

# Bibliography of NBO Applications, 2000

Drablos F

*Ab initio simulation of chemical shift effects from metal ion binding in bacitracin A*  
J COMPUT CHEM 21 (1): 1-7 JAN 15 2000

Del Rio E, Lopez R, Menendez MI, et al.

*A theoretical study of the reaction of HCO+ with C2H2*  
J COMPUT CHEM 21 (1): 35-42 JAN 15 2000

Fathalla W, Cajan M, Pazdera P

*Regioselectivity of electrophilic attack on 4-methyl-1-thioxo-1,2,4,5-tetrahydro[1,2,4]triazolo[4,3-a]quinazolin-5-one - Part 2: Reactions on nitrogen atom*  
MOLECULES 5 (12): 1210-1223 DEC 2000

Moudgil R, Kaur D, Vashisht R, et al.

*Theoretical studies on the conformations of selenamides*  
P INDIAN AS-CHEM SCI 112 (6): 623-629 DEC 2000

Glaser R, Wu Z, Lewis M

*A higher level ab initio quantum-mechanical study of the quadrupole moment tensor components of carbon dioxide*  
J MOL STRUCT 556 (1-3): 131-141 Sp. Iss. SI DEC 12 2000

Sohn CK, Chun YI, Rhee SK, et al.

*Transmission of substituent effects through five-membered heteroaromatic rings. III. Addition equilibria of hydroxide anion to benzaldehyde analogues*  
B KOR CHEM SOC 21 (12): 1202-1206 DEC 20 2000

Qu ZW, Li ZS, Ding YH, et al.

*Theoretical study of the gas-phase reaction of diborane(3) anion B2H3- with CO2*  
J PHYS CHEM A 104 (51): 11952-11960 DEC 28 2000

Pejov L, Ristova M, Soptrajanov B

*A gradient-corrected density functional study of structure, harmonic vibrational frequencies and charge distribution of benzenesulfonate anion on the ground-state potential energy surface*  
J MOL STRUCT 555: 341-349 NOV 28 2000

Eshdat L, Ayalon A, Beust R, et al.

*Up to six units of charge and twist-boat benzene moieties: Alkali metal reduction of phenyl-perisubstituted benzenes*  
J AM CHEM SOC 122 (51): 12637-12645 DEC 27 2000

Fabian J, Krebs A, Schonemann D, et al.

*1,3-heterocumulene-to-alkyne [3+2] cycloaddition reactions: A theoretical and experimental study*

J ORG CHEM 65 (26): 8940-8947 DEC 29 2000

Mire LW, Marynick DS

*Bonding preferences of C<sub>2</sub>X<sub>4</sub>-bridged bimetallic transition metal complexes of Ti, Cu, and Ag*  
INORG CHEM 39 (26): 5970-5975 DEC 25 2000

Brady ED, Hanusa TP, Pink M, et al.

*The first noncoordinated phosphonium diylide, [Me<sub>2</sub>P(C<sub>13</sub>H<sub>8</sub>)<sub>2</sub>](-), and its ylidic and cationic counterparts: Synthesis, structural characterization, and interaction with the heavy group 2 metals*  
INORG CHEM 39 (26): 6028-6037 DEC 25 2000

Nazmutdinov RR, Pobelov IV, Tsirlina GA, et al.

*Nature of the 'current pit' in concentrated solutions - Part I. Microscopic modelling of the interaction of Pt(II) aquachlorocomplexes with a mercury electrode*  
J ELECTROANAL CHEM 491 (1-2): 126-138 SEP 8 2000

Tossell JA, Sahai N

*Calculating the acidity of silanols and related oxyacids in aqueous solution*  
GEOCHIM COSMOCHIM AC 64 (24): 4097-4113 DEC 2000

Pulkkinen S, Noguera M, Rodriguez-Santiago L, et al.

*Gas phase intramolecular proton transfer in cationized glycine and chlorine substituted derivatives (M-gly, M = Na<sup>+</sup>, Mg<sup>2+</sup>, Cu<sup>+</sup>, Ni<sup>+</sup>, and Cu<sup>2+</sup>): Existence of zwitterionic structures?*  
CHEM-EUR J 6 (23): 4393-4399 DEC 1 2000

Szabo KJ

*Umpolung of the allylpalladium reactivity: Mechanism and regioselectivity of the electrophilic attack on bis-allylpalladium complexes formed in palladium-catalyzed transformations*  
CHEM-EUR J 6 (23): 4413-4421 DEC 1 2000

Deubel DV, Frenking G, Senn HM, et al.

*On the electronic character of oxygen-transfer reactions*  
CHEM COMMUN (24): 2469-2470 2000

Weiss D, Winter M, Fischer RA, et al.

*[Pt-2(GaCp<sup>\*</sup>)(2)(μ(2)-GaCp<sup>\*</sup>)(3)]: structure and bonding situation of the first homoleptic platinum complex with terminal and bridging Cp<sup>\*</sup>Ga ligands*  
CHEM COMMUN (24): 2495-2496 2000

Hieringer W, Eppinger J, Anwander R, et al.

*C-2-symmetric ansa-lanthanidocene complexes. Theoretical evidence for a symmetric Ln center*

*dot center dot center dot(Si--H) beta-diagnostic interaction*  
J AM CHEM SOC 122 (48): 11983-11994 DEC 6 2000

Fuentealba P, Savin A

*Electronic structure and bonding of the ground state of alkaline-earth-metal monoxides and carbides*  
J PHYS CHEM A 104 (46): 10882-10886 NOV 23 2000

George P, Glusker JP, Bock CW

*Cyclization/fission and fragmentation/recombination mechanisms for the 1,2 shift in free radicals: A computational study of H<sub>2</sub>C(center dot)-CH<sub>2</sub>X (X = -C equivalent to CH, -C equivalent to N, -CH=CH<sub>2</sub>, and -CH=NH) and H<sub>2</sub>C center dot-CH<sub>2</sub>CY=O (Y = -H, -F, -Cl, . . .)*  
J PHYS CHEM A 104 (48): 11347-11354 DEC 7 2000

Dore L, Puzzarini C, Cazzoli G, et al.

*Nuclear quadrupole tensors for Cl-35 and Cl-37 in cis-1-chloro-2-fluoroethylene obtained by detection of perturbation-allowed Delta J=2 and Delta J=3 transitions*  
J MOL SPECTROSC 204 (2): 262-267 DEC 2000

Firsov DA, Granovsky AA, Nemukhin AV

*Ab initio calculations of Cl-(HF)(n), n <= 6 clusters*  
IZV AKAD NAUK FIZ+ 64 (8): 1499-1501 SEP 2000

Li JS, Xiao HM, Dong HS

*A theoretical study on the intermolecular interaction of energetic system - Nitromethane dimer*  
CHINESE J CHEM 18 (6): 815-819 NOV-DEC 2000

Feil F, Harder S

*alpha,alpha-bis(trimethylsilyl)-substituted benzyl complexes of potassium and calcium*  
ORGANOMETALLICS 19 (24): 5010-5015 NOV 27 2000

Nolan EM, Linck RG

*Charge variations in substituted alkanes: Evidence for a through-space effect*  
J AM CHEM SOC 122 (46): 11497-11506 NOV 22 2000

Geise CM, Hadad CM

*Computational study of the electronic structure of substituted phenylcarbene in the gas phase*  
J ORG CHEM 65 (24): 8348-8356 DEC 1 2000

Portmann S, Inauen A, Luthi HP, et al.

*Chiral discrimination in hydrogen-bonded complexes*  
J CHEM PHYS 113 (21): 9577-9585 DEC 1 2000

Ohm M, Schulz A, Severin K

*Asymmetric halogeno-bridged complexes of the late transition metals - A computational and*

*experimental study*

EUR J INORG CHEM (12): 2623-2629 DEC 2000

Takahashi M, Veszpremi T, Hajgato B, et al.

*Theoretical study on stereochemical diversity in the addition of water to disilene*  
ORGANOMETALLICS 19 (23): 4660-4662 NOV 13 2000

Landis CR, Feldgus S, Uddin J, et al.

*Computational assessment of the effect of sigma-pi bonding synergy and reorganization energies on experimental trends in rhodium-phosphine bond enthalpies*  
ORGANOMETALLICS 19 (23): 4878-4886 NOV 13 2000

Bharatam PV, Moudgil R, Kaur D

*Se-N interactions in selenohydroxylamine: a theoretical study*  
J CHEM SOC PERK T 2 (12): 2469-2474 2000

Andrews L, Manceron L, Alikhani ME, et al.

*Observed and calculated infrared spectrum of Pd(H-2) in solid argon: A ligand-free side-bonded molecular hydrogen complex*  
J AM CHEM SOC 122 (44): 11011-11012 NOV 8 2000

Wang XF, Andrews L

*Reactions of laser-ablated ruthenium atoms with CO and H-2 mixtures: Infrared spectra and density functional theory calculations of H<sub>2</sub>Ru(CO)(x) (x=2-4) and (H-2)RuCO*  
J PHYS CHEM A 104 (44): 9892-9900 NOV 9 2000

Kar T, Angyan JG, Sannigrahi AB

*Comparison of ab initio Hartree-Fock and Kohn-Sham orbitals in the calculation of atomic charge, bond index, and valence*  
J PHYS CHEM A 104 (44): 9953-9963 NOV 9 2000

Sakata K

*Electron reorganization along the intrinsic reaction coordinate in 1,3-dipolar cycloaddition*  
J PHYS CHEM A 104 (44): 10001-10008 NOV 9 2000

Zimmerman HE, Lapin YA, Nesterov EE, et al.

*Rodlike molecules and singlet energy transfer*  
J ORG CHEM 65 (23): 7740-7746 NOV 17 2000

Kim KS, Tarakeshwar P, Lee JY

*Molecular clusters of pi-systems: Theoretical studies of structures, spectra, and origin of interaction energies*  
CHEM REV 100 (11): 4145-4185 NOV 2000

Hobza P, Havlas Z

*Blue-shifting hydrogen bonds*

CHEM REV 100 (11): 4253-4264 NOV 2000

Anbauer C, Davidge K, Klapotke TM, et al.

*Crystal structures of the phosphorus-boron adducts n-Pr<sub>3</sub>P center dot BBr<sub>3</sub> and I<sub>3</sub>P center dot BBr<sub>3</sub>*

Z ANORG ALLG CHEM 626 (11): 2373-2378 NOV 2000

Bailly F, Barthen P, Frohn HJ, et al.

