NEIGHBOURS

Program release 4.12

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A utility program for setting up input files for DMAREL, which models crystals of rigid organic molecules using anisotropic atom-atom intermolecular potentials.

For the online manual for DMAREL, visit this web site:

http://www.ucl.ac.uk/~uccahht/dmarelmanual/index.html

Contents

Neighbours should compile and run on any platform with a FORTRAN compiler, it is not FORTRAN 77 standard but the extensions are all part of the FORTRAN 90 standard.

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1. Introduction

NEIGHBOURS is a program for setting up input files in the format that DMAREL 3.02 requires.

The program converts crystallographic data files (CSD FDAT (http://www.ccdc.cam.ac.uk) and SHELX (http://shelx.uni-ac.gwdg.de/SHELX)) to a cartesian coordinate system. The molecular fragments are treated as

rigid identities. It sets up the molecule fixed local axis system on each molecule. The first run of NEIGHBOURS is usually performed to obtain the coordinates of the molecule in the local axis system prior to

ab initio calculations. This sets the origin at centre of mass and the local molecular axes parallel to specified

intramolecular bonds. The coordinates can be used to calculate the atomic multipoles (DMA) for the electrostatic, or for an *ab initio* optimisation on the geometry. The program can combine an anisotropic multipoles (DMA), with repulsion-dispersion model. Anisotropic repulsion potentials, requiring definition of

local atomic axes at present partly required to be edited in manually.

The program in principle accepts all atom types, with 32 default types currently available. It also has this function to allow pasting of a molecular structure (i.e. *ab initio* derived geometry) into an experimental crystal

structure. Two different crystallographic files are accepted as input, they are CSD FDAT file and SHELX file.

Note: DMAREL 3.02 cannot handle linear molecules or very high symmetry space groups occupied by high

symmetry molecule.

DMAREL is a lattice energy minimisation program for molecular structures, using a realistic anisotropic atomatom

model for the intermolecular forces, electrostatic model, along with anisotropic repulsion and simple dispersion models. DMAREL needs inverted molecules, and NEIGHBOURS will set them up accordingly.

There is a need to convert labels, so that $Z' < 1$, where there is no inverted and non-inverted atoms in the same

molecule. Symmetry information are generated from the FDAT file, using the symmetry information, but also

the first letter for the space group is needed to be specified.

2. Input files required

In order to run NEIGHBOURS, the following files are required. (See **6. Example of input file (formic acid)**)

fdat or shelx - crystallographic data file
cutoff - covalent bonds specification
punch - atomic multipoles from DMA
axis or axes - local axis set up for molecule
potential - repulsion-dispersion potential

Standard input (Unit 5)

If running in interactive mode, the program must read in the character 'I' or 'i' as the first character read in. If this
is what is read, the rest of the screen input is read from standard input. The FDAT or SHELX input is read from
unit 11.

If running from default values using the UNIX file redirection, the input file ,must be in FDAT format. The
program detects FDAT format files using the first character which is always '#'. Standard input (unit 5) is used
for the FDAT file input. fort.22 file must exists in order for this to run.

Running from default values using an FDAT filename which is the same as the refcode is treated the same as
interactive mode.

If running in non-interactive mode, the program will read any other character as its first character. In this case,
the rest of the normal screen input is read from fort.22 (written from a previous run). The FDAT or SHELX file
input is read form standard input (unit 5).

fdat or shelx - crystallographic data file

The input file can be either an FDAT format file (Cambridge Crystallographic Database), or a SHELX format
file for providing the crystal structure information. The are 32 types of atoms that can be included
automatically.

Here below are examples of the file format for SHELX and FDAT.

