|  |  |
| --- | --- |
| **1.** | **Index of Function & Subroutine Calls** |

This section contains an alphabetical cross index listing of the routines called by each TINKER program, subroutine and function. Routines not present in this list do not make calls to any other portion of the TINKER package.

**Routine List of Source Code Units called by this Routine**

**ACTIVE** GETTEXT UPCASE

**ADDBASE** ADDBOND FINDATM JACOBI NEWATM OLDATM OVERLAP PIALTER PIMOVE PITILT

**ADDSIDE** ADDBASE ADDBOND FATAL FINDATM FREEUNIT JACOBI NEWATM OLDATM OVERLAP PIALTER PIMOVE PITILT PRTSEQ VERSION

**ALCHEMY** ENERGY FINAL FREEUNIT GETTEXT GETXYZ HATOM HYBRID INITIAL MECHANIC NUMERAL READXYZ UPCASE VERSION

**ANALYSIS** BOUNDS EANGANG3 EANGLE3 EBOND3 EBUCK3 ECHARGE3 ECHGDPL3 EDIPOLE3 EGAUSS3 EGEOM3 EHAL3 EIMPROP3 EIMPTOR3 ELJ3 EMETAL3 EMM3HB3 EMPOLE3 EOPBEND3 EOPDIST3 EPITORS3 ERXNFLD3 ESOLV3 ESTRBND3 ESTRTOR3 ETORS3 ETORTOR3 EUREY3 EXTRA3 PISCF REPLICA

**ANALYZE** ANALYZ4 ANALYZ6 ANALYZ8 ATOMYZE ENRGYZE FINAL FREEUNIT GETXYZ INITIAL MECHANIC NEXTARG PARAMYZE PROPYZE READXYZ SUFFIX TRIMTEXT UPCASE VERSION

**ANGLES** FATAL

**ANNEAL** BEEMAN FINAL GETTEXT GETXYZ INITIAL MDINIT MDREST MECHANIC NEXTARG RGDSTEP SDSTEP SHAKEUP SIGMOID UPCASE VERLET

**ARCHIVE** ACTIVE BASEFILE FINAL FREEUNIT GETTEXT INITIAL NEXTARG NUMERAL PRTARC PRTCAR PRTXMOL PRTXYZ READXYZ SUFFIX TRIMTEXT UPCASE VERSION

**ATTACH** FATAL SORT

**BASEFILE** CONTROL GETKEY TRIMTEXT

**BCUINT** BCUCOF

**BCUINT1** BCUCOF

**BCUINT2** BCUCOF

**BEEMAN** GRADIENT KINETIC MDSAVE MDSTAT PRESSURE RATTLE RATTLE2 TEMPER TEMPER2

**BETAI** BETACF GAMMLN

**BIGBLOCK** CELLATOM

**BITORS** FATAL

**BONDS** FATAL

**BORN** SURFATOM

**BSET** BMAX

**BSSTEP** FATAL MMID PZEXTR

**CALENDAR** DATE\_AND\_TIME

**CERROR** FATAL TRIMTEXT

**CFFTB** CFFTB1

**CFFTB1** PASSB PASSB2 PASSB3 PASSB4 PASSB5

**CFFTF** CFFTF1

**CFFTF1** PASSF PASSF2 PASSF3 PASSF4 PASSF5

**CFFTI** CFFTI1

**CHKTREE** LOCALXYZ

**CIRPLN** ANORM DOT VCROSS VNORM

**CLIMBER** ENERGY GETREF LOCALMIN MAKEINT MAKEXYZ

**CLIMBRGD** ENERGY LOCALRGD RIGIDXYZ

**CLIMBROT** ENERGY LOCALROT MAKEXYZ

**CLIMBTOR** CHKTREE ENERGY GETREF LOCALXYZ MAKEINT MAKEXYZ

**CLIMBXYZ** CHKTREE ENERGY GETREF LOCALXYZ

**CLUSTER** CUTOFFS FATAL GETNUMB GETTEXT SORT SORT3 UPCASE

**COMMAND** GETARG UPCASE

**COMPRESS** CERROR GETTOR

**CONNECT** SORT

**CONNOLLY** COMPRESS CONTACT NEIGHBOR PLACE SADDLES TORUS VAM

**CONTACT** ANORM CERROR PTINCY

**CONTROL** GETTEXT UPCASE

**COORDS** GYRATE RMSERROR

**CORRELATE** FINAL INITIAL NEXTARG PROPERTY READBLK TRIMTEXT

**CRYSTAL** BIGBLOCK BOUNDS FIELD FINAL FREEUNIT GETTEXT GETXYZ INITIAL KATOM LATTICE MOLECULE NEXTARG PRTXYZ SYMMETRY UNITCELL UPCASE VERSION

**CUTOFFS** GETTEXT UPCASE

**CYTSY** CYTSYP CYTSYS

**DEPTH** DOT VCROSS VNORM

**DIAGQ** GETIME SETIME

**DIFFEQ** BSSTEP GDASTAT GVALUE

**DIFFUSE** BASEFILE FATAL FIELD FINAL FREEUNIT INITIAL KATOM MOLECULE NEXTARG READXYZ SUFFIX UNITCELL VERSION

**DISTGEOM** ACTIVE ANGLES ATTACH BONDS EMBED FATAL FINAL FREEUNIT GEODESIC GETIME GETTEXT GETXYZ GRAFIC IMPOSE INITIAL KCHIRAL KGEOM MAKEREF NEXTARG NUMERAL PRTXYZ SETIME TORSIONS TRIFIX UPCASE VERSION