*Pentafluorophenyl iodine(III) compounds. 4 [1]*

*Aryl(pentafluorophenyl)iodoniumtetrafluoroborates: General method of synthesis, typical properties, and structural features*

Z ANORG ALLG CHEM 626 (11): 2419-2427 NOV 2000

Riedmiller F, Schmidbaur H

*Trihydrogermyl-substituted thiophenes*

J CHEM SOC DALTON (22): 4117-4121 2000

Gumienna-Kontecka E, Berthon G, Fritsky IO, et al.

*2-(Hydroxyimino)propanohydroxamic acid, a new effective ligand for aluminium*

J CHEM SOC DALTON (22): 4201-4208 2000

Lee I, Kim CK, Li HG, et al.

*Acyl-transfer mechanisms involving various acyl functional groups: > X-Y with X = C, S, P and Y = O, S*

J AM CHEM SOC 122 (45): 11162-11172 NOV 15 2000

Matxain JM, Fowler JE, Ugalde JM

*Small clusters of II-VI materials: Zni<sub>i</sub>O<sub>i</sub>, i=1-9 - art. no. 053201*

PHYS REV A 6205 (5): 3201-- NOV 2000

Broadus KM, Kass SR

*The electron as a protecting group. 2. Generation of benzocyclobutadiene radical anion in the gas phase and an experimental determination of the heat of formation of benzocyclobutadiene*

J AM CHEM SOC 122 (43): 10697-10703 NOV 1 2000

Carballeira L, Perez-Juste I

*Ab initio study and NBO interpretation of the anomeric effect in CH<sub>2</sub>(XH<sub>2</sub>)<sub>2</sub> (X = N, P, As) compounds*

J PHYS CHEM A 104 (41): 9362-9369 OCT 19 2000

Clericuzio M, Alagona G, Ghio C, et al.

*Ab initio and density functional evaluations of the molecular conformations of beta-caryophyllene and 6-hydroxycaryophyllene*

J ORG CHEM 65 (21): 6910-6916 OCT 20 2000

Carda M, Portoles R, Murga J, et al.

*Stereoselective 1,3-dipolar cycloadditions of a chiral nitrone derived from erythrulose. An experimental and DFT theoretical study*

J ORG CHEM 65 (21): 7000-7009 OCT 20 2000

Chao I, Shih JH, Wu HJ

*Quantum mechanical study on the facial selectivity of dioxa and trioxa cage molecules*

J ORG CHEM 65 (22): 7523-7533 NOV 3 2000

Van der Vaart A, Gogonea V, Dixon SL, et al.

*Linear scaling molecular orbital calculations of biological systems using the semiempirical divide and conquer method*

J COMPUT CHEM 21 (16): 1494-1504 DEC 2000

Kong J, White CA, Krylov AI, et al.

*Q-chem 2.0: A high-performance ab initio electronic structure program package*

J COMPUT CHEM 21 (16): 1532-1548 DEC 2000

Bach A, Coussan S, Muller A, et al.

*Water-wire clusters: Vibronic spectra of 7-hydroxyquinoline center dot(H<sub>2</sub>O)(3)*

J CHEM PHYS 113 (20): 9032-9043 NOV 22 2000

Gross KC, Seybold PG

*Substituent effects on the physical properties and pK(a) of aniline*

INT J QUANTUM CHEM 80 (4-5): 1107-1115 NOV-DEC 2000

Edder C, Piguet C, Bernardinelli G, et al.

*Unusual electronic effects of electron-withdrawing sulfonamide groups in optically and magnetically active self-assembled noncovalent heterodimetallic d-f podates*

INORG CHEM 39 (22): 5059-5073 OCT 30 2000

Minkwitz R, Berkei M, Ludwig R

*Synthesis and characterization of novel iodine(III) compounds; Crystal structures of methoxy(trifluoromethyl)iodine(III) chloride [CF<sub>3</sub>I(Cl)OCH<sub>3</sub>] and dimethoxy(trifluoromethyl)iodine(III) [CF<sub>3</sub>I(OCH<sub>3</sub>)<sub>2</sub>]*

EUR J INORG CHEM (11): 2387-2392 NOV 2000

Weiss D, Steinke T, Winter M, et al.

*[(dcpe)Pt(ECp\*)(2)] (E = Al, Ga): Synthesis, structure, and bonding situation of the first aluminum(I) and gallium(I) complexes of phosphine-substituted transition metal centers*

ORGANOMETALLICS 19 (22): 4583-4588 OCT 30 2000

Blum O, Carmielli R, Martin JML, et al.

*Why does the tetrakis(trimethylphosphine)iridium(III) hydridochloride cation adopt the sterically*

*and electronically unfavorable cis geometry?*

ORGANOMETALLICS 19 (22): 4608-4612 OCT 30 2000

Peschke M, Blades AT, Kebarle P

*Binding energies for doubly-charged ions  $M2+ = Mg2+, Ca2+$  and  $Zn2+$  with the ligands  $L = H2O$ , acetone and N-methylacetamide in complexes  $MLn2+$  for  $n=1$  to 7 from gas phase equilibria determinations and theoretical calculations*

J AM CHEM SOC 122 (42): 10440-10449 OCT 25 2000

Wang CC, Tang TH, Wang Y

*Theoretical and experimental characterization of Cr-L multiple bonds ( $L = O, N$ , and C)*

J PHYS CHEM A 104 (42): 9566-9572 OCT 26 2000

Arulmozhiraja S, Fujii T

*$Li^+$  ion affinities of global-warming perfluorocarbons*

J PHYS CHEM A 104 (42): 9613-9618 OCT 26 2000

Bentley J

*Electron density as a descriptor of thermal molecular size*

J PHYS CHEM A 104 (42): 9630-9635 OCT 26 2000

Groen P, Oskam A, Kovacs A

*Theoretical study of mixed  $LiCeX4$  ( $X = F, Cl, Br, I$ ) rare earth/alkali halide complexes*

J MOL STRUC-THEOCHEM 531: 23-31 OCT 23 2000

Han YK, Hirao K

*Structure and stability of  $Na6Pb$  clusters*

J CHEM PHYS 113 (16): 6613-6617 OCT 22 2000

van der Vaart A, Bursulaya BD, Brooks CL, et al.

*Are many-body effects important in protein folding?*

J PHYS CHEM B 104 (40): 9554-9563 OCT 12 2000

Hommes NJRV, Heidrich D, Schleyer PVR

*Ab initio models for six-center multiple proton exchange and ion pair formation assisted by Lewis acids*

J MOL MODEL 6 (9): 563-574 2000

Goldenberg LM, Skabara PJ, Roberts DM, et al.

*Electrochemical molecular recognition of silver cation by electropolymerised thieno[3',4':5,6][1,4]dithiino[2,3-b]quinoxaline: a joint experimental and theoretical study*

J MATER CHEM 10 (11): 2458-2465 2000

Srinivas GN, Chen Z, Hamilton TP, et al.

*A theoretical study of  $B2Li6$*

CHEM PHYS LETT 329 (3-4): 239-247 OCT 20 2000

Fleischer H, Schollmeyer D

*Functionalized tellurium(II) thiolates: Tellurium bis(2-hydroxyethanethiolate) hydrate, the first H<sub>2</sub>O-Te-II complex*

ANGEW CHEM INT EDIT 39 (20): 3705-3706 2000

Minkin VI, Minyaev RM

*Aromatic stabilization of organochalcogen compounds with the intramolecular X <- O (X = S, Se, Te) coordination*

MENDELEEV COMMUN (5): 171-172 2000

Yoshimura T, Fujii T, Murotani S, et al.

*The structures of [Ph<sub>2</sub>XS-N-SPh<sub>2</sub>NH](+) cations (X=NH, O)*

J ORGANOMET CHEM 611 (1-2): 272-279 OCT 6 2000

Sakaki S, Biswas B, Musashi Y, et al.

*Bonding nature and reaction behavior of inter-element linkages with transition metal complexes. A theoretical study*

J ORGANOMET CHEM 611 (1-2): 288-298 OCT 6 2000

He Y, Grafenstein J, Kraka E, et al.

*What correlation effects are covered by density functional theory?*

MOL PHYS 98 (20): 1639-1658 OCT 20 2000

Takahashi A, Yang FH, Yang RT

*Aromatics/aliphatics separation by adsorption: New sorbents for selective aromatics adsorption by pi-complexation*

IND ENG CHEM RES 39 (10): 3856-3867 OCT 2000

Jeong M, Kwon Y

*The molecular structures and conformation of o-selenobenzyl fluoride derivatives, ArSeX (Ar = C<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>F; X = CN, Cl, Me): ab initio and DFT calculations*

CHEM PHYS LETT 328 (4-6): 509-515 OCT 6 2000

Peralta JE, Conteras RH, Snyder JP

*Natural bond orbital dissection of fluorine-fluorine through-space NMR coupling (*J(F,F)*) in polycyclic organic molecules*

CHEM COMMUN (20): 2025-2026 2000

Lee I, Rhee SK, Kim CK, et al.

*Transmission of substituent effects through 5-membered heteroaromatic rings*

B KOR CHEM SOC 21 (9): 882-890 SEP 20 2000

Sohn CK, Lim SH, Rhee SK, et al.

*Transmission of substituent effects through five-membered heteroaromatic rings, II. Deprotonation equilibria of phenol analogues*  
B KOR CHEM SOC 21 (9): 891-895 SEP 20 2000

Broadus KM, Kass SR

*Benzocyclobutadienyl anion: Formation and energetics of an antiaromatic molecule*  
J ORG CHEM 65 (20): 6566-6571 OCT 6 2000

Li GM, Niu S, Segi M, et al.

*On the behavior of alpha,beta-unsaturated thioaldehydes and thioketones in the Diels-Alder reaction*  
J ORG CHEM 65 (20): 6601-6612 OCT 6 2000

Gu Y, Kar T, Scheiner S

*Comparison of the CH center dot center dot center dot N and CH center dot center dot center dot O interactions involving substituted alkanes*  
J MOL STRUCT 552: 17-31 Sp. Iss. SI SEP 26 2000

Hakimelahi GH, Moosavi-Movahedi AA, Tsay SC, et al.

