Acronyms in Quantum Chemistry (March 2001)

AH	Alternating Hydrocarbon
AIM	Atoms in Molecules, W.Moffitt, Proc.Roy.Soc. (London), **A210**, 245 (1951)
AM1	Austin Model 1, newly parametrized MNDO version, M.J.S.Dewar, E.G.Zoebisch, E.F.Healy, J.J.P.Stewart, J.Am.Chem.Soc. **107**, 3902 (1985)
AMO	Antibonding MO
AO	Atomic Orbital
ASMO	Antisymmetrized MO, B3
BIGGMOLI	ab initio program name
BLYP	Functional in DFT
B3LYP	Functional in DFT
BMO	Bonding MO
BO	Born-Oppenheimer (-Approximation)
BSSE	Basis Set Superposition Error, D2
CADPAC	ab initio program name (CAMbridge Derivative PAckage)
CASSCF	Complete Active Space SCF (Version of MCSCF)
CC	Coupled Cluster, R.J. Bartlett, Ann.Rev.Phys.Chem. **32**, 359 (1981)
cc	correlation consistent, T. H. Dunning, J.Chem.Phys. **90**, 1007 (1989)
CEPA	Coupled Electron Pair Approximation, D2, W.Meyer, J.Chem.Phys. **58**,1017 (1973), Int.J.Quantum Chem. **S5**, 341 (1971)
CGTF	Contracted GTF (=CGTO), D
CGTO	Contracted GTO (=CGTF), D
CHF	Coupled Hartree-Fock method, D3, R.M.Stevens, R.M.Pitzer, W.N.Lipscomb, J.Chem.Phys. **38**, 550 (1963), R.Mc Weeney, Phys.Rev.**126**, 1028 (1962)
CI	Configuration Interaction, A,D
CI-SD	CI with all Singly and Doubly Excited Configurations, D2,D3
CI-SDQ	CI-SD with all Quadruply Excited Configurations, D2
CNDO	Complete Neglect of Differential Overlap, C
CNDO/1	CNDO, 1.Version, C, J.A.Pople, D.P.Santry, G.A.Segal, J.Chem.Phys. **43**, S129 (1965), J.A.Pople, G.A.Segal, J.Chem.Phys. **43**, S136 (1965)
CNDO/2	CNDO, 2.Version, C, J.A.Pople, G.A.Segal, J.Chem.Phys. **44**, 3289 (1966),
CNDO/S	CNDO parametrized for spectra (including correlation), J.Del Bene, H.H.Jaffe, J.Chem.Phys. **48**, 1807 (1968)
CMO	Canonical MO, A
CPHF	Coupled Perturbed Hartree-Fock, J.Gerratt, I.M.Mills, J.Chem.Phys. **49**, 1719 (1968), Y.Osamura, Y.Yamaguchi, P.Saxe, M.A.Vincent, J.F.Gaw, H.F.Schaefer, Chem.Phys. **72**, 131 (1982)
CPMET	Coupled Pair MET, D2, J.Cizek, J.Chem.Phys. **45**, 4256 (1966)
DE	Delocalisation Energy, B
DFT	Density Functional Theory, G. Parr, W. Yang, "Density-functional theory of atoms and molecules", Clarendon, Oxford 1989
DIIS	Direct Inversion of the Iterative Subspace (convergence accelerator)
DIM	Diatomics in Molecules, F.O.Ellison, J.Am.Chem.Soc. **85**, 3540 (1963), J.C.Tully, J.Chem.Phys. **58**,1396 (1973), E.Steiner, P.R.Certain, P.J.Kuntz, J.Chem.Phys. **59**, 47 (1973)
DODS	Different Orbitals for Different Spins (=UHF), A
DZ	Double-Zeta Basis Set , A, D
DZ+P	DZ plus Polarization Basis Set, A, D
ECP	Effective Core Potential, L.R.Kahn, P.Baybutt, D.G.Truhlar, J.Chem.Phys. **65**, 3826 (1976)
ECPMET	Extended CPMET, D2, J.Paldus, J.Cizek, I.Shavitt, Phys.Rev. **A5**, 50 (1972)
EFV	Electric Field Variant (Basis Set), A.J.Sadlej, Chem.Phys.Letters **47**, 50 (1977)
EHT	Extended Hueckel Theory, A, R.Hoffmann, J.Chem.Phys. **39**, 1397(1963), S.Z.Engelke, Ch.L.Beckel, Int.J.Quant.Chem. **Symp. 8**, 209 (1974)