**DMDUMP** GRAFIC

**DOCUMENT** FINAL FREEUNIT GETPRM GETTEXT GETWORD INITIAL LOWCASE NEXTARG NEXTTEXT PRTPRM SORT10 SORT6 SORT7 SUFFIX TRIMTEXT UPCASE VERSION

**DSTMAT** GETIME GETNUMB GETTEXT INVBETA RANDOM SETIME SORT2 TRIFIX UPCASE

**DYNAMIC** BEEMAN FINAL GETXYZ INITIAL MDINIT MDREST MECHANIC NEXTARG RGDSTEP SDSTEP SHAKEUP VERLET

**EANGANG** GROUPS IMAGE

**EANGANG1** GROUPS IMAGE

**EANGANG2** EANGANG2A GROUPS

**EANGANG2A** IMAGE

**EANGANG3** GROUPS IMAGE

**EANGLE** GROUPS IMAGE

**EANGLE1** GROUPS IMAGE

**EANGLE2** EANGLE2A EANGLE2B GROUPS

**EANGLE2A** GROUPS IMAGE

**EANGLE2B** IMAGE

**EANGLE3** GROUPS IMAGE

**EBOND** GROUPS IMAGE

**EBOND1** GROUPS IMAGE

**EBOND2** GROUPS IMAGE

**EBOND3** GROUPS IMAGE

**EBUCK** EBUCK0A EBUCK0B EBUCK0C FATAL

**EBUCK0A** GROUPS IMAGE SWITCH

**EBUCK0B** GROUPS LIGHTS SWITCH

**EBUCK0C** EGAUSS

**EBUCK1** EBUCK1A EBUCK1B EBUCK1C FATAL

**EBUCK1A** GROUPS IMAGE SWITCH

**EBUCK1B** GROUPS LIGHTS SWITCH

**EBUCK1C** EGAUSS1

**EBUCK2** EBUCK2A EBUCK2B FATAL

**EBUCK2A** GROUPS IMAGE SWITCH

**EBUCK2B** EGAUSS2

**EBUCK3** EBUCK3A EBUCK3B EBUCK3C FATAL

**EBUCK3A** GROUPS IMAGE SWITCH

**EBUCK3B** GROUPS LIGHTS SWITCH

**EBUCK3C** EGAUSS3

**ECHARGE** ECHARGE0A ECHARGE0B ECHARGE0C ECHARGE0D ECHARGE0E

**ECHARGE0A** GROUPS IMAGE SWITCH

**ECHARGE0B** GROUPS LIGHTS SWITCH

**ECHARGE0C** ERF GROUPS

**ECHARGE0D** EPME ERFC GROUPS IMAGE SWITCH

**ECHARGE0E** EPME ERFC GROUPS LIGHTS SWITCH

**ECHARGE1** ECHARGE1A ECHARGE1B ECHARGE1C ECHARGE1D

**ECHARGE1A** GROUPS IMAGE SWITCH

**ECHARGE1B** GROUPS LIGHTS SWITCH

**ECHARGE1C** ERF GROUPS

**ECHARGE1D** EPME1 ERFC GROUPS IMAGE SWITCH

**ECHARGE2** ECHARGE2A ECHARGE2B ECHARGE2C

**ECHARGE2A** GROUPS IMAGE SWITCH

**ECHARGE2B** ERF GROUPS

**ECHARGE2C** ERFC GROUPS IMAGE

**ECHARGE3** ECHARGE3A ECHARGE3B ECHARGE3C ECHARGE3D ECHARGE3E

**ECHARGE3A** GROUPS IMAGE SWITCH

**ECHARGE3B** GROUPS LIGHTS SWITCH

**ECHARGE3C** ERF GROUPS

**ECHARGE3D** EPME3 ERFC GROUPS IMAGE SWITCH

**ECHARGE3E** EPME3 ERFC GROUPS LIGHTS SWITCH

**ECHGDPL** GROUPS IMAGE SWITCH

**ECHGDPL1** GROUPS IMAGE SWITCH

**ECHGDPL2** GROUPS IMAGE SWITCH

**ECHGDPL3** GROUPS IMAGE SWITCH

**EDIPOLE** GROUPS IMAGE SWITCH

**EDIPOLE1** GROUPS IMAGE SWITCH

**EDIPOLE2** GROUPS IMAGE SWITCH

**EDIPOLE3** GROUPS IMAGE SWITCH

**EGAUSS** EGAUSS0A EGAUSS0B

**EGAUSS0A** GROUPS SWITCH

**EGAUSS0B** ERF GROUPS

**EGAUSS1** EGAUSS1A EGAUSS1B

**EGAUSS1A** GROUPS SWITCH

**EGAUSS1B** ERF GROUPS

**EGAUSS2** EGAUSS2A EGAUSS2B

**EGAUSS2A** GROUPS SWITCH

**EGAUSS2B** GROUPS

**EGAUSS3** EGAUSS3A EGAUSS3B

**EGAUSS3A** GROUPS SWITCH

**EGAUSS3B** ERF GROUPS

**EGBSA0A** GROUPS SWITCH

**EGBSA0B** ERF GROUPS