*Design, synthesis, and SAR of novel carbapenem antibiotics with high stability to Xanthomonas maltophilia oxyminocephalosporinase type II*  
J MED CHEM 43 (20): 3632-3640 OCT 5 2000

Adamo C, Barone V

*Structures and properties of lanthanide and actinide complexes by a new density functional approach: Lanthanum, gadolinium, lutetium, and thorium halides as case studies*  
J COMPUT CHEM 21 (13): 1153-1166 OCT 2000

Kaplan IG, Roszak S, Leszczynski J

*Nature of binding in the alkaline-earth clusters: Be-3, Mg-3, and Ca-3*  
J CHEM PHYS 113 (15): 6245-6252 OCT 15 2000

Fores M, Duran M, Sola M

*Substituent effects on the intramolecular proton transfer in the ground and lowest-lying singlet excited states of salicylaldimine*  
CHEM PHYS 260 (1-2): 53-64 OCT 1 2000

Plug C, Wallfisch B, Andersen HG, et al.

*Mesoionic pyridopyrimidinylium and pyridooxazinylium olates and non-mesoionic pyridopyrimidinones. Structures in the solid state, solution, and matrices*  
J CHEM SOC PERK T 2 (10): 2096-2108 2000

Gudat D, Haghverdi A, Hupfer H, et al.

*Stability and electrophilicity of phosphorus analogues of Arduengo carbenes - An experimental and computational study*

CHEM-EUR J 6 (18): 3414-3425 SEP 15 2000

Ashkenazi N, Vigalok A, Parthiban S, et al.

*Discovery of the first metallaquinone*

J AM CHEM SOC 122 (36): 8797-8798 SEP 13 2000

Piffl M, Weston J, Gunther W, et al.

*On the structure of sulfur-stabilized allyllithium compounds in solution*

J ORG CHEM 65 (19): 5942-5950 SEP 22 2000

Remko M, Sefcikova J

*Structure, reactivity and vibrational spectra of formohydroxamic and silaformohydroxamic acids: a comparative ab initio study*

J MOL STRUC-THEOCHEM 528: 287-296 AUG 25 2000

Kozlov ES, Kapustin EG, Soifer GB

*Cl-35 NQR spectra of phosphorus chlorides and their molecular conformations in crystals. Part 1.*

*Phosphorus (III) chlorides R<sub>2</sub>PCl<sub>2</sub>*

J MOL STRUCT 550: 167-175 Sp. Iss. SI SEP 5 2000

Kraka E, Cremer D

*Computer design of anticancer drugs. A new enediyne warhead*

J AM CHEM SOC 122 (34): 8245-8264 AUG 30 2000

Asthagiri D, Schure MR, Lenhoff AM

*Calculation of hydration effects in the binding of anionic ligands to basic proteins*

J PHYS CHEM B 104 (36): 8753-8761 SEP 14 2000

Ayers AE, Marynick DS, Dias HVR

*Azido derivatives of low-valent group 14 elements: Synthesis, characterization, and electronic structure of [(n-Pr)(2)ATI]GeN<sub>3</sub> and [(n-Pr)(2)ATI]SnN<sub>3</sub> featuring heterobicyclic 10-pi-electron ring systems*

INORG CHEM 39 (18): 4147-4151 SEP 4 2000

Harcourt RD

*Increased-valence structures for qualitative valence-bond representations of electronic structure for electron-rich molecules*

EUR J INORG CHEM (9): 1901-1916 SEP 2000

Buhl M, Gaemers S, Elsevier CJ

*Density-functional computation of Ru-99 NMR parameters*

CHEM-EUR J 6 (17): 3272-3280 SEP 1 2000

Arca M, Demartin F, Devillanova FA, et al.

*An experimental and theoretical approach to the study of the properties of parabanic acid and*

*related compounds: synthesis and crystal structure of diethylimidazolidine-2-selone-4,5-dione*  
CAN J CHEM 78 (9): 1147-1157 SEP 2000

Park HY, Kim CK, Lee BS, et al.

*Theoretical studies on gas-phase reactions of negative ions with alkyl nitrites*  
B KOR CHEM SOC 21 (8): 823-827 AUG 20 2000

Muller T, Meyer R, Lennartz D, et al.

*Unusually stable vinyl cations*  
ANGEW CHEM INT EDIT 39 (17): 3074-3077 2000

Heckmann G, Gorbunowa-Jonas E, Plank S, et al.

*Protonation of 1,1,3,3,5,5-hexakis(dimethylamino)-lambda(5)-[1,3,5] triphosphinine. Cyclotrimethylenetriphosphinic acid. NMR data, crystal structures, and quantum chemical calculations*  
Z ANORG ALLG CHEM 626 (9): 1974-1984 SEP 2000

Bickelhaupt FM, Baerends EJ

*Kohn-Sham density functional theory: Predicting and understanding chemistry*  
REV COMP CH 15: 1-86 2000

Pezacki JP, Loncke PG, Ross JP, et al.

*Silicon migration from oxygen to carbon and decarbonylation in methoxytriphenylsiloxycarbene*  
ORG LETT 2 (18): 2733-2736 SEP 7 2000

Yudanov IV, Di Valentin C, Gisdakis P, et al.

*Olefin epoxidation by mono and bisperoxo complexes of Mo(VI): a density functional model study*  
J MOL CATAL A-CHEM 158 (1): 189-197 SEP 8 2000

Anders E, Wermann K, Vanden Eynde JJ

*Chemistry of N-(1-haloalkyl)heteroarylium salts*  
ADV HETEROCYCL CHEM 77: 183-219 2000

Alder RW, Read D

*Remarkable in/out inversions at bridgehead phosphorus atoms*  
ANGEW CHEM INT EDIT 39 (16): 2879-2882 2000

Zhang YF, Xiang SC, Li JQ

*A density functional study on the geometries and bond dissociation energies of Mo(CO)(n)(+) (n = 1 similar to 6) compounds*  
ACTA CHIM SINICA 58 (8): 962-970 2000

Gonzalez-Luque R, Garavelli M, Bernardi F, et al.

*Computational evidence in favor of a two-state, two-mode model of the retinal chromophore photoisomerization*

P NATL ACAD SCI USA 97 (17): 9379-9384 AUG 15 2000

Shishkin OV, Gorb L, Leszczynski J

*Does the hydrated cytosine molecule retain the canonical structure? A DFT study*

J PHYS CHEM B 104 (22): 5357-5361 JUN 8 2000

de Oliveira AE, Haiduke RLA, Bruns RE

*Atomic mean dipole moment derivatives and GAPT charges*

J PHYS CHEM A 104 (22): 5320-5327 JUN 8 2000

Pacios LF, Galvez O, Gomez PC

*Structures and bonding in silane derivatives with one alkali atom*

J PHYS CHEM A 104 (32): 7617-7624 AUG 17 2000

Bogdanov B, McMahon TB

*An ab initio and density functional theory investigation of the structures and energetics of halide ion-alcohol complexes in the gas phase*

J PHYS CHEM A 104 (33): 7871-7880 AUG 24 2000

Wu S, Greer A

*Attractive through-space S-O interaction in the DNA-cleaving antitumor antibiotic leinamycin*

J ORG CHEM 65 (16): 4883-4887 AUG 11 2000

Dias HVR, Polach SA, Goh SK, et al.

*Copper and silver complexes containing organic azide ligands: Syntheses, structures, and theoretical investigation of [HB(3,5-(CF<sub>3</sub>)(2)Pz)(3)]CuNNN(1-Ad) and [HB(3,5-*

*(CF<sub>3</sub>)(2)Pz)(3)]AgN(1-Ad)NN (where Pz = pyrazolyl and 1-Ad=1-adamantyl)*

INORG CHEM 39 (17): 3894-3901 AUG 21 2000

Diaz N, Suarez D, Merz KM

*Hydration of zinc ions: theoretical study of [Zn(H<sub>2</sub>O)(4)](H<sub>2</sub>O)(8)(2+)* and

*[Zn(H<sub>2</sub>O)(6)](H<sub>2</sub>O)(6)(2+)*

CHEM PHYS LETT 326 (3-4): 288-292 AUG 18 2000

Zitto ME, Caputo MC, Ferraro MB, et al.

*Thomas-Reiche-Kuhn populations in X-CH<sub>3</sub> and X-C<sub>2</sub>H<sub>5</sub> series of molecules*

CHEM PHYS 259 (1): 1-9 SEP 1 2000

Tattershall BW, Blachnik R, Hepp A

*Phosphorus NMR and ab initio study of pentaphosphorus dichalcogenide halides*

J CHEM SOC DALTON (15): 2551-2558 2000

Domingo LR

*A density functional theory study of the chemoselectivity and regioselectivity of the domino cycloaddition reactions of nitroalkenes with substituted alkenes*

THEOR CHEM ACC 104 (3-4): 240-246 JUL 2000

Mori S, Nakamura E, Morokuma K

*Mechanism of S(N)2 alkylation reactions of lithium organocuprate clusters with alkyl halides and epoxides. Solvent effects, BF3 effects, and trans-diaxial epoxide opening*  
J AM CHEM SOC 122 (30): 7294-7307 AUG 2 2000

Semenov SG

*Additive overlap populations of atomic orbitals*  
J STRUCT CHEM+ 41 (1): 19-27 JAN-FEB 2000

Bienati M, Bonacic-Koutecky V, Fantucci P

*Theoretical study of the reactivity of bismuth oxide cluster cations with ethene in the presence of molecular oxygen*  
J PHYS CHEM A 104 (30): 6983-6992 AUG 3 2000

Arulmozhiraja S, Fujii T, Tokiwa H

*Electron affinity for the most toxic 2,3,7,8-tetrachlorodibenzo-p-dioxin (TCDD): A density functional theory study*  
J PHYS CHEM A 104 (30): 7068-7072 AUG 3 2000

Cao ZX, Niu SQ, Hall MB

*Theoretical studies of inorganic and organometallic reaction mechanisms. 16. Oxidative promotion of the migratory insertion of carbon monoxide in cyclopentadienylmethyldicarbonyliron (II)*  
J PHYS CHEM A 104 (31): 7324-7332 AUG 10 2000

Misiaszek T, Szostak MM

*Atomic charge distribution in 4-isopropylphenol molecule derived from atomic polar tensors*  
J MOL STRUCT 526: 303-308 AUG 10 2000

McKee ML

*Theoretical study of hydrogen exchange in the reaction of FeC5H6+ with H-2*  
INT J MASS SPECTROM 201 (1-3): 143-149 2000

Impronta R, Scalmani G, Barone V

*Radical cations of DNA bases: some insights on structure and fragmentation patterns by density functional methods*  
INT J MASS SPECTROM 201 (1-3): 321-336 2000

Gade LH

*Highly polar metal - Metal bonds in "early-late" heterodimetallic complexes*  
ANGEW CHEM INT EDIT 39 (15): 2659-2678 2000

Topol IA, Nemukhin AV, Chao M, et al.