EMZDO	Exchange Modified ZDO, R.N.Dixon, Mol.Phys.**12**, 83 (1967)
EPCE	Effective Pair Correlation Energy, D2, O.Sinanoglu, H.Oe.Pamuk, Theor.Chim.Acta **27**, 289 (1972)
EPCE-F2	EPCE with F2-approximation extended to skeleton, H.O.Pamuk, Theor.Chim.Acta **28**, 85 (1972), O.Sinanoglu, H.O.Pamuk, J.Am.Chem.Soc. **95**, 5435 (1973)
EPV	Exclusion Principle Violating, D2,
FE	Frees Electron
FIM	Fragments-in-Molecules, M.Klessinger, Theor.Chim.Acta **49**, 77 (1978)
FOGO	Floating Orbital Geometry Optimization, H.Huber, Chem.Phys.Letters **62**, 95 (1979), Theor.Chim.Acta **55**, 117 (1980)
FORS	Full Optimized Reaction Space, D.F.Feller, M.W.Schmidt, K.J.Ruedenberg, J.Am.Chem.Soc. **104**, 960 (1982)
FP-INDO	Finite Perturbation INDO, G.E.Maciel,J.W.Mc Iver, N.S.Ostlund, J.A.Pople, J.Am.Chem.Soc. **92**, 1 (1970)
FRC	Frozen Core, M.Jungen, Theor.Chim.Acta **60**, 369 (1981)
FSGO	Floating Spherical Gaussian Orbitals, D2, D3, A.A.Frost, J.Chem.Phys. **47**, 3707, 3714 (1967), A.A.Frost, R.A.Rouse, L.Vescelius, nt.J.Quant.Chem. **2S**, 43 (1968)
G2	GAUSSIAN-2, L.A.Curtiss, K.Raghavachari, G.W.Trucks, J.A.Pople, J.Chem.Phys. **94**, 7221 (1991)
GAUSSIAN	ab initio program name
GGA	Generalized Gradient Approach (DFT approximation)
GIAO	Gauge Invariant AO, R.Ditchfield, J.Chem.Phys. **56**, 5688 (1972)
GTF	Gaussian Type Function (=GTO), A, D
GTO	Gaussian Type Orbital (=GTF), A, D
GVB	Generalized VB
HAM	Hydrogenic Atoms in Molecules, L.Asbrink, C.Fridh, E.Lindholm, Chem.Phys.Letters **52**, 63, 69, 72 (1977), **66**, 411(1979)
HF	Hartree-Fock, A, C, D
HFR	HF-Roothaan, A, C, D
HMO	Hueckel Molecular Orbital Method, A, B, E.Hueckel, Z.Physik, **70**, 204 (1931), **72**, 310 (1931), **76**, 628 (1932)
HOMO	Highest Occupied MO
HONDO	ab initio program name, D2, M.Dupuis, J.Rys, H.F.King, J.Chem.Phys. **65**, 111 (1976)
IBMOL	ab initio program name, D2
IEPA	Independent Electron Pair Approximation, D2, R.Ahlrichs, H.Lischka, V.Staemmler, W.Kutzelnigg, J.Chem. Phys. **62**, 1225 (1975), M.Jungen, R.Ahlrichs, Theor.Chim. Acta **17**, 339 (1970)
IGLO	Individual Gauge for Localized Orbitals, Method for the Calculation of NMR-Shifts, W.Kutzelnigg, U.Fleischer, M.Schindler, in "NMR, Basic Principles and Progress 23", ed. P.Diehl et.al., Springer, Berlin, 1991
IMOA	Iterative Maximum Overlap Approximation, A, Z.B.Maksic, K.Kovacevic, A.Mogus, Theor.Chim.Acta **55**, 127 (1980)
INDO	Intermediate Neglect of Differential Overlap, A, C, J.A.Pople, D.L.Beveridge, P.A.Dobosh, J.Chem.Phys. **47**, 2026 (1967)
INDO/S	INDO parametrized for spectra (including correlation), J.Ridley, M.Zerner, Theor.Chim.Acta **32**, 111 (1973)
INO	Iterative Natural Orbital Method, D2, C.F.Bender, E.R.Davidson, J.Phys.Chem. **70**, 2675 (1966)
IRDO	Intermediate Retention of Differential Overlap, C3
IVO	Improved Virtual Orbitals (s.a. FRC), W.Hunt,W.J.Goddard, Chem.Phys.Letters **3**, 414 (1969)
