

NBO (1980-1997) – 1176 references

Search run on 2/18/2013– Ariel Neff

- Andersson, M.; Blomquist, J.; Folkesson, B.; Larsson, R.; Sundberg, P.
ESCA, MOSSBAUER AND INFRARED SPECTROSCOPIC INVESTIGATIONS OF A SERIES OF TIN COMPLEXES
Journal of Electron Spectroscopy and Related Phenomena, (40): 385-396 1986.
- Arteca, G. A.; Mezey, P. G.
MOLECULAR SIMILARITY AND MOLECULAR SHAPE CHANGES ALONG REACTION PATHS - A TOPOLOGICAL ANALYSIS AND CONSEQUENCES ON THE HAMMOND POSTULATE
Journal of Physical Chemistry, (93): 4746-4751 1989.
- Bachrach, S. M.
TOPOLOGICAL ELECTRON-DENSITY ANALYSIS OF PHOSPHINES, PHOSPHAALKENES AND PHOSPHAALKYNES
Journal of Computational Chemistry, (10): 392-406 1989.
- Bachrach, S. M.; Ritchie, J. P.
AMIDE COORDINATION EFFECTS IN ORGANOLITHIUMS
Journal of the American Chemical Society, (111): 3134-3140 1989.
- Bachrach, S. M.; Streitwieser, A.
APPLICATION OF VARIOUS POPULATION METHODS TO SOME OXYGENATED COMPOUNDS
Journal of Computational Chemistry, (10): 514-519 1989.
- Bader, R. F. W.; Larouche, A.; Gatti, C.; Carroll, M. T.; Macdougall, P. J.; Wiberg, K. B.
PROPERTIES OF ATOMS IN MOLECULES - DIPOLE-MOMENTS AND TRANSFERABILITY OF PROPERTIES
Journal of Chemical Physics, (87): 1142-1152 1987.
- Baker, J.; Buckingham, A. D.
AN ABINITIO INVESTIGATION OF N-2= CO+
Journal of the Chemical Society-Faraday Transactions Ii, (83): 1609-1614 1987.
- Baldwin, M. A.; Welham, K. J.
CHARGE LOCALIZATION BY MOLECULAR-ORBITAL CALCULATIONS .2. FORMAMIDE, THIOFORMAMIDE AND N-METHYLATED ANALOGS
Organic Mass Spectrometry, (23): 425-428 1988.
- Bauer, W.; Winchester, W. R.; Schleyer, P. V.
MONOMERIC ORGANOLITHIUM COMPOUNDS IN TETRAHYDROFURAN - TERT-BUTYL LITHIUM, SEC-BUTYL LITHIUM, SUPERMESITYL LITHIUM, MESITYL LITHIUM, AND PHENYL LITHIUM - CARBON LITHIUM COUPLING-CONSTANTS AND THE NATURE OF CARBON LITHIUM BONDING
Organometallics, (6): 2371-2379 1987.
- Benzel, M. A.; Dykstra, C. E.

CONFORMATIONAL ENERGETICS IN HYDROGEN-BONDED DIMERS - THE UNOBSERVED CO-HF COMPLEX
Chemical Physics, (80): 273-278 1983.

Bernholdt, D. E.; Liu, S. Y.; Dykstra, C. E.
A THEORETICAL-STUDY OF THE STRUCTURE, BONDING, AND VIBRATIONAL FREQUENCY-SHIFTS OF THE H₂-HF COMPLEX
Journal of Chemical Physics, (85): 5120-5127 1986.

Bestmann, H. J.; Kos, A. J.; Witzgall, K.; Schleyer, P. V.
PHOSPHINE ALKYLENES .47. HETEROSUBSTITUENT INFLUENCE ON PHOSPHONIUM YLIDES - AN ABINITIO MO STUDY
Chemische Berichte-Recueil, (119): 1331-1349 1986.

Bingel, W. A.; Luttko, W.
HYBRID ORBITALS AND THEIR APPLICATIONS IN STRUCTURAL CHEMISTRY
Angewandte Chemie-International Edition in English, (20): 899-911 1981.

Blair, J. T.; Kroghjespersen, K.; Levy, R. M.
SOLVENT EFFECTS ON OPTICAL-ABSORPTION SPECTRA - THE 1A1- 1A2 TRANSITION OF FORMALDEHYDE IN WATER
Journal of the American Chemical Society, (111): 6948-6956 1989.

Blair, J. T.; Levy, R. M.; Kroghjespersen, K.
MOLECULAR MECHANICS PARAMETERS FOR ELECTRONICALLY EXCITED-STATES - THE (N, PI-STAR) SINGLET-STATE OF FORMALDEHYDE
Chemical Physics Letters, (166): 429-436 1990.

Blair, J. T.; Weisshaar, J. C.; Carpenter, J. E.; Weinhold, F.
PHOTODISSOCIATION OF (CO)₂⁺ - THEORETICAL-STUDIES OF GROUND 2BU AND EXCITED 2BG POTENTIAL-ENERGY SURFACES
Journal of Chemical Physics, (87): 392-410 1987.

Bond, D.
AN ABINITIO STUDY OF VINYLALLENE CONFORMATIONS
Journal of Organic Chemistry, (55): 661-665 1990.

Bond, D.; Schleyer, P. V.
CONFORMATIONS OF UNSATURATED ETHERS
Journal of Organic Chemistry, (55): 1003-1013 1990.

Bremer, M.; Schleyer, P. V.; Schotz, K.; Kausch, M.; Schindler, M.
4-CENTER 2-ELECTRON BONDING IN A TETRAHEDRAL TOPOLOGY - EXPERIMENTAL REALIZATION OF 3-DIMENSIONAL HOMOAROMATICITY IN THE 1,3-DEHYDRO-5,7-ADAMANTANEDIYL DICATION
Angewandte Chemie-International Edition in English, (26): 761-763 1987.

Buncel, E.; Venkatachalam, T. K.

CARBANION MECHANISMS .15. CONCERNING THE Si-Li BONDING IN PHENYLSILYL LITHIUMS AS STUDIED BY VARIABLE TEMPERATURE Li-7 NUCLEAR-MAGNETIC-RESONANCE
Canadian Journal of Chemistry-Revue Canadienne De Chimie, (64): 1674-1676 1986.

Burley, S. K.; Petsko, G. A.
WEAKLY POLAR INTERACTIONS IN PROTEINS
Advances in Protein Chemistry, (39): 125-189 1988.