*Quantum chemical studies of reactions of the cyclic disulfides with the zinc finger domains in the HIV-1 nucleocapsid protein (NCp7)*

J AM CHEM SOC 122 (29): 7087-7094 JUL 26 2000

Sundermann A, Uzan O, Milstein D, et al.

*Selective C-C vs C-H bond activation by rhodium(I) PCP pincer complexes. A computational study*

J AM CHEM SOC 122 (29): 7095-7104 JUL 26 2000

Marsman AW, Havenith RWA, Bethke S, et al.

*Long-range sigma-pi interactions in Tetrahydro-4H-thiopyran end-capped oligo(cyclohexylidenes). Photo-electron spectroscopy, ab initio SCF MO calculations, and natural bond orbital analyses*

J ORG CHEM 65 (15): 4584-4592 JUL 28 2000

Lammertsma K, Bharatam PV

*Keto reversible arrow enol, imine reversible arrow enamine, and nitro reversible arrow aci-nitro tautomerism and their interrelationship in substituted nitroethylenes. Keto, imine, nitro, and vinyl substituent effects and the importance of H-bonding*

J ORG CHEM 65 (15): 4662-4670 JUL 28 2000

Cundari TR, Deng J, Pop HF, et al.

*Structural analysis of transition metal beta-X substituent interactions. Toward the use of soft computing methods for catalyst modeling*

J CHEM INF COMP SCI 40 (4): 1052-1061 JUL-AUG 2000

Lim CC, Xu ZP, Huang HH, et al.

*The alternative thermal decomposition mode of 2-oxetanone and 2-azetidinone: a DFT and PES study*

CHEM PHYS LETT 325 (4): 433-439 JUL 28 2000

Levy JB

*Quantum chemical study of hydroxy- and formyl-substituted benzenonium ions*

STRUCT CHEM 11 (2-3): 141-144 JUN 2000

Lewars E

*Pyramidane 2. Further computational studies: potential energy surface, basicity and acidity, electron-withdrawing and electron-donating power, ionization energy and electron affinity, heat of formation and strain energy, and NMR chemical shifts*

J MOL STRUC-THEOCHEM 507: 165-184 JUL 24 2000

Tanaka H, Yokoyama K, Kudo H

*Ionization energies of hyperlithiated and electronically segregated isomers of Li-n(OH)(n-1) (n=2-5) clusters*

J CHEM PHYS 113 (5): 1821-1830 AUG 1 2000

Platts JA

*Theoretical prediction of hydrogen bond basicity*  
PHYS CHEM CHEM PHYS 2 (14): 3115-3120 2000

Boronat M, Viruela P, Corma A

*Ab initio and density-functional theory study of zeolite-catalyzed hydrocarbon reactions: hydride transfer, alkylation and disproportionation*  
PHYS CHEM CHEM PHYS 2 (14): 3327-3333 2000

Chen Y, Petz W, Frenking G

*Is it possible to synthesize a low-valent transition metal complex with a neutral carbon atom as terminal ligand? A theoretical study of (CO)(4)FeC*  
ORGANOMETALLICS 19 (14): 2698-2706 JUL 10 2000

Grunenberg J, Goldberg N

*How strong is the gallium equivalent to gallium triple bond? Theoretical compliance matrices as a probe for intrinsic bond strengths*  
J AM CHEM SOC 122 (25): 6045-6047 JUN 28 2000

Vivanco S, Lecea B, Arrieta A, et al.

*Origins of the loss of concertedness in pericyclic reactions: Theoretical prediction and direct observation of stepwise mechanisms in [3+2] thermal cycloadditions*  
J AM CHEM SOC 122 (25): 6078-6092 JUN 28 2000

Thompson WH, Hynes JT

*Frequency shifts in the hydrogen-bonded OH stretch in halide-water clusters. The importance of charge transfer*  
J AM CHEM SOC 122 (26): 6278-6286 JUL 5 2000

Wong MW

*Prediction of a metastable helium compound: HHeF*  
J AM CHEM SOC 122 (26): 6289-6290 JUL 5 2000

Hobza P, Sponer J, Cubero E, et al.

*C-H center dot center dot O contacts in the adenine center dot center dot center dot uracil Watson-Crick and uracil center dot center dot center dot uracil nucleic acid base pairs: Nonempirical ab initio study with inclusion of electron correlation . . .*  
J PHYS CHEM B 104 (26): 6286-6292 JUL 6 2000

Thomson LM, Hall MB

*Theoretical study of the thermal decomposition of N,N'-diacyl-N,N'-dialkoxyhydrazines: A comparison of HF, MP2, and DFT*  
J PHYS CHEM A 104 (26): 6247-6252 JUL 6 2000

Zhang HG, Schelly ZA, Marynick DS

*Theoretical study of the molecular and electronic structures of neutral silver bromide clusters (AgBr)(n), n=1-9*  
J PHYS CHEM A 104 (26): 6287-6294 JUL 6 2000

Harcourt RD, Schulz A

*Valence bond structures for N<sub>2</sub>O and HCNO with apparently pentavalent nitrogen atoms*  
J PHYS CHEM A 104 (27): 6510-6516 JUL 13 2000

Kraka E, Cremer D

*Structure and stability of enediynes containing heteroatoms - a quantum chemical investigation*  
J MOL STRUC-THEOCHEM 506: 191-211 Sp. Iss. SI JUL 14 2000

Roy RK, Hirao K, Pal S

*On non-negativity of Fukui function indices. II*  
J CHEM PHYS 113 (4): 1372-1379 JUL 22 2000

Cossio FP, de la Cruz P, de la Hoz A, et al.

*Determination of syn/anti isomerism in DCNQI derivatives by 2D exchange spectroscopy: Theoretical underpinning*  
EUR J ORG CHEM (13): 2407-2415 JUL 2000

Benisch C, Bethke S, Gleiter R, et al.

*Syntheses and structural properties of cyclic tetrathiadiynes*  
EUR J ORG CHEM (13): 2479-2488 JUL 2000

Joubert L, Silvi B, Picard G

*Topological approach in the structural and bonding characterization of lanthanide trihalide molecules*  
THEOR CHEM ACC 104 (2): 109-115 JUN 2000

Couturier-Tamburelli I, Aycard JP, Wong MW, et al.

*A stable ketene-pyridine prereactive intermediate: Experimental and theoretical identifications of the C<sub>3</sub>O<sub>2</sub> center dot center dot center dot pyridine complex*  
J PHYS CHEM A 104 (16): 3466-3471 APR 27 2000

Alabugin IV

*Stereoelectronic interactions in cyclohexane, 1,3-dioxane, 1,3-oxathiane, and 1,3-dithiane: W-effect, sigma(C-X) (<->) sigma\*(C-H) interactions, anomeric effect - What is really important?*  
J ORG CHEM 65 (13): 3910-3919 JUN 30 2000

Park YS, Kim WK, Kim YB, et al.

*Theoretical studies of hetero-Diels-Alder reactions involving N-sulfinyl dienophiles*  
J ORG CHEM 65 (13): 3997-4002 JUN 30 2000

Anane H, Jarid A, Boutalib A, et al.

*G2(MP2) molecular orbital study of the substituent effect in the H<sub>3</sub>BPH<sub>3-n</sub>F<sub>n</sub> (n=0-3) donor-acceptor complexes*

CHEM PHYS LETT 324 (1-3): 156-160 JUN 30 2000

Jeong M, Kwon Y

*The molecular structure and conformation of tetrabromoformaldazine: ab initio and DFT calculations*

CHEM PHYS LETT 324 (1-3): 183-188 JUN 30 2000

Rousseau B, Peeters A, Van Alsenoy C

*Systematic study of the parameters determining stockholder charges*

CHEM PHYS LETT 324 (1-3): 189-194 JUN 30 2000

Bailly F, Barthen P, Breuer W, et al.

*Pentafluorophenyliodine (III) compounds. 3 - Pentafluorophenyliodinedifluoride: Alternative preparations, molecular structure, and properties*

Z ANORG ALLG CHEM 626 (6): 1406-1413 JUN 2000

Isaeva EV, Nemukhin AV, Monastyrskii OI

*Comparison of structural and dynamic properties of aluminium, chromium, and iron phenylsiloxanes*

VESTN MOSK U KHIM+ 41 (2): 94-97 MAR-APR 2000

Bogdan TV, Granovskii AA, Nemukhin AV

*Structure of hydrogen bonded molecular clusters: Hydrogen fluoride oligomers*

VESTN MOSK U KHIM+ 41 (2): 98-100 MAR-APR 2000

Masamura M

*Error of atomic charges derived from electrostatic potential*

STRUCT CHEM 11 (1): 41-45 FEB 2000

Wang YS, Gaspar PP, Taylor JS

*Quantum chemical study of the electron-transfer-catalyzed splitting of oxetane and azetidine intermediates proposed in the photoenzymatic repair of (6-4) photoproducts of DNA*

J AM CHEM SOC 122 (23): 5510-5519 JUN 14 2000

Atheaux I, Donnadieu B, Rodriguez V, et al.

*A unique coordination of SiH<sub>4</sub>: Isolation, characterization, and theoretical study of (PR<sub>3</sub>)<sub>2</sub>H<sub>2</sub>Ru(SiH<sub>4</sub>)RuH<sub>2</sub>(PR<sub>3</sub>)<sub>2</sub>*

J AM CHEM SOC 122 (23): 5664-5665 JUN 14 2000

Chui KL, Yang QC, Mak TCW, et al.

*Synthesis, structure, and bonding of d(0)/f(n) metallacarboranes incorporating the eta(7)-carboranyl ligand*

J AM CHEM SOC 122 (24): 5758-5764 JUN 21 2000

Liu KT, Chen HI, Lin YS, et al.

