

XP commands

ARAD a b s key | a=rad b=rad s=space r
ATYP t c key | t=-4 to 10 c= 1 to 15
BACK c i | c= 1 to 15 i=0 to 3
BANG key | bond & angle
CELL λ a b c α β γ
CENT key | centroid
CENT/X key | add to coords
DEMO
DIAG key | diagonal drawing
DIAG/B | BOX diagonal
DRAW plotfile | send plotfile to print/file
ECHO text
EDEN key | electron density
EGSD path | path for example files
END
ENVI d key | enviroment r1+r1+d [d=0.5]
<Esc> | stop
EXAM template | template=DOS or UNIX command
EXIT file | filename (opt) print output
EYES n | n=1 mono n=2 stereo
FILE file | write *.ins file=*
FMOL key, d | make mole r1+r2+d [d=0.5]
FMOL REST | make molecule less current
FMOL/N | not listing to screen
FUSE | complement of GROW
GAPS o s | o=gap bond/atom s=shade gap
GROW d key | r1+r2+d [d=0.5]
HADD t d U key | t=1 to 9 d=0.96(0.08)U=-1.2
HIMP d key | d=distance [d=0.96]
HLPD path | path to help files
INFO key | atom info
INVT x y z key | invert atoms thru x,y,z
ISOT key | make isotropic
JOIN t key | t= 1 to 7
KILL key | delete
LABL c s | c=0 to 4 : s [s=600]
LIBR key | libration
LINE two atoms | l.s. line thru atoms
LINK t key | t=0 to 7
LITE I d s p | I=2 to 20 d=0 to 1 p=4 to 20
LOSE filename | delete filename
MATR p11 p12 p13 p21 p22 p23 p31 p32 p33
MATR n | n=1(a); n=2(b); n=3(c)
MATR h,k,l | perp. to h,k,l
MGEN k dX dY dZ X Y Z
MODL key s d | s=[def=3.0A] d=[def=0.25]
MOVE dx dy dz sign
MPLN key | least-square plane
MPLN/N | no output
NAME old new c | c=sfaccode
NEWM two atoms | newman projection
NEXT filename | read save file
NOPL | clear plane info
OFIT key | orthogonal fit
ORTH filename | orthogonal file
ORTH/F filename | include unit-cell, symmetry
PACK d2 d1 d key | packing diagram
PAGE | form feed
PART n | n=part number
PART/S n atom | change part number of atom
PAWS | pause
PBOX w d x y z | w=[def=20] d=[def=8]
PERS br key | br=[def=0.05]
PGEN key dX dY dZ X Y Z
PICK key | atom pick
POLP key | polyhedral fill (plotter)
POLY key | polyhedral fill (screen)
POST plotfile | poster/plotfile maker
PREV | previous matrix
PRIN | print buffer
PROJ d k | d=rotation degree

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PROJ/P | alpha-carbon traces
PRUN nb key | nb=max. # of bonds
PRUN d1 d2 key | prun below d1 above d2
PUSH dx dy dz sign
QUIT
RASD code | rast device code=L,F,C,D
RAST filename | raster file
READ filetitle | read file to END
REAP filetitle | read file to EOF
RESI n c | n=number c=class
RESI/S n c atom | chage class number of atom
RIDE key | riding model
RING c key | find rings c = bondtype
ROTA n,p; ... | n=1(x),2(y),3(z) p=degrees
ROTA two atoms | about axis
SAVE filename | save snapshot (see NEXT)
SFIL s d key | space s=-3,0,3; d=[def=50]
SGEN sym key | symmetry expansion
SORT al a2...an | atom sort
SORT/H | hydrogens sorted with rest
SORT/N | sorts in numerical order
SORT/R | sorts in numeric residue
order
SORT/P | sorts in residue order
SPIX key | space fill screen
SPOT I m p | I=4 to 20; m=deg p=deg
SRCH keys d | search r1+r2+d
SYMM symmetry operator
TELP s p b d key | s=-3,0,3 p=% b=br d=view d
TELP/P | alpha-carbon traces
TITL text
TORS key | torsion angle
UNDO key | undo BOND
UNIQ key d | r1+r2+d
USER path | change path
VIEW plotfile | screen view
WAIT wt key | atom weights
WIPE | screen clear
ZOOM scal | scale value

key : keywords

keywords :

atom names, **TYPE**n, **ALL**, **TO**, **LESS** and **LPT**.

ALL means all atoms in the list
TO defines a string of consecutive atoms
'>' is equivalent to 'TO'
LESS is used to omit atoms from the list
LPT creates (additional) lineprinter output
The switch/L has the same effect as LPT
TYPEn (n=1,2,...,9) means all atoms of SFAC
atom names
dollar sign (\$) by element name=
all atoms of that element
question mark (?) may be used in place
of any character

Other keywords : **REST CELL**

REST = all atoms not in the current list
CELL = include unit cell