SHELX
```
TITL file.dmain
CELL 1.0 24.8344 6.2757 6.2856 90.0000 96.6956 90.0000
ZERR 4 0.0 0.0 0.0 0.0 0.0 0.0
LATT 1
SYMM -X +1/2, +Y +1/2, -Z
SFAC CL N C
CLR2 1 0.16380157 0.41246903 0.24583555
CLR4 1 0.18382651 -0.12393270 -0.40565023
CLR5 1 0.08712042 -0.39771688 -0.27714111
CLR6 1 0.02957807 -0.25777906 0.11842632
NIT1 2 0.05183901 0.18108460 0.48480173
NIT3 2 0.24807347 0.35136593 -0.18193694
CAR1 3 0.09972236 0.06908985 0.16033453
CAR2 3 0.14265604 0.18909242 0.10164472
CAR3 3 0.16853027 0.12879765 -0.07342343
CAR4 3 0.15120442 -0.05274196 -0.19000470
CAR5 3 0.10828502 -0.17403983 -0.13276038
CAR6 3 0.08270618 -0.11218192 0.04272150
CBR7 3 0.07292869 0.13175419 0.34190008
CBR8 3 0.21304191 0.25334000 -0.13414060
END
```
FDAT
```
#BAWNIW0123 20 9 44 0 0 2 3 14 0 0 14102200000000000000000000
86953 60293 92518 9000 11613 9000444222101010 0 6 0 0 0 4P21 040
R=0.0000 CREATED BY WMIN2FDAT K.S.WIBLEY 1995
211 0121 0112 0011 0121 6110 0
CL 99N 68C 68
CL1 60474 0 5645 CL2 44232 0 55307 CL3 5165 0 31303
CL4 -5658 0 -5801 N1 18755 0 -28595 N2 82226 0 49149
C1 27943 0 1946 C2 45225 0 12720 C3 50198 0 29204
C4 37764 0 34888 C5 20435 0 24220 C6 15609 0 7752
C7 22802 0 -15143 C8 68129 0 40360
0 0 0 0 0 0 0 0 0 0 0 0 0 0
```
cutoff - covalent bonds specification

This file is used to establish the covalent bonds and assumed atoms within the specified distances are bonded.

There is an entry for every type of covalent bond in molecule, set at just slightly larger than the maximum likely

value. Only the first 2 character of the atoms needs to be specified. The cutoff filename should be cutoff or file.cutoff, otherwise its name will be asked for.

Example of **cutoff** file

```
CA CL 1.80
CA NI 1.50
CA CA 1.55
ENDS
```

punch - multipoles from DMA

This contains the atomic multipoles derive by DMA of an *ab initio* wavefunction of the isolated molecule. It is

essential that the calcultation uses the same orientation of the molecule as in the defined axes file.It is essentially

the same definition of atomic multipole moments, as multipole expansion of electrostatic energy programmed in

DMAREL.

The atomic multipoles from the distributed multipole analysis (DMA) punch file, this can be calculated using

either CADPAC (http://ket.ch.cam.ac.uk/software/cadpac.html) or from GAUSSIAN

(http://www.gaussian.com) files using GDMA (http://fandango.ch.cam.ac.uk/programs.html#GDMA). The GDMA file is converted into the correct punch format using a utility code.

Here below are examples of the punch file format obtained from CADPAC and GDMA.