*Solvolytic of N,N-diphenylcarbamoyl chloride revisited. Extended positive charge delocalization on phenyl rings in the transition state and possible contribution of non-canonical resonance structure*

J PHYS ORG CHEM 13 (6): 322-329 JUN 2000

Taurian OE, Contreras RH

*Interactions that define the alkylamine side-chain conformation in phenylalkylamine hallucinogens: an ab initio study*

J MOL STRUC-THEOCHEM 504: 119-126 JUN 12 2000

Hatch FT, Lightstone FC, Colvin ME

*Quantitative structure-activity relationship of flavonoids for inhibition of heterocyclic amine mutagenicity*

ENVIRON MOL MUTAGEN 35 (4): 279-299 2000

Li XH, Zhang BW, Cao Y

*Aggregation of bis(2,4,6-trihydroxyphenyl) squaraine in different solutions*

DYES PIGMENTS 45 (3): 209-217 JUN 2000

Kendall RA, Apra E, Bernholdt DE, et al.

*High performance computational chemistry: An overview of NWChem a distributed parallel application*

COMPUT PHYS COMMUN 128 (1-2): 260-283 JUN 2000

Tomoda S, Zhang J, Kaneno D, et al.

*Reversal of pi-facial diastereoselection in the hydride reduction of selenanones. Further application of the exterior frontier orbital extension model*

TETRAHEDRON LETT 41 (23): 4597-4601 JUN 12 2000

Hermann H, Lohrenz JCW, Kuhn A, et al.

*The influence of the leaving group X (X=F, Cl, Br, I, OH) on the carbenoid nature of the carbenoids LiCH<sub>2</sub>X and XZnCH<sub>2</sub>X - A theoretical study*

TETRAHEDRON 56 (25): 4109-4115 JUN 16 2000

Della EW, Lochert IJ, Peralta JE, et al.

*A DFT/GIAO/NBO and experimental study of C-13 SCSs in 1-X-bicyclo[1.1.1]pentanes*

MAGN RESON CHEM 38 (6): 395-402 JUN 2000

Ishii A, Mikami K

*Catalytic asymmetric synthesis of organofluorine compounds using fluoral*

J SYN ORG CHEM JPN 58 (4): 324-333 APR 2000

Kingsbury CA, Lee KH

*IR and computational studies of alkyl chloride conformations*

J PHYS ORG CHEM 13 (5): 244-252 MAY 2000

Cossio FP, Arrieta A, Lecea B, et al.

*Highly efficient induction of chirality in intramolecular [2+2] cycloadditions between ketenimines and imines*

J ORG CHEM 65 (12): 3633-3643 JUN 16 2000

Palmer MH

*On the charge distribution in ethanes and disilanes and correlations with equilibrium bond lengths; an ab initio study*

J MOL STRUC-THEOCHEM 500: 225-243 APR 3 2000

Buschel M, Stadler C, Lambert C, et al.

*Heterocyclic quinones as core units for redox switches: UV-vis/NIR, FTIR spectroelectrochemistry and DFT calculations on the vibrational and electronic structure of the radical anions*

J ELECTROANAL CHEM 484 (1): 24-32 APR 7 2000

Kim KS, Oh KS, Lee JY

*Catalytic role of enzymes: Short strong H-bond-induced partial proton shuttles and charge redistributions*

P NATL ACAD SCI USA 97 (12): 6373-6378 JUN 6 2000

Saarenketo P, Suontamo R, Jodicke T, et al.

*Ab initio MO study of silver ion complexation in [2.2.2]cyclophane pi-prisms*

ORGANOMETALLICS 19 (12): 2346-2353 JUN 12 2000

Fuster F, Silvi B

*Does the topological approach characterize the hydrogen bond?*

THEOR CHEM ACC 104 (1): 13-21 MAY 2000

Wang YG, Sun CJ, Bian WS, et al.

*Ab initio studies on MCH<sub>2</sub>(OH) and CH<sub>3</sub>OM(M=H, -, Li, Na)*

CHEM RES CHINESE U 16 (2): 136-140 MAY 2000

Rodriguez D, Navarro A, Castedo L, et al.

*Intramolecular [4+2] cycloaddition reactions of diarylacetylenes: Synthesis of benzo[b]fluorene derivatives via cyclic allenes*

ORG LETT 2 (11): 1497-1500 JUN 1 2000

Fokin AA, Kushko AO, Kirij AV, et al.

*Direct transformations of ketones to gamma-unsaturated thiols via [2,3]-sigmatropic rearrangement of allyl sulfinyl carbanions: A combined experimental and computational study*

J ORG CHEM 65 (10): 2984-2995 MAY 19 2000

Di Valentin C, Gisdakis P, Yudanov IV, et al.

*Olefin epoxidation by peroxy complexes of Cr, Mo, and W. A comparative density functional study*  
J ORG CHEM 65 (10): 2996-3004 MAY 19 2000

Serrar C, Es-sofi A, Boutalib A, et al.

*Synthesis, structural characterization, and theoretical calculations of a new copper(I)-octahydrotriborate complex*

INORG CHEM 39 (10): 2224--+ MAY 15 2000

Kar T, Sannigrahi AB

*Local reactivity indices of free radicals: Ab initio Hartree-Fock and Kohn-Sham density functional calculations*

INDIAN J CHEM A 39 (1-3): 68-74 JAN-MAR 2000

Kumar A, Mishra PC

*An ab initio study of molecular charge distribution and electrostatic potentials: Role of hybridization displacement charge*

INDIAN J CHEM A 39 (1-3): 180-188 JAN-MAR 2000

Mitzel NW, Losehand U, Wu A, et al.

*(N,N-dimethylaminoxy)trifluorosilane: Strong, dipole moment driven changes in the molecular geometry studied by experiment and theory in solid, gas, and solution phases*

J AM CHEM SOC 122 (18): 4471-4482 MAY 10 2000

Sundermann A, Schoeller WW

*Phosphorane-iminato complexes of transition metals with heterocubane structure: A computational study*

J AM CHEM SOC 122 (19): 4729-4734 MAY 17 2000

Pejov L, Ristova M, Zdravkovski Z, et al.

*Ab initio quantum chemical and experimental study of structure, harmonic vibrational frequencies and internal Ph-SO<sub>3</sub> torsion of benzenesulfonate anion*

J MOL STRUCT 524: 179-188 JUN 13 2000

Wang FH, Wang X, Jin FQ, et al.

*Theoretical studies on the structure and spectral properties of cycloocta-1,5-diene-3,7-diyne*  
ACTA CHIM SINICA 58 (3): 347-350 2000

Frash MV, Hopkinson AC, Bohme DK

*A quantum-chemical study of the geometries and electronic structures of ArO and [Ar,O,H](+): proton affinities of singlet and triplet ArO*

PHYS CHEM CHEM PHYS 2 (10): 2271-2274 2000

Kim CK, Li HG, Lee HW, et al.

*Ab initio study of the X-+RCOY displacement reactions with R = H, CH<sub>3</sub> and X, Y = Cl, Br*

J PHYS CHEM A 104 (17): 4069-4076 MAY 4 2000

Ma NL, Wong MW

*A theoretical study of the properties and reactivities of ketene, thioketene, and selenoketene*  
EUR J ORG CHEM (8): 1411-1421 APR 2000

Lee MS, Head-Gordon M

*Absolute and relative energies from polarized atomic orbital self-consistent field calculations and a second order correction. Convergence with size and composition of the secondary basis*  
COMPUT CHEM 24 (3-4): 295-301 MAY 2000

Fokin AA, Kiran B, Bremer M, et al.

*Which electron count rules are needed for four-center three-dimensional aromaticity?*  
CHEM-EUR J 6 (9): 1615-1628 MAY 2 2000

Garcia-Yebra C, Lopez-Mardomingo C, Fajardos M, et al.

*Facile synthesis of alkynyl- and vinylidene-niobocene complexes. Unexpected eta(1)-vinylidene-eta(2)-alkyne isomerization*  
ORGANOMETALLICS 19 (9): 1749-1765 MAY 1 2000

Musashi Y, Sakaki S

*Theoretical study of ruthenium-catalyzed hydrogenation of carbon dioxide into formic acid. Reaction mechanism involving a new type of sigma-bond metathesis*  
J AM CHEM SOC 122 (16): 3867-3877 APR 26 2000

Huelskopf M, Ludwig R

*Temperature dependence of hydrogen bonding in alcohols*  
J MOL LIQ 85 (1-2): 105-125 Sp. Iss. SI APR 2000

Rocha WR, De Almeida WB

*Carbonyl insertion reaction into the Pt-C bond in heterobimetallic Pt(SnCl<sub>3</sub>)(PH<sub>3</sub>)<sub>2</sub>(CO)(CH<sub>3</sub>) compound: Theoretical study*  
J COMPUT CHEM 21 (8): 668-674 JUN 2000

Li M, Xie RG, Hu CW, et al.

*Quantum chemical study on enantioselective reduction of aromatic ketones catalyzed by chiral cyclic sulfur-containing oxazaborolidines. Part 1. Structures and properties of catalysts*  
INT J QUANTUM CHEM 78 (4): 245-251 JUN 15 2000

Li M, Xie RG, Tian SH, et al.

*Quantum chemical study on enantioselective reduction of aromatic ketones catalyzed by chiral cyclic sulfur-containing oxazaborolidines. Part 2. Structures of catalyst-borane-ketone adducts*  
INT J QUANTUM CHEM 78 (4): 252-260 JUN 15 2000

Li M, Xie RG, Hu XR, et al.

*Quantum chemical study on enantioselective reduction of aromatic ketones catalyzed by chiral cyclic sulfur-containing oxazaborolidines. Part 3. Structures of catalyst-alkoxyborane adducts*  
INT J QUANTUM CHEM 78 (4): 261-268 JUN 15 2000

Tomoda S, Kaneno D, Senju T

*Origin of pi-facial diastereoselection in carbonyl addition. Application of the exterior frontier orbital extension model to 1,3-diheteran-5-ones (heteroatom = O, S)*  
HETEROCYCLES 52 (3): 1435-- MAR 1 2000

Aumann R, Kossmeier M, Muck-Lichtenfeld C, et al.

