 2006.
- Parnaiba-da Silva, A. J.; da Silva, J. B. P.; da Gama, A. A. S.; Ramos, M. N.
Comparative study of Green's function matrix elements and charge transfers obtained from different partitioning schemes of molecular charge in hydrogen-bonded complexes
Journal of the Brazilian Chemical Society, (17): 237-242 2006.
- Parra, R. D.; Yoo, B.; Wemhoff, M.
Conformational stability of a model macrocycle tetraamide: An ab initio study
Journal of Physical Chemistry A, (110): 4487-4494 2006.
- Parreira, R. L. T.; Galembeck, S. E.

Computational study of pyrylium cation-water complexes: hydrogen bonds, resonance effects, and aromaticity

Journal of Molecular Structure-Theochem, (760): 59-73 2006.

Parthasarathi, R.; Elango, M.; Padmanabhan, J.; Subramanian, V.; Roy, D. R.; Sarkar, U.; Chattaraj, P. K.

Application of quantum chemical descriptors in computational medicinal chemistry and chemoinformatics

Indian Journal of Chemistry Section a-Inorganic Bio-Inorganic Physical Theoretical & Analytical Chemistry, (45): 111-125 2006.

Pathak, B.; Pandian, S.; Hosmane, N.; Jemmis, E. D.

Reversal of stability on metalation of pentagonal-bipyramidal (1-MB6H72-, 1-M-2-CB5H71-, and 1-M-2,4-C2B4H7) and icosahedral (1-MB11H122-, 1-M-2-CB10H121-, and 1-M-2,4-C2B9H12) Boranes (M = Al, Ga, In, and Tl): Energetics of condensation and relationship to binuclear metallocenes

Journal of the American Chemical Society, (128): 10915-10922 2006.

Patil, M. P.; Sunoj, R. B.

Density functional theory and atoms-in-molecule study on the role of two-electron stabilizing interactions in retro Diels-Alder reaction of cycloadducts derived from substituted cyclopentadiene and p-benzoquinone

Organic & Biomolecular Chemistry, (4): 3923-3930 2006.

Pavelka, M.; Simanek, M.; Sponer, J.; Burda, J. V.

Copper cation interactions with biologically essential types of ligands: A computational DFT study

Journal of Physical Chemistry A, (110): 4795-4809 2006.

Pejov, L.; Solimannejad, M.; Stefov, V.

The pi-type hydrogen bond with triple C-C bond acting as a proton-acceptor. A gradient-corrected hybrid HF-DFT and MP2 study of the phenol-acetylene dimer in the neutral S-O ground state

Chemical Physics, (323): 259-270 2006.

Pellegrinet, S. C.; Goodman, J. M.

Asymmetric conjugate addition of alkynylboronates to enones: Rationale for the intriguing catalysis exerted by binaphthols

Journal of the American Chemical Society, (128): 3116-3117 2006.

Pendas, A. M.; Blanco, M. A.; Francisco, E.

The nature of the hydrogen bond: A synthesis from the interacting quantum atoms picture

Journal of Chemical Physics, (125) 2006.

Perez, M.; Peakman, T. M.; Alex, A.; Higginson, P. D.; Mitchell, J. C.; Snowden, M. J.; Morao, M.

Accuracy vs time dilemma on the prediction of NMR chemical shifts: A case study (chloropyrimidines)

Journal of Organic Chemistry, (71): 3103-3110 2006.

- Petit, L.; Adamo, C.; Maldivi, P.
Toward a clear-cut vision on the origin of 2,6-di(1,2,4-triazin-3-yl)pyridine selectivity for trivalent actinides: Insights from theory
Inorganic Chemistry, (45): 8517-8522 2006.
- Petit, L.; Joubert, L.; Maldivi, P.; Adamo, C.
A comprehensive theoretical view of the bonding in actinide molecular complexes
Journal of the American Chemical Society, (128): 2190-2191 2006.
- Piacenza, M.; Rakow, J.; Hyla-Kryspin, I.; Grimme, S.
Theoretical study of the effects of phosphane substituents, on the bonding properties of acetylene with Ni(PR₃)(2) (R = H, CH₃, F, CF₃, C₆H₅)
European Journal of Inorganic Chemistry: 213-221 2006.
- Pigot, T.; Foucat, S.; Pfister-Guillouzo, G.
Gas phase characterization by photoelectron spectroscopy of unhindered alpha-heterosubstituted germylenes 1
Journal of Molecular Structure, (782): 36-43 2006.
- Pillet, S.; Souhassou, M.; Lecomte, C.; Rabu, P.; Drillon, M.; Massobrio, C.
Electron density analysis of the layered antiferromagnetic compound Cu-2(OH)(3)NO₃: Relationship with the magnetic interaction mechanism
Physical Review B, (73) 2006.
- Pineda, L. W.; Jancik, V.; Oswald, R. B.; Roesky, H. W.
Preparation of LGe(Se)OH: A germanium analogue of a selenocarboxylic acid (L=H C(CMe)(NAr)(2), Ar=2,6-iPr(2)C(6)H(3))
Organometallics, (25): 2384-2387 2006.
- Pineda, L. W.; Jancik, V.; Starke, K.; Oswald, R. B.; Roesky, H. W.
Stable monomeric germanium(II) and tin(II) compounds with terminal hydrides
Angewandte Chemie-International Edition, (45): 2602-2605 2006.
- Pirani, F.; Maciel, G. S.; Cappelletti, D.; Aquilanti, V.
Experimental benchmarks and phenomenology of interatomic forces: open-shell and electronic anisotropy effects
International Reviews in Physical Chemistry, (25): 165-199 2006.
- Plutecka, A.; Hoffmann, M.; Rychlewska, U.; Kucybala, Z.; Paczkowski, J.; Pyszka, I.
Relationship between structure and photoinitiating abilities of selected bromide salts of 2-oxo-2,3dihydro-1H-imidazo 1,2-a pyridine (IMP): influence of the solvent and the substitution in benzaldehyde on the course of its reaction with IMP
Acta Crystallographica Section B-Structural Science, (62): 135-142 2006.
- Poater, A.; Solans-Monfort, X.; Clot, E.; Coperet, C.; Eisenstein, O.
DFT calculations of d(0) M(NR)(CHtBu)(X)(Y) (M = Mo, W; R = CPh₃, 2,6-iPr-C₆H₃; X and Y=CH(2)tBu, OtBu, OSi(OtBu)(3)) olefin metathesis catalysts: structural, spectroscopic and electronic properties

Dalton Transactions: 3077-3087 2006.

Poater, J.; Sola, M.; Bickelhaupt, F. M.

A model of the chemical bond must be rooted in quantum mechanics, provide insight, and possess predictive power

Chemistry-a European Journal, (12): 2902-2905 2006.

Pogodin, S.; Rae, I. D.; Agranat, I.

The effects of fluorine and chlorine substituents across the fjords of bifluorenylidenes:

Overcrowding and stereochemistry

European Journal of Organic Chemistry: 5059-5068 2006.

Pointner, B. E.; Suontamo, R. J.; Schrobilgen, G. J.

Syntheses and X-ray crystal structures of alpha- and beta- $XeO_2F SbF_6$, $XeO_2F AsF_6$, $FO_2XeFXeO_2F AsF_6$, and $XeF_5 SbF_6$ center dot $XeOF_4$ and computational studies of the XeO_2F^+ and $FO_2XeFXeO_2F^+$ cations and related species

Inorganic Chemistry, (45): 1517-1534 2006.

Porsev, V. V.; Tulub, A. V.

Cluster quantum-chemical study of Grignard reagent formation

Doklady Physical Chemistry, (409): 237-241 2006.

Prakash, G. K. S.; Panja, C.; Vaghoo, H.; Surampudi, V.; Kultyshev, R.; Mandal, M.; Rasul, G.; Mathew, T.; Olah, G. A.

Facile synthesis of TMS-protected trifluoromethylated alcohols using trifluoromethyltrimethylsilane (TMSCF₃) and various nucleophilic catalysts in DMF

Journal of Organic Chemistry, (71): 6806-6813 2006.

Prakash, R.; Gotz, A. W.; Heinemann, F. W.; Gorling, A.; Sellmann, D.

Hydrazine nitrosation of a metal-bound nitric oxide: Structural evidence for the formation of an ammine complex

Inorganic Chemistry, (45): 4661-4667 2006.

Pramod, G.; Mohan, H.; Manoj, P.; Manojkumar, T. K.; Manoj, V. M.; Mittal, J. P.; Aravindakumar, C. T.

Redox chemistry of 8-azaadenine: a pulse radiolysis study

Journal of Physical Organic Chemistry, (19): 415-424 2006.

Pratuangdejkul, J.; Jaudon, P.; Ducrocq, C.; Nosoongnoen, W.; Guerin, G. A.; Conti, M.; Loric, S.; Launay, J. M.; Manivet, P.

Cation-pi interactions in serotonin: Conformational, electronic distribution, and energy decomposition analysis

Journal of Chemical Theory and Computation, (2): 746-760 2006.

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

Theoretical insights on O-2 and CO adsorption on neutral and positively charged gold clusters

Journal of Physical Chemistry B, (110): 12240-12248 2006.

Provasi, P. F.; Sauer, S. P. A.

On the angular dependence of the vicinal fluorine-fluorine coupling constant in 1,2-difluoroethane: Deviation from a Karplus-like shape
Journal of Chemical Theory and Computation, (2): 1019-1027 2006.

Puskas, I.; Fleisch, T. H.; Full, P. R.; Kaduk, J. A.; Marshall, C. L.; Meyers, B. L.
Novel aspects of the physical chemistry of CO/SiO₂ Fischer-Tropsch catalyst preparations - The chemistry of cobalt silicate formation during catalyst preparation or hydrogenation
Applied Catalysis a-General, (311): 146-154 2006.

Qi, X. J.; Liu, L.; Fu, Y.; Guo, Q. X.
Ab initio calculations of pK(a) values of transition-metal hydrides in acetonitrile
Organometallics, (25): 5879-5886 2006.