KS	Kohn-Sham (-orbitals or theory; -> DFT)
LCAO	Linear Combination of AO's
LCBO	Linear Combination of Bond Orbitals, A, G.G.Hall, Proc.Roy.Soc. (London) **A205**,

LCBO	Linear Combination of Bond Orbitals, A, G.G.Hall, Proc.Roy.Soc. (London) **A205**, 541 (1951)
LCMO	Linear Combination of MO's, B1,C2, M.J.S.Dewar, Proc.Cambridge Phil.Soc. **45**, 639 (1949)
LDA	Local Densitiy Approximation (DFT approximation)
LEMAOnG	Least Energy Minimal Atomic Orbitals (Basis Set), R.Ditchfield, W.J.Hehre, J.A.Pople, J.Chem.Phys. **52**, 5001(1970)
LMO	Localized MO, W.England, L.S.Salmon, K.Ruedenberg, Fortschr.chem.Forschung **23**, 31 (1971), S.F.Boys, Rev.mod.Phys. **32**, 296 (1960), W.v.Niessen, J.Chem.Phys. **56**, 4290 (1972), Theor.Chim.Acta **27**, 9 (1972)
LNDO/S	Local Neglect of Differential Overlap (including correlation), G.Lauer, K.W.Schulte, A.Schweig, J.Am.Chem.Soc. **100**, 4925 (1978)
LO	Localized Orbital (s.a. LMO), C2
LSD	Local Spin Density (DFT approximation)
LSDA	Local Spin Density Approximation (DFT approximation)
LUMO	Lowest Unoccupied MO
MAO	Modified AO, R.Heinzmann, R.Ahlrichs, Theor.Chim.Acta **42**, 33 (1976)
MB	Minimal Basis, A, D
MBPT	Many Body Perturbation Theory, D3, J.Goldstone, Proc.Roy.Soc.(London) **A239**, 267 (1957), H.P.Kelly, Advan.Chem.Phys. **14**, 129 (1969)
MB-RSPT	Many Body Raleigh-Schroedinger Perturbation Theory, D2, I.Hubac, P.Carsky, Fortschr.chem.Forschung **75**, 97 (1978)
MCSCF	Multi Configuration SCF, D2, D3, D.R.Hartree, W.Hartree, B.Swirles, Phil.Trans.Roy.Soc. (London) **A238**, 229 (1939)
MET	Many Electron Theory, D2, O.Sinanoglu, J.Chem.Phys. **36**, 706 (1962)
MINDO	Modified INDO (s.a. MINDO/1) A, C2, C3
MINDO/1	1.Version of MINDO, N.C.Baird, M.J.S.Dewar, J.Chem.Phys. **50**, 1262 (1969)
MINDO/2	2.Version of MINDO, M.J.S.Dewar, E.Haselbach, J.Am.Chem.Soc. **92**, 590 (1970)
MINDO/3	3.Version of MINDO, R.C.Bingham, M.J.S.Dewar, D.H.Lo, J.Am.Chem.Soc. **97**, 1285 (1975)
MIM	Molecules-in-Molecules, W.von Niessen, J.Chem.Phys. **55**, 1948 (1971)
MM	Molecular Mechanics; not a quantum chemial method. (Force-Field-Calculations)
MNDDO	Modified NDDO (s.MNDO)
MNDO	Modified Neglect of Diatomic Overlaps (New name for MNDDO), A , M.J.S.Dewar, W.Thiel, J.Am.Chem.Soc. **99**, 4899, 4907 (1977); Extension to d-orbitals: W.Thiel, A.A. Voitynk, J.Phys.Chem. **100**, 616 (1996)
MNDOC	MNDO including correlation (as 2. order perturbation), W.Thiel, J.Am.Chem.Soc. **103**, 1413, 1420, 1425 (1981)
MO	Molecular Orbital
MP	Moeller-Plesset (-Störungsrechnung), A, C2, C3, C.Moeller, M.S.Plesset, Phys.Rev. **46**, 618 (1934)
MRCI	Multi-Reference CI
MS X	Multiple Scattering X, (Semiempirical Method), J.C.Slater, The SCF for Molecules and Solids, Vol.4, McGraw Hill, N.Y., 1974, Phys.bibl.Th175, K.H.Johnson, Adv.Quant.Chem. **7**, 143 (1973)
NAH	Non-AH
NBMO	Non-Bonding MO
NBO	Natural Bond Orbitals, A.E. Reed, L.A. Curtiss, F.Weinhold, Chem.Rev. 88, 899 (1988)