punch file from CADPAC

```
UREA from UREAXX12 neutron study
1 CAR1 0.102858 0.000000 0.000000 Next 2 Limit 4
1.142734
0.000000 0.163569 0.000000
-0.115661 0.000000 0.000000 0.213489 0.000000
0.000000 -0.452037 0.000000 0.000000 0.000000 -1.755088 0.000000
0.288890 0.000000 0.000000 0.011036 0.000000 0.000000 0.000000
-0.557763 0.000000
2 OXY1 2.486560 0.000000 0.000000 Next 3 Limit 4
-0.942585
0.000000 0.395975 0.000000
0.330669 0.000000 0.000000 0.312420 0.000000
0.000000 -0.062567 0.000000 0.000000 0.000000 -0.552782 0.000000
0.034192 0.000000 0.000000 -0.612699 0.000000 0.000000 0.000000
1.062039 0.000000
3 NIT1 -1.219552 -2.169872 0.000000 Next 4 Limit 4
-0.702845
0.000000 0.097093 -0.021555
-0.409123 0.000000 0.000000 0.226010 0.053068
0.000000 -0.084590 0.080790 0.000000 0.000000 2.053346 0.306773
-0.897911 0.000000 0.000000 -0.363623 0.277733 0.000000 0.000000
0.016630 1.220312
4 HPD1 -0.280411 -3.829624 0.000000 Next 5 Limit 4
0.319084
0.000000 0.060251 -0.097863
0.001509 0.000000 0.000000 0.008894 0.018881
0.000000 0.003705 -0.008955 0.000000 0.000000 -0.003279 0.000303
0.008741 0.000000 0.000000 0.005165 0.006545 0.000000 0.000000
-0.002919 0.000306
5 HPD2 -3.119080 -2.143102 0.000000 Next 6 Limit 4
0.283687
0.000000 -0.107948 -0.001013
0.001371 0.000000 0.000000 -0.015800 -0.000800
0.000000 -0.010229 0.003014 0.000000 0.000000 -0.001783 0.001932
0.004046 0.000000 0.000000 -0.015559 -0.000022 0.000000 0.000000
-0.006394 -0.003327
6 NIT2 -1.219552 2.169872 0.000000 Next 7 Limit 4
-0.702845
0.000000 0.097093 0.021555
-0.409123 0.000000 0.000000 0.226010 -0.053068
0.000000 -0.084590 -0.080790 0.000000 0.000000 2.053346 -0.306773
-0.897911 0.000000 0.000000 -0.363623 -0.277733 0.000000 0.000000
0.016630 -1.220312
7 HPD3 -0.280411 3.829624 0.000000 Next 8 Limit 4
0.319084
```

```
0.000000 0.060251 0.097863
0.001509 0.000000 0.000000 0.008894 -0.018881
0.000000 0.003705 0.008955 0.000000 0.000000 -0.003279 -0.000303
0.008741 0.000000 0.000000 0.005165 -0.006545 0.000000 0.000000
-0.002919 -0.000306
8 HPD4 -3.119080 2.143102 0.000000 Next 0 Limit 4
0.283687
0.000000 -0.107948 0.001013
0.001371 0.000000 0.000000 -0.015800 0.000800
0.000000 -0.010229 -0.003014 0.000000 0.000000 -0.001783 -0.001932
0.004046 0.000000 0.000000 -0.015559 0.000022 0.000000 0.000000
-0.006394 0.003327
```
punch file from GDMA
```
urea (MP2(fc)/6-31G**) + ChelpG
C01 0.0000000000 0.0000000000 0.0000000000 Rank 4
1.1447943435
0.0000000000 0.1627860177 0.0000000000
-0.1174227029 0.0000000000 0.0000000000 0.2147702637 0.0000000000
0.0000000000 -0.4514517479 0.0000000000 0.0000000000 0.0000000000
-1.7578918216 0.0000000000
0.2896125980 0.0000000000 0.0000000000 0.0112548351 0.0000000000
0.0000000000 0.0000000000 -0.5570962336 0.0000000000
O02 2.3837026300 0.0000000000 0.0000000000 Rank 4
-0.9432973732
0.0000000000 0.3964067424 0.0000000000
0.3302489865 0.0000000000 0.0000000000 0.3136883602 0.0000000000
0.0000000000 -0.0617674727 0.0000000000 0.0000000000 0.0000000000
-0.5567138694 0.0000000000
0.0350620093 0.0000000000 0.0000000000 -0.6156676822 0.0000000000
0.0000000000 0.0000000000 1.0692901565 0.0000000000
N03 -1.3224105900 2.1698729000 0.0000000000 Rank 4
-0.7032398248
0.0000000000 0.0971222097 0.0223257344
-0.4094599141 0.0000000000 0.0000000000 0.2267814252 -0.0540072273
0.0000000000 -0.0857313669 -0.0802374866 0.0000000000 0.0000000000
2.0513481203 -0.3089219094
-0.8967796466 0.0000000000 0.0000000000 -0.3635415507 -0.2741894155
0.0000000000 0.0000000000 0.0108184671 -1.2160218300
N04 -1.3224105900 -2.1698729000 0.0000000000 Rank 4
-0.7032398248
0.0000000000 0.0971222097 -0.0223257344
-0.4094599141 0.0000000000 0.0000000000 0.2267814252 0.0540072273
0.0000000000 -0.0857313669 0.0802374866 0.0000000000 0.0000000000
2.0513481203 0.3089219094
-0.8967796466 0.0000000000 0.0000000000 -0.3635415507 0.2741894155
0.0000000000 0.0000000000 0.0108184671 1.2160218300
H05 -0.3832689340 3.8296248800 0.0000000000 Rank 4
0.3189680135
0.0000000000 0.0602681099 0.0979012760
0.0015130789 0.0000000000 0.0000000000 0.0089058984 -0.0188947758
0.0000000000 0.0037060430 0.0089539382 0.0000000000 0.0000000000
-0.0032914010 -0.0003036204
0.0087468839 0.0000000000 0.0000000000 0.0051668117 -0.0065533191
0.0000000000 0.0000000000 -0.0029148867 -0.0003025211
H06 -3.2219374600 2.1431027000 0.0000000000 Rank 4
0.2835233217
0.0000000000 -0.1079818824 0.0010096560
0.0013702413 0.0000000000 0.0000000000 -0.0158238424 0.0008021915
0.0000000000 -0.0102277825 -0.0030041475 0.0000000000 0.0000000000
-0.0017938979 -0.0019164778
0.0040668876 0.0000000000 0.0000000000 -0.0155429240 0.0000182452
0.0000000000 0.0000000000 -0.0063673254 0.0033250818
H07 -0.3832689340 -3.8296248800 0.0000000000 Rank 4
0.3189680135
0.0000000000 0.0602681099 -0.0979012760
0.0015130789 0.0000000000 0.0000000000 0.0089058984 0.0188947758
0.0000000000 0.0037060430 -0.0089539382 0.0000000000 0.0000000000
-0.0032914010 0.0003036204
0.0087468839 0.0000000000 0.0000000000 0.0051668117 0.0065533191
0.0000000000 0.0000000000 -0.0029148867 0.0003025211
H08 -3.2219374600 -2.1431027000 0.0000000000 Rank 4
0.2835233217
0.0000000000 -0.1079818824 -0.0010096560
0.0013702413 0.0000000000 0.0000000000 -0.0158238424 -0.0008021915
0.0000000000 -0.0102277825 0.0030041475 0.0000000000 0.0000000000
-0.0017938979 0.0019164778
0.0040668876 0.0000000000 0.0000000000 -0.0155429240 -0.0000182452
0.0000000000 0.0000000000 -0.0063673254 -0.0033250818
```
axis - local axis set up for molecule