Cammi, R.; Hofmann, H. J.; Tomasi, J.
DECOMPOSITION OF THE INTERACTION ENERGY BETWEEN METAL-CATIONS AND WATER OR AMMONIA WITH INCLUSION OF COUNTERPOISE CORRECTIONS TO THE INTERACTION ENERGY TERMS
Theoretica Chimica Acta, (76): 297-313 1989.

Cao, Y.; Wang, Y. L.
FRONTIER HYBRID ORBITALS .1. PRINCIPLES
Croatica Chemica Acta, (62): 669-676 1990.

Carpenter, J. E.; McGrath, M. P.; Hehre, W. J.
EFFECT OF ELECTRON CORRELATION ON ATOMIC ELECTRON POPULATIONS
Journal of the American Chemical Society, (111): 6154-6156 1989.

Carpenter, J. E.; Weinhold, F.
ANALYSIS OF THE GEOMETRY OF THE HYDROXYMETHYL RADICAL BY THE DIFFERENT HYBRIDS FOR DIFFERENT SPINS NATURAL BOND ORBITAL PROCEDURE
Journal of Molecular Structure-Theochem, (46): 41-62 1988.

Carpenter, J. E.; Weinhold, F.
TORSION VIBRATION INTERACTIONS IN HYDROGEN-PEROXIDE .2. NATURAL BOND ORBITAL ANALYSIS
Journal of Physical Chemistry, (92): 4306-4313 1988.

Carpenter, J. E.; Weinhold, F.
TRANSFERABILITY OF NATURAL BOND ORBITALS
Journal of the American Chemical Society, (110): 368-372 1988.

Charkin, O. P.; Klabo, A.; Shloier, P. F. R.; Zyubin, A. S.
THEORETICAL-STUDY OF STABILITY AND STRUCTURE OF Li₂BEH₄, Li₂MGH₄, Li₂BH₄⁺ AND Li₂AlH₄⁺ COMPLEX HYDRIDES
Koordinatsionnaya Khimiya, (16): 309-317 1990.

Cioslowski, J.
A NEW POPULATION ANALYSIS BASED ON ATOMIC POLAR TENSORS
Journal of the American Chemical Society, (111): 8333-8336 1989.

Cioslowski, J.; Hamilton, T.; Scuseria, G.; Hess, B. A.; Hu, J.; Schaad, L. J.; Dupuis, M.
APPLICATION OF THE GAPT POPULATION ANALYSIS TO SOME ORGANIC-MOLECULES AND TRANSITION STRUCTURES

Journal of the American Chemical Society, (112): 4183-4186 1990.

Cioslowski, J.; Hay, P. J.; Ritchie, J. P.

*CHARGE-DISTRIBUTIONS AND EFFECTIVE ATOMIC CHARGES IN TRANSITION-METAL COMPLEXES
USING GENERALIZED ATOMIC POLAR TENSORS AND TOPOLOGICAL ANALYSIS*

Journal of Physical Chemistry, (94): 148-151 1990.

Colbert, D. T.; Sibert, E. L.

VARIABLE CURVATURE COORDINATES FOR MOLECULAR VIBRATIONS

Journal of Chemical Physics, (91): 350-363 1989.

Curtiss, L. A.; Blander, M.

THERMODYNAMIC PROPERTIES OF GAS-PHASE HYDROGEN-BONDED COMPLEXES

Chemical Reviews, (88): 827-841 1988.

Curtiss, L. A.; Jurgens, R.

NONADDITIVITY OF INTERACTION IN HYDRATED CU⁺ AND CU⁻²⁺ CLUSTERS

Journal of Physical Chemistry, (94): 5509-5513 1990.

Curtiss, L. A.; Melendres, C. A.; Reed, A. E.; Weinhold, F.

THEORETICAL-STUDIES OF O₂(-)-(H₂O)_N CLUSTERS

Journal of Computational Chemistry, (7): 294-305 1986.

Curtiss, L. A.; Pochatko, D. J.; Reed, A. E.; Weinhold, F.

INVESTIGATION OF THE DIFFERENCES IN STABILITY OF THE OC ... HF AND CO ... HF COMPLEXES

Journal of Chemical Physics, (82): 2679-2687 1985.

Czech, P. T.; Gladysz, J. A.; Fenske, R. F.

*THE ROLE OF VIRTUAL HALOGEN D ORBITALS IN THE STABILITY AND REACTIVITY OF RHENIUM
ALKYL HALIDE-COMPLEXES OF THE FORM (ETA-5-C₅H₅)RE(NO)(PPH₃)(XR) +*

Organometallics, (8): 1806-1810 1989.

Czech, P. T.; Ye, X. Q.; Fenske, R. F.

*APPLICATION OF THE FENSKE-HALL MOLECULAR-ORBITAL METHOD TO THE CALCULATION OF C-
13 NMR SHIFTS IN ORGANOMETALLIC COMPOUNDS - CORRELATION BETWEEN CALCULATED
SIGMA-P VALUES AND THE OBSERVED CHEMICAL-SHIFT, SIGMA*

Organometallics, (9): 2016-2022 1990.

Dannenberg, J. J.; Vinson, L. K.

*AM1 MOLECULAR-ORBITAL STUDY OF HYDROGEN-BONDING - GAS-PHASE HYDRATION OF
PROTONATED DIAMINES*

Journal of Physical Chemistry, (92): 5635-5639 1988.

Dionne, P.; Stjacques, M.

*MECHANISM OF THE GAUCHE CONFORMATIONAL EFFECT IN 3-HALOGENATED 1,5-
BENZODIOXEPINS*

Journal of the American Chemical Society, (109): 2616-2623 1987.