*Organic syntheses via transition metal complexes, CI - Uncovering reaction pathways of 1-aminocyclohexenes with [(1-alkynyl)carbene]tungsten complexes leading to cyclopentadienes and dihydropyrroles*  
EUR J ORG CHEM (1): 37-49 JAN 2000

Esser M, Neumuller B, Petz W, et al.

*Preparation, structure, and quantum chemical calculation of [C(NMe<sub>2</sub>)(3)](2)[(CO)(4)FeInCl<sub>3</sub>]*  
Z ANORG ALLG CHEM 626 (4): 915-920 APR 2000

Solans-Monfort X, Branchadell V, Sodupe M

*Theoretical study of the structure of ZCu(NO<sub>2</sub>)(NO). A proposed intermediate in the NO<sub>x</sub> decomposition by Cu-ZSM-5*  
J PHYS CHEM A 104 (14): 3225-3230 APR 13 2000

Pophristic V, Goodman L

*Influence of protonation on internal rotation of dimethyl ether*  
J PHYS CHEM A 104 (14): 3231-3238 APR 13 2000

Crawford MJ, Harcourt RD, Klapotke TM

*Nitrosodifluoroamine, F<sub>2</sub>N<sub>2</sub>O*  
J PHYS CHEM A 104 (15): 3406-3409 APR 20 2000

Villa A, Cosentino U, Pitea D, et al.

*Force field parametrization for gadolinium complexes-based on ab initio potential energy surface calculations*  
J PHYS CHEM A 104 (15): 3421-3429 APR 20 2000

Omoto K, Fujimoto H

*Theoretical study of activation of oxirane by bidentate acids*  
J ORG CHEM 65 (8): 2464-2471 APR 21 2000

Li JS, Xiao HM, Dong HS

*Theoretical study on intermolecular interaction of epoxyethane dimer*  
INT J QUANTUM CHEM 78 (2): 94-98 MAY 20 2000

Baldridge KK, Uzan O, Martin JML

*The silabenzenes: Structure, properties, and aromaticity*

ORGANOMETALLICS 19 (8): 1477-1487 APR 17 2000

Fu ZW, Zhang LN, Qin QZ, et al.

*An experimental and ab initio study of hypervalent LiOZn*

J PHYS CHEM A 104 (13): 2980-2984 APR 6 2000

Mo YR, Gao JL

*An ab initio molecular orbital-valence bond (MOVB) method for simulating chemical reactions in solution*

J PHYS CHEM A 104 (13): 3012-3020 APR 6 2000

Chiu SW, Lau KC, Li WK

*Structures, energetics, and reactions of [C<sub>2</sub>H<sub>3</sub>S] radicals and [C<sub>2</sub>H<sub>3</sub>S](+) ions: A Gaussian-2 ab initio study*

J PHYS CHEM A 104 (13): 3028-3037 APR 6 2000

Franchetti P, Marchetti S, Cappellacci L, et al.

*Synthesis, conformational analysis, and biological activity of C-thioribonucleosides related to tiazofurin*

J MED CHEM 43 (7): 1264-1270 APR 6 2000

Freeman F, Tsegai ZM, Kasner ML, et al.

*A comparison of the ab initio calculated and experimental conformational energies of alkylcyclohexanes*

J CHEM EDUC 77 (5): 661-667 MAY 2000

Jackson P, Srinivas R, Blanksby SJ, et al.

*A mass spectrometry study of XCO+, X = Si, Ge: Is SiCO+ a main group carbonyl? Comments on the bonding in ground state SiCO and the [Si,C,O](+) potential energy surface*

CHEM-EUR J 6 (7): 1236-1242 APR 3 2000

Zanchini C

*Silylcyanides and silylisocyanides: a comparative theoretical study*

CHEM PHYS 254 (2-3): 187-202 APR 1 2000

Sushko PV, Shluger AL, Catlow CRA

*Relative energies of surface and defect states: ab initio calculations for the MgO(001) surface*

SURF SCI 450 (3): 153-170 APR 10 2000

Sproviero EM, Burton G

*Stereoelectronic contributions to H-1-H-1 coupling constants*

MOLECULES 5 (3): 539-540 MAR 2000

Meyer F, Hyla-Kryspin I, Kaifer E, et al.

*Cooperative binding of nitrile moieties within a bimetallic pocket: Enforcing side-on pi-interaction with a high-spin nickel(II) site*

EUR J INORG CHEM (4): 771-781 APR 2000

Hernandez MG, Beste A, Frenking G, et al.

*Charge decomposition analysis of the chemisorption bond*

CHEM PHYS LETT 320 (3-4): 222-228 APR 7 2000

Braden DA, Tyler DR

*Density functional studies on 19-electron metal sandwich complexes: Electronic structures of CpFe(eta(6)-C<sub>6</sub>H<sub>6</sub>), CpFe(eta(6)-C<sub>6</sub>Me<sub>6</sub>), and (C<sub>5</sub>Me<sub>5</sub>)Fe(eta(6)-C<sub>6</sub>H<sub>6</sub>)*

ORGANOMETALLICS 19 (6): 1175-1181 MAR 20 2000

Olah GA, Rasul G, Hachoumy M, et al.

*Diprotonated hydrogen halides (H<sub>3</sub>X<sub>2</sub><sup>+</sup>) and gitonic protio methyl and dimethylhalonium dications (CH<sub>3</sub>XH<sub>2</sub><sup>+</sup> and (CH<sub>3</sub>)<sub>2</sub>XH<sub>2</sub><sup>+</sup>): Theoretical and hydrogen-deuterium exchange studies*

J AM CHEM SOC 122 (12): 2737-2741 MAR 29 2000

Weiser PS, Wild DA, Wolyne PP, et al.

*Infrared and ab initio study of the chloride-ammonia anion complex*

J PHYS CHEM A 104 (12): 2562-2566 MAR 30 2000

Kim CK, Hyun KH, Kim CK, et al.

*Nucleophilic substitution at unactivated vinylic carbon. Factors conducive to the energetic preference for the in-plane S(N)2 pathway*

J AM CHEM SOC 122 (10): 2294-2299 MAR 15 2000

Yamasaki T, Mainz DT, Goddard WA

*Correlation analysis of chemical bonds (CACB) II: Quantum mechanical operators for classical chemical concepts*

J PHYS CHEM A 104 (11): 2221-2229 MAR 23 2000

Frash MV, van Santen RA

*Activation of small alkanes in Ga-exchanged zeolites: A quantum chemical study of ethane dehydrogenation*

J PHYS CHEM A 104 (11): 2468-2475 MAR 23 2000

Glasovac Z, Eckert-Maksic M, Broadus KM, et al.

*Benzocyclobutene: The impact of fusing a strained ring onto benzene*

J ORG CHEM 65 (6): 1818-1824 MAR 24 2000

Diez RP, Jubert AH

*A conformational study of 3,3,6,6-tetramethyl-1,2,4,5-tetroxane using molecular dynamics and*

*density functional theory*

J MOL STRUC-THEOCHEM 499: 85-89 MAR 17 2000

Klapotke TM

*Ab initio calculations of the open-chain N-6 diazide molecule*

J MOL STRUC-THEOCHEM 499: 99-104 MAR 17 2000

Wang SP, Chang TC

*The split of the electron pairs and the UV photoelectron spectra of open-shell species*

J MOL STRUC-THEOCHEM 499: 127-135 MAR 17 2000

Borosky GL, Nishimoto S, Pierini AB

*Radical anions from 5-fluorouracil derivatives. A theoretical study of their cleavage and orbital isomerism*

J MOL STRUC-THEOCHEM 499: 151-160 MAR 17 2000

Carballeira L, Perez-Juste I

*An ab initio interpretation in gas phase and aqueous solution of the generalized anomeric effect in R-O-CR<sub>2</sub>-NR<sub>2</sub> (R = H, CH<sub>3</sub>)*

J COMPUT CHEM 21 (6): 462-477 APR 30 2000

Bachler V, Schaffner K

*The photochemistry of 1,3-butadiene rationalized by means of theoretical resonance structures and their weights*

CHEM-EUR J 6 (6): 959-970 MAR 17 2000

Mikami K

*Catalytic asymmetric synthesis of diastereomeric alpha- or beta-CF<sub>3</sub> liquid crystalline molecules - Conformational probe for anti-ferroelectricity and self-assembly for spontaneous chiral resolution of the racemates*

ACS SYM SER 746: 255-269 2000

Niyomura O, Kato S, Inagaki S

*An unusual planar diacyl ditelluride (2-MeOC<sub>6</sub>H<sub>4</sub>COTe)(2): The origin of its planarity*

J AM CHEM SOC 122 (9): 2132-2133 MAR 8 2000

Papai I, Jancso G

*Hydrogen bonding in methyl-substituted pyridine-water complexes: A theoretical study*

J PHYS CHEM A 104 (10): 2132-2137 MAR 16 2000

Muck-Lichtenfeld C

*Theoretical prediction of the stability and intramolecular rearrangement reactions of heteroanalogues of cyclopropylcarbene: 2-oxiranyl-, 2-aziridinyl-, and 1-aziridinylcarbene*

J ORG CHEM 65 (5): 1366-1375 MAR 10 2000

Rozhenko AB, Schoeller WW, Povolotskii MI

*Conjugation in phosphabutadienes: ab initio investigation and NMR spectral manifestation*

J MOL STRUC-THEOCHEM 498: 1-20 FEB 28 2000

Benassi R, Bertarini C, Kleinpeter E, et al.

*Exocyclic push-pull conjugated compounds. Part 1. Theoretical study of the effect of ring size on the structure, electronic properties and rotational barriers of cyclic analogues of 1,1-diamino-2,2-dicyanoethylene*

J MOL STRUC-THEOCHEM 498: 201-215 FEB 28 2000

Benassi R, Bertarini C, Kleinpeter E, et al.

*Exocyclic push-pull conjugated compounds. Part 2. The effect of donor and acceptor substituents on the rotational barrier of push-pull ethylenes*

J MOL STRUC-THEOCHEM 498: 217-225 FEB 28 2000

Mo YR, Gao JL, Peyerimhoff SD

*Energy decomposition analysis of intermolecular interactions using a block-localized wave function approach*

J CHEM PHYS 112 (13): 5530-5538 APR 1 2000

Kovacs A

*Theoretical study of rare earth trihalide dimers Ln(2)X(6) (Ln = La, Dy; X = F, Cl, Br, I)*

CHEM PHYS LETT 319 (3-4): 238-246 MAR 17 2000

Mo YR, Lin MH, Wu W, et al.