This is set up to define the molecular axis system for running in DMAREL, and used for DMAs. The axis input

file is in free format as shown below.

Where the integer after `MOLX` gives the number of types of molecule in the cell. Enantiomers should not be

given separately, although NEIGHBOURS will generate separate `AXES` for DMAREL. DMA and enantiomers

defined by right handed axis system.

In the example above, the X axis runs from CLR1 to CAR2 which is a first earliest neighbour. The Y axis is in

the plane formed by `CLR1`, `CAR2` (first earliest neighbour) and `CAR3` (second nearest neighbour). The Z axis

always makes a right-handed set. NEIGHBOURS avoids this difficulty by setting them up as two different molecules. The multipole expansions from the punch file are changed so that all odd-z components on the inverted molecule have the sign changed. NEIGHBOURS3.01 processes this information to work out the local

axis system of the molecules, previously it was necessary to run DMAREL to do this. The output is printed in

fort.21, in both Angstroms and AU. While DMAREL can run with any of X, Y or Z forming the first (`LINE`)

axis, this is not recommended as the fix for enantiomers only works if Z is the third axis. Enantiomers are automatically added. When a molecule is generated by inversion etc. (i.e. an enantiomer) then we need to ensure

multipoles and axes are still right handed.

Example of an **axis** file
```
MOLX 1
X LINE CLR1 CODA CAR2 CODA 1
Y PLANE CLR1 CODA CAR2 CODA 1 CAR3 CODA 2
```
potential: repulsion-dispersion potential

This is the file where the repulsion-dispersion potential is set up. The default is the Buckingham potential (BUCK). For details of the format and other types of potential formats, see DMAREL 3.02 manual (http://www.ucl.ac.uk/~uccahht/dmarelmanual/dmarel.html). A set of recommended potentials along with references will be given in the DMAREL manual. Here below are the examples of the repulsion-dispersion in

the form of a Buckingham potential, isotropic and anisotropic.

For anisotropic, follow the link for full detailed of the format. In addition to the potential, axes need to be set up

for each atom. At present, the axes for the anisotropic atoms need to be inserted manually.

Here below are examples of file format for isotropic and anisotropic repulsion-dispersion potential.