- Dykstra, C. E.; Kirtman, B.
LOCAL QUANTUM-CHEMISTRY
Annual Review of Physical Chemistry, (41): 155-174 1990.
- Eckertmaksic, M.
PROTONATION OF 4H-PYRAN-4-ONE AND ITS SULFUR ANALOGS - MNDO STUDY
Zeitschrift Fur Naturforschung Section a-a Journal of Physical Sciences, (39): 267-275 1984.
- Fan, Q.; Pfeiffer, G. V.
THEORETICAL-STUDY OF LINEAR LIC₂-8LI MOLECULES
Chemical Physics Letters, (162): 479-485 1989.
- Frenking, G.; Cremer, D.
THE CHEMISTRY OF THE NOBLE-GAS ELEMENTS HELIUM, NEON, AND ARGON - EXPERIMENTAL FACTS AND THEORETICAL PREDICTIONS
Structure and Bonding, (73): 17-95 1990.
- Frenking, G.; Koch, W.; Schwarz, H.
THEORETICAL INVESTIGATIONS ON FLUORINE-SUBSTITUTED ETHYLENE DICATIONS C₂HNF₄₋N₂⁺(N = 0-4)
Journal of Computational Chemistry, (7): 406-416 1986.
- Fujimoto, H.
PAIRED INTERACTING ORBITALS - A WAY OF LOOKING AT CHEMICAL INTERACTIONS
Accounts of Chemical Research, (20): 448-453 1987.
- Fujimoto, H.; Yamasaki, T.
A THEORETICAL-ANALYSIS OF CATALYTIC ROLES BY PAIRED INTERACTING ORBITALS - PD(II)-CATALYZED NUCLEOPHILIC ADDITIONS TO C=C BONDS
Journal of the American Chemical Society, (108): 578-581 1986.
- Fujimoto, H.; Yamasaki, T.; Mizutani, H.; Koga, N.
A THEORETICAL-STUDY OF OLEFIN INSERTIONS INTO Ti-C AND Ti-H BONDS - AN ANALYSIS BY PAIRED INTERACTING ORBITALS
Journal of the American Chemical Society, (107): 6157-6161 1985.
- Glaser, R.
THE DENSITY INTEGRATION APPROACH TO POPULATIONS - A CRITICAL COMPARISON OF PROJECTION POPULATIONS TO POPULATIONS DEFINED BY THE THEORY OF ATOMS IN MOLECULES
Journal of Computational Chemistry, (10): 118-135 1989.
- Goldshtain, I. P.; Fedotov, A. N.
INTERMOLECULAR CHARGE-TRANSFER UNDER ELECTRON-DONOR-ACCEPTOR MOLECULAR-INTERACTIONS
Zhurnal Fizicheskoi Khimii, (62): 2667-2686 1988.
- Gopinathan, M. S.

DETERMINATION OF ATOMIC HYBRIDIZATION IN MOLECULAR-ORBITAL THEORY - A VALENCY METHOD

Theochem-Journal of Molecular Structure, (46): 379-388 1988.

Gopinathan, M. S.; Jug, K.

VALENCY .1. A QUANTUM CHEMICAL DEFINITION AND PROPERTIES

Theoretica Chimica Acta, (63): 497-509 1983.

Gopinathan, M. S.; Jug, K.

VALENCY .2. APPLICATIONS TO MOLECULES WITH 1ST-ROW ATOMS

Theoretica Chimica Acta, (63): 511-527 1983.

Gronert, S.; Glaser, R.; Streitwieser, A.

CHARGE TRANSFERS AND POLARIZATIONS IN BONDS TO SILICON - ORGANOSILANES AND THE SN₂(Si) REACTION OF SiH₄+F⁻ - AN ABINITIO STUDY

Journal of the American Chemical Society, (111): 3111-3117 1989.

Hobza, P.; Schleyer, P. V.

ON THE NATURE OF THE BONDING IN HE-BE-O, NE-BE-O, AR-BE-O MOLECULES

Collection of Czechoslovak Chemical Communications, (53): 2230-2238 1988.

Hobza, P.; Zahradník, R.

INTERMOLECULAR INTERACTIONS BETWEEN MEDIUM-SIZED SYSTEMS - NONEMPIRICAL AND EMPIRICAL CALCULATIONS OF INTERACTION ENERGIES - SUCCESSES AND FAILURES

Chemical Reviews, (88): 871-897 1988.

Holmer, B. K.; Certain, P. R.

NATURAL ORBITAL ANALYSIS OF VIBRATION-ROTATION WAVE-FUNCTIONS

Journal of Physical Chemistry, (89): 4464-4472 1985.

Horn, H.; Ahlrichs, R.

ENERGETIC MEASURE FOR THE IONIC CHARACTER OF BONDS

Journal of the American Chemical Society, (112): 2121-2124 1990.

Huheey, J. E.

BENT'S RULE - ENERGETICS, ELECTRONEGATIVITY, AND THE STRUCTURES OF NONMETAL FLUORIDES

Inorganic Chemistry, (20): 4033-4035 1981.

Jug, K.; Fasold, E.; Gopinathan, M. S.

A CONCEPT OF CHARGE AND VALENCE FOR ABINITIO WAVE-FUNCTIONS

Journal of Computational Chemistry, (10): 965-974 1989.

Kanis, D. R.; Fenske, R. F.

BONDING IN TRANSITION-METAL POLYSULFIDES - A MOLECULAR-ORBITAL AND NATURAL BOND ORBITAL ANALYSIS

Abstracts of Papers of the American Chemical Society, (198): 268-INOR 1989.

- Kar, T.; Behera, L.; Sannigrahi, A. B.
EFFECT OF A GENERAL NONSINGULAR TRANSFORMATION OF THE AO BASIS SET ON MO CALCULATIONS OF VALENCY
Chemical Physics Letters, (163): 157-164 1989.
- Kar, T.; Sannigrahi, A. B.; Mukherjee, D. C.
COMPARISON OF ATOMIC CHARGES, VALENCIES AND BOND ORDERS IN SOME HYDROGEN-BONDED COMPLEXES CALCULATED FROM MULLIKEN AND LOWDIN SCF DENSITY-MATRICES
Theochem-Journal of Molecular Structure, (38): 93-101 1987.
- Kar, T.; Sannigrahi, A. B.; Niyogi, B. G.
AN ABINITIO STUDY OF HYDROGEN, LITHIUM AND SODIUM BONDING ON THE BASIS OF ATOMIC CHARGES, VALENCIES, BOND ORDERS AND OVERLAP POPULATIONS
Indian Journal of Chemistry Section a-Inorganic Bio-Inorganic Physical Theoretical & Analytical Chemistry, (26): 989-993 1987.
- Kaufmann, E.; Raghavachari, K.; Reed, A. E.; Schleyer, P. V.
METHYLLITHIUM AND ITS OLIGOMERS - STRUCTURAL AND ENERGETIC RELATIONSHIPS
Organometallics, (7): 1597-1607 1988.
- Kaufmann, E.; Schleyer, P. V.
DILITHIODIBORANE(6) (Li₂B₂H₄) - AN EXPERIMENTALLY VIABLE SPECIES WITH A B=B DOUBLE-BOND - PLANAR NO-BOND DOUBLE-BOND ISOMERS WITH PENTACOORDINATE BORON
Inorganic Chemistry, (27): 3987-3992 1988.
- Kaufmann, E.; Schleyer, P. V.
DEGENERATE LITHIUM-HYDROGEN EXCHANGE-REACTIONS - ABINITIO MODELS FOR METALATION MECHANISMS INVOLVING H-2, CH₄, NH₃, H₂O, AND HF
Journal of Computational Chemistry, (10): 437-448 1989.
- Kaufmann, E.; Schleyer, P. V.; Gronert, S.; Streitwieser, A.; Halpern, M.
THE STRUCTURES AND ENERGIES OF MAIN GROUP METAL FORMYL COMPLEXES - THE MECHANISM OF THE REACTION OF LIH WITH CO - AN ABINITIO STUDY
Journal of the American Chemical Society, (109): 2553-2559 1987.
- Kaufmann, E.; Sieber, S.; Schleyer, P. V.
ABINITIO MODELS FOR METALATION AND HYDROGENOLYSIS REACTIONS INVOLVING ORGANOLITHIUM COMPOUNDS
Journal of the American Chemical Society, (111): 121-125 1989.
- Kaufmann, E.; Sieber, S.; Schleyer, P. V.
CARBOXYLATION OF LITHIUM COMPOUNDS - ABINITIO MECHANISMS
Journal of the American Chemical Society, (111): 4005-4008 1989.
- Kaufmann, E.; Tidor, B.; Schleyer, P. V.
THE REMARKABLY INVARIANT INTERACTION ENERGIES OF LITHIUM 1ST-ROW COMPOUNDS WITH WATER AND WITH AMMONIA
Journal of Computational Chemistry, (7): 334-344 1986.