Qiao, Q. A.; Yang, C. L.; Qu, R. J.; Jin, Y. Q.; Wang, M. S.; Zhang, Z. H.; Xu, Q.; Yu, Z. X.
A density functional theory study on the role of His-107 in arylamine N-acetyltransferase 2 acetylation
Biophysical Chemistry, (122): 215-220 2006.

Qu, Y. H.; Ma, W. Y.; Bian, X. F.; Tang, H. W.; Tian, W. X.
Electronic structure and stability of BP clusters: Theoretical calculations for (BP)(n) (n=2-4)
International Journal of Quantum Chemistry, (106): 960-967 2006.

Rai, V.; Namboothiri, I. N. N.
A theoretical evaluation of the Michael-acceptor ability of conjugated nitroalkenes
European Journal of Organic Chemistry: 4693-4703 2006.

Raissi, H.; Nowroozi, A.; Mohammdi, R.; Hakimi, M.
Intramolecular hydrogen bond, molecular structure and vibrational assignment of tetra-acetylene - A density functional study
Spectrochimica Acta Part a-Molecular and Biomolecular Spectroscopy, (65): 605-615 2006.

Ramalingam, M.; Ramasami, K.; Venuvanalingam, P.
Transition states and charge analyses along the IRC for the singlet chlorocarbenes insertions into C-H bond of alkanes
Chemical Physics Letters, (430): 414-419 2006.

Ramirez-Solis, A.; Zicovich-Wilson, C. M.; Kirtman, B.
Periodic Hartree-Fock and density functional theory calculations for Li-doped polyacetylene chains
Journal of Chemical Physics, (124) 2006.

Ramos, D. R.; Castillo, R.; Canle, M.; Garcia, M. V.; Andres, J.; Santaballa, J. A.
Density functional study of the Hoffmann elimination of (N-Cl),N-methylethanolamine in gas phase and in aqueous solution
Chemical Physics Letters, (429): 425-429 2006.

Ran, J.; Wong, M. W.
Saturated hydrocarbon-benzene complexes: Theoretical study of cooperative CH/pi interactions

Journal of Physical Chemistry A, (110): 9702-9709 2006.

Range, K.; Ayala, I.; York, D.; Barry, B. A.

Normal modes of redox-active tyrosine: Conformation dependence and comparison to experiment

Journal of Physical Chemistry B, (110): 10970-10981 2006.

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

Ab initio/GIAO-CCSD(T) study of propenoyl ($H_2C=CH-CO+$) and isopentenoyl ($(CH_3)_2C=CH-CO+$) cations and their superelectrophilic protonated dications

Journal of Physical Chemistry A, (110): 1041-1045 2006.

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

Theoretical study of $AlH_2((+n)n=1-7)$ dications

Journal of Molecular Modeling, (12): 559-562 2006.

Rawe, S. L.; Doyle, D.; Zaric, V.; Rozas, I.; McMahon, K.; Tosin, M.; Bunz, H. M.; Murphy, E. P.; O'Boyle, K. M.; Murphy, P. V.

N-glycosyl-thiophene-2-carboxamides: synthesis, structure and effects on the growth of diverse cell types

Carbohydrate Research, (341): 1370-1390 2006.

Raynaud, C.; Perrin, L.; Maron, L.

A DFT study of stannane dehydrocoupling catalyzed by Cp_2LaH

Organometallics, (25): 3143-3151 2006.

Rayon, V. M.; Redondo, P.; Barrientos, C.; Largo, A.

Structure and bonding in first-row transition-metal dicarbides: Are they related to the stability of met-cars?

Chemistry-a European Journal, (12): 6963-6975 2006.

Redfern, P. C.; Zapol, P.; Sternberg, M.; Adiga, S. P.; Zygmunt, S. A.; Curtiss, L. A.

Quantum chemical study of mechanisms for oxidative dehydrogenation of propane on vanadium oxide

Journal of Physical Chemistry B, (110): 8363-8371 2006.

Regas, D.; Ruiz, J. M.; Afonso, M. M.; Palenzuela, J. A.

Hetero Diels-Alder reaction of vinyl allenes and aldehydes. An experimental and computational study

Journal of Organic Chemistry, (71): 9153-9164 2006.

Remacle, F.; Levine, R. D.

Electrical transport in saturated and conjugated molecular wires

Faraday Discussions, (131): 45-67 2006.

Remenyi, C.; Reviakine, R.; Kaupp, M.

Density functional study of electron paramagnetic resonance parameters and spin density distributions of dicopper(I) complexes with bridging azo and tetrazine radical-anion ligands

Journal of Physical Chemistry A, (110): 4021-4033 2006.

Ren, H.; Qu, Y. X.; Zhao, S. H.

Reinforcement of styrene-butadiene rubber with silica modified by silane coupling agents: Experimental and theoretical chemistry study
Chinese Journal of Chemical Engineering, (14): 93-98 2006.

Ren, J.

Polar group enhanced gas-phase acidities of carboxylic acids: An investigation of intramolecular electrostatic interaction
Journal of Physical Chemistry A, (110): 13405-13411 2006.

Ren, Y.; Li, M.; Wong, N. B.; Chu, S. Y.

Ab initio computational insight into the ion-pair S(N)2 reaction of lithium isothiocyanate and methyl fluoride in the gas phase and in acetone solution
Journal of Molecular Modeling, (12): 182-189 2006.

Rincon, E.; Jaque, P.; Toro-Labbe, A.

Reaction force analysis of the effect of Mg(II) on the 1,3 intramolecular hydrogen transfer in thymine
Journal of Physical Chemistry A, (110): 9478-9485 2006.

Rios-Font, R.; Bertran, J.; Rodriguez-Santiago, L.; Sodupe, M.

Effects of ionization, metal cationization and protonation on 2'-Deoxyguanosine: Changes on sugar puckering and stability of the N-glycosidic bond
Journal of Physical Chemistry B, (110): 5767-5772 2006.

Rodriguez, A. H.; Branda, M. M.; Castellani, N. J.

DFT studies of the adsorption and interaction of two methanol molecules on a MgO edge
Journal of Molecular Structure-Theochem, (769): 249-254 2006.

Rodriguez-Dieguez, A.; Kivekas, R.; Sillanpaa, R.; Cano, J.; Lloret, F.; McKee, V.; Stoeckli-Evans, H.; Colacio, E.

Structural and magnetic diversity in cyano-bridged bi- and trimetallic complexes assembled from cyanometalates and M(rac-CTH) (n+) building blocks (CTH = d, I-5,5,7,12,12,14-hexamethyl-1,4,8,11-tetraazacyclotetradecane)
Inorganic Chemistry, (45): 10537-10551 2006.

Rogachev, A. Y.; Mironov, A. V.; Troyanov, S. I.; Kuzmina, N. P.; Nemukhin, A. V.

Synthesis, crystal structures and theoretical study of mixed ligand complexes of lanthanides acetylacetones with o-phenanthroline and 2,2'-dipyridyl: The unexpected inverted electrostatic trend in stability
Journal of Molecular Structure, (789): 187-194 2006.

Roger, M.; Barros, N.; Arliguie, T.; Thuery, P.; Maron, L.; Ephritikhine, M.

U(SMes)(n), (n=3, 4) and Ln(SMes*)(3) (Ln = La, Ce, Pr, Nd): Lanthanide(III)/actinide(III) differentiation in agostic interactions and an unprecedented eta(3) Ligation mode of the arylthiolate ligand, from x-ray diffraction and DFT analysis*

Journal of the American Chemical Society, (128): 8790-8802 2006.

Romano, R. M.; Picone, A. L.; Downs, A. J.

*Matrix-isolated van der Waals complexes formed between CS₂ and dihalogen molecules XY,
where XY = Cl-2, Br-2, BrCl, ICl, or IBr*

Journal of Physical Chemistry A, (110): 12129-12135 2006.

Roohi, H.; Ebrahimi, A.; Habibi, S. M.; Jarahi, E.

NBO and AIM analyses of the anomeric effect in fluoromethanethiol

Journal of Molecular Structure-Theochem, (772): 65-73 2006.

Roohi, H.; Ebrahimi, A.; Mackiabadi, B.; Hagealirezahi, M.

Evaluation of the origin of rotational barrier in NH₂-X (X = NO, NS)

Journal of Molecular Structure-Theochem, (778): 63-67 2006.

Roos, G.; Loverix, S.; Brosens, E.; Van Belle, K.; Wyns, L.; Geerlings, P.; Messens, J.

The activation of electrophile, nucleophile and leaving group during the reaction catalysed by p1258 arsenate reductase

Chembiochem, (7): 981-989 2006.

Rosokha, S. V.; Lu, J. J.; Dibrov, S. M.; Kochi, J. K.

2,3,4,5,6-Pantanitroaniline 1,2-dichloroethane disolvate: 'push-pull' deformation of aromatic rings by intramolecular charge transfer

Acta Crystallographica Section C-Crystal Structure Communications, (62): O464-O466 2006.

Roux, M. V.; Temprado, M.; Jimenez, P.; Foces-Foces, C.; Notario, R.; Verevkin, S. P.; Liebman, J. F.

Thermochemistry of 2,5-thiophenedicarboxylic acid

Journal of Physical Chemistry A, (110): 12477-12483 2006.

Roux, M. V.; Temprado, M.; Jimenez, P.; Notario, R.; Guzman-Mejia, R.; Juaristi, E.

Calorimetric and computational study of 1,4-dithiacyclohexane 1,1-dioxide (1,4-dithiane sulfone)

Journal of Organic Chemistry, (71): 2581-2586 2006.

Roy, D.; Corminboeuf, C.; Wannere, C. S.; King, R. B.; Schleyer, P. V.

Planar tetracoordinate carbon atoms centered in bare four-membered rings of late transition metals

Inorganic Chemistry, (45): 8902-8906 2006.