isotropic
```
BUCK CA CODA CA CODA
3832.147036 0.277778 25.286949 0.0 70.0
ENDS
BUCK NI CODA NI CODA
2638.028450 0.264550 14.286224 0.0 70.0
ENDS
BUCK CL CODA CL CODA
9583.579675 0.284900 80.224453 0.0 70.0
ENDS
BUCK CA CODA NI CODA
3179.514571 0.271003 19.006710 0.0 70.0
ENDS
BUCK CA CODA CL CODA
6060.172118 0.281317 44.799129 0.0 70.0
ENDS
BUCK NI CODA CL CODA
5028.096689 0.274537 33.849123 0.0 70.0
ENDS
```
anisotropic
```
BUCK CL CODA CL CODA
39279.474707 0.251090 73.204 0.0 70.0
ANIS CL CODA CL CODA
0 0 1 0 1 0.049824
0 0 0 1 1 0.049824
```

```
0 0 2 0 2 -0.128090
0 0 0 2 2 -0.128090
ENDS
BUCK CL CODA CA CODA
15209.716098 0.257807 35.399 0.0 70.0
ANIS CL CODA CA CODA
0 0 1 0 1 0.049824
0 0 0 1 1 0.000000
0 0 2 0 2 -0.128090
0 0 0 2 2 0.0000000
ENDS
BUCK CL CODA CB CODA
13352.561124 0.250420 35.399 0.0 70.0
ANIS CL CODA CB CODA
0 0 1 0 1 0.049824
0 0 0 1 1 0.000000
0 0 2 0 2 -0.128090
0 0 0 2 2 0.0000000
ENDS
BUCK CL CODA NI CODA
24248.092691 0.250115 34.571 0.0 70.0
ANIS CL CODA NI CODA
0 0 1 0 1 0.049824
0 0 0 1 1 -0.147641
0 0 2 0 2 -0.128090
0 0 0 2 2 0.120118
ENDS
BUCK CA CODA CA CODA
4950.350673 0.215561 17.170 0.0 70.0
ENDS
BUCK CA CODA CB CODA
3794.071843 0.224029 17.170 0.0 70.0
ENDS
BUCK CA CODA NI CODA
6190.707698 0.257639 16.842 0.0 70.0
ANIS CA CODA NI CODA
0 0 1 0 1 0.000000
0 0 0 1 1 -0.147641
0 0 2 0 2 0.000000
0 0 0 2 2 0.120118
ENDS
BUCK CB CODA CB CODA
3281.982135 0.239850 17.170 0.0 70.0
ENDS
BUCK CB CODA NI CODA
5517.272582 0.249234 16.842 0.0 70.0
ANIS CB CODA NI CODA
0 0 1 0 1 0.000000
0 0 0 1 1 -0.147641
0 0 2 0 2 0.000000
0 0 0 2 2 0.120118
ENDS
BUCK NI CODA NI CODA
11647.681230 0.251382 16.625 0.0 70.0
ANIS NI CODA NI CODA
0 0 1 0 1 -0.147641
0 0 0 1 1 -0.147641
0 0 2 0 2 0.120118
0 0 0 2 2 0.120118
ENDS
```

3. Running NEIGHBOURS

NEIGHBOURS 3.01 may be run in the following 3 ways:

(i) Running interactively without default values - useful for initial setups for geometry

(ii) Running with default values

(iii) Running non-interactively - useful for repeated setups

(i) Running interactively without default values

The input file can be either an FDAT format file (Cambridge Crystallographic Database), or a SHELX format

file. The interactive input is exactly the same in both cases, except that SHELX files must be run interactively

(there is no option 2.). A NEIGHBOURS read the first character of the first record, if it is # it is assumed to be

an FDAT file, anything else is assumed to be SHELX. If the file is in FDAT format, then characters 2-9 are the

refcod. Some of the input and output files from neighbours can use this refcod as part of the filename. The FDAT filename must not be the same as the refcod to run interactively. The cutoff filename should be cutoff or

file_1.cutoff, otherwise its name will be asked for.

Below is a typical interactive run. > indicates output from NEIGHBOURS

```
> TYPE I FOR INTERACTIVE MODE
i
> File name containing basis set?
filename.fdat
> Filename differs from csd refcod, interactive mode
> Used
> cutoff
> as file with standard bond lengths
> Maximum required inter-molecular contact?
4.0
> nbonds= 4
> Do you want to standardise bond lengths to hydrogen?
y
> Do you wish to insert any bond centre sites (Y/N) ?
n
> CVECTOR
> 14.861000000000
> Input zero for no symmetry subgroup or n to remove representation n
0
> Do you have a punch file yet (y/n)
y
> File name for punch file
filename.punch
> Labelled basis to be written to
> filename.dmain
> This file will be overwritten
> Do you have an axis definition file?
y
> Enter filename for axis definition file.
filename.axis
> Do you want to paste coordinates?
n
> Do you have a potential input file?
y
> Enter filename for potential input file.
pote.dat
> Labelled nearest neighbour list to be written to filename.nnl
> This file will be overwritten
> Labelled close contact list to be written to filename.ccl
> This file will be overwritten
> MACROMODEL file to be written to filename.mac
> This file will be overwritten
> NEMESIS file to be written to filename.nem
> This file will be overwritten
```

Notes on responses to questions

```
> TYPE I FOR INTERACTIVE MODE
i
```

I or i will run interactively, if response is N or n it will run according to option 3.

```
> File name containing basis set ?
filename.fdat
> Filename differs from csd refcod, interactive mode
```

If the filename is refcod.fdat, then it would proceed to run as option 2 for running with default values. This message is not printed if the file is in SHELX format

```
> Used
> cutoff
> as file with standard bond lengths
```

The file name with the bond cutoff should be cutoff or file_1.cutoff. This will then be used with message. If this

file does not exist NEIGHBOURS will prompt for a name. (> File name with standard bond lengths ?)

```
> Maximum required inter-molecular contact?
4.0
```

This prints the intermolecular atom-atom contacts less than 4 Å in the output. Usually 4.0 is large enough.

```
> nbonds= 4
```

Number of records read from cutoff file, i.e. number of types of covalent bond.

```
> Do you want to standardise bond lengths to hydrogen?
y
```

This is necessary when X-ray hydrogen positions are used to correct for the appointment of shortening of bonds.