**EGBSA1A** GROUPS SWITCH

**EGBSA1B** ERF GROUPS

**EGBSA2A** SWITCH

**EGBSA2B** ERF

**EGBSA3A** GROUPS SWITCH

**EGBSA3B** ERF GROUPS

**EGEOM** GROUPS IMAGE

**EGEOM1** GROUPS IMAGE

**EGEOM2** GROUPS IMAGE

**EGEOM3** GROUPS IMAGE

**EHAL** EHAL0A EHAL0B

**EHAL0A** GROUPS IMAGE SWITCH

**EHAL0B** GROUPS LIGHTS SWITCH

**EHAL1** EHAL1A EHAL1B

**EHAL1A** GROUPS IMAGE SWITCH

**EHAL1B** GROUPS LIGHTS SWITCH

**EHAL2** GROUPS IMAGE SWITCH

**EHAL3** EHAL3A EHAL3B

**EHAL3A** GROUPS IMAGE SWITCH

**EHAL3B** GROUPS LIGHTS SWITCH

**EIGEN** GETIME POWER SETIME

**EIGENRGD** DIAGQ HESSRGD

**EIGENROT** DIAGQ HESSROT

**EIGENROT** DIAGQ HESSROT

**EIGENTOR** DIAGQ HESSROT

**EIGENXYZ** DIAGQ HESSIAN

**EIMPROP** GROUPS IMAGE

**EIMPROP1** GROUPS IMAGE

**EIMPROP2** GROUPS IMAGE

**EIMPROP3** GROUPS IMAGE

**EIMPTOR** GROUPS IMAGE

**EIMPTOR1** GROUPS IMAGE

**EIMPTOR2** GROUPS IMAGE

**EIMPTOR3** GROUPS IMAGE

**ELJ** ELJ0A ELJ0B ELJ0C ELJ0D

**ELJ0A** GROUPS IMAGE SWITCH

**ELJ0B** GROUPS LIGHTS SWITCH

**ELJ0C** EGAUSS

**ELJ0D** GROUPS

**ELJ1** ELJ1A ELJ1B ELJ1C ELJ1D

**ELJ1A** GROUPS IMAGE SWITCH

**ELJ1B** GROUPS LIGHTS SWITCH

**ELJ1C** EGAUSS1

**ELJ1D** GROUPS

**ELJ2** ELJ2A ELJ2B

**ELJ2A** GROUPS IMAGE SWITCH

**ELJ2B** EGAUSS2

**ELJ2C** GROUPS

**ELJ3** ELJ3A ELJ3B ELJ3C ELJ3D

**ELJ3A** GROUPS IMAGE SWITCH

**ELJ3B** GROUPS LIGHTS SWITCH

**ELJ3C** EGAUSS3

**ELJ3D** GROUPS

**EMBED** BNDERR CHIRER CHKSIZE COORDS DMDUMP DSTMAT EIGEN EXPLORE FRACDIST FREEUNIT GETIME GYRATE IMPOSE LOCERR MAJORIZE METRIC NUMERAL PRTXYZ REFINE RMSERROR SETIME TORSER VDWERR

**EMETAL** FATAL

**EMETAL1** FATAL

**EMETAL3** EMETAL

**EMM3HB** EMM3HB0A EMM3HB0B

**EMM3HB0A** GROUPS IMAGE SWITCH

**EMM3HB0B** GROUPS LIGHTS SWITCH

**EMM3HB1** EMM3HB1A EMM3HB1B

**EMM3HB1A** GROUPS IMAGE SWITCH

**EMM3HB1B** GROUPS LIGHTS SWITCH

**EMM3HB2** GROUPS IMAGE SWITCH

**EMM3HB3** EMM3HB3A EMM3HB3B

**EMM3HB3A** GROUPS IMAGE SWITCH

**EMM3HB3B** GROUPS LIGHTS SWITCH

**EMPOLE** EMPOLE0A EMPOLE0B

**EMPOLE0A** CHKPOLE GROUPS IMAGE INDUCE ROTPOLE SWITCH

**EMPOLE0B** CHKPOLE EREAL ERECIP INDUCE ROTPOLE

**EMPOLE1** EMPOLE1A EMPOLE1B

**EMPOLE1A** CHKPOLE GROUPS IMAGE INDUCE ROTPOLE SWITCH TORQUE TORQUE1

**EMPOLE1B** CHKPOLE EREAL1 ERECIP1 INDUCE ROTPOLE TORQUE

**EMPOLE2** EMPOLE2A

**EMPOLE2A** GROUPS IMAGE SWITCH TORQUE

**EMPOLE3** EMPOLE3A EMPOLE3B

**EMPOLE3A** CHKPOLE GROUPS IMAGE INDUCE ROTPOLE SWITCH

**EMPOLE3B** CHKPOLE EREAL3 ERECIP3 INDUCE ROTPOLE

**ENERGY** BOUNDS EANGANG EANGLE EBOND EBUCK ECHARGE ECHGDPL EDIPOLE EGAUSS EGEOM EHAL EIMPROP EIMPTOR ELJ EMETAL EMM3HB EMPOLE EOPBEND EOPDIST EPITORS ERXNFLD ESOLV ESTRBND ESTRTOR ETORS ETORTOR EUREY EXTRA PISCF REPLICA