Roy, D.; Sunoj, R. B.

Quantification of intramolecular nonbonding interactions in organochalcogens

Journal of Physical Chemistry A, (110): 5942-5947 2006.

Roy, D. R.; Parthasarathi, R.; Subramanian, V.; Chattaraj, P. K.

An electrophilicity based analysis of toxicity of aromatic compounds towards Tetrahymena pyriformis

Qsar & Combinatorial Science, (25): 114-122 2006.

Roy, D. R.; Sarkar, U.; Chattaraj, P. K.; Mitra, A.; Padmanabhan, J.; Parthasarathi, R.; Subramanian, V.; Van Damme, S.; Bultinck, P.

Analyzing toxicity through electrophilicity

Molecular Diversity, (10): 119-131 2006.

Rozas, I.; Alkorta, I.; Elguero, J.

Stereoisomer discrimination in complexes of halogen-substituted difuranes and Li or Na cations

Journal of Physical Chemistry A, (110): 13310-13316 2006.

Ruiz, A. J.; Lorono, M.; Cordova, T.; Chuchani, G.

Theoretical study of the gas phase unimolecular elimination kinetics of 2-substituted electron-withdrawing groups of ethyl N,N-dimethylcarbamates

Journal of Molecular Structure-Theochem, (769): 193-199 2006.

Rusanova, J.; Rusanov, E.; Gorelsky, S. I.; Christendat, D.; Popescu, R.; Farah, A. A.; Beaulac, R.; Reber, C.; Lever, A. B. P.

*The very covalent diammino(*o*-benzoquinonediimine) dichlororuthenium(II). An example of very strong pi-back-donation*

Inorganic Chemistry, (45): 6246-6262 2006.

Ruzsinszky, A.; Perdew, J. P.; Csonka, G. I.; Vydrov, O. A.; Scuseria, G. E.

Spurious fractional charge on dissociated atoms: Pervasive and resilient self-interaction error of common density functionals

Journal of Chemical Physics, (125) 2006.

Saczewski, J.; Frontera, A.; Gdaniec, M.; Brzozowski, Z.; Saczewski, F.; Tabin, P.; Quinonero, D.; Deya, P. M.

Synthesis, X-ray structure analysis and computational studies of novel bis(thiocarbamoyl) disulfides with non-covalent S center dot center dot center dot N and S center dot center dot center dot S interactions

Chemical Physics Letters, (422): 234-239 2006.

Sadekov, I. D.; Abakarov, G. M.; Minkin, V. I.

Five-membered heterocycles with vicinal Te and O heteroatoms

Advances in Heterocyclic Chemistry, Vol 92, (92): 55-82 2006.

Saenz, P.; Cachau, R. E.; Seoane, G.; Kieninger, M.; Ventura, O. N.

A new perspective in the Lewis acid catalyzed ring opening of epoxides. Theoretical study of some complexes of methanol, acetic acid, dimethyl ether, diethyl ether, and ethylene oxide with boron trifluoride

Journal of Physical Chemistry A, (110): 11734-11751 2006.

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

A computational and conceptual density functional theory study of the properties of Re and Tc tricarbonyl complexes

Journal of Physical Chemistry A, (110): 9240-9246 2006.

Sahnoun, R.; Fujimura, Y.; Kabuto, K.; Takeuchi, Y.; Noyori, R.

Hyperconjugative electron-delocalization mechanism controlling the conformational preference of fluoroacetaldehyde and methyl fluoroacetate
Bulletin of the Chemical Society of Japan, (79): 555-560 2006.

Sahnoun, R.; Nakai, K.; Sato, Y.; Kono, H.; Fujimura, Y.; Tanaka, M.
Theoretical investigation of the stability of highly charged C-60 molecules produced with intense near-infrared laser pulses
Journal of Chemical Physics, (125) 2006.

Sajan, D.; Fischer, A.; Joe, I. H.; Jayakumar, V. S.
Dimerisation and vibrational spectroscopic properties of (RS)-phenylsuccinic acid
Journal of Raman Spectroscopy, (37): 1307-1318 2006.

Saloni, J.; Roszak, S.; Hilpert, K.; Popovic, A.; Miller, M.; Leszczynski, J.
Mass spectrometric and quantum chemical studies of the thermodynamics and bonding of neutral and ionized LnCl, LnCl(2), and LnCl(3) species (Ln = Ce, Lu)
Inorganic Chemistry, (45): 4508-4517 2006.

Saloni, J.; Roszak, S.; Miller, M.; Leszczynski, J.
Theoretical thermodynamics and the nature of interactions of the quasi-binary NaCl-SnCl₂ system
Journal of Physical Chemistry A, (110): 12535-12539 2006.

Samantaray, M. K.; Katiyar, V.; Roy, D.; Pang, K. L.; Nanavati, H.; Stephen, R.; Sunoj, R. B.; Ghosh, P.
A cationic (N-Heterocyclic carbene)silver complex as catalyst for bulk ring-opening polymerization of (L)-lactides
European Journal of Inorganic Chemistry: 2975-2984 2006.

Samantaray, M. K.; Roy, D.; Patra, A.; Stephen, R.; Saikh, M.; Sunoj, R. B.; Ghosh, P.
Experimental and theoretical studies of a silver complex of O-functionalized N-heterocyclic carbene
Journal of Organometallic Chemistry, (691): 3797-3805 2006.

Sanz, M. E.; Lesarri, A.; Pena, M. I.; Vaquero, V.; Cortijo, V.; Lopez, J. C.; Alonso, J. L.
The shape of beta-alanine
Journal of the American Chemical Society, (128): 3812-3817 2006.

Sarangi, R.; Aboelella, N.; Fujisawa, K.; Tolman, W. B.; Hedman, B.; Hodgson, K. O.; Solomon, E. I.
X-ray absorption edge spectroscopy and computational studies on LCuO₂ species: Superoxide-Cu-II versus peroxide-Cu-III bonding
Journal of the American Chemical Society, (128): 8286-8296 2006.

Sargent, A. L.; Mosley, B. J.; Sibert, J. W.
A theoretical investigation on the Wurster's crown analogue of 18-crown-6
Journal of Physical Chemistry A, (110): 3826-3837 2006.

Sarkar, U.; Padmanabhan, J.; Parthasarathi, R.; Subramanian, V.; Chattaraj, P. K.
Toxicity analysis of polychlorinated dibenzofurans through global and local electrophilicities

Journal of Molecular Structure-Theochem, (758): 119-125 2006.

Sarma, B. K.; Mugesh, G.

Biomimetic studies on selenoenzymes: Modeling the role of proximal histidines in thioredoxin reductases

Inorganic Chemistry, (45): 5307-5314 2006.

Sasanuma, Y.; Kumagai, R.; Nakata, K.

Prediction of structures, properties, and functions of alternating copolymers of ethylene imine and ethylene oxide as an example of molecular design for polymers

Macromolecules, (39): 6752-6764 2006.

Sasanuma, Y.; Sugita, K.

The attractive gauche effect of ethylene oxides

Polymer Journal, (38): 983-988 2006.

Sasanuma, Y.; Watanabe, A.

Conformational characteristics of poly(trimethylene sulfide) and structure-property relationships of representative polysulfides and polyethers

Macromolecules, (39): 1646-1656 2006.

Scalmani, G.; Frisch, M. J.; Mennucci, B.; Tomasi, J.; Cammi, R.; Barone, V.

Geometries and properties of excited states in the gas phase and in solution: Theory and application of a time-dependent density functional theory polarizable continuum model

Journal of Chemical Physics, (124) 2006.

Schofield, M. H.; Sorel, M. A.; Manalansan, R. J.; Richardson, D. P.; Markgraf, J. H.

Substituent effects on N-15 and C-13 NMR chemical shifts of 3-phenylisoxazoles: a theoretical and spectroscopic study

Magnetic Resonance in Chemistry, (44): 851-855 2006.

Selvarengan, P.; Kolandaivel, P.

Theoretical study of CH...O hydrogen bond in proton transfer reaction of glycine

International Journal of Quantum Chemistry, (106): 1001-1008 2006.

Semenov, S. G.; Aleksandrova, A. V.; Dogadina, A. V.; Sigolaev, Y. F.; Belyakov, A. V.; Ionin, B. I.

Quantum-chemical investigation of reactions of (dialkylamino)ethynylphosphonates with amines

Russian Journal of General Chemistry, (76): 895-905 2006.

Semenov, S. G.; Sigolaev, Y. F.

Affinity of xenon(II) and carbon in the (heptafluorocyclohexa-1,4-dien-1-yl)xenonium ion for fluoride ion and acetonitrile

Russian Journal of Organic Chemistry, (42): 1789-1791 2006.

Semenov, S. G.; Sigolaev, Y. F.

Quantumchemical investigation of borabenzene adduct with pyridine

Russian Journal of General Chemistry, (76): 1925-1929 2006.

Semenov, S. G.; Sigolaev, Y. F.
trans-Difluoro(pentafluorophenyl)xenonium(IV) in acetonitrile: A quantum-chemical study
Russian Journal of Organic Chemistry, (42): 936-937 2006.

Semenov, S. G.; Sigolaev, Y. F.; Belyakov, A. V.
*(Pentafluorophenyl)xenonium(II) cyanide, isocyanide, and fluoride in dichloromethane: A
PCM/DFT study*
Russian Journal of General Chemistry, (76): 1729-1731 2006.

Senthilkumar, K.; Raman, M. S.; Kolandaivel, P.
Effect of substitution of electron-donating and -withdrawing groups on the stability of flavin-diaminepyridine complexes - a density functional theory study
Journal of Molecular Structure-Theochem, (758): 107-112 2006.

Senthilkumar, L.; Ghanty, T. K.; Ghosh, S. K.; Kolandaivel, P.
Hydrogen bonding in substituted formic acid dimers
Journal of Physical Chemistry A, (110): 12623-12628 2006.