A few defaults are C...H 1.08 Å, N...H 1.01 Å and O...H 1.02 Å. See options for more details.

```
> Do you wish to insert any bond centre sites (Y/N)?
n
```

Normally n, but for high accuracy work on small polyatomics, e.g. N_2, then an additional multipole site at the

centre of bond will provide a more accurate description of the close contact list.

```
> CVECTOR
> 14.861000000000
> Input zero for no symmetry subgroup or n to remove representation n
0
```

Normally 0 to use crystallographic symmetry. When DMAREL shows that the minimum has a lower symmetry,

then a number of the representation with negative values is given.

```
> Do you have a punch file yet (y/n)
y
```

n only used for runs to establish molecular geometry in local axis system.

```
> File name for punch file
filename.punch
```

If n is typed, dmain file is set up with LEVEL 0 multipoles. Note that charges of free ions are not read from the

punch file, the dmain file will need to be changed. If more than one type of molecule in crystal, then the punch

file will need to be constructed from punch files from individual *ab initio* calculation. Free ions, e.g. Cl- needs

to be added manually.

```
> Labelled basis to be written to
> filename.dmain
> This file will be overwritten if file exists
> Do you have an axis definition file?
y
```

n is only useful to print out the atomic numbering and intramolecular connectively table if you do not have a

chemical diagram from which to choose your axis definition.

```
> Enter filename for axis definition file.
filename.axis
```

This must correspond to the axis definition used for calculating DMAs.

```
> Do you want to paste coordinates?
n
```

Normally n. This option can be used to paste another molecular structure into the crystal, so that the centre of

mass matches and the molecular local axes are parallel. It is particularly useful for comparing the minimum structure with an *ab initio* optimised version of the experimental structure. Type y if you want to paste coordinates over an experimental structure.

```
> Do you have a potential input file?
y
> Enter filename for potential input file.
pote.dat
```

NEIGHBOURS 3.01 can insert Buckingham potentials from a file into the dmain dataset. pote.dat should contain any number of Buckingham potentials in the same format as used in the dmain file, beginning with BUCK and ending with ENDS. Only Buckingham potentials needed for the structure are copied to the dmain

file. Missing potentials are set to zero.

```
> Labelled nearest neighbour list to be written to filename.nnl
> This file will be overwritten
> Labelled close contact list to be written to filename.ccl
> This file will be overwritten
> MACROMODEL file to be written to filename.mac
> This file will be overwritten
> NEMESIS file to be written to filename.nem
> This file will be overwritten
```

These files can be used to find atoms to define the axis system if a graphics program is not available.

(ii) Running with default values

The input file must be an FDAT format file. The first record has a first character #, then characters 2-9 are the

refcod, in the example below BAWNIW01. Most of the input and output files from neighbours will use this

refcod as part of the filename.

Again responses to the terminal from NEIGHBOURS are indicated by >

(ii) a. Redirecting the input from a file

Start the program by typing the following at the unix prompt

```
neigh.exe < BAWNIW01.fdat
>TYPE I FOR INTERACTIVE MODE
```

Ignore this message.

Neighbours will run only if fort.22 file exits, and it will not be expecting any more user input assuming the default values and file names described below

(ii) b. Using an FDAT filename which is the same as the refcod

Start the program by typing the following at the unix prompt

```
prompt> neigh3.01
>TYPE I FOR INTERACTIVE MODE
I or i
>File name containing basis set ?
BAWNIW01.fdat
```

Neighbours will run without expecting any more user input assuming the default values and file names described below. Start the program by typing the following at the unix prompt.

```
prompt> neigh3.01
>TYPE I FOR INTERACTIVE MODE
I or i
>File name containing basis set ?
BAWNIW01.fdat
```

Neighbours will run without expecting any more user input assuming the default values and file names described below.

INPUT FILES USED Fortran unit Use Required input

BAWNIW01.fdat 11 or 5 FDAT input Yes

BAWNIW01.cutoff or cutoff 12 cutoffs Yes

BAWNIW01.punch 19 multipoles No

BAWNIW01.axis or BAWNIW01.axes 13 molecule axis No

pote.dat 15 BUCK potentials No

If no punch file is present, multipoles are written as `LEVEL  0`. If no axes file is present, no axes are written to

dmain. If no pote.dat file is present, `BUCK` potentials are written as zero.