**ENRGYZE** ANALYSIS

**EOPBEND** GROUPS IMAGE

**EOPBEND1** GROUPS IMAGE

**EOPBEND2** EOPBEND2A GROUPS

**EOPBEND2A** IMAGE

**EOPBEND3** GROUPS IMAGE

**EOPDIST** GROUPS IMAGE

**EOPDIST1** GROUPS IMAGE

**EOPDIST2** GROUPS IMAGE

**EOPDIST3** GROUPS IMAGE

**EPITORS** GROUPS IMAGE

**EPITORS1** GROUPS IMAGE

**EPITORS2** EPITORS2A GROUPS

**EPITORS2A** IMAGE

**EPITORS3** GROUPS IMAGE

**EPME** BSPLINE FFTFRONT

**EPME1** BSPLINE1 FFTBACK FFTFRONT

**EPME3** BSPLINE FFTFRONT

**EPUCLC** ANORM

**EREAL** ERFC IMAGE SWITCH

**EREAL1** ERFC IMAGE SWITCH TORQUE TORQUE1

**EREAL3** ERFC IMAGE SWITCH

**ERECIP1** TORQUE

**ERF** ERFCORE

**ERFC** ERFCORE

**ERFIK** D1D2 RFINDEX

**ERFINV** ERF FATAL

**ERXNFLD** CHKPOLE ERFIK IJKPTS ROTPOLE SWITCH

**ERXNFLD3** CHKPOLE ERFIK IJKPTS ROTPOLE SWITCH

**ESOLV** BORN EGBSA0A EGBSA0B SURFACE

**ESOLV1** BORN BORN1 EGBSA1A EGBSA1B SURFACE

**ESOLV2** EGBSA2A EGBSA2B

**ESOLV3** BORN EGBSA3A EGBSA3B SURFACE

**ESTRBND** GROUPS IMAGE

**ESTRBND1** GROUPS IMAGE

**ESTRBND2** GROUPS IMAGE

**ESTRBND3** GROUPS IMAGE

**ESTRTOR** GROUPS IMAGE

**ESTRTOR1** GROUPS IMAGE

**ESTRTOR2** GROUPS IMAGE

**ESTRTOR3** GROUPS IMAGE

**ETORS** ETORS0A ETORS0B

**ETORS0A** GROUPS IMAGE

**ETORS0B** GROUPS

**ETORS1** ETORS1A ETORS1B

**ETORS1A** GROUPS IMAGE

**ETORS1B** GROUPS

**ETORS2** ETORS2A ETORS2B

**ETORS2A** GROUPS IMAGE

**ETORS2B** GROUPS

**ETORS3** ETORS3A ETORS3B

**ETORS3A** GROUPS IMAGE

**ETORS3B** GROUPS

**ETORTOR** BCUINT GROUPS IMAGE

**ETORTOR1** BCUINT1 GROUPS IMAGE

**ETORTOR2** BCUINT2 GROUPS IMAGE

**ETORTOR3** BCUINT GROUPS IMAGE

**EUREY** GROUPS IMAGE

**EUREY1** GROUPS IMAGE

**EUREY2** GROUPS IMAGE

**EUREY3** GROUPS IMAGE

**EWALDCOF** ERFC

**EXPLORE** INITERR MIDERR SIGMOID TOTERR

**FFTBACK** CFFTB

**FFTFRONT** CFFTF

**FFTSETUP** CFFTI

**FIELD** GETPRM PRMKEY

**FINAL** SKTKILL

**FRACDIST** DIST2 TRIMTEXT

**FREEUNIT** FATAL

**GDA** DIFFEQ FINAL FREEUNIT GDASTAT GETTEXT GETXYZ INITIAL MECHANIC NEXTARG NUMERAL PRTXYZ RANDOM TNCG UPCASE VERSION

**GDA1** GRADIENT HESSIAN

**GDA2** GRADIENT

**GDA3** HESSIAN

**GDASTAT** ENERGY GYRATE OPTSAVE

**GEODESIC** MINPATH SORT3

**GETBASE** PDBATM

**GETIME** CLOCK

**GETINT** BASEFILE CHKXYZ CONNECT FATAL FREEUNIT MAKEXYZ NEXTARG READINT SUFFIX VERSION

**GETKEY** FATAL FREEUNIT GETTEXT SUFFIX TRIMTEXT UPCASE

**GETMOL2** BASEFILE FREEUNIT NEXTARG READMOL2 SUFFIX VERSION

**GETNUCH** PDBATM

**GETNUMB** TRIMTEXT

**GETPDB** BASEFILE FREEUNIT NEXTARG READPDB SUFFIX VERSION

**GETPRB** DIST2 DOT GETTOR VCROSS

**GETPRM** FATAL FREEUNIT GETTEXT INITPRM NEXTARG READPRM SUFFIX TRIMTEXT UPCASE VERSION

**GETPROH** PDBATM

**GETSEQ** GETWORD TRIMTEXT UPCASE

**GETSEQN** GETTEXT GETWORD TRIMTEXT UPCASE

**GETSIDE** PDBATM

**GETTOR** DIST2

**GETXYZ** BASEFILE FATAL FREEUNIT NEXTARG READXYZ SUFFIX VERSION

**GRADIENT** BOUNDS EANGANG1 EANGLE1 EBOND1 EBUCK1 ECHARGE1 ECHGDPL1 EDIPOLE1 EGAUSS1 EGEOM1 EHAL1 EIMPROP1 EIMPTOR1 ELJ1 EMETAL1 EMM3HB1 EMPOLE1 EOPBEND1 EOPDIST1 EPITORS1 ERXNFLD1 ESOLV1 ESTRBND1 ESTRTOR1 ETORS1 ETORTOR1 EUREY1 EXTRA1 PISCF REPLICA

**GRADRGD** GRADIENT

**GRADROT** GRADIENT ROTLIST

**HANGLE** NUMERAL

**HBOND** NUMERAL

**HDIPOLE** NUMERAL

**HESSIAN** BORN BOUNDS CHKPOLE EANGANG2 EANGLE2 EBOND2 EBUCK2 ECHARGE2 ECHGDPL2 EDIPOLE2 EGAUSS2 EGEOM2 EHAL2 EIMPROP2 EIMPTOR2 ELJ2 EMETAL2 EMM3HB2 EMPOLE2 EOPBEND2 EOPDIST2 EPITORS2 ERXNFLD2 ESOLV2 ESTRBND2 ESTRTOR2 ETORS2 ETORTOR2 EUREY2 EXTRA2 FATAL INDUCE PISCF REPLICA ROTPOLE