Senthilkumar, L.; Kolandaivel, P.
Molecular interaction study of formohydroxamic acid (FHA) with water
Journal of Molecular Structure, (791): 149-157 2006.

Sereda, G. A.
*A sequence of linked experiments, suitable for practical courses of inorganic, organic,
computational chemistry, and NMR spectroscopy*
Journal of Chemical Education, (83): 931-933 2006.

Sevryugina, Y.; Rogachev, A. Y.; Jackson, E. A.; Scott, L. T.; Petrukhina, M. A.
*Ray and density functional theory structural study of 1,3,5,7,9-penta-tert-butylcorannulene,
C₄₀H₅₀*
Journal of Organic Chemistry, (71): 6615-6618 2006.

Shao, Y.; Molnar, L. F.; Jung, Y.; Kussmann, J.; Ochsenfeld, C.; Brown, S. T.; Gilbert, A. T. B.; Slipchenko, L. V.; Levchenko, S. V.; O'Neill, D. P.; DiStasio, R. A.; Lochan, R. C.; Wang, T.; Beran, G. J. O.; Besley, N. A.; Herbert, J. M.; Lin, C. Y.; Van Voorhis, T.; Chien, S. H.; Sodt, A.; Steele, R. P.; Rassolov, V. A.; Maslen, P. E.; Korambath, P. P.; Adamson, R. D.; Austin, B.; Baker, J.; Byrd, E. F. C.; Dachsel, H.; Doerksen, R. J.; Dreuw, A.; Dunietz, B. D.; Dutoi, A. D.; Furlani, T. R.; Gwaltney, S. R.; Heyden, A.; Hirata, S.; Hsu, C. P.; Kedziora, G.; Khalliulin, R. Z.; Klunzinger, P.; Lee, A. M.; Lee, M. S.; Liang, W.; Lotan, I.; Nair, N.; Peters, B.; Proynov, E. I.; Pieniazek, P. A.; Rhee, Y. M.; Ritchie, J.; Rosta, E.; Sherrill, C. D.; Simonett, A. C.; Subotnik, J. E.; Woodcock, H. L.; Zhang, W.; Bell, A. T.; Chakraborty, A. K.; Chipman, D. M.; Keil, F. J.; Warshel, A.; Hehre, W. J.; Schaefer, H. F.; Kong, J.; Krylov, A. I.; Gill, P. M. W.; Head-Gordon, M.
Advances in methods and algorithms in a modern quantum chemistry program package
Physical Chemistry Chemical Physics, (8): 3172-3191 2006.

Sharma, M.; Kumar, P.; Singh, H.; Chakraborty, T. K.
*Preferential cyclotrimerization of 5-(aminomethyl)-2-furancarboxylic acid (AMFC): Electrostatic
and orbital interactions studies*
Journal of Molecular Structure-Theochem, (764): 109-115 2006.

Shchavlev, A. E.; Pankratov, A. N.; Shalabay, A. V.
DFT computational studies on rotation barriers, tautomerism, intramolecular hydrogen bond, and solvent effects in 8-hydroxyquinoline
International Journal of Quantum Chemistry, (106): 876-886 2006.

Shen, W.; Li, M.; Huang, H.; Li, Y.; Wang, S.
Thieno 3,4-f isothianaphthene and its N-substitutes: a theoretical insight
Molecular Simulation, (32): 457-464 2006.

Sheng, L.; Cohen, A.; Gerber, R. B.
Theoretical prediction of chemically bound compounds made of argon and hydrocarbons
Journal of the American Chemical Society, (128): 7156-7157 2006.

Sheng, L.; Gerber, R. B.
High coordination chemically bound compounds of noble gases with hydrocarbons: Ng(CCH)(4) and Ng(CCH)(6), (Ng=Xe or Kr)
Journal of Chemical Physics, (124) 2006.

Sheng, L.; Gerber, R. B.
Stability and structure of oligomers and polymers made of xenon and hydrocarbons: Theoretical predictions
Journal of Chemical Physics, (125) 2006.

Shindo, M.; Yoshikawa, T.; Itou, Y.; Mori, S.; Nishii, T.; Shishido, K.
Heteroatom-guided torqueselective olefination of alpha-oxy and alpha-amino ketones via ynolates
Chemistry-a European Journal, (12): 524-536 2006.

Shishkin, O. V.; Zubatyuk, R. I.; Shtamburg, V. G.; Tsygankov, A. V.; Klots, E. A.; Mazepa, A. V.; Kostyanovsky, R. G.
Pyramidal amide nitrogen in N-acyloxy-N-alkoxyureas and N-acyloxy-N-alkoxycarbamates
Mendeleev Communications: 222-223 2006.

Siboulet, B.; Marsden, C. J.; Vitorge, P.
A theoretical study of uranyl solvation: Explicit modelling of the second hydration sphere by quantum mechanical methods
Chemical Physics, (326): 289-296 2006.

Sidorkin, V. E.; Belogolova, E. F.; Pestunovich, V. A.
Molecular design of neutral intramolecular complexes bearing two silicon atoms anchored by a carbonyl oxygen atom: N,N'-bis(silylmethyl)propylene ureas
Chemistry-a European Journal, (12): 2021-2031 2006.

Silva, L. C.; Gomes, P. T.; Veiros, L. F.; Pascu, S. I.; Duarte, M. T.; Namorado, S.; Ascenso, J. R.; Dias, A. R.
Synthesis, structure, and solution dynamics of neutral allylnickel complexes of N-heterocyclic carbenes
Organometallics, (25): 4391-4403 2006.

- Singh, P. C.; Patwari, G. N.
Theoretical investigation of C-H center dot center dot center dot H-B dihydrogen bonded complexes of acetylenes with borane-trimethylamine
Chemical Physics Letters, (419): 5-9 2006.
- Sinha, R. K.; Pradhan, B.; Singh, B. P.; Kundu, T.; Biswas, P.; Chakraborty, T.
Origin of threefold symmetric torsional potential of methyl group in 4-methylstyrene
Journal of Chemical Physics, (124) 2006.
- Sirijaraensre, J.; Limtrakul, J.
Vapor-phase beckmann rearrangement of oxime molecules over H-faujasite zeolite
Chemphyschem, (7): 2424-2432 2006.
- Sivasankar, C.; Baskaran, C.; Samuelson, A. G.
Synthesis, spectroscopic characterization and electronic structure of some new Cu(I) carbene complexes
Journal of Chemical Sciences, (118): 237-242 2006.
- Sizova, O. V.
The valence structure analysis for dirhodium(II) tetracarboxylato, complexes with nitric oxide as axial ligand
Journal of Molecular Structure-Theochem, (760): 183-187 2006.
- Sizova, O. V.; Ivanova, N. V.
Electronic structure and spectra of rhodium(II) tetracarboxylate complexes
Russian Journal of Coordination Chemistry, (32): 444-450 2006.
- So, C. W.; Roesky, H. W.; Magull, J.; Oswald, R. B.
Synthesis and characterization of PhC(NtBu)(2) SiCl: A stable monomeric chlorosilylene
Angewandte Chemie-International Edition, (45): 3948-3950 2006.
- Solomon, E. I.; Gorelsky, S. I.; Dey, A.
Metal-thiolate bonds in bioinorganic chemistry
Journal of Computational Chemistry, (27): 1415-1428 2006.
- Song, H. J.; Xiao, H. M.; Dong, H. S.
Cooperative effects, strengths of hydrogen bonds, and intermolecular interactions in circular cis, trans-cyclotriazane clusters ($n=3-8$)
Journal of Chemical Physics, (125) 2006.
- Song, H. J.; Xiao, H. M.; Dong, H. S.
Density functional theory study of the properties of N-H center dot center dot center dot N, noncooperativities, and intermolecular interactions in linear trans-diazene clusters up to ten molecules
Journal of Physical Chemistry A, (110): 6178-6183 2006.
- Song, H. J.; Xiao, H. M.; Dong, H. S.

Theoretical study of properties of H bonds and intermolecular interactions in linear cis-,trans-cyclotriazane clusters (n=2-8)
Journal of Chemical Physics, (124) 2006.

Song, H. J.; Xiao, H. M.; Dong, H. S.; Zhu, W. H.
Cooperative effects and strengths of hydrogen bonds in open-chain cis-triaziridine clusters (n=2-8): A DFT investigation
Journal of Physical Chemistry A, (110): 2225-2230 2006.

Song, J. R.; Ren, Y. H.; Huang, J.; Ma, H. X.; Xu, K. Z.; Hu, H. M.
Synthesis, crystal structure and theoretical calculation of 4-(1,2,4-triazole-5-one-4-yl)-3-thiourea carboxylic acid ethyl ester
Acta Chimica Sinica, (64): 1334-1340 2006.

Song, J. W.; Lee, H. J.; Choi, Y. S.; Yoon, C. J.
Origin of rotational barriers of the N-N bond in hydrazine: NBO analysis
Journal of Physical Chemistry A, (110): 2065-2071 2006.

Song, Z. Q.; Li, Y. X.; Liu, M.; Cong, L. Q.; Liu, Y. H.
Regio- and stereoselective coupling of heteroaryl-substituted alkynes: New insights into the mechanism of zirconium-mediated cyclodimerization of alkynes and a facile route to 3-methylenecyclobutenes
Organometallics, (25): 5035-5044 2006.

Soriano, E.; Marco-Contelles, J.
Mechanisms of the transition metal-mediated hydroarylation of alkynes and allenes
Organometallics, (25): 4542-4553 2006.

Sorokin, V. I.; Ozeryanskii, V. A.; Borodkin, G. S.; Chernyshev, A. V.; Muir, M.; Baker, J.
Preparation of dialkylamino-substituted benzenes and naphthalenes by nucleophilic replacement of fluorine in the corresponding perfluoroaromatic compounds
Zeitschrift Fur Naturforschung Section B-a Journal of Chemical Sciences, (61): 615-625 2006.