*The block-localized wavefunction method and its application*

ACTA CHIM SINICA 58 (2): 218-221 2000

Maranzana A, Ghigo G, Tonachini G

*Diradical and peroxirane pathways in the [pi 2+pi 2] cycloaddition reactions of (1)Delta(g) dioxygen with ethene, methyl vinyl ether, and butadiene: A density functional and multireference perturbation theory study*

J AM CHEM SOC 122 (7): 1414-1423 FEB 23 2000

Srinivas GN, Hamilton TP, Jemmis ED, et al.

*Will an eta(3)-Si3H3 ligand form sandwich compounds with main group elements?*

J AM CHEM SOC 122 (8): 1725-1728 MAR 1 2000

Nakamura E, Yamanaka M, Mori S

*Complexation of Lewis acid with trialkylcopper(III): On the origin of BF3-acceleration of cuprate conjugate addition*

J AM CHEM SOC 122 (8): 1826-1827 MAR 1 2000

da Silva MAVR, Matos MAR, Rio CA, et al.

*A thermochemical and theoretical study of the phenylpyridine isomers*

J PHYS CHEM A 104 (8): 1774-1778 MAR 2 2000

Domingo LR, Asensio A

*A DFT study of the domino inter [4+2]/intra [3+2] cycloaddition reactions of nitroalkenes with enol ethers*

J ORG CHEM 65 (4): 1076-1083 FEB 25 2000

Brauer M, Weston J, Anders E

*Fixation of heterocumulenes. 1. A theoretical study on the irreversible reaction of CO<sub>2</sub> with a 2-lithio-1,3-dithiane*

J ORG CHEM 65 (4): 1193-1199 FEB 25 2000

Miqueu K, Sotiropoulos JM, Pfister-Guillouzo G, et al.

*Application of photoelectron spectroscopy to molecular properties, 55 - Low-coordinate arsenic chemistry: Studies of amino(iminoarsanes) using UV photoelectron spectroscopy and density functional theory*

EUR J INORG CHEM (3): 477-483 MAR 2000

Uddin J, Boehme C, Frenking G

*Nature of the chemical bond between a transition metal and a group-13 element: Structure and bonding of transition metal complexes with terminal group-13 diyl ligands ER (E = B to Tl; R = Cp, N(SiH<sub>3</sub>)<sub>2</sub>, Ph, Me)*

ORGANOMETALLICS 19 (4): 571-582 FEB 21 2000

Niu X, Gopal L, Masingale MP, et al.

*Experimental and theoretical investigation of Z-E alkene isomerization in [(Cy<sub>3</sub>P)<sub>2</sub>Cl<sub>2</sub>Ru](2)(μ-CHCH=CHCH) and related vinylalkylidenes*

ORGANOMETALLICS 19 (4): 649-660 FEB 21 2000

Aubauer C, Klapotke TM, Schulz A

*An experimental and theoretical study on the novel tetraphosphorus triselenide boron triiodide (P<sub>4</sub>Se<sub>3</sub>)center dot(BI<sub>3</sub>) adduct*

J MOL MODEL 6 (2): 76-85 2000

Glaser R, Lewis M, Wu ZY

*Stereochemistry and stereoelectronics of azines. 13. Conformational effects on the quadrupolarity of azines. An ab initio quantum-mechanical study of a lateral synthon*

J MOL MODEL 6 (2): 86-98 2000

Hofmann M, Scheschkewitz D, Ghaffari A, et al.

*Two-electron aromatics with classical and non-classical homobridges*

J MOL MODEL 6 (2): 257-271 2000

Stefan T, Janoschek R

*How relevant are S=O and P=O double bonds for the description of the acid molecules H<sub>2</sub>SO<sub>3</sub>,*

*H<sub>2</sub>SO<sub>4</sub>, and H<sub>3</sub>PO<sub>4</sub>, respectively?*  
J MOL MODEL 6 (2): 282-288 2000

Castillo R, Moliner V, Andres J

*A theoretical study on the molecular mechanism for the normal Reimer-Tiemann reaction*  
CHEM PHYS LETT 318 (1-3): 270-275 FEB 18 2000

Platts JA

*Theoretical prediction of hydrogen bond donor capacity*  
PHYS CHEM CHEM PHYS 2 (5): 973-980 2000

Frash MV, van Santen RA

*Activation of ethane in Zn-exchanged zeolites: a theoretical study*  
PHYS CHEM CHEM PHYS 2 (5): 1085-1089 2000

Dobado JA, Martinez-Garcia H, Molina JM, et al.

*Chemical bonding in hypervalent molecules revised. 3. Application of the atoms in molecules theory to Y<sub>3</sub>X-CH<sub>2</sub> (X = N, P, or As ; Y = H or F) and H<sub>2</sub>X-GH(2) (X = O, S, or Se) ylides*  
J AM CHEM SOC 122 (6): 1144-1149 FEB 16 2000

Minkin VI, Dorogan IV, Minyaev RM

*Computational modeling of the mechanisms and stereochemistry of circumambulatory rearrangements of formyl-cyclopropene and 4-hydroxycyclobut enyl cation*  
J PHYS ORG CHEM 13 (1): 3-12 JAN 2000

Citra A, Andrews L

*Reactions of laser-ablated osmium and ruthenium atoms with nitrogen. Matrix infrared spectra and density functional calculations of osmium and ruthenium nitrides and dinitrides*  
J PHYS CHEM A 104 (6): 1152-1161 FEB 17 2000

Rodriguez-Santiago L, Sodupe M, Oliva A, et al.

*Intramolecular proton transfer in glycine radical cation*  
J PHYS CHEM A 104 (6): 1256-1261 FEB 17 2000

Saunders WH

*Effects of the leaving group and of ion pairing on the stereochemistry of E2 reactions. An ab initio study*  
J ORG CHEM 65 (3): 681-684 FEB 11 2000

Glaser R, Nichols GR

*Conformational preferences and pathways for enantiomerization and diastereomerization of benzyl alcohol. Data mining and ab initio quantum-mechanical study*  
J ORG CHEM 65 (3): 755-766 FEB 11 2000

Lee MS, Maslen PE, Head-Gordon M

*Closely approximating second-order Moller-Plesset perturbation theory with a local triatomics in molecules model*

J CHEM PHYS 112 (8): 3592-3601 FEB 22 2000

Buhl M

*NMR properties of polylithiated C-60*

Z ANORG ALLG CHEM 626 (2): 332-337 FEB 2000

Breidung J, Thiel W

*Equilibrium structure and fundamental vibrational wavenumbers in difluorosilanone: An ab initio study*

Z ANORG ALLG CHEM 626 (2): 362-367 FEB 2000

Sandig N, Dargel TK, Koch W

*Quantum chemical investigation of the initial steps of the yttrium-mediated polymerization of ethene and propene*

Z ANORG ALLG CHEM 626 (2): 392-399 FEB 2000

Zimmerman HE, Alabugin IV

*Excited state energy distribution and redistribution and chemical reactivity; Mechanistic and exploratory organic photochemistry*

J AM CHEM SOC 122 (5): 952-953 FEB 9 2000

Muller-Dethlefs K, Hobza P

*Noncovalent interactions: A challenge for experiment and theory*

CHEM REV 100 (1): 143-167 JAN 2000

Levin MD, Kaszynski P, Michl J

*Bicyclo[1.1.1]pentanes, [n]staffanes, [1.1.1]propellanes, and tricyclo[2.1.0.0(2,5)]pentanes*

CHEM REV 100 (1): 169-234 JAN 2000

Frenking G, Frohlich N

*The nature of the bonding in transition-metal compounds*

CHEM REV 100 (2): 717-774 FEB 2000

Ohshima K, Misaizu F, Ohno K

*Anionic oligomerization of acrylonitrile molecules initiated by intracluster electron transfer from alkali metal atoms: Photoionization mass spectrometry of M(CH<sub>2</sub>=CHCN)(n) (M = Li, Na, and K)*

J PHYS CHEM A 104 (4): 765-770 FEB 3 2000

Sannigrahi AB, Kar T

*Ab initio theoretical study of three-centre bonding on the basis of bond index*

J MOL STRUC-THEOCHEM 496: 1-17 JAN 7 2000

Freeman F, Kasner JA, Kasner ML, et al.

*An ab initio molecular orbital study of the conformational energies of 2-alkyltetrahydro-2H-pyrans (tetrahydropyrans, oxacyclohexanes, oxanes)*  
J MOL STRUC-THEOCHEM 496: 19-39 JAN 7 2000

Chung G, Kwon Y

*Molecular structures of gauche and trans conformers for oxalyl chloride: ab initio and DFT calculations*  
J MOL STRUC-THEOCHEM 496: 199-206 JAN 7 2000

Kwon Y

*Theoretical studies on o-aminofuranaldehyde and o-aminofuranthioaldehyde in reaction field: C-C rotational barriers and intramolecular hydrogen bonding*  
J MOL STRUC-THEOCHEM 496: 217-226 JAN 7 2000

Van der Vaart A, Merz KM

*Charge transfer in biologically important molecules: Comparison of high-level ab initio and semiempirical methods*  
INT J QUANTUM CHEM 77 (1): 27-43 MAR 5 2000

Bagno A, Bonchio M

*Effective core potential DFT calculations of nuclear shielding as a tool for the prediction and assignment of the tungsten chemical shift in mono- and polynuclear complexes*  
CHEM PHYS LETT 317 (1-2): 123-128 JAN 28 2000

Xie YM, Schaefer HF, Robinson GH

*The gallium-gallium triple bond in a realistic model. A density functional theory study of Na-2[(C<sub>6</sub>H<sub>5</sub>)<sub>2</sub>C<sub>6</sub>H<sub>3</sub>GaGaC<sub>6</sub>H<sub>3</sub>(C<sub>6</sub>H<sub>5</sub>)<sub>2</sub>]*  
CHEM PHYS LETT 317 (1-2): 174-180 JAN 28 2000

Bharatam PV, Uppal P, Kaur A, et al.

*Theoretical investigation on the conformational preferences of sulfinimines*  
J CHEM SOC PERK T 2 (1): 43-50 JAN 2000

Laali KK, Hollenstein S, Galembeck SE, et al.