- Kirtman, B.; Demelo, C. P.
ACCURATE LOCAL-SPACE TREATMENT OF HYDROGEN-BONDING IN LARGE SYSTEMS
International Journal of Quantum Chemistry, (29): 1209-1222 1986.
- Klusener, P. A. A.; Hanekamp, J. C.; Brandsma, L.; Schleyer, P. V.
*EXPERIMENTAL AND THEORETICAL-STUDY OF THE DIMETALLATION OF PHENYLACETYLENE AND
(1-NAPHTHYL)ACETYLENE*
Journal of Organic Chemistry, (55): 1311-1321 1990.
- Kovacevic, K.; Maksic, Z. B.; Mogusmilankovic, A.
*GEOMETRY OF MOLECULES .7. INTERATOMIC DISTANCES, BOND ANGLES AND STRAIN ENERGIES
IN SOME ROTENES AND RELATED SPIROCOMPOUNDS BY THE IMO METHOD*
Croatica Chemica Acta, (57): 187-200 1984.
- Kovacevic, K.; Maksic, Z. B.; Vuckovic, D. L.; Vujisic, L.
*GEOMETRY OF MOLECULES .8. INTERATOMIC DISTANCES, BOND ANGLES AND HYBRIDIZATION
IN SOME BASKETANES BY THE IMO METHOD*
Theochem-Journal of Molecular Structure, (36): 233-243 1987.
- Krijn, M.; Feil, D.
*ELECTRON-DENSITY DISTRIBUTIONS IN HYDROGEN-BONDS - A LOCAL DENSITY-FUNCTIONAL
STUDY OF ALPHA-OXALIC ACID DIHYDRATE AND COMPARISON WITH EXPERIMENT*
Journal of Chemical Physics, (89): 4199-4208 1988.
- Krijn, M.; Feil, D.
*A LOCAL DENSITY-FUNCTIONAL STUDY OF THE ELECTRON-DENSITY DISTRIBUTION IN THE H₂O
DIMER*
Journal of Chemical Physics, (89): 5787-5793 1988.
- Kroghjespersen, K.; Zhang, X. H.; Westbrook, J. D.; Fikar, R.; Nayak, K.; Kwik, W. I.; Potenza, J. A.; Schugar, H. J.
*CRYSTAL, MOLECULAR, AND ELECTRONIC-STRUCTURES OF PENTAAMMINERUTHENIUM(III)-
THIOETHER COMPLEXES*
Journal of the American Chemical Society, (111): 4082-4091 1989.
- Kunze, K. L.; Hall, M. B.
*WHY THE ACCUMULATION OF ELECTRON-DENSITY APPEARS WEAK OR ABSENT IN CERTAIN
COVALENT BONDS*
Journal of the American Chemical Society, (108): 5122-5127 1986.
- Kutzelnigg, W.
ORTHOGONAL AND NON-ORTHOGONAL HYBRIDS
Theochem-Journal of Molecular Structure, (46): 403-419 1988.
- Lammertsma, K.; Guner, O. F.; Drewes, R. M.; Reed, A. E.; Schleyer, P. V.
REMARKABLE STRUCTURES OF DIALANE(4), AL₂H₄
Inorganic Chemistry, (28): 313-317 1989.

- Lammertsma, K.; Leszczynski, J.
ABINITIO STUDY ON DIGALLANE(4), GA₂H₄
Journal of Physical Chemistry, (94): 5543-5548 1990.
- Laube, T.
CONSTRUCTION OF THE BEST SET OF 4 ORTHONORMAL 2S-2P HYBRID ORBITALS BY LEAST-SQUARES METHODS
Journal of Computational Chemistry, (9): 356-361 1988.
- Lazzeretti, P.; Zanasi, R.; Raynes, W. T.
ON THE CH BOND DIPOLE-MOMENT IN ALKANES
Journal of Chemical Physics, (87): 1681-1684 1987.
- Levy, R. M.; Kitchen, D. B.; Blair, J. T.; Kroghjespersen, K.
MOLECULAR-DYNAMICS SIMULATION OF TIME-RESOLVED FLUORESCENCE AND NONEQUILIBRIUM SOLVATION OF FORMALDEHYDE IN WATER
Journal of Physical Chemistry, (94): 4470-4476 1990.
- Lopez, J. P.
STATIONARY-POINTS ON THE POTENTIAL-ENERGY SURFACE OF O₂-HF AND O₂-H₂O
Journal of Computational Chemistry, (10): 55-62 1989.
- Lugert, G.; Manero, J.; Feigel, M.; Bremer, M.
CRYSTAL-STRUCTURE OF 2-(CHLOROMETHYL)-5-(PHTHALIMIDOMETHYL)THIOPHENE - NO EVIDENCE FOR INTRAMOLECULAR 1,4-S=N ATTRACTION
Journal of the Chemical Society-Chemical Communications: 1395-1396 1988.
- Magnasco, V.; Musso, G. F.; Costa, C.; Figari, G.
A MINIMAL BASIS BOND ORBITAL INVESTIGATION OF THE LINEAR WATER DIMER
Molecular Physics, (56): 1249-1269 1985.
- Magnusson, E.
SP HYBRIDIZATION RECONSIDERED - THE COMPOSITION OF ORBITALS IN MAIN-GROUP HYDRIDES
Journal of the American Chemical Society, (106): 1177-1185 1984.
- Maksic, Z. B.
SYMMETRY, HYBRIDIZATION AND BONDING IN MOLECULES
Computers & Mathematics with Applications-Part B, (12): 697-723 1986.
- Maksic, Z. B.; Eckertmaksic, M.; Rupnik, K.
MODEL DESCRIPTION OF SOME MOLECULAR-PROPERTIES BY THE MODIFIED-ATOM-IN-MOLECULE (MAM) APPROACH
Croatica Chemica Acta, (57): 1295-1353 1984.
- Millar, T. J.; Defrees, D. J.; McLean, A. D.; Herbst, E.

