Full List of Keywords Used in MOPAC Version 6

&	Turn next line into keywords
+	Add another line of keywords
0SCF	Read in data, then stop
1ELECTRON	Print final one-electron matrix
1SCF	Do one SCF and then stop
AIDER	Read in ab initio derivatives
AIGIN	Geometry must be in gaussian format
AIGOUT	In arc file, include ab-initio geometry
ANALYT	Use analytical derivatives of energy W.R.T. geometry
AM1	Use the AM1 Hamiltonian
BAR=N.N	Reduce bar length by a maximum of N.N
BIRADICAL	System has two unpaired electrons
BONDS	Print final bond-order matrix
C.I.	A multi-electron configuration interaction specified
CHARGE=N	Charge on system = N (e.g. NH4 => CHARGE=1)
COMPFG	Print heat of formation calculated in COMPFG
CONNOLLY	Use Connolly surface
DEBUG	Debug option turned on
DENOUT	Density matrix output (channel 10)
DENSITY	Print final density matrix
DEP	Generate Fortran code for parameters for new elements
DEPVAR=N	Translation vector is a multiple of bond-length
DERIV	Print part of working in deriv
DFORCE	Force calculation specified, also print force matrix.
DFP	Use Davidon-Fletcher-Powell method to optimize geometry
DIPOLE	Fit the ESP to the calculated dipole
DIPX	X component of dipole to be fitted
DIPY	Y component of dipole to be fitted
DIPZ	Z component of dipole to be fitted
DMAX	Maximum stepsize in eigenvector following
DOUBLET	Doublet state required
DRC	Dynamic reaction coordinate calculation
DUMP=N	Write restart files every N seconds
ECHO	Data are echoed back bEFore calculation starts
EF	Use EF routine for minimum search
EIGINV	

EIGS	Print all eigenvalues in iter
ENPART	Partition energy into components
ESP	Electrostatic potential calculation
ESPRST	Restart of electrostatic potential
ESR	Calculate RHF unpaired spin density
EXCITED	Optimize first excited singlet state
EXTERNAL	Read parameters off disk
FILL=N	In RHF open and closed shell, force m.o. N to be filled
FLEPO	Print details of geometry optimization
FMAT	Print details of working in FMAT
FOCK	Print last Fock matrix
FORCE	Force calculation specified
GEO-OK	Override interatomic distance check
GNORM=N.N	Exit when gradient norm drops below N.N
GRADIENTS	Print all gradients
GRAPH	Generate file for graphics
HCORE	Print details of working in HCORE
HESS=N	Options for calculating Hessian matrices in EF
H-PRIO	Heat of formation takes priority in DRC
HYPERFINE	Hyperfine coupling constants to be calculated
IRC	Intrinsic reaction coordinate calculation
ISOTOPE	Force matrix written to disk (channel 9)
ITER	Print details of working in ITER
ITRY=N	Set limit of number of SCF iterations to N.
IUPD	Mode of Hessian update in eigenvector following
K=(N,N)	Brillouin zone structure to be calculated
KINETIC	Excess kinetic energy added to DRC calculation
LINMIN	Print details of line minimization
LARGE	Print expanded output
LET	Override certain safety checks
LOCALIZE	Print localized orbitals
MAX	Prints maximum grid size (23*23)
MECI	Print details of MECI calculation
MICROS	Use specific microstates in the C.I.
MINDO/3	Use the MINDO/3 Hamiltonian
MMOK	Use molecular mechanics correction to CONH bonds
MODE=N	In EF, follow Hessian mode no. N

MOLDAT	Print details of working in MOLDAT
MS=N	In MECI, magnetic component of spin
MULLIK	Print the Mulliken population analysis
NLLSQ	Minimize gradients using NLLSQ
NOANCI	Do not use analytical C.I. derivatives
NODIIS	Do not use DIIS geometry optimizer
NOINTER	Do not print interatomic distances
NOLOG	Suppress log file trail, where possible
NOMM	Do not use molecular mechanics correction to CONH bond
NONR	
NOTHIEL	Do not use thiel's FSTMIN technique
NSURF=N	Number of surfaces in an ESP calculation
NOXYZ	Do not print cartesian coordinates
NSURF	Number of layers used in electrostatic potential
OLDENS	Read initial density matrix off disk
OLDGEO	Previous geometry to be used
OPEN	Open-shell RHF calculation requested
ORIDE	
PARASOK	In AM1 calculations some MNDO parameters are to be use
PI	Resolve density matrix into sigma and pi bonds
PL	Monitor convergence of density matrix in iter
PM3	Use the MNDO-PM3 Hamiltonian
POINT=N	Number of points in reaction path
POINT1=N	Number of points in first direction in grid calculatio
POINT2=N	Number of points in second direction in grid calculati
POLAR	Calculate first, second and third order polarizabiliti
POTWRT	In ESP write out electrostatic potential to unit 21
POWSQ	Print details of working in POWSQ
PRECISE	Criteria to be increased by 100 times
PULAY	Use pulay's converger to obtain a SCF
QUARTET	Quartet state required
QUINTET	Quintet state required
RECALC=N	In EF, recalculate Hessian every n steps
RESTART	Calculation restarted
ROOT=N	Root N to be optimized in a C.I. calculation
ROT=N	The symmetry number of the system is n.
SADDLE	Optimize transition state

SCALE	Scaling factor for van der waals distance in esp
SCFCRT=N	Default SCF criterion replaced by the value supplied
SCINCR	Increment between layers in esp
SETUP	Extra keywords to be read of setup file
SEXTET	Sextet state required
SHIFT=N	A damping factor of n defined to start SCF
SIGMA	Minimize gradients using sigma
SINGLET	Singlet state required
SLOPE	Multiplier used to scale MNDO charges
SPIN	Print final UHF spin matrix
STEP	Step size in path
STEP1=N	Step size N for first coordinate in grid calculation
STEP2=N	Step size N for second coordinate in grid calculation
STO-3G	Deorthogonalize orbitals in STO-3G basis
SYMAVG	Average symmetry equivalent esp charges
SYMMETRY	Impose symmetry conditions
T=N	A time of n seconds requested
THERMO	Perform a thermodynamics calculation
TIMES	Print times of various stages
T-PRIO	Time takes priority in DRC
TRANS	The system is a transition state (used in thermodynamics calculation)
TRIPLET	Tiplet state required
TS	Using EF routine for TS search
UHF	Unrestricted Hartree-Fock calculation
VECTORS	Print final eigenvectors
VELOCITY	Supply the initial velocity vector in a DRC calculatio
WILLIAMS	Use Williams surface
X-PRIO	Geometry changes take priority in DRC
XYZ	Do all geometric operations in cartesian coordinates.