**HESSRGD** GRADRGD RIGIDXYZ

**HESSROT** GRADROT MAKEXYZ

**HIMPTOR** NUMERAL

**HSTRTOR** NUMERAL

**HTORS** NUMERAL

**HYBRID** HANGLE HATOM HBOND HCHARGE HDIPOLE HIMPTOR HSTRBND HSTRTOR HTORS HVDW

**IMPOSE** CENTER QUATFIT RMSFIT

**INDUCE** INDUCE0A INDUCE0B

**INDUCE0A** FATAL GROUPS IMAGE PRTERR SWITCH

**INDUCE0B** FATAL PRTERR UDIRECT1 UDIRECT2 UMUTUAL1 UMUTUAL2

**INEDGE** CERROR

**INERTIA** JACOBI

**INITERR** LOCERR TORSER

**INITIAL** COMMAND INITRES PRECISE PROMO

**INITROT** FATAL NEXTARG ROTCHECK ROTLIST

**INTEDIT** FIELD FINAL FREEUNIT GEOMETRY GETINT GETWORD INITIAL MAKEXYZ NUMBER PRTINT TRIMTEXT UPCASE VERSION ZHELP ZVALUE

**INTXYZ** FINAL FREEUNIT GETINT INITIAL PRTXYZ VERSION

**INVBETA** BETAI GAMMLN

**INVERT** FATAL

**IPEDGE** CERROR

**ISPLPE** CYTSY CYTSYS

**KANGANG** GETTEXT UPCASE

**KANGLE** GETTEXT NUMERAL UPCASE

**KATOM** GETNUMB GETSTRING GETTEXT UPCASE

**KBOND** GETTEXT KENEG NUMERAL UPCASE

**KCHARGE** GETTEXT UPCASE

**KDIPOLE** GETTEXT NUMERAL UPCASE

**KENEG** GETTEXT NUMERAL UPCASE

**KEWALD** EWALDCOF FATAL FFTSETUP GETTEXT MODULI UPCASE

**KGEOM** FATAL GEOMETRY GETTEXT GETWORD IMAGE UPCASE

**KIMPROP** GETTEXT NUMERAL UPCASE

**KIMPTOR** GETTEXT NUMERAL TORPHASE UPCASE

**KMPOLE** CHKPOLE GETTEXT NUMBER NUMERAL RANDOM SORT3 UPCASE

**KOPBEND** GETTEXT NUMBER NUMERAL UPCASE

**KOPDIST** GETTEXT NUMERAL UPCASE

**KORBIT** GETTEXT NUMERAL UPCASE

**KPITORS** GETTEXT NUMERAL UPCASE

**KPOLAR** CHKPOLE GETTEXT POLARGRP UPCASE

**KSOLV** GETTEXT GETWORD KANGLE KBOND UPCASE

**KSTRBND** GETTEXT UPCASE

**KSTRTOR** GETTEXT NUMERAL UPCASE

**KTORS** GETTEXT NUMERAL TORPHASE UPCASE

**KTORTOR** GETTEXT ISPLPE NUMERAL SORT9 UPCASE

**KUREY** GETTEXT NUMERAL UPCASE

**KVDW** GETTEXT NUMBER NUMERAL UPCASE

**LBFGS** COMMENT' GETTEXT OPTSAVE SEARCH UPCASE

**LIGASE** FINDATM

**LIGHTS** FATAL SORT2 SORT5

**LMSTEP** PRECISE QRSOLVE

**LOCALMIN** GRADIENT TNCG

**LOCALRGD** OCVM

**LOCALROT** OCVM

**LOCALXYZ** TNCG

**MAJORIZE** GETIME GYRATE RMSERROR SETIME

**MAKEINT** ADJACENT FATAL GEOMETRY GETTEXT UPCASE

**MAKEPDB** ATTACH FREEUNIT GETBASE GETNUCH GETPROH GETSIDE NUMERAL PDBATM READSEQ VERSION

**MAKEXYZ** XYZATM

**MAPCHECK** FREEUNIT NUMERAL PRTXYZ VERSION

**MAXWELL** ERFINV RANDOM

**MCM1** GRADIENT

**MCM2** HESSIAN

**MCMSTEP** TNCG

**MDINIT** FREEUNIT GETTEXT GETWORD GRADIENT GRPLINE LATTICE MAXWELL MDREST NUMERAL RANVEC READDYN UPCASE VERSION

**MDREST** INVERT

**MDSAVE** FATAL FREEUNIT NUMERAL OPENEND PRTDYN PRTXYZ SKTDYN SUFFIX TRIMTEXT VERSION

**MEASFN** CERROR TRIPLE VCROSS VECANG VNORM

**MEASFP** CERROR DOT VCROSS VECANG VNORM

**MEASFS** CERROR DOT VECANG VNORM

**MEASPM** VCROSS

**MECHANIC** ACTIVE ANGLES ATTACH BITORS BONDS CLUSTER CUTOFFS FATAL FIELD KANGANG KANGLE KATOM KBOND KCHARGE KDIPOLE KEWALD KGEOM KIMPROP KIMPTOR KMETAL KMPOLE KOPBEND KOPDIST KORBIT KPITORS KPOLAR KSOLV KSTRBND KSTRTOR KTORS KTORTOR KUREY KVDW LATTICE MOLECULE MUTATE ORBITAL POLYMER RINGS SMOOTH TORSIONS UNITCELL