THE SENSITIVITY OF GAS-PHASE MODELS OF DENSE INTERSTELLAR CLOUDS TO CHANGES IN DISSOCIATIVE RECOMBINATION BRANCHING RATIOS
Astronomy and Astrophysics, (194): 250-256 1988.

Moberg, R.; Yuan, Z. C.; Holmberg, S.; Bokman, F.; Ahlberg, P.; Bohman, O.; Siegbahn, H.
ESCA STUDIES OF CARBANIONIC COMPOUNDS - BUTYLLITHIUM IN HEPTANE SOLUTION AND DIBUTYLMERCURY IN THE GAS-PHASE
Journal of Physical Organic Chemistry, (2): 417-424 1989.

Moss, R. A.; Wilk, B.; Kroghjespersen, K.; Blair, J. T.; Westbrook, J. D.
ORGANOIODINANE REAGENTS FOR PHOSPHATE CLEAVAGE - EXPERIMENTAL AND COMPUTATIONAL STUDIES
Journal of the American Chemical Society, (111): 250-258 1989.

Moss, R. A.; Wilk, B.; Kroghjespersen, K.; Westbrook, J. D.
SYNTHESIS AND PROPERTIES OF THE VALENCE TAUTOMER OF CIS-IODOSOCYCLOPROPANECARBOXYLIC ACID - 4,5-METHANO-1-HYDROXYIODOXOL-3(1H)-ONE
Journal of the American Chemical Society, (111): 6729-6734 1989.

Mullay, J.
CALCULATION OF GROUP ELECTRONEGATIVITY
Journal of the American Chemical Society, (107): 7271-7275 1985.

Mullay, J.
A SIMPLE METHOD FOR CALCULATING ATOMIC CHARGE IN MOLECULES
Journal of the American Chemical Society, (108): 1770-1775 1986.

Musso, G. F.; Costa, C.; Magnasco, V.
THE INTRODUCTION OF POLARIZATION FUNCTIONS IN THE SINGLE-ZETA BOND-ORBITAL METHOD AND AN APPLICATION TO THE GROUND-STATE OF THE WATER MOLECULE
Theochem-Journal of Molecular Structure, (28): 267-278 1986.

Nelson, J. T.; Pietro, W. J.
NATURAL BOND ORBITAL (NBO) ANALYSIS OF SUBSTITUENT EFFECTS IN BORAZINE DERIVATIVES
Inorganic Chemistry, (28): 544-548 1989.

Newton, M. D.
ELECTRONIC-STRUCTURE ANALYSIS OF ELECTRON-TRANSFER MATRIX-ELEMENTS FOR TRANSITION-METAL REDOX PAIRS
Journal of Physical Chemistry, (92): 3049-3056 1988.

Paddonrow, M. N.; Jordan, K. D.
AN ABINITIO MO STUDY OF 7-SILANORBORNADIENE AND 7,7-DIMETHYL-7-SILANORBORNADIENE - EXAMPLES OF NORBORNADIENES IN WHICH THE PI-ORBITALS INTERACT LARGEMLY THROUGH BONDS RATHER THAN THROUGH-SPACE
Journal of the Chemical Society-Chemical Communications: 1508-1510 1988.

Paddonrow, M. N.; Wong, S. S.; Jordan, K. D.

ABINITIO SCF-MO AND NATURAL BOND ORBITAL STUDIES OF 7-SILANORBORNADIENE AND 7,7-DIMETHYL-7-SILANORBORNADIENE - 2 MOLECULES POSSESSING AN INVERTED SEQUENCE OF PI-ORBITALS

Journal of the American Chemical Society, (112): 1710-1722 1990.

Paddonrow, M. N.; Wong, S. S.; Jordan, K. D.

AN ABINITIO SCF-MO STUDY OF THE ELECTRONIC-STRUCTURE OF 7-GERMANORBORNADIENE AND 7-STANNANORBORNADIENE - 2 MOLECULES PREDICTED TO HAVE AN INVERTED SEQUENCE OF PI-LEVELS

Journal of the Chemical Society-Perkin Transactions 2: 417-423 1990.

Paddonrow, M. N.; Wong, S. S.; Jordan, K. D.

A CAUTIONARY COMMENT ON THE USE OF ORTHOGONAL LOCALIZED MOLECULAR-ORBITALS FOR THE QUANTITATIVE-ANALYSIS OF THROUGH-SPACE AND THROUGH-BOND ORBITAL INTERACTIONS

Journal of the Chemical Society-Perkin Transactions 2: 425-430 1990.

Panina, N. S.; Yakovlev, V. N.; Kukushkin, Y. N.

THEORETICAL-STUDY OF PROTON AFFINITY OF PHOSPHORUS(III) COMPOUNDS

Journal of Structural Chemistry, (25): 682-687 1984.

Peterson, K. A.; Woods, R. C.

AN INVESTIGATION OF THE HBCL+-BCLH+ SYSTEM BY MOLLER-PLESSET PERTURBATION-THEORY

Journal of Chemical Physics, (88): 1074-1079 1988.

Peterson, K. A.; Woods, R. C.

PREDICTIONS OF THE ROTATIONAL AND VIBRATIONAL-SPECTRA OF SIF+, PO+, AND NS+ BY MOLLER-PLESSET PERTURBATION-THEORY

Journal of Chemical Physics, (89): 4929-4944 1988.

Peterson, K. A.; Woods, R. C.

GROUND-STATE SPECTROSCOPIC AND THERMODYNAMIC PROPERTIES OF ALO-, SIN-, CP-, BS-, BO-, AND CN- FROM MOLLER-PLESSET PERTURBATION-THEORY

Journal of Chemical Physics, (90): 7239-7250 1989.