Sparkes, H. A.; Raithby, P. R.; Clot, E.; Shields, G. P.; Chisholm, J. A.; Allen, F. H.
Carbonyl/(center dot center dot center dot)carbonyl interactions in first-row transition metal complexes
CrystEngComm, (8): 563-570 2006.

Spencer, L. P.; Beddie, C.; Hall, M. B.; Fryzuk, M. D.
Synthesis, reactivity, and DFT studies of tantalum complexes incorporating diamido-N-heterocyclic carbene ligands. Facile endocyclic C-H bond activation
Journal of the American Chemical Society, (128): 12531-12543 2006.

Sporea, C.; Rabilloud, F.; Allouche, A. R.; Frecon, M.
Ab initio study of neutral and charged SinNap(+) (n <= 6, p <= 2) clusters
Journal of Physical Chemistry A, (110): 1046-1051 2006.

Sporea, C.; Rabilloud, F.; Cosson, X.; Allouche, A. R.; Aubert-Frecon, M.

Theoretical study of mixed silicon-lithium clusters SinLip(+) (n=1-6, p=1-2)
Journal of Physical Chemistry A, (110): 6032-6038 2006.

Srinivas, G. N.; Lu, Y.; Schwartz, M.
Ge2H2 a pi-ligand in organometallic chemistry
Journal of Organometallic Chemistry, (691): 2503-2511 2006.

Srinivas, G. N.; Schwartz, M.
A computational study of bond dissociation enthalpies in haloethenes
Journal of Molecular Structure-Theochem, (760): 121-129 2006.

Steudel, R.; Steudel, Y.
Geometries, thermodynamic properties and reactions of methylzinc alkoxide clusters studied by density functional theory calculations
Journal of Physical Chemistry A, (110): 8912-8924 2006.

Steudel, R.; Steudel, Y.
Interaction of zinc oxide clusters with molecules related to the sulfur vulcanization of polyolefins ("rubber")
Chemistry-a European Journal, (12): 8589-8602 2006.

Steudel, R.; Steudel, Y.; Mak, A. M.; Wong, M. W.
Homolytic dissociation of the vulcanization accelerator tetramethylthiuram disulfide (TMTD) and structures and stabilities of the related radicals Me2NCSn center dot (n=1-4)
Journal of Organic Chemistry, (71): 9302-9311 2006.

Strohmeier, M.; Barich, D. H.; Grant, D. M.; Miller, J. S.; Pugmire, R. J.; Simons, J.
Solid-state NMR spectra and long intradimer bonds in the pi- TCNE (2)(2-) dianion
Journal of Physical Chemistry A, (110): 7962-7969 2006.

Studt, F.; Lehnert, N.; Wiesler, B. E.; Scherer, A.; Beckhaus, R.; Tuczek, F.
Spectroscopic comparison of dinuclear Ti+ and Ti2+ mu-eta(1):eta(1) dinitrogen complexes with Cp/pentafulvene and amine/amide ligation: Moderate versus strong activation of N-2*
European Journal of Inorganic Chemistry: 291-297 2006.

Studt, F.; MacKay, B. A.; Fryzuk, M. D.; Tuczek, F.
N-N splitting of a functionalized mu-eta(1):eta(2) coordinated N-2 ligand leading to a mu-nitrido mu-imido core: mechanistic insight from DFT
Dalton Transactions: 1137-1140 2006.

Stueber, D.
The embedded ion method: A new approach to the electrostatic description of crystal lattice effects in chemical shielding calculations
Concepts in Magnetic Resonance Part A, (28A): 347-368 2006.

Su, Z. S.; Hu, C. W.; Qin, S.; Feng, X. M.
A quantum chemical study on the mechanism of chiral N-oxides-catalyzed Strecker reaction
Tetrahedron, (62): 4071-4080 2006.

- Su, Z. S.; Qin, S.; Tang, D. Y.; Yang, H. Q.; Hu, C. W.
Theoretical study on the reaction of methane and zinc oxide in gas phase
Journal of Molecular Structure-Theochem, (778): 41-48 2006.
- Sun, J.; Lu, W. C.; Wang, H.; Li, Z. S.; Sun, C. C.
Theoretical study of Al-n and AlnO (n=2-10) clusters
Journal of Physical Chemistry A, (110): 2729-2738 2006.
- Sun, Y. X.; Ren, Y.; Wong, N. B.; Chu, S. Y.; Xue, Y.
Comprehensive mechanistic study of ion pair S(N)2 reactions of lithium isocyanate and methyl halides
International Journal of Quantum Chemistry, (106): 1653-1663 2006.
- Sun, Y. X.; Zhang, R.; Ding, D. J.; Liu, S.; Wang, B. L.; Wang, Y. L.; Lin, Y. X.
Experimental and density functional studies on two structurally similar antipyrine derivatives: 4-(2-hydroxy-5-nitrobenzylidene-amino)-1,2-dihydro-1,5-dimethyl-2-phenyl pyrazol-3-one and 4-(3-bromo-5-chloro-2-hydroxybenzylideneamino)-1,2-dihydro-1,5-dimethyl- 2-phenylpyrazol-3-one
Structural Chemistry, (17): 655-665 2006.
- Sundberg, M. R.; Ponec, R.
The nature of M-O bond in MOX4 compounds (M = Os, Ru; X = F, Cl, Br, I)
Inorganica Chimica Acta, (359): 899-906 2006.
- Sung, D. D.; Koo, I. S.; Yang, K.; Lee, I.
Effects of atom pairs O and S on the stability of zwitterionic tetrahedral intermediate: A theoretical study
Chemical Physics Letters, (432): 426-430 2006.
- Sushko, P. V.; Shluger, A. L.; Hayashi, K.; Hirano, M.; Hosono, H.
Mechanisms of oxygen ion diffusion in a nanoporous complex oxide 12CaO center dot 7Al(2)O(3)
Physical Review B, (73) 2006.
- Szaleniec, M.; Witko, M.; Tadeusiewicz, R.; Goclon, J.
Application of artificial neural networks and DFT-based parameters for prediction of reaction kinetics of ethylbenzene dehydrogenase
Journal of Computer-Aided Molecular Design, (20): 145-157 2006.
- Szatmari, I.; Toth, D.; Koch, A.; Heydenreich, M.; Kleinpeter, E.; Fulop, F.
Study of the substituent-influenced anomeric effect in the ring-chain tautomerism of 1-alkyl-3-aryl-naphth 1,2-e 1,3 oxazines
European Journal of Organic Chemistry: 4670-4675 2006.
- Szymczak, J. J.; Gora, R. W.; Roszak, S.; Majumdar, D.; Wang, J.; Grabowski, S. J.; Leszczynski, J.
Proton bound open shell systems - theoretical studies on O2H+(O-2)(n) (n=1-6) complexes
Molecular Physics, (104): 2327-2336 2006.
- Szymczak, J. J.; Urban, J.; Roszak, S.; Leszczynski, J.

The nature of variations of ammonia proton affinity in an argon environment
Journal of Physical Chemistry A, (110): 13099-13105 2006.

Takahashi, M.; Kawazoe, Y.

Ab initio quantum chemical investigation of several isomers of anionic Si-6
Chemical Physics Letters, (418): 475-480 2006.

Talarico, G.; Cavallo, L.

Living propene polymerization with bis(phenoxy-imine) group 4 metal catalysts: A theoretical study
Kinetics and Catalysis, (47): 289-294 2006.

Talbot-Eeckelaers, C. E.; Rajaraman, G.; Cano, J.; Aromi, G.; Ruiz, E.; Brechin, E. K.

Encouraging chromium(III) ions to form larger clusters: Syntheses, structures, magnetic properties and theoretical studies of di- and octametallic Cr clusters
European Journal of Inorganic Chemistry: 3382-3392 2006.

Tamilmani, V.; Daul, C.; Jenny, T.

Possible ring structures of armchair single-walled carbon nanotubes
Chimia, (60): 228-230 2006.

Tautermann, C. S.; Clary, D. C.

Comparative study of cluster- and supercell-approaches for investigating heterogeneous catalysis by electronic structure methods: Tunneling in the reaction N+H → NH on Ru(0001)
Physical Chemistry Chemical Physics, (8): 1437-1444 2006.

Taylor, D. E.; Bunte, S. W.; Runge, K.

A pseudoatom approach to molecular truncation: Application in ab initio MBPT methods
Journal of Physical Chemistry A, (110): 6279-6284 2006.

Tayyari, S. F.; Emampour, J. S.; Vakili, M.; Nekoei, A. R.; Eshghi, H.; Salemi, S.; Hassanpour, M.

Vibrational assignment and structure of benzoylacetone: A density functional theoretical study
Journal of Molecular Structure, (794): 204-214 2006.

Tayyari, S. F.; Moosavi-Tekyeh, Z.; Zahedi-Tabrizi, M.; Eshghi, H.; Emampour, J. S.; Rahemi, H.; Hassanpour, M.

Intramolecular hydrogen bonding in 2-nitromalonaldehyde: Infrared spectrum and quantum chemical calculations
Journal of Molecular Structure, (782): 191-199 2006.

Thakur, T. S.; Desiraju, G. R.

Misassigned C-H center dot center dot center dot Cu agostic interaction in a copper(II) ephedrine derivative is actually a weak, multicentred hydrogen bond
Chemical Communications: 552-554 2006.

Tian, S. X.

Ab initio study of structures and energies of Al₂H₄ and Al₂H₄
Theoretical Chemistry Accounts, (115): 291-297 2006.