**MERGE** FATAL GETREF

**MIDERR** BNDERR CHIRER LOCERR TORSER

**MINIMIZ1** GRADIENT

**MINIMIZE** FINAL FREEUNIT GETTEXT GETXYZ GRADIENT INITIAL LBFGS MECHANIC NEXTARG PRTXYZ UPCASE VERSION

**MINIROT** FINAL FREEUNIT GETINT GETTEXT GRADROT INITIAL INITROT LBFGS MECHANIC NEXTARG PRTINT UPCASE VERSION

**MINIROT1** GRADROT MAKEXYZ

**MINRIGID** FINAL FREEUNIT GETTEXT GETXYZ GRADRGD INITIAL LBFGS MECHANIC NEXTARG ORIENT PRTXYZ UPCASE VERSION

**MINRIGID1** GRADRGD RIGIDXYZ

**MMID** GVALUE

**MODECART** CLIMBXYZ EIGENXYZ GETREF IMPOSE MAKEREF

**MODEROT** CLIMBROT EIGENROT MAKEXYZ

**MODESRCH** CLIMBER EIGENROT MAKEINT MAKEREF MAPCHECK

**MODETORS** CLIMBTOR EIGENTOR GETREF IMPOSE MAKEINT MAKEREF

**MODULI** BSPLINE DFTMOD

**MOLECULE** SORT SORT3

**MOLUIND** UFIELD

**MOMENTS** CHKPOLE INDUCE JACOBI ROTPOLE

**MONTE** CHKCLASH FREEUNIT GETREF GETTEXT GETXYZ INITIAL INITROT MAKEINT MAKEREF MAKEXYZ MCMSTEP MECHANIC NEXTARG PRTXYZ RANDOM RANVEC UPCASE VERSION

**MUTATE** GETTEXT UPCASE

**NEIGHBOR** CERROR DIST2

**NEWATM** ADDBOND XYZATM

**NEWTON** FINAL FREEUNIT GETTEXT GETXYZ GRADIENT INITIAL MECHANIC NEXTARG PRTXYZ TNCG UPCASE VERSION

**NEWTON1** GRADIENT

**NEWTON2** HESSIAN

**NEWTROT** FINAL FREEUNIT GETINT GETTEXT GRADROT INITIAL INITROT MECHANIC NEXTARG PRTINT TNCG UPCASE VERSION

**NEWTROT1** GRADROT MAKEXYZ

**NEWTROT2** HESSROT MAKEXYZ

**NORMAL** RANDOM

**NUCBASE** OCVM ORIENT POTOFF ZATOM

**NUCCHAIN** NUCBASE OCVM ORIENT ZATOM

**NUCLEIC** BASEFILE CONNECT DELETE FIELD FREEUNIT GETKEY GETSEQN INITIAL MAKEINT MAKEXYZ MOLECULE NEXTARG NUCCHAIN PRTINT PRTSEQ PRTXYZ TRIMTEXT VERSION WATSON

**NUMBER** TRIMTEXT

**OCVM** GETTEXT OPTSAVE PRECISE UPCASE

**OLDATM** ADDBOND FATAL

**OPTIMIZ1** GRADIENT

**OPTIMIZE** FATAL FINAL FREEUNIT GETTEXT GETXYZ GRADIENT INITIAL MECHANIC NEXTARG OCVM PRTXYZ UPCASE VERSION

**OPTIROT** FATAL FINAL FREEUNIT GETINT GETTEXT GRADROT INITIAL INITROT MECHANIC NEXTARG OCVM PRTINT UPCASE VERSION

**OPTIROT1** GRADROT MAKEXYZ

**OPTRIGID** FATAL FINAL FREEUNIT GETTEXT GETXYZ GRADRGD INITIAL MECHANIC NEXTARG OCVM ORIENT PRTXYZ UPCASE VERSION

**OPTRIGID1** GRADRGD RIGIDXYZ

**OPTSAVE** FATAL FREEUNIT MAKEXYZ NUMERAL OPENEND PRTINT PRTXYZ SKTOPT SUFFIX VERSION

**ORBITAL** FATAL GETTEXT PIPLANE UPCASE

**ORIENT** XYZRIGID

**OVERLAP** SLATER

**PATH** FINAL GETXYZ IMPOSE INITIAL INVERT LBFGS MECHANIC NEXTARG OPTSAVE ORTHOG POTNRG

**PATH1** POTNRG

**PATHPNT** OCVM

**PATHSCAN** PATHPNT SADDLE1 TANGENT

**PATHVAL** IMPOSE

**PDBXYZ** CHKXYZ DELETE FIELD FINAL FREEUNIT GETNUMB GETPDB INITIAL LIGASE PRTXYZ RIBOSOME SORT UPCASE VERSION

**PIPLANE** FATAL

**PISCF** NEWATM

**PITILT** OLDATM

**PLACE** CERROR DIST2 GETPRB GETTOR INEDGE

**POLARGRP** SORT SORT8

**POLARIZE** FATAL GETXYZ INITIAL JACOBI MECHANIC MOLUIND

**POLYMER** FATAL GETTEXT IMAGE UPCASE

**POTNRG** GRADIENT

**POWER** RANDOM

**PRECOND** CHOLESKY COLUMN

**PRESSURE** LATTICE

**PRMKEY** GETTEXT GETWORD POTOFF UPCASE

**PROCHAIN** GETTEXT PROSIDE UPCASE ZATOM

**PROJCT** DOT

**PROPYZE** GRADIENT GYRATE INERTIA MOMENTS

**PROSIDE** FREEUNIT PRTINT PRTXYZ VERSION ZATOM

**PROTEIN** BASEFILE CHKXYZ CONNECT DELETE FIELD FINAL FREEUNIT GETKEY GETSEQ INITIAL MAKEINT MAKEXYZ NEXTARG PROCHAIN PRTINT PRTSEQ PRTXYZ TRIMTEXT VERSION