Peterson, K. A.; Woods, R. C.

AN ABINITIO INVESTIGATION OF THE SPECTROSCOPIC PROPERTIES OF CLF, ARF+, SF-, AND CLO- IN THEIR GROUND ELECTRONIC STATES

Journal of Chemical Physics, (92): 7412-7417 1990.

Peterson, K. A.; Woods, R. C.

AN ABINITIO STUDY OF THE 24 ELECTRON RADICALS PF, SO, NCL, SF+, CLO+, SIF-, PO-, NS-, AND CCL- IN THEIR X3SIGMA- ELECTRONIC STATES

Journal of Chemical Physics, (93): 1876-1888 1990.

Poirier, R. A.; Surjan, P. R.

THE APPLICATION OF STRICTLY LOCALIZED GEMINALS TO THE DESCRIPTION OF CHEMICAL-BONDS

Journal of Computational Chemistry, (8): 436-441 1987.

Raghavachari, K.; Sapse, A. M.; Jain, D. C.

STRUCTURES OF LINH₂ HEXAMERS - REPLY

Inorganic Chemistry, (27): 3862-3863 1988.

Rajca, A.; Streitwieser, A.; Tolbert, L. M.

ABINITIO STUDY OF 2,3-DILITHIOPROPENE

Journal of the American Chemical Society, (109): 1790-1792 1987.

Rajca, A.; Wang, P.; Streitwieser, A.; Schleyer, P. V.

*UNUSUAL STRUCTURES OF DILITHIOSILANES AND DISODIOSILANES - IONICITY OF THE SILICON
ALKALI-METAL BOND*

Inorganic Chemistry, (28): 3064-3070 1989.

Ramos, M. N.; Gussoni, M.; Castiglioni, C.; Zerbi, G.

CORRECTED MULLIKEN CHARGES FOR SMALL MOLECULES

Croatica Chemica Acta, (62): 595-602 1990.

Reed, A. E.; Clark, T.

*A NATURAL BOND ORBITAL ANALYSIS OF THE BONDING IN SOLVATED ELECTRONS WITHIN A
LOCALIZED ELECTRON MODEL*

Faraday Discussions, (85): 365-372 1988.

Reed, A. E.; Curtiss, L. A.; Weinhold, F.

*INTERMOLECULAR INTERACTIONS FROM A NATURAL BOND ORBITAL, DONOR-ACCEPTOR
VIEWPOINT*

Chemical Reviews, (88): 899-926 1988.

Reed, A. E.; Schade, C.; Schleyer, P. V.; Kamath, P. V.; Chandrasekhar, J.

ANOMERIC EFFECTS INVOLVING SILICON CENTERS - SILANOLS

Journal of the Chemical Society-Chemical Communications: 67-69 1988.

Reed, A. E.; Schleyer, P. V.

*THE ANOMERIC EFFECT WITH CENTRAL ATOMS OTHER THAN CARBON .1. STRONG-
INTERACTIONS BETWEEN NONBONDED SUBSTITUENTS IN POLYFLUORINATED 1ST-ROW AND
2ND-ROW HYDRIDES*

Journal of the American Chemical Society, (109): 7362-7373 1987.

Reed, A. E.; Schleyer, P. V.

*THE NATURE AND DECOMPOSITION PATHWAYS OF SIH₅-, PH₅, AND SH₅⁺, THE SIMPLEST VIABLE
PENTAVALENT MOLECULES*

Chemical Physics Letters, (133): 553-561 1987.

Reed, A. E.; Schleyer, P. V.

*THE ANOMERIC EFFECT WITH CENTRAL ATOMS OTHER THAN CARBON .2. STRONG-
INTERACTIONS BETWEEN NONBONDED SUBSTITUENTS IN MONOFLUORINATED AND
POLYFLUORINATED 1ST-ROW AND 2ND-ROW AMINES, FNAHMNH₂*

Inorganic Chemistry, (27): 3969-3987 1988.

Reed, A. E.; Schleyer, P. V.

CHEMICAL BONDING IN HYPERVALENT MOLECULES - THE DOMINANCE OF IONIC BONDING AND NEGATIVE HYPERCONJUGATION OVER D-ORBITAL PARTICIPATION

Journal of the American Chemical Society, (112): 1434-1445 1990.

Reed, A. E.; Weinhold, F.

NATURAL BOND ORBITAL ANALYSIS OF NEAR-HARTREE-FOCK WATER DIMER

Journal of Chemical Physics, (78): 4066-4073 1983.

Reed, A. E.; Weinhold, F.

NATURAL LOCALIZED MOLECULAR-ORBITALS

Journal of Chemical Physics, (83): 1736-1740 1985.

Reed, A. E.; Weinhold, F.

A THEORETICAL-MODEL OF BONDING IN HYPERLITHIATED CARBON-COMPOUNDS

Journal of the American Chemical Society, (107): 1919-1921 1985.

Reed, A. E.; Weinhold, F.

ON THE ROLE OF D ORBITALS IN SF₆

Journal of the American Chemical Society, (108): 3586-3593 1986.

Reed, A. E.; Weinhold, F.

SOME REMARKS ON THE C-H BOND DIPOLE-MOMENT

Journal of Chemical Physics, (84): 2428-2430 1986.

Reed, A. E.; Weinhold, F.; Curtiss, L. A.; Pochatko, D. J.

NATURAL BOND ORBITAL ANALYSIS OF MOLECULAR-INTERACTIONS - THEORETICAL-STUDIES OF BINARY COMPLEXES OF HF, H₂O, NH₃, N-2, O-2, F₂, CO, AND CO₂ WITH HF, H₂O, AND NH₃

Journal of Chemical Physics, (84): 5687-5705 1986.

Reed, A. E.; Weinhold, F.; Weiss, R.; Macheleid, J.

NATURE OF THE CONTACT ION-PAIR CCL₃+CL⁻ - A THEORETICAL-STUDY

Journal of Physical Chemistry, (89): 2688-2694 1985.

Rensberger, K. J.; Blair, J. T.; Weinhold, F.; Crim, F. F.

EXPERIMENTAL AND THEORETICAL-STUDY OF THE RELAXATION OF VIBRATIONALLY EXCITED HF BY NO AND CO

Journal of Chemical Physics, (91): 1688-1696 1989.

Ritchie, J. P.; Bachrach, S. M.

BOND PATHS AND BOND PROPERTIES OF CARBON LITHIUM BONDS

Journal of the American Chemical Society, (109): 5909-5916 1987.