*Stable ion study of protonated cyclopenta[a]phenanthrenes. Structure-reactivity relationships and charge delocalization in the carbocations*  
J CHEM SOC PERK T 2 (2): 211-220 2000

Crnugelj M, Dukhan D, Barascut JL, et al.

*How S-C-N anomeric effects and energetic preference across [S-C-C-O] fragments steer conformational equilibria in 4'-thionucleosides. H-1 NMR and ab initio MO study*  
J CHEM SOC PERK T 2 (2): 255-262 2000

Arnaud R, Adamo C, Cossi M, et al.

*Theoretical study of the addition of hydrogen cyanide to methanimine in the gas phase and in*

*aqueous solution*

J AM CHEM SOC 122 (2): 324-330 JAN 19 2000

Hernandez V, Losada SC, Casado J, et al.

*Combined theoretical and vibrational study of dihexylbithienoquinonoid derivatives with regioregular head-to-head, head-to-tail, and tail-to-tail orientations*

J PHYS CHEM A 104 (3): 661-672 JAN 27 2000

Czerw M, Goldman AS, Krogh-Jespersen K

*Addition of ammonia to AlH<sub>3</sub> and BH<sub>3</sub>. Why does only aluminum form 2 : 1 adducts?*

INORG CHEM 39 (2): 363-369 JAN 24 2000

Schoeller WW

*On the electronic properties of substituted phosphanylcarbenes*

EUR J INORG CHEM (2): 369-374 FEB 2000

Tsunoyama H, Ohshima K, Yamakita Y, et al.

*Photoionization and density functional theory study of clusters of acetone containing an alkali metal atom, M((CH<sub>3</sub>)<sub>2</sub>CO)(n) (M = Li, Na): intracluster electron transfer from metal to acetone in 1 : 1 complexes*

CHEM PHYS LETT 316 (5-6): 442-448 JAN 21 2000

Irigoras A, Elizalde O, Silanes I, et al.

*Reactivity of Co+(F-3,F-5), Ni+(D-2,F-4), and Cu+(S-1,D-3): Reaction of Co+, Ni+, and Cu+ with water*

J AM CHEM SOC 122 (1): 114-122 JAN 12 2000

Fabian WMF, Kappe CO, Bakulev VA

*Ab initio and density functional calculations on the pericyclic vs pseudopericyclic mode of conjugated nitrile ylide 1,5-electrocyclizations*

J ORG CHEM 65 (1): 47-53 JAN 14 2000

Pratt LM, Streitwieser A

*Ab initio analysis of pentadienyllithium, pentadienylsodium, and the pentadienyl ions*

J ORG CHEM 65 (2): 290-294 JAN 28 2000

Nelson PG

*Quantifying molecular character*

J CHEM EDUC 77 (2): 245-248 FEB 2000

Petrie S

*Do branched structures exist for cyanide-containing magnesium compounds? Computational studies on a range of mixed-ligand compounds XMg(CN) (X = F, Cl, OH, SH, NH<sub>2</sub>, CH<sub>3</sub>, CN)*

INT J QUANTUM CHEM 76 (5): 626-642 FEB 15 2000

- Milburn RK, Bohme DK, Hopkinson AC  
*Small-ring carbenes carrying a positive charge: the effects of substituting by CN in c-C<sub>4</sub>H<sub>3</sub>+*  
INT J MASS SPECTROM 196: 393-399 Sp. Iss. SI JAN 21 2000
- Nakayama N, Takahashi O, Kikuchi O, et al.  
*Ab initio molecular orbital study of dications of 1,5-dichalcogenacyclooctanes*  
HETEROATOM CHEM 11 (1): 31-41 2000
- Korchowiec J, Uchimaru T  
*New energy partitioning scheme based on the self-consistent charge and configuration method for subsystems: Application to water dimer system*  
J CHEM PHYS 112 (4): 1623-1633 JAN 22 2000
- Tarakeshwar P, Kim KS, Brutschy B  
*Interaction of the water dimer with pi-systems: A theoretical investigation of structures, energies, and vibrational frequencies*  
J CHEM PHYS 112 (4): 1769-1781 JAN 22 2000
- Fathalla W, Cajan M, Pazdera P  
*Regioselectivity of electrophilic attack on 4-methyl-1-thioxo-1,2,4,5-tetrahydro[1,2,4]triazolo[4,3-a]quinazolin-5-one - Part 2: Reactions on nitrogen atom*  
MOLECULES 5 (12): 1210-1223 DEC 2000
- Yu ZH, Peng XQ, Xuan ZQ  
*The controversy over the nature of aromaticity and conjugation*  
CHINESE J ORG CHEM 20 (6): 882-888 DEC 2000
- Moudgil R, Kaur D, Vashisht R, et al.  
*Theoretical studies on the conformations of selenamides*  
P INDIAN AS-CHEM SCI 112 (6): 623-629 DEC 2000
- Meda L, Nicastro C, Conte F, et al.  
*Experimental valuation of net atomic charge via XPS*  
SURF INTERFACE ANAL 29 (12): 851-855 DEC 2000
- Diedenhofen M, Jonas V, Frenking G  
*Tetracyclo[3.1.0.0(1.3).0(3.5)]hexane: a new C<sub>6</sub>H<sub>6</sub> isomer with an unusual bonding situation*  
J MOL STRUCT 556 (1-3): 23-32 Sp. Iss. SI DEC 12 2000
- Glaser R, Wu Z, Lewis M  
*A higher level ab initio quantum-mechanical study of the quadrupole moment tensor components of carbon dioxide*  
J MOL STRUCT 556 (1-3): 131-141 Sp. Iss. SI DEC 12 2000
- Contreras RH, Taurian OE, Ortiz FS, et al.

*The polar bond-polarizable bond interaction in 1-X,2-methoxy naphthalenes. An experimental and theoretical study*

J MOL STRUCT 556 (1-3): 263-273 Sp. Iss. SI DEC 12 2000

Sohn CK, Chun YI, Rhee SK, et al.

*Transmission of substituent effects through five-membered heteroaromatic rings. III. Addition equilibria of hydroxide anion to benzaldehyde analogues*

B KOR CHEM SOC 21 (12): 1202-1206 DEC 20 2000

Buhl M, Hakansson M, Mahmoudkhani AH, et al.

*X-ray structures and DFT calculations on rhodium-olefin complexes: Comments on the Rh-103 NMR shift-stability correlation*

ORGANOMETALLICS 19 (26): 5589-5596 DEC 25 2000

Qu ZW, Li ZS, Ding YH, et al.

*Theoretical study of the gas-phase reaction of diborane(3) anion B2H3- with CO2*

J PHYS CHEM A 104 (51): 11952-11960 DEC 28 2000

Pejov L, Ristova M, Soptrajanov B

*A gradient-corrected density functional study of structure, harmonic vibrational frequencies and charge distribution of benzenesulfonate anion on the ground-state potential energy surface*

J MOL STRUCT 555: 341-349 NOV 28 2000

Eshdat L, Ayalon A, Beust R, et al.

*Up to six units of charge and twist-boat benzene moieties: Alkali metal reduction of phenyl-perisubstituted benzenes*

J AM CHEM SOC 122 (51): 12637-12645 DEC 27 2000

Le Bras J, Jiao HJ, Meyer WE, et al.

*Synthesis, crystal structure, and reactions of the 17-valence-electron rhenium methyl complex [(eta(5)-C5Me5)Re(NO)(P(4-C6H4CH3)(3))(CH3)](center dot+) B(3,5-C6H3(CF3)(2))(4)(-): experimental and computational bonding comparisons with 18-electron methyl and . . .*

J ORGANOMET CHEM 616 (1-2): 54-66 DEC 15 2000

Fabian J, Krebs A, Schonemann D, et al.

*1,3-heterocumulene-to-alkyne [3+2] cycloaddition reactions: A theoretical and experimental study*

J ORG CHEM 65 (26): 8940-8947 DEC 29 2000

Mire LW, Marynick DS

*Bonding preferences of C2X4-bridged bimetallic transition metal complexes of Ti, Cu, and Ag*

INORG CHEM 39 (26): 5970-5975 DEC 25 2000

Groen CP, Oskam A, Kovacs A

*Theoretical study of mixed LiLnX(4) (Ln = La, Dy; X = F, Cl, Br, I) rare earth/alkali halide*

*complexes*

INORG CHEM 39 (26): 6001-6008 DEC 25 2000

Brady ED, Hanusa TP, Pink M, et al.

*The first noncoordinated phosphonium diylide, [Me<sub>2</sub>P(C<sub>13</sub>H<sub>8</sub>)(2)](-), and its ylidic and cationic counterparts: Synthesis, structural characterization, and interaction with the heavy group 2 metals*  
INORG CHEM 39 (26): 6028-6037 DEC 25 2000

Contreras RH, Peralta JE

*Angular dependence of spin-spin coupling constants*

PROG NUCL MAG RES SP 37 (4): 321-425 NOV 27 2000

Kaupp M, Metz B, Stoll H

*Breakdown of bond length-bond strength correlation: A case study*

ANGEW CHEM INT EDIT 39 (24): 4607-+ 2000

Cameron TS, Deeth RJ, Dionne I, et al.

*Bonding, structure, and energetics of gaseous E-8(2+) and of solid E-8(AsF<sub>6</sub>)(2) (E = S, Se)*

INORG CHEM 39 (25): 5614-5631 DEC 11 2000

Buchhold K, Reimann B, Djafari S, et al.

*Fluorobenzene and p-difluorobenzene microsolvated by methanol: An infrared spectroscopic and ab initio theoretical investigation*

J CHEM PHYS 112 (4): 1844-1858 JAN 22 2000

Ludwig R

*Cooperative hydrogen bonding in amides and peptides*

J MOL LIQ 84 (1): 65-75 JAN 2000

Scalmani G, Bredas JL, Barone V

*Ab initio study of the gas-phase structure and electronic properties of M-CH<sub>3</sub> (M=Li, Na) and M-CCH (M=Li, Na, K): A combined post-Hartree-Fock and density functional theory study*

J CHEM PHYS 112 (3): 1178-1191 JAN 15 2000

Lee MS, Head-Gordon M

*Extracting polarized atomic orbitals from molecular orbital calculations*

INT J QUANTUM CHEM 76 (2): 169-184 JAN 15 2000

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