DEFAULT VALUES OF CONSTANTS AND ANSWERS TO QUESTIONS

which are input interactively using option (i).

```
>Maximum required inter-molecular contact?
4.0
>Do you want to standardise bond lengths to hydrogen?
y
>Do you wish to insert any bond centre sites (Y/N) ?
n
>Input zero for no symmetry subgroup or n to remove representation n
0
>Do you want to paste coordinates?
n
```

(iii) Running non-interactively

Running NEIGHBOURS using option (i) produces a file fort.22 which has the user responses to the questions

written to it. You can now use this option if you have previously used either option (i) or option (ii) b., but not

option (ii) a.

```
> TYPE I FOR INTERACTIVE MODE
n
```

NEIGHBOURS will read fort.22 and interpret this as the user input. Here is a typical fort.22 file

```
file_1.fdat
4.0000000000000
y
n
0
y
file_1.punch
y
file_1.axis
n
y
pote.dat
```

fort.22 may be edited to
a) change the input fdat file
b) change the options that NEIGHBOURS uses
This way of running NEIGHBOURS is useful for running a series of cells where the default options are not used.

4. Contents of output files
Here are the output files produced by NEIGHBOURS (e.g. examples for formic acid)
fort.7
fort.8
fort.10
fort.20
fort.21
fort.22
fort.23
file.dmain
file.ccl
file.mac
file.nem
file.nnl

Standard output (Unit 6)

Interactive mode
Questions which require a user response are written here, normally to the screen.

Non-interactive mode
Only the instruction TYPE I FOR INTERACTIVE MODE is written, and can be ignored (See also fort.23).

fort.7
Write out of fdat information as read in.

fort.8
Symmetry operations of system.

fort.10
An spf file. A fairly free format used by CSD PLUTO and PLATON to deduce reduced cell.

fort.20
Symmetry interface file for DMAREL 3.01. Essential for DMAREL run, a file containing the crystal information.

fort.21
Information about symmetry analysis.

fort.22
It writes an input file that can be used to run NEIGHBOURS non-interactively.

fort.23
This is a file to which the screen output is written if you use non-interactive mode.

file.dmain
DMAREL input file.

file.ccl
A file containing close contacts list.

file.mac
A MACRO file.

file.nem
A NEMESIS file.

file.nnl
A file containing nearest neighbours list within molecule. In the molecule, the nth nearest neighbouring atoms
are separated by a covalent bond.

5. Options
There are a few options that could be applied in NEIGHBOURS.
Pasting molecular structure in experimental crystal structure
Standardising bond lengths

Atom types
Pasting molecular structure in experimental crystal structure
Pasting is an option, where an ab intio molecular structure can be pasted into an experimental crystal structure in

the same axis system. For example using experimental molecular structure and optimised it using an *ab initio*

program such as CADPAC (or GAUSSIAN). The opposite could also be done, that is pasting in an experimental molecular structure into an *ab initio* optimised crystal structure. An example of this is when a blind prediction is needed, when the experimental structure is known, in order to check that the predicted structure is of reasonable quality, the experimental molecular structure can be pasted into the predicted structure

for minimisation.

The procedures are as follow:
1. Run NEIGHBOURS using the CSD FDAT (or SHELX) to get the molecular structure in the local axis system from the output file fort.21.
2. Optimise the molecular structure in CADPAC (or GAUSSIAN) to give an *ab initio* molecular structure.
3. Use the *ab initio* molecular structure to calculate a new DMA punch file in CADPAC (or GAUSSIAN with

GDMA).
4. Run NEIGHBOURS again (See below).

The format of the paste input dataset is:
```
TITLE
NMOLECULES NATOMS NATOMS
(5 Blank Lines)
I4,7X,A4,3F13.6
Index, Label, Coordinates
(5 Blank Lines)
I4,7X,A4,3F13.6
Index, Label, Coordinates
```
NMOLECULES is the number of molecules in the unit cell. NATOMS are the corresponding number of atoms

for each molecule. The second set of labels and coordinates are for the inverted molecule for which the z coordinate has the sign changed. The coordinates are input in AU.