**PRTARC** VERSION

**PRTCAR** VERSION

**PRTDYN** ZATOM

**PRTERR** ZATOM

**PRTINT** VERSION

**PRTMOL2** NUMBER VERSION

**PRTPDB** VERSION

**PRTPRM** NUMBER

**PRTSEQ** VERSION

**PRTXMOL** VERSION

**PRTXYZ** VERSION

**PSS** ACTIVE FINAL GETTEXT GETXYZ IMPOSE INITIAL INITROT LOCALXYZ MAKEINT MAKEREF MECHANIC MODECART MODETORS NEXTARG PSSWRITE SIGMOID UPCASE

**PSS1** GRADIENT

**PSS2** HESSIAN

**PSSRGD1** GRADRGD RIGIDXYZ

**PSSRIGID** FINAL FREEUNIT GETTEXT GETXYZ IMPOSE INITIAL MAKEREF MECHANIC NEXTARG NUMERAL OCVM ORIENT PRTXYZ RGDSRCH RIGIDXYZ SIGMOID UPCASE VERSION

**PSSROT** FINAL FREEUNIT GETTEXT GETXYZ IMPOSE INITIAL INITROT MAKEREF MAKEXYZ MECHANIC MODEROT NEXTARG NUMERAL OCVM PRTXYZ UPCASE VERSION

**PSSROT1** GRADROT MAKEXYZ

**PSSWRITE** FREEUNIT NUMERAL PRTXYZ VERSION

**PTINCY** DOT EPUCLC PROJCT ROTANG

**QUATFIT** JACOBI

**RADIAL** BASEFILE FATAL FINAL FREEUNIT GETTEXT GETWORD IMAGE INITIAL LATTICE MOLECULE NEXTARG READXYZ SUFFIX UNITCELL UPCASE VERSION

**RANDOM** CALENDAR GETTEXT UPCASE

**RANVEC** RANDOM

**RATTLE** FATAL IMAGE PRTERR

**RATTLE2** FATAL IMAGE PRTERR

**READBLK** FATAL FREEUNIT GETWORD NUMERAL

**READDYN** FATAL VERSION

**READINT** FATAL GETTEXT GETWORD NEXTTEXT TRIMTEXT VERSION

**READMOL2** FATAL GETTEXT GETWORD SORT TRIMTEXT UPCASE VERSION

**READPDB** FATAL FIXPDB GETTEXT NEXTARG TRIMTEXT UPCASE VERSION

**READPRM** FATAL GETNUMB GETSTRING GETTEXT GETWORD NUMERAL PRMKEY SORT9 TORPHASE TRIMTEXT UPCASE

**READSEQ** FATAL GETNUMB GETTEXT GETWORD TRIMTEXT VERSION

**READXYZ** CHKXYZ FATAL GETTEXT GETWORD NEXTTEXT SORT TRIMTEXT VERSION

**REFINE** LBFGS

**REPLICA** FATAL

**RGDSRCH** CLIMBRGD EIGENRGD RIGIDXYZ

**RGDSTEP** CHOLESKY GRADIENT KINETIC LINBODY MDSAVE MDSTAT PRESSURE ROTRGD TEMPER2

**RIBOSOME** ADDBOND ADDSIDE FATAL FINDATM FREEUNIT NEWATM OLDATM PRTSEQ VERSION

**RINGS** ANGLES BITORS BONDS FATAL TORSIONS

**RMSERROR** TRIMTEXT

**ROTANG** DOT VCROSS

**ROTCHECK** ROTLIST

**ROTLIST** FATAL

**ROTPOLE** ROTMAT ROTSITE

**SADDLE** COMMENT' FATAL FINAL FREEUNIT GETTEXT GETXYZ IMPOSE INITIAL MAKEINT MAKEXYZ MECHANIC NEXTARG PATHPNT PATHSCAN PATHVAL PRTXYZ READXYZ SADDLE1 SEARCH TANGENT UPCASE VERSION

**SADDLE1** GRADIENT

**SADDLES** CERROR IPEDGE TRIPLE

**SCAN** ACTIVE FINAL FREEUNIT GETXYZ INITIAL INITROT LOCALMIN MAKEINT MAPCHECK MECHANIC MODESRCH NEXTARG NUMERAL READXYZ VERSION

**SCAN1** GRADIENT

**SCAN2** HESSIAN

**SDAREA** SURFATOM

**SDSTEP** GRADIENT KINETIC MDSAVE MDSTAT PRESSURE RATTLE RATTLE2 SDTERM

**SDTERM** NORMAL SDAREA

**SETIME** CLOCK

**SHAKEUP** CHKRING GETNUMB GETTEXT GETWORD UPCASE

**SKTDYN** CREATEUPDATE GETMONITOR NEEDUPDATE RELEASEMONITOR SETACCELERATION SETCOORDINATES SETENERGY SETINDUCED SETTIME SETUPDATED SETVELOCITY SKTINIT

**SKTINIT** CREATEJVM CREATESERVER CREATESYSTEM SETATOMIC SETATOMTYPES SETCHARGE SETCONNECTIVITY SETCOORDINATES SETFILE SETFORCEFIELD SETKEYWORD SETMASS SETNAME SETSTORY

**SKTKILL** DESTROYJVM DESTROYSERVER SKTDYN SKTOPT

**SKTOPT** CREATEUPDATE GETMONITOR NEEDUPDATE RELEASEMONITOR SETCOORDINATES SETENERGY SETGRADIENTS SETINDUCED SETSTEP SETUPDATED SKTINIT

**SLATER** ASET BSET CJKM POLYP

**SMOOTH** GETTEXT GETWORD NEXTARG UPCASE

**SNIFFER** FINAL FREEUNIT GETREF GETXYZ GRADIENT INITIAL MAKEREF MECHANIC NEXTARG OPTSAVE PRTXYZ SNIFFER1 VERSION

**SNIFFER1** GRADIENT

**SOAK** DELETE FREEUNIT IMAGE LATTICE MAKEREF MERGE MOLECULE READXYZ SUFFIX UNITCELL VERSION

**SPACEFILL** ACTIVE CONNOLLY FIELD FINAL FREEUNIT GETTEXT GETXYZ INITIAL KATOM KVDW NEXTARG READXYZ SUFFIX UPCASE VERSION