- Tian, S. X.
Conformation effects on the electronic structures of beta-alanine
Journal of Physical Chemistry A, (110): 3961-3966 2006.
- Tian, S. X.; Yang, J. L.
Effects of intramolecular hydrogen bonding on the ionization energies of proline
Angewandte Chemie-International Edition, (45): 2069-2072 2006.
- Tian, W. Q.; Ge, M. F.; Gu, F. L.; Yamada, T.; Aoki, Y.
Binary clusters AuPt and Au6Pt: Structure and reactivity within density functional theory
Journal of Physical Chemistry A, (110): 6285-6293 2006.
- Tian, W. Q.; Liu, L. V.; Wang, Y. A.
Electronic properties and reactivity of Pt-doped carbon nanotubes
Physical Chemistry Chemical Physics, (8): 3528-3539 2006.
- Tiwari, S. K.; Gais, H. J.; Lindenmaier, A.; Babu, G. S.; Raabe, G.; Reddy, L. R.; Kohler, F.; Gunter, M.; Koep, S.; Iska, V. B. R.
Functionalized chiral vinyl aminosulfoxonium salts: Asymmetric synthesis and application to the synthesis of enantiopure unsaturated prolines, beta,gamma-dehydro amino acids, and cyclopentanoid keto aminosulfoxonium ylides
Journal of the American Chemical Society, (128): 7360-7373 2006.
- Toma, L. M.; Lescouezec, R.; Pasan, J.; Ruiz-Perez, C.; Vaissermann, J.; Cano, J.; Carrasco, R.; Wernsdorfer, W.; Lloret, F.; Julve, M.
Fe(bpym)(CN)(4) (-): A new building block for designing single-chain magnets
Journal of the American Chemical Society, (128): 4842-4853 2006.
- Toma, L. M.; Toma, L. D.; Delgado, F. S.; Ruiz-Perez, C.; Sletten, J.; Cano, J.; Clemente-Juan, J. M.; Lloret, F.; Julve, M.
Trans-dicyanobis(acetylacetonato)ruthenate(III) as a precursor to build novel cyanide-bridged Ru-III-M-II bimetallic compounds M = Co and Ni
Coordination Chemistry Reviews, (250): 2176-2193 2006.
- Toom, L.; Kutt, A.; Kaljurand, I.; Leito, I.; Ottosson, H.; Grennberg, H.; Gogoll, A.
Substituent effects on the basicity of 3,7-diazabicyclo 3.3.1 nonanes
Journal of Organic Chemistry, (71): 7155-7164 2006.
- Torrent-Sucarrat, M.; Anglada, J. M.
On the gas phase hydrogen bond complexes between formic acid and hydroperoxyl radical. A theoretical study
Journal of Physical Chemistry A, (110): 9718-9726 2006.
- Torrent-Sucarrat, M.; Sola, M.; Toro-Labbe, A.
Gas-phase structures, rotational barriers, and conformational properties of hydroxyl and mercapto derivatives of cyclohexa-2,5-dienone and cyclohexa-2,5-dienethione
Journal of Physical Chemistry A, (110): 8901-8911 2006.

- Trapp, M. L.; Watts, J. K.; Weinberg, N.; Pinto, B. M.
Component analysis of the X-C-Y anomeric effect (X = O, S ; Y=F, OMe, NHMe) by DFT molecular orbital calculations and natural bond orbital analysis
Canadian Journal of Chemistry-Revue Canadienne De Chimie, (84): 692-701 2006.
- Trujillo, C.; Lamsabhi, A. M.; Mo, O.; Yanez, M.
Reactions of F+(P-3) and F+(D-1) with silicon oxide. Possibility of spin-forbidden processes
Journal of Physical Chemistry A, (110): 7130-7137 2006.
- Tsai, Y. C.; Lin, Y. M.; Yu, J. S. K.; Hwang, J. K.
A three-coordinate and quadruply bonded Mo-Mo complex
Journal of the American Chemical Society, (128): 13980-13981 2006.
- Tsipis, A. C.
Exploring the forces that control the P-C bond length in phosphamides and their complexes: The key role of hyperconjugation
Organometallics, (25): 2774-2781 2006.
- Tsuda, M.; Arboleda, N. B.; Kasai, H.
Initial driving force for proton transfer in Nafion
Chemical Physics, (324): 393-397 2006.
- Tsuda, M.; David, M.; Kasai, H.
O₂ binding to cytochrome c oxidase-inspired nanomaterials
Surface Science, (600): 3992-3994 2006.
- Tsuda, M.; Dino, W. A.; Kasai, H.; Nakanishi, H.; Aikawa, H.
Mg-H dissociation of magnesium hydride MgH₂ catalyzed by 3(d) transition metals
Thin Solid Films, (509): 157-159 2006.
- Tsuda, M.; Dy, E. S.; Kasai, H.
Side-on O₂ interaction with heme-based nanomaterials
European Physical Journal D, (38): 139-141 2006.
- Tsuda, M.; Kasai, H.
Ab initio study of alloying and straining effects on CO interaction with Pt
Physical Review B, (73) 2006.
- Tsuda, M.; Kasai, H.
Solvent effects on anionic and acid forms of Nafion side chain
Japanese Journal of Applied Physics Part 1-Regular Papers Brief Communications & Review Papers, (45): 5121-5125 2006.
- Tsuge, M.; Hamatani, S.; Kawai, A.; Tsuji, K.; Shibuya, K.
Jet spectroscopy of arylmethyl radicals in the visible region: assignment of low-frequency vibrational modes in diphenylmethyl and chlorodiphenylmethyl radicals
Physical Chemistry Chemical Physics, (8): 256-263 2006.

- Tsutsui, S.; Tanaka, H.; Kwon, E.; Matsumoto, S.; Sakamoto, K.
Experimental evidence and bond characterization of a cyclopropenylgermylene
Journal of Organometallic Chemistry, (691): 595-603 2006.
- Tunell, I.; Lim, C.
Factors governing the metal coordination number in isolated group IA and IIA metal hydrates
Inorganic Chemistry, (45): 4811-4819 2006.
- Uchida, N.; Miyazaki, T.; Kanayama, T.
Stabilization mechanism of Si-12 cage clusters by encapsulation of a transition-metal atom: A density-functional theory study
Physical Review B, (74) 2006.
- Uchimaru, T.; Tsuzuki, S.; Sugie, M.; Tokuhashi, K.; Sekiya, A.
A theoretical study on the strength of two-center three-electron bonds in the NO₃ radical adducts of reduced sulfur molecules, H₂S, CH₃SH, CH₃SCH₃, and CH₃SSCH₃
Chemical Physics, (324): 465-473 2006.
- Uddin, J.; Morales, C. M.; Maynard, J. H.; Landis, C. R.
Computational studies of metal-ligand bond enthalpies across the transition metal series
Organometallics, (25): 5566-5581 2006.
- Vaganova, T. A.; Yuferov, P. S.; Goryunov, L. L.; Panteleeva, E. V.; Sal'nikov, G. E.; Shchegoleva, L. N.; Mamatyuk, V. L.; Shteingarts, V. D.
Reductive activation of arenes 20. Anionic products of two-electron reduction of tolunitriles in liquid ammonia: the nature and electronic structure
Russian Chemical Bulletin, (55): 976-980 2006.
- Varga, Z.; Hargittai, M.
The NaDyBr₄ complex; its molecular structure and thermodynamic properties
Structural Chemistry, (17): 225-233 2006.
- Veiro, L. F.
Substituent effects on haptotropic rearrangements of bis(indenyl)zirconium sandwich complexes
Organometallics, (25): 2266-2273 2006.
- Veiro, L. F.
Tuning indenyl hapticity in zirconium bis(indenyl) complexes with the nature of complementary ligands
Organometallics, (25): 4698-4701 2006.
- Veiro, L. F.; Prazeres, A.; Costa, P. J.; Romao, C. C.; Kuhn, F. E.; Calhorda, M. J.
Olefin epoxidation with tert-butyl hydroperoxide catalyzed by MoO₂X₂L complexes: a DFT mechanistic study
Dalton Transactions: 1383-1389 2006.
- Veroni, I.; Makedonas, C.; Rontogianni, A.; Mitsopoulou, C. A.

An experimental and DFT computational study of a novel zerovalent tetracarbonyl tungsten complex of 2-(2'-pyridyl)quinoxaline
Journal of Organometallic Chemistry, (691): 267-281 2006.

Vianello, R.; Maksic, Z. B.
Triadic analysis of substituent effects - gas-phase acidity of para-substituted phenols
Tetrahedron, (62): 3402-3411 2006.

Vianello, R.; Peran, N.; Maksic, Z. B.
Hydride affinities of some substituted alkynes: Prediction by DFT calculations and rationalization by triadic formula
Journal of Physical Chemistry A, (110): 12870-12881 2006.

Villamena, F. A.; Locigno, E. J.; Rockenbauer, A.; Hadad, C. M.; Zweier, J. L.
Theoretical and experimental studies of the spin trapping of inorganic radicals by 5,5-dimethyl-1-pyrroline N-oxide (DMPO). 1. Carbon dioxide radical anion
Journal of Physical Chemistry A, (110): 13253-13258 2006.

Villingen, A.; Mayer, P.; Schulz, A.
GaCl₃-assisted 2+3 cycloaddition: A route to tetrazaphospholes
Chemical Communications: 1236-1238 2006.

Vitillo, J. G.; Damin, A.; Zecchina, A.; Ricchiardi, G.
Theoretical characterization of dihydrogen adducts with halide anions
Journal of Chemical Physics, (124) 2006.

Vogel, P.; Sordo, J. A.
Hetero-Diels-Alder an cheletropic additions of sulfur dioxide to conjugated dienes. Experimental facts and theoretical analysis
Current Organic Chemistry, (10): 2007-2036 2006.

Vrcek, V.; Buhl, M.
Conformational analysis of ferrocene-containing alcohols. A density functional study of weak OH center dot center dot center dot Fe interactions
Organometallics, (25): 358-367 2006.

Vyboishchikov, S. F.; Salvador, P.
Ab initio energy partitioning at the correlated level
Chemical Physics Letters, (430): 204-209 2006.

Waller, M. P.; Howard, S. T.; Platts, J. A.; Piltz, R. O.; Willock, D. J.; Hibbs, D. E.
Novel properties from experimental charge densities: An application to the zwitterionic neurotransmitter taurine
Chemistry-a European Journal, (12): 7603-7614 2006.