NDDO	Neglect of Diatomic Differential Overlap, A, C
NO	Natural Orbital, A
OAO	Orthogonal AO's, A
OCE	One Center Expansions
ω-Methode	A, B3, C2, G.W.Wheland, D.W.Mann, J.Chem.Phys.17,264(1949)
PCILO	Perturbational CI of LO's, A , S.Diner, J.P.Malrieu, F.Jordan, M.Gilbert, Theor.Chim.Acta **15**, 100 (1969)
	Theor.Chim.Acta **15**, 100 (1969)
PERTCI	CI and second order Brillouin-Wigner PERTurbation, H-L.Hase, G.Lauer, K-W.Schulte, A.Schweig, Theor.Chim.Acta **48**, 47 (1978)
PES	Potential Energy Surface
PHANTOM	ab initio program name D2
PM3	J.J.P.Stewart, J.Comp.Chem.**10**, 209, 221 (1989)
PMO	Perturbational MO Method (perturbation calculation, usually used for a specially simplified version by Dewar), A, C2
PNDO	Partial Neglect of Differential Overlap, C2, C3, M.J.S.Dewar, G.Klopman, J.Am.Chem.Soc. **89**, 3089 (1967)
PNO	Pair NO (=PSNO), A, D2, D3, C.Edmiston, M.Krauss, J.Chem.Phys. **45**, 1833 (1966), W.Meyer, Int.J.Quant.Chem. **S5**, 341 (1971)
POLYATOM	ab initio program name, D2
POLYCAL	STO-Integral-Program Name, D2, R.M.Stevens, J.Chem.Phys. **52**, 1397 (1970)
PPP	Pariser-Parr-Pople Method, A, C2, C3
PRDDO	Partial Retention of Diatomic Differential Overlap, T.A.Halgren, W.N.Lipscomb, J.Chem.Phys. **58**, 1569 (1973)
PSNO	Pseudo NO (=PNO)
PUHF	Projected UHF, D3, W.A.Goddard, Phys.Rev. **182**, 48 (1969)
QCPE	Quantum Chemical Program Exchange
QM/MM	Quanten Mechanics combined with Molecular Mechanics, M.J. Field, P.A. Bash, M. Karplus, J.Comp.Chem. **11**, 700 (1990)
REPE	Resonance Energy per Electron, B.A.Hess, L.J.Schaad, J.Am.Chem.Soc. **93**, 305 (1971)
RHF	Restricted HF Method, A, C, D
SAMO	Simulated ab initio MO, J.E.Eilers, D.R.Whitman, J.Am.Chem.Soc. **95**, 2067 (1973), B.J.Duke, B.O'Leary, J.Chem.Phys. **79**, 3424 (1983)
S.C.E.	Self Consistent Electronegativity (=VESCF)
SCF	Self Consistent Field, A, C, D
SEHF	Spin Extended HF, D3, W.A.Goddard, Phys.Rev. **182**, 48 (1969)
SD-CI	(=CI-SD)
SDQ-CI	(=CI-SDQ)
SINDO	Symmetrically Orthogonalized INDO, P.Coffey, K.Jug, J.Am.Chem.Soc. **95**, 7575 (1973)
SINDO1	New Version of SINDO, K.Jug,D.N.Nanda, Theor.Chim.Acta **57**, 95, 107, 131 (1980)
SOHF	Spin Optimized HF, D3, U.Kaldor, F.E.Harris, Phys.Rev. **183**, 1 (1969)
SPINDO	Spectroscopic Potentials adjusted INDO, L.Asbrink, C.Fridh, E.Lindholm, J.Am.Chem.Soc. **94**, 5501 (1972)
SPO	Split-p-Orbital, C2, M.J.S.Dewar, N.L.Hojvat, J.Chem.Phys. **34**, 1232 (1961), M.J.S.Dewar, N.L.Sabelli, J.Chem. Phys. **36**, 2310 (1962)
STO	Slater Type Orbital
STO-nG	n=2,3,4,5,6 Basis of STO's expanded by n Gaussian functions, A, D2
SUHF	Spin UHF (=UHF)
SV	Split Valence (Basis), D2
SZO	Slater-Zener-Orbitals (=STO)
TEXAS	ab initio program name
UHF	Unrestricted HF, A, C, D
VB	Valence Bond Method, A
VESCF	Variable Electronegativity SCF, C3, R.D.Brown, M.L.Heffernan, Trans.Farad.Soc. **54**, 757 (1958)
WF	Wave function
X	(= MS X)
ZDO	Zero Differential Overlap, A, C