Rives, A. B.

CORRECTION

International Journal of Quantum Chemistry: 555-555 1981.

- Rives, A. B.; Xiaozeng, Y.; Fenske, R. F.
SOME ASPECTS OF THE ELECTRONIC-STRUCTURES OF A SERIES OF TRIMERIC TRANSITION-METAL CLUSTER COMPLEXES
Inorganic Chemistry, (21): 2286-2294 1982.
- Ruedenberg, K.; Schmidt, M. W.; Gilbert, M. M.
ARE ATOMS INTRINSIC TO MOLECULAR ELECTRONIC WAVEFUNCTIONS .2. ANALYSIS OF FORS ORBITALS
Chemical Physics, (71): 51-64 1982.
- Saethre, L. J.; Siggel, M. R. F.; Thomas, T. D.
EFFECT OF HALOGEN SUBSTITUENTS ON CARBON-1S IONIZATION ENERGIES IN HALOETHENES AND HALOETHANES
Journal of Electron Spectroscopy and Related Phenomena, (49): 119-137 1989.
- Salzner, U.; Schleyer, P. V.
ARE THERE ANOMERIC EFFECTS INVOLVING SELENIUM
Journal of the Chemical Society-Chemical Communications: 190-192 1990.
- Sannigrahi, A. B.; Kar, T.
ABINITIO INVESTIGATION OF THE NATURE OF BONDING IN LIX DIMERS WITH 1ST ROW SUBSTITUENTS
Theochem-Journal of Molecular Structure, (49): 149-160 1988.
- Sapse, A. M.; Raghavachari, K.; Schleyer, P. V.; Kaufmann, E.
THEORETICAL-STUDIES OF LIF, LIOH, AND LINH₂ TETRAMERS
Journal of the American Chemical Society, (107): 6483-6486 1985.
- Schade, C.; Schleyer, P. V.
SODIUM, POTASSIUM, RUBIDIUM, AND CESIUM - X-RAY STRUCTURAL-ANALYSIS OF THEIR ORGANIC-COMPOUNDS
Advances in Organometallic Chemistry, (27): 169-278 1987.
- Schade, C.; Schleyer, P. V.; Gregory, P.; Dietrich, H.; Mahdi, W.
COMPETITION AMONG MULTIHAPTO BONDING, SOLVATION, AND AGGREGATION - THE ETA-1 ETA-2 INFINITE-CHAIN X-RAY STRUCTURE OF INDENYLSODIUM.N,N,N',N'-TETRAMETHYL-1,2-DIAMINOETHANE
Journal of Organometallic Chemistry, (341): 19-38 1988.
- Schiffer, H.; Ahlrichs, R.
THE C-LI BOND IN METHYLLITHIUM - BINDING-ENERGY AND IONIC CHARACTER
Chemical Physics Letters, (124): 172-176 1986.
- Schleyer, P. V.
REEXAMINATION OF THE STRUCTURES OF C₂Li₂ AND OF C₄Li₄
Journal of Physical Chemistry, (94): 5560-5563 1990.

- Schleyer, P. V.; Buhl, M.
ON THE NATURE OF PYRAZOLYLBORANE - AN ABINITIO IGLO NMR-STUDY
Angewandte Chemie-International Edition in English, (29): 304-306 1990.
- Schleyer, P. V.; Buhl, M.; Fleischer, U.; Koch, W.
THEORETICAL REFINEMENT OF THE B5H11 STRUCTURE - APPLICATION OF IGLO CHEMICAL-SHIFT CALCULATIONS
Inorganic Chemistry, (29): 153-155 1990.
- Schleyer, P. V.; Clark, T.
THE MOST STABLE SIH3LI STRUCTURE IS INVERTED
Journal of the Chemical Society-Chemical Communications: 1371-1373 1986.
- Schleyer, P. V.; Janoschek, R.
PENTASILA 1.1.1 PROPELLANE - PREDICTIONS CONCERNING STRUCTURE, BONDING, AND STRAIN-ENERGY
Angewandte Chemie-International Edition in English, (26): 1267-1268 1987.
- Schleyer, P. V.; Kost, D.
A COMPARISON OF THE ENERGIES OF DOUBLE-BONDS OF 2ND-ROW ELEMENTS WITH CARBON AND SILICON
Journal of the American Chemical Society, (110): 2105-2109 1988.
- Schleyer, P. V.; Pople, J. A.
THE REACTION OF LITHIUM WITH HYDROGEN - A MODEL ABINITIO STUDY
Chemical Physics Letters, (129): 475-481 1986.
- Schleyer, P. V.; Reed, A. E.
THE NONTETRAHEDRAL STRUCTURE AND FLUXIONAL CHARACTER OF SILI4 - A VIOLATION OF BOTH VANTHOFF AND ELECTROSTATIC BONDING PRINCIPLES
Journal of the American Chemical Society, (110): 4453-4454 1988.
- Schleyer, P. V.; Sawaryn, A.; Reed, A. E.; Hobza, P.
THE REMARKABLE STRUCTURE OF LITHIUM CYANIDE ISOCYANIDE
Journal of Computational Chemistry, (7): 666-672 1986.
- Schleyer, P. V.; Stout, P. D.
ON THE NATURE OF THE SI=N DOUBLE-BOND AND THE EASE OF BENDING AT NITROGEN
Journal of the Chemical Society-Chemical Communications: 1373-1374 1986.
- Seebach, D.; Maetzke, T.; Haynes, R. K.; Paddonrow, M. N.; Wong, S. S.
LOW-TEMPERATURE X-RAY CRYSTAL-STRUCTURE ANALYSIS OF THE THERMALLY UNSTABLE LITHIATED 2-BUTENYL TERT-BUTYL SULFIDE - A COMPARISON WITH MODEL ABINITIO MO CALCULATIONS
Helvetica Chimica Acta, (71): 299-311 1988.
- Siggel, M. R. F.; Streitwieser, A.; Thomas, T. D.
THE ROLE OF RESONANCE AND INDUCTIVE EFFECTS IN THE ACIDITY OF CARBOXYLIC-ACIDS

Journal of the American Chemical Society, (110): 8022-8028 1988.

Singh, U. C.; Kollman, P. A.

ABINITIO CALCULATIONS ON THE STRUCTURE AND NATURE OF THE HYDROGEN-BONDED COMPLEX H₂S ... HF

Journal of Chemical Physics, (80): 353-355 1984.

Smits, G. F.; Krol, M. C.; Altona, C.