Wang, H. M.; Yang, C. L.; Wan, B. S.; Han, K. L.
The peculiar electronic structure of the di-metallocene: The evidence for the stability and the character of metal-metal bond

Journal of Theoretical & Computational Chemistry, (5): 461-473 2006.

Wang, J.; Gu, J. D.; Leszczynski, J.

A model study of interactions between TcAChE peripheral site segment Tyr70Val71 and Loop 1 of fasciculin 2

Journal of Biomolecular Structure and Dynamics, (24): 139-148 2006.

Wang, J.; Gu, J. D.; Leszczynski, J.

Modelling interactions between Loop1 of Fasciculin2 (Fas2) and Torpedo californica acetylcholinesterase (TcAChE)

Chemical Physics Letters, (431): 149-154 2006.

Wang, J.; Gu, J. D.; Leszczynski, J.

Phosphonylation mechanisms of sarin and acetylcholinesterase: A model DFT study

Journal of Physical Chemistry B, (110): 7567-7573 2006.

Wang, J. Y.; Fu, X. H.; Wu, T.; Wang, J.; Xiao, S. X.; Hu, C. W.

Ab initio study on the Michael addition reaction mechanism of indole with dimethyl alkylidene malonate

Acta Chimica Sinica, (64): 727-732 2006.

Wang, S. G.; Qiu, Y. X.; Fang, H.; Schwarz, W. H. E.

The challenge of the so-called electron configurations of the transition metals

Chemistry-a European Journal, (12): 4101-4114 2006.

Wang, W. G.; Ge, M. F.; Wang, D. X.

A density functional study on iodine dioxide-water complexes

Chemical Physics, (328): 165-172 2006.

Wang, X. F.; Andrews, L.

Infrared spectra and density functional calculations for M(OH)(2,3) and HOMO molecules and M(OH)(2)(+) cations (M = Y, La)

Journal of Physical Chemistry A, (110): 4157-4168 2006.

Wang, Y.; Huang, Y. H.; Liu, R. Z.

Hexa- and octacoordinate carbon in hydrocarbon cages: Theoretical design and characterization

Chemistry-a European Journal, (12): 3610-3616 2006.

Wang, Y.; Huang, Y. H.; Liu, R. Z.

Squeezing carbon dimers into the smallest fullerenes: DFT prediction of new carbon clusters containing double hypercoordinate carbons

Journal of Molecular Structure-Theochem, (775): 61-65 2006.

Wang, Y.; Li, H. R.; Han, S. J.

The chemical nature of the C-circle plus-H center dot center dot center dot center dot X- (X=Cl or Br) interaction in imidazolium halide ionic liquids

Journal of Chemical Physics, (124) 2006.

- Wang, Z. X.; Zhang, J. C.; Cao, W. L.
Study on the cation-pi interactions between ammonium ion and aromatic pi systems
Chinese Journal of Chemistry, (24): 1523-1530 2006.
- Wei, L. X.; Yang, B.; Wang, J.; Huang, C. Q.; Sheng, L. U.; Zhang, Y. W.; Qi, F.; Lam, C. S.; Li, W. K.
Vacuum ultraviolet photoionization mass spectrometric study of ethylenediamine
Journal of Physical Chemistry A, (110): 9089-9098 2006.
- Weinhold, F.
Resonance character of hydrogen-bonding interactions in water and other H-bonded species
Peptide Solvation and H-Bonds, (72): 121-+ 2006.
- Wiberg, K. B.; Wang, Y. G.; Sklenak, S.; Deutsch, C.; Trucks, G.
Permanganate oxidation of alkenes. Substituent and solvent effects. Difficulties with MP2 calculations
Journal of the American Chemical Society, (128): 11537-11544 2006.
- Wielgus, P.; Gora, R. W.; Szefczyk, B.; Roszak, S.; Leszczynski, J.
On the influence of microsolvation by argon atoms on the electron affinity properties of water dimer
Journal of Chemical Physics, (124) 2006.
- Wierzejewska, M.; Saldyka, M.
Theoretical study of hydrogen bonded complexes of dimethyl disulfide or dimethyl peroxide with nitric acid
Journal of Molecular Structure, (786): 33-38 2006.
- Wilke, J. J.; Weinhold, F.
Resonance bonding patterns of peroxide chemistry: Cyclic three-center hyperbonding in "phosphadioxirane" intermediates
Journal of the American Chemical Society, (128): 11850-11859 2006.
- Winkler, M.; Sander, W.
Generation and reactivity of the phenyl cation in cryogenic argon matrices: Monitoring the reactions with nitrogen and carbon monoxide directly by IR spectroscopy
Journal of Organic Chemistry, (71): 6357-6367 2006.
- Wu, C. W.; Ho, J. J.
Calculated effect of substitutions on the regioselectivity of cyclization of alpha-sulfenyl-, alpha-sulfinyl-, and alpha-sulfonyl-(5R)-5-hexenyl radicals
Journal of Organic Chemistry, (71): 9595-9601 2006.
- Wu, J.; Hagelberg, F.
Equilibrium geometries and associated energetic properties of mixed metal-silicon clusters from global optimization
Journal of Physical Chemistry A, (110): 5901-5908 2006.
- Wysokinski, R.; Kuduk-Jaworska, J.; Michalska, D.

Electronic structure, Raman and infrared spectra, and vibrational assignment of carboplatin. Density functional theory studies
Journal of Molecular Structure-Theochem, (758): 169-179 2006.

Xie, J.; Feng, D. C.; Feng, S. Y.
Insertion of the p-complex structure of silylenoid H₂SiLiF into X-H bonds (X = C, Si, N, P, O, S, and F)
Journal of Organometallic Chemistry, (691): 208-223 2006.

Xie, J.; Feng, D. C.; Feng, S. Y.
Theoretical study on the isomeric structures and the stability of silylenoid (Tsi)Cl₂SiLi (Tsi = C(SiMe₃)(3))
Journal of Computational Chemistry, (27): 933-940 2006.

Xie, J.; Feng, D. C.; Feng, S. Y.; Zhang, J.
Theoretical study on the reaction of silylenoid H₂SiLiF with HF
Chemical Physics, (323): 185-192 2006.

Xiu, H. Z.; Se, L.; Qian, S. L.
Characterizations of novel binuclear alkaline-earth metal compounds: M-2(eta(n)-N-5)(2)(M=Be and Mg, n=1, 2; M=Ca, n=2,5)
Journal of Theoretical & Computational Chemistry, (5): 475-487 2006.

Xu, J. H.
Probing the mechanism of Morita-Baylis-Hillman reaction in dichloromethane by density functional theory
Journal of Molecular Structure-Theochem, (767): 61-66 2006.

Xu, W. G.; Jin, B.
Aromaticity of regular heptagonal P-7(3-) trianion in the MP72- (M = Li, Na, K, Rb, and Cs) species
Chemical Physics Letters, (419): 439-443 2006.

Xu, W. G.; Jin, B.
Aromaticity of the planar pentagonal As-5(-) anion in the MAs5 (M = Li, Na, K, Rb, and Cs) and MAs5+ (M = Be, Mg, Ca, Sr, and Ba) clusters
Journal of Molecular Structure-Theochem, (759): 101-107 2006.

Xue, Z. M.; Chen, C. H.
The relationship between structure and electrochemical property of cyanoimino derivatives of squaric acid
Molecular Simulation, (32): 401-408 2006.

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 2006.

Yadav, V. K.; Gupta, A.; Balamurugan, R.; Sriramurthy, V.; Kumar, N. V.
*Distinguishing the early and late transition states and exploring the validity of sigma ->sigma *#, sigma#->sigma *, and sigma ->pi * (C=O) concepts in diastereoselection from NBO analysis*
Journal of Organic Chemistry, (71): 4178-4182 2006.

Yamakita, Y.; Isogai, Y.; Ohno, K.
Large Raman-scattering activities for the low-frequency modes of substituted benzenes: Induced polarizability and stereo-specific ring-substituent interactions
Journal of Chemical Physics, (124) 2006.

Yamashita, M.; Takamiya, I.; Jin, K.; Nozaki, K.
Syntheses and characterizations of methylpalladium complexes bearing a biphenyl-based bulky phosphine ligand: Weak interactions suggested by NBO and QTAIM analyses
Journal of Organometallic Chemistry, (691): 3189-3195 2006.

Yan, S. H.; Bu, Y. X.; Cukier, R. I.
Electron bridging dihydrogen bond in the imidazole-contained anion derivatives
Journal of Chemical Physics, (124) 2006.

Yang, H. Q.; Hu, C. W.; Qin, S.
Theoretical study on the reaction mechanism of CH4 with CaO
Chemical Physics, (330): 343-348 2006.

Yang, Y.; Zhang, W. J.; Gao, X. M.
Blue-shifted and red-shifted hydrogen bonds: Theoretical study of the CH3CHO center dot center dot center dot HNO complexes
International Journal of Quantum Chemistry, (106): 1199-1207 2006.

Yang, Y.; Zhang, W. J.; Gao, X. M.
Theoretical study on N-H center dot O blue-shifted H-bond for HNO center dot center dot center dot H2O2 complex
Chinese Journal of Chemistry, (24): 887-893 2006.

Yang, Z.; Ma, X. L.; Oswald, R. B.; Roesky, H. W.; Cui, C. M.; Schmidt, H. G.; Noltemeyer, M.
An unprecedented example of a heterotrimetallic main-group L2Al2Ge4Li2S7 cluster containing a Ge-II-Ge-II donor-acceptor bond
Angewandte Chemie-International Edition, (45): 2277-2280 2006.

Yang, Z.; Ma, X. L.; Oswald, R. B.; Roesky, H. W.; Noltemeyer, M.
Synthesis of an aluminum spirocyclic hybrid with an inorganic B2O3 and an organic C3N2 core
Journal of the American Chemical Society, (128): 12406-12407 2006.