**SPECTRUM** BASEFILE FREEUNIT INITIAL NEXTARG SUFFIX VERSION

**SQUARE** GETTEXT LMSTEP LSQWRITE PRECISE QRFACT RSDVALUE TRUST UPCASE

**SUFFIX** TRIMTEXT

**SUPERPOSE** FIELD FINAL FREEUNIT GETTEXT GETXYZ IMPOSE INITIAL KATOM NEXTARG PRTXYZ READXYZ SUFFIX TRIMTEXT UPCASE VERSION

**SURFACE** FATAL SORT2

**SURFATOM** FATAL SORT2

**SWITCH** REPLICA

**SYBYLXYZ** FINAL FREEUNIT GETMOL2 INITIAL PRTXYZ VERSION

**SYMMETRY** CELLATOM

**TANGENT** PATHPNT SADDLE1

**TEMPER** KINETIC

**TEMPER2** MAXWELL RANDOM RANVEC

**TESTGRAD** ENERGY FINAL GETTEXT GETXYZ GRADIENT INITIAL MECHANIC NEXTARG UPCASE

**TESTHESS** FINAL FREEUNIT GETTEXT GETXYZ GRADIENT HESSIAN INITIAL MECHANIC NEXTARG NUMGRAD UPCASE VERSION

**TESTLIGHT** EBUCK EBUCK1 ECHARGE ECHARGE1 EGAUSS EGAUSS1 EHAL EHAL1 ELJ ELJ1 EMM3HB EMM3HB1 FINAL GETIME GETXYZ INITIAL LIGHTS MECHANIC NEXTARG SETIME

**TESTROT** ENERGY FINAL GETINT GRADROT INITIAL INITROT MAKEXYZ MECHANIC NEXTARG

**TIMER** ENERGY FINAL GETIME GETTEXT GETXYZ GRADIENT HESSIAN INITIAL MECHANIC NEXTARG SETIME UPCASE

**TIMEROT** ENERGY FINAL GETIME GETINT GETTEXT GRADROT HESSROT INITIAL INITROT MECHANIC NEXTARG SETIME UPCASE

**TNCG** GETTEXT HMATRIX OPTSAVE PISCF SEARCH TNSOLVE UPCASE

**TNSOLVE** PRECOND

**TORSIONS** FATAL

**TORUS** CERROR GETTOR

**TOTERR** BNDERR CHIRER LOCERR TORSER VDWERR

**TRIANGLE** FATAL

**TRIPLE** DOT VCROSS

**TRUST** PRECISE RSDVALUE

**UDIRECT2** ERFC IMAGE SWITCH

**UMUTUAL2** ERFC IMAGE SWITCH

**UNITCELL** FATAL GETTEXT GETWORD UPCASE

**VAM** CERROR CIRPLN DEPTH DIST2 DOT GENDOT MEASFN MEASFP MEASFS MEASPM TRIPLE VCROSS VNORM

**VDWERR** LIGHTS

**VECANG** ANORM DOT TRIPLE

**VERLET** GRADIENT KINETIC MDSAVE MDSTAT PRESSURE RATTLE RATTLE2 TEMPER TEMPER2

**VERSION** LOWCASE NEXTARG TRIMTEXT

**VIBRATE** DIAGQ FATAL FINAL FREEUNIT GETXYZ HESSIAN INITIAL MECHANIC NEXTARG NUMERAL PRTXYZ VERSION

**VIBRIGID** DIAGQ FINAL GETXYZ HESSRGD INITIAL MECHANIC ORIENT

**VIBROT** DIAGQ FINAL GETINT HESSROT INITIAL INITROT MECHANIC

**VNORM** ANORM

**VOLUME** CONNOLLY

**VOLUME1** FATAL

**VOLUME2** FATAL

**WATSON** ZATOM

**WATSON1** GRADRGD RIGIDXYZ

**XTALERR** ENERGY XTALMOVE XTALPRM

**XTALFIT** FINAL GETXYZ INITIAL MECHANIC NEXTARG POTOFF SQUARE XTALPRM

**XTALLAT1** ENERGY LATTICE

**XTALMIN** FINAL FREEUNIT GETXYZ GRADIENT INITIAL LATTICE MECHANIC NEXTARG OCVM PRTXYZ TNCG VERSION XTALLAT1

**XTALMOL1** GRADIENT

**XTALMOL2** HESSIAN

**XTALMOVE** LATTICE

**XTALPRM** BOUNDS LATTICE MOLECULE

**XYZEDIT** ACTIVE BOUNDS CUTOFFS DELETE FIELD FINAL FREEUNIT GETXYZ IMAGE INERTIA INITIAL INSERT KATOM LATTICE MAKEREF MERGE MOLECULE PRTXYZ RANDOM SOAK SORT SORT4 UNITCELL VERSION

**XYZINT** FINAL FREEUNIT GETTEXT GETXYZ INITIAL MAKEINT NEXTARG PRTINT READINT UPCASE VERSION

**XYZPDB** FIELD FINAL FREEUNIT GETXYZ INITIAL KATOM MAKEPDB MOLECULE PRTPDB VERSION

**XYZRIGID** JACOBI ROTEULER

**XYZSYBYL** BONDS FINAL FREEUNIT GETXYZ INITIAL PRTMOL2 VERSION

**ZATOM** FATAL

**ZVALUE** MAKEXYZ TRIMTEXT