THEORETICAL INVESTIGATIONS ON THE NATURE OF INTRAMOLECULAR INTERACTIONS .3. APPLICATION OF THE ENERGY DECOMPOSITION SCHEME TO THE STUDY OF THE ANOMERIC EFFECT IN CH₃CH₂OH, NH₂CH₂OH, HOCH₂OH AND FCH₂OH

Molecular Physics, (65): 513-529 1988.

Sowa, T.; Kawamura, T.; Yamabe, T.; Yonezawa, T.

ELECTRON-SPIN RESONANCE OF RE₂(MU-H)₂(CO)₈⁻. AND RE₂(MU-H)₂(CO)₆(MU-(PH₂P)CH₂)⁻ - AN INDICATION OF LARGE 5D-6P MIXING IN THE ODD-ELECTRON ORBITAL

Journal of the American Chemical Society, (107): 6471-6475 1985.

Spackman, M. A.

A SIMPLE QUANTITATIVE MODEL OF HYDROGEN-BONDING

Journal of Chemical Physics, (85): 6587-6601 1986.

Spackman, M. A.

A SIMPLE QUANTITATIVE MODEL OF HYDROGEN-BONDING - APPLICATION TO MORE COMPLEX-SYSTEMS

Journal of Physical Chemistry, (91): 3179-3186 1987.

Stams, D. A.; Thomas, T. D.; Maclaren, D. C.; Ji, D.; Morton, T. H.

EMPIRICAL AND ABINITIO ESTIMATES OF THE STABILITIES OF FLUORINE-CONTAINING CATIONS

Journal of the American Chemical Society, (112): 1427-1434 1990.

Steinke, T.; Hansele, E.; Clark, T.

THE SOLVENT EFFECT ON THE ELECTRONIC NATURE OF 1,3-DIPOLES - AN ABINITIO SCRF STUDY

Journal of the American Chemical Society, (111): 9107-9109 1989.

Stevens, W. J.; Fink, W. H.

FROZEN FRAGMENT REDUCED VARIATIONAL SPACE ANALYSIS OF HYDROGEN-BONDING INTERACTIONS - APPLICATION TO THE WATER DIMER

Chemical Physics Letters, (139): 15-22 1987.

Streitwieser, A.; Vorpagel, E. R.

ELECTRON-DENSITY ANALYSIS OF SUBSTITUENT EFFECTS IN SUBSTITUTED BENZENES

Collection of Czechoslovak Chemical Communications, (53): 1961-1980 1988.

Stucky, G. D.; Eddy, M. M.; Harrison, W. H.; Lagow, R.; Kawa, H.; Cox, D. E.

SOME OBSERVATIONS CONCERNING THE STRUCTURE OF DILITHIOMETHANE

Journal of the American Chemical Society, (112): 2425-2427 1990.

Sundberg, P.; Larsson, R.; Folkesson, B.
ON THE CORE ELECTRON-BINDING ENERGY OF CARBON AND THE EFFECTIVE CHARGE OF THE CARBON-ATOM
Journal of Electron Spectroscopy and Related Phenomena, (46): 19-29 1988.

Surjan, P. R.
THE REPRESENTATION OF THE CHEMICAL-BOND IN QUANTUM CHEMICAL CALCULATIONS
Croatica Chemica Acta, (57): 833-854 1984.

Surjan, P. R.
THE ROLE OF HYBRIDIZATION IN PERTURBATIVE BOND THEORIES - THE EXISTENCE OF EXACT STRICTLY LOCALIZED ORBITALS IN SMALL MOLECULES
Theochem-Journal of Molecular Structure, (46): 95-104 1988.

Thomas, R. D.; Clarke, M. T.; Young, T. C.
C-13 CHEMICAL-SHIFT SUBSTITUENT PARAMETERS FOR ALKYL-LITHIUM COMPOUNDS IN HYDROCARBON SOLVENTS
Journal of Organometallic Chemistry, (328): 239-248 1987.

Thomas, T. D.; Siggel, M. R. F.; Saethre, L. J.
CORE-IONIZATION ENERGIES AND CHEMICAL-PROPERTIES
Journal of Electron Spectroscopy and Related Phenomena, (51): 417-438 1990.

Ugliengo, P.; Saunders, V. R.; Garrone, E.
SILANOL AS A MODEL FOR THE FREE HYDROXYL OF AMORPHOUS SILICA - ABINITIO CALCULATIONS OF THE INTERACTION WITH FORMALDEHYDE
Chemical Physics Letters, (169): 501-508 1990.

Vedejs, E.; Dent, W. H.
AN EVALUATION OF SIGMA-SIGMA-STAR AND TORSIONAL EFFECTS IN THE OSMYLATION AND EPOXIDATION OF 4-TERT-BUTYLMETHYLENECYCLOHEXANE DERIVATIVES
Journal of the American Chemical Society, (111): 6861-6862 1989.

Weinhold, F.; Carpenter, J. E.
SOME REMARKS ON NONORTHOGONAL ORBITALS IN QUANTUM-CHEMISTRY
Theochem-Journal of Molecular Structure, (42): 189-202 1988.

Weiss, E.; Lambertsen, T.; Schubert, B.; Cockcroft, J. K.; Wiedenmann, A.
METAL ALKYL AND ARYL COMPOUNDS .40. STRUCTURE REFINEMENT OF METHYL LITHIUM BY NEUTRON-DIFFRACTION OF (LiCD₃)₄ AT 1.5-K AND 290-K
Chemische Berichte, (123): 79-81 1990.

Williams, D. E.
REPRESENTATION OF THE MOLECULAR ELECTROSTATIC POTENTIAL BY ATOMIC MULTIPOLE AND BOND DIPOLE MODELS
Journal of Computational Chemistry, (9): 745-763 1988.

Wong, S. S.; Paddonrow, M. N.

THEORETICAL EVIDENCE IN SUPPORT OF THE ANH-EISENSTEIN ELECTRONIC MODEL IN CONTROLLING PI-FACIAL STEREOSELECTIVITY IN NUCLEOPHILIC ADDITIONS TO CARBONYL-COMPOUNDS

Journal of the Chemical Society-Chemical Communications: 456-458 1990.

Yadav, L. S.; Yadav, J. S.

BOND ORDER AND VALENCE - ANALOGY BETWEEN THE MAYER AND THE EIGENVALUE TREATMENTS

Theochem-Journal of Molecular Structure, (42): 289-295 1988.

Yang, C.

THE 6 DECADES OF THE HYBRID CONCEPT

Theochem-Journal of Molecular Structure, (46): 1-31 1988.