Yassin, F. H.; Marynick, D. S.
Computational study of matrix-peptide interactions in MALDI mass spectrometry: Interactions of 2,5-and 3,5-dihydroxybenzoic acid with the tripeptide valine-proline-leucine
Journal of Physical Chemistry A, (110): 3820-3825 2006.

Ye, A. J.; Autschbach, J.

Study of static and dynamic first hyperpolarizabilities using time-dependent density functional quadratic response theory with local contribution and natural bond orbital analysis
Journal of Chemical Physics, (125) 2006.

Yeo, G. A.; Ford, T. A.
Conformational preferences of the structures, and energetics of the molecular complexes of boron trifluoride with some hydrogen halides, halogens and interhalogens
Journal of Molecular Structure-Theochem, (771): 157-164 2006.

Yerushalmi, R.; Brandis, A.; Rosenbach-Belkin, V.; Baldridge, K. K.; Scherz, A.
Modulation of fragmental charge transfer via hydrogen bonds. Direct measurement of electronic contributions
Journal of Physical Chemistry A, (110): 412-421 2006.

Yesudas, K.; Chaitanya, G. K.; Prabhakar, C.; Bhanuprakash, K.; Rao, V. J.
Structure, bonding, and lowest energy transitions in unsymmetrical squaraines: A computational study
Journal of Physical Chemistry A, (110): 11717-11729 2006.

Yi, H. B.; Diefenbach, M.; Choi, Y. C.; Lee, E. C.; Lee, H. M.; Hong, B. H.; Kim, K. S.
Interactions of neutral and cationic transition metals with the redox system of hydroquinone and quione: Theoretical characterization of the binding topologies, and implications for the formation of nanomaterials
Chemistry-a European Journal, (12): 4885-4892 2006.

Yoshikai, N.; Yamanaka, M.; Ojima, I.; Morokuma, K.; Nakamura, E.
Bimetallic synergism in alkyne silylformylation catalyzed by a cobalt-rhodium mixed-metal cluster
Organometallics, (25): 3867-3875 2006.

Yu, W. B.; Lin, Z. J.; Huang, Z. J.
Coexistence of dihydrogen, blue- and red-shifting hydrogen bonds in an ultrasmall system: Valine
Chemphyschem, (7): 828-830 2006.

Yu, Y. M.; Feng, S. Y.
Theoretical investigations on thermal rearrangement reactions of (aminomethyl)silane
Journal of Physical Chemistry A, (110): 12463-12469 2006.

Zade, S. S.; Bendikov, M.
Theoretical study of long oligothiophene dications: Bipolaron vs polaron pair vs triplet state
Journal of Physical Chemistry B, (110): 15839-15846 2006.

Zampieri, M.; Lazaro, S. R.; Paskocimas, C. A.; Ferreira, A. G.; Longo, E.; Varela, J. A.
Structural analysis of Ti and Pb citrate using NMR and FT-Raman signals and quantum mechanics simulations
Journal of Sol-Gel Science and Technology, (37): 9-17 2006.

Zborowski, K.; Alkorta, I.; Elguero, J.

Effect of dimerization and racemization processes on the electron density and the optical rotatory power of hydrogen peroxide derivatives
Journal of Physical Chemistry A, (110): 7247-7252 2006.

Zeng, X. Q.; Wang, W. G.; Liu, F. Y.; Ge, M. F.; Sun, Z.; Wang, D. X.
Electronic structure of binary phosphoric and arsenic triazides
European Journal of Inorganic Chemistry: 416-421 2006.

Zhang, J. D.; Xie, Y.; Schaefer, H. F.
Successive attachment of electrons to protonated guanine: (G+H)(center dot) radicals and (G+H)(-) anions
Journal of Physical Chemistry A, (110): 12010-12016 2006.

Zhang, R. B.; Eriksson, L. A.
The role of nucleobase carboradical and carbanion on DNA lesions: A theoretical study
Journal of Physical Chemistry B, (110): 23583-23589 2006.

Zhang, S. G.; Li, H.; Yang, P.
Quantum-chemical study on the structures and properties of uracil-BX3 (X= F, Cl) complexes
Chinese Journal of Structural Chemistry, (25): 947-956 2006.

Zhang, X.; Du, H. F.; Wang, Z.; Wu, Y. D.; Ding, K. L.
Experimental and theoretical studies on the hydrogen-bond-promoted enantioselective hetero-Diels-alder reaction of Danishefsky's diene with benzaldehyde
Journal of Organic Chemistry, (71): 2862-2869 2006.

Zhang, Y. X.; Zhang, X. X.; Liu, Z. Q.; Xu, H.; Jiang, J. Z.
Comparative density functional theory study of the structures and properties of metallophthalocyanines of group IVB
Vibrational Spectroscopy, (40): 289-298 2006.

Zhao, H. T.; Ariaftard, A.; Lin, Z. Y.
In-depth insight into metal-alkene bonding interactions
Inorganica Chimica Acta, (359): 3527-3534 2006.

Zhao, H. T.; Lin, Z. Y.; Marder, T. B.
Density functional theory studies on the mechanism of the reduction of CO₂ to CO catalyzed by copper(I) boryl complexes
Journal of the American Chemical Society, (128): 15637-15643 2006.

Zhao, L. M.; Guo, W. Y.; Zhang, R. R.; Wu, S. J.; Lu, X. Q.
Theoretical investigation of the decarbonylation of acetaldehyde Fe+ and Cr+
Chemphyschem, (7): 1345-1354 2006.

Zhao, L. M.; Zhang, R. R.; Guo, W. Y.; Lu, X. Q.
The oxidation pathways of Ti+ by acetaldehyde in the gas phase: A density functional theory investigation
Chemical Physics Letters, (431): 56-61 2006.

- Zhao, P. S.; Li, R. Q.; Zhang, L. L.; Jian, F. F.
*Density functional calculations on a double hydrogen bonded dimer of (*p*-methoxyphenyl)thiosemicarbazide*
Polish Journal of chemistry, (80): 2031-2039 2006.
- Zhao, S.; Liu, Z. P.; Li, Z. H.; Wang, W. N.; Fan, K. N.
Density functional study of small neutral and charged silver cluster hydrides
Journal of Physical Chemistry A, (110): 11537-11542 2006.
- Zhao, Y.; Truhlar, D. G.
Comparative assessment of density functional methods for 3d transition-metal chemistry
Journal of Chemical Physics, (124) 2006.
- Zheng, W. J.; Zhang, G. Z.; Fan, K. N.
Synthesis and characterization of eta(5)-1,2,4-diazaphospholide complexes of ruthenium
Organometallics, (25): 1548-1550 2006.
- Zheng, W. X.; Wong, N. B.; Li, W. K.; Tian, A. M.
Theoretical studies on the nonlinear optical properties of octupolar tri-s-triazines
Journal of Chemical Theory and Computation, (2): 808-814 2006.
- Zhou, D. H.; Wang, Y. Q.; He, N.; Yang, G.
The pi-complexation mechanisms of Cu(I), Ag(I)/zeolites for desulfurization
Acta Physico-Chimica Sinica, (22): 542-547 2006.
- Zhou, G.; Pu, X. M.; Wong, N. B.; Tian, A. M.; Zhou, H. W.
Theoretical investigation on the replacement of CH groups by n atoms in caged structure (CH)(8)
Journal of Physical Chemistry A, (110): 4107-4114 2006.
- Zhou, H.; Li, Z. H.; Wang, W. N.; Fan, K. N.
Density functional study of the interaction of molecular oxygen with small neutral and charged silver clusters
Chemical Physics Letters, (421): 448-452 2006.
- Zhou, J.; Li, Z. H.; Wang, W. N.; Fan, K. N.
Density functional study of the interaction of carbon monoxide with small neutral and charged silver clusters
Journal of Physical Chemistry A, (110): 7167-7172 2006.
- Zhou, J.; Wang, W. N.; Fan, K. N.
Novel compounds with cobalt, copper, and nickel dimers sandwiched between benzene molecules: A DFT study
Chemical Physics Letters, (424): 247-251 2006.
- Zhou, S. Q.; Ju, X. H.; Fan, X. W.
Intermolecular interactions of sulfur trioxide and sulfuric acid dimers studied by the DFT method
Journal of Chemical Research-S: 790-793 2006.

- Zhu, H. Y.; Zhou, L. J.; Wang, Y. Y.; Wen, Z. Y.; Wang, Y. B.
A polymer { Cu-II(Hpb)(mal) H₂O}(n): Magnetic studies and quantum chemical calculation for its monomer
Chinese Journal of Chemistry, (24): 321-325 2006.
- Zhu, Z. L.; Wright, R. J.; Olmstead, M. M.; Rivard, E.; Brynda, M.; Power, P. P.
A zinc-zinc-bonded compound and its derivatives bridged by one or two hydrogen atoms: A new type of Zn-Zn bonding
Angewandte Chemie-International Edition, (45): 5807-5810 2006.
- Zierkiewicz, W.; Michalska, D.; Cerny, J.; Hobza, P.
Cation-pi complexes between alkali metal cation and para-halogenophenols. Structures, binding energies and thermodynamic properties: DFT study and CCSD(T) complete basis set limit calculations
Molecular Physics, (104): 2317-2325 2006.
- Zimmerman, H. E.; Mitkin, O. D.
Conical intersection control of heterocyclic photochemical bond scission
Journal of the American Chemical Society, (128): 12743-12749 2006.
- Zolfigol, M. A.; Niknam, K.; Nazari, F.
Molybdatophosphoric acid/NaNO₂ as an efficient procedure for the chemoselective N-nitrosation of secondary amines
Journal of the Chinese Chemical Society, (53): 669-676 2006.
- Zubarev, D. Y.; Alexandrova, A. N.; Boldyreva, A. I.; Cui, L. F.; Li, X.; Wang, L. S.
On the structure and chemical bonding of Si-6(2-) and Si-6(2-) in NaSi6- upon Na⁺ coordination
Journal of Chemical Physics, (124) 2006.