Here below is an example of the paste file.
```
pyrene (D2h RHF/6-31G** structure) in PYRENE02 (cryst. struct.)
2 26 26
1 CAR1 -6.615739 0.000000 0.000000
2 CARa 2.688476 -2.309989 0.000000
3 CARb 1.265503 -4.643900 0.000000
4 CARc -1.265503 -4.643900 0.000000
5 CARd -2.688476 -2.309989 0.000000
6 CARe -5.318119 -2.271274 0.000000
7 CARf -1.353904 0.000000 0.000000
8 CARg 1.353904 0.000000 0.000000
9 CAR2 -5.318119 2.271274 0.000000
10 CAR3 -2.688476 2.309989 0.000000
11 CAR4 -1.265503 4.643900 0.000000
12 CAR5 1.265503 4.643900 0.000000
13 CAR6 2.688476 2.309989 0.000000
14 CAR7 5.318119 2.271274 0.000000
15 CAR8 6.615739 0.000000 0.000000
16 CAR9 5.318119 -2.271274 0.000000
17 HYD1 -8.649170 0.000000 0.000000
18 HYDb 2.294913 -6.398497 0.000000
19 HYDc -2.294913 -6.398497 0.000000
20 HYDe -6.344427 -4.027802 0.000000
21 HYD2 -6.344427 4.027802 0.000000
22 HYD4 -2.294913 6.398497 0.000000
23 HYD5 2.294913 6.398497 0.000000
24 HYD7 6.344427 4.027802 0.000000
25 HYD8 8.649170 0.000000 0.000000
26 HYD9 6.344427 -4.027802 0.000000
27 CAI1 -6.615739 0.000000 0.000000
28 CAIa 2.688476 -2.309989 0.000000
29 CAIb 1.265503 -4.643900 0.000000
30 CAIc -1.265503 -4.643900 0.000000
31 CAId -2.688476 -2.309989 0.000000
32 CAIe -5.318119 -2.271274 0.000000
33 CAIf -1.353904 0.000000 0.000000
```

```
34 CAIg 1.353904 0.000000 0.000000
35 CAI2 -5.318119 2.271274 0.000000
36 CAI3 -2.688476 2.309989 0.000000
37 CAI4 -1.265503 4.643900 0.000000
38 CAI5 1.265503 4.643900 0.000000
39 CAI6 2.688476 2.309989 0.000000
40 CAI7 5.318119 2.271274 0.000000
41 CAI8 6.615739 0.000000 0.000000
42 CAI9 5.318119 -2.271274 0.000000
43 HYI1 -8.649170 0.000000 0.000000
44 HYIb 2.294913 -6.398497 0.000000
45 HYIc -2.294913 -6.398497 0.000000
46 HYIe -6.344427 -4.027802 0.000000
47 HYI2 -6.344427 4.027802 0.000000
48 HYI4 -2.294913 6.398497 0.000000
49 HYI5 2.294913 6.398497 0.000000
50 HYI7 6.344427 4.027802 0.000000
51 HYI8 8.649170 0.000000 0.000000
52 HYI9 6.344427 -4.027802 0.000000
```

Here is an example running NEIGHBOURS to insert paste file:

```
prompt> neigh3.01
>TYPE I FOR INTERACTIVE MODE
i
>File name containing basis set ?
file.fdat
>Filename differs from csd refcod, interactive mode
>Used
>cutoff
>as file with standard bond lengths
>Maximum required inter-molecular contact?
4.0
>nbonds= 2
>Do you want to standardise bond lengths to hydrogen?
n
>Do you wish to insert any bond centre sites (Y/N) ?
n
>CVECTOR
>8.470000000000001
>Input zero for no symmetry subgroup or n to remove representation n
0
>Do you have a punch file yet (y/n)
y
>File name for punch file
file.punch
>Labelled basis to be written to
>pyrene.dmain
>This file will be overwritten
>Do you have an axis definition file?
y
>Enter filename for axis definition file.
axis
>Do you want to paste coordinates?
y
>Enter filename for coordinate pasting file.
paste
>Do you have a potential input file?
y
>Enter filename for potential input file.
pote.dat
>Labelled nearest neighbour list to be written to file.nnl
>This file will be overwritten
>Labelled close contact list to be written to file.ccl
>This file will be overwritten
>MACROMODEL file to be written to file.mac
>This file will be overwritten
>NEMESIS file to be written to file.nem
>This file will be overwritten
```

Standardising bond lengths

Standardising bond lengths is needed where the C-H bondlengths in the experimental crystal structure (all are

0.950 Å) must be corrected to the standard 1.08Å, as X-ray diffraction has reduced the C-H bondlengths.

Currently only C...H, N...H, O...H and water are recognised and set to a standard length, of 1.08 Å, 1.01 Å and

1.02 Å respectively.

Subroutine FUNGRP will recognise a number of additional functional groups, but no bond length is reset.

Modifications can be made in the subroutine NORMBL for automatic normalising the bond lengths for the atom
types below.
Below is a list.
101 H SP3 C
102 H SP1 C
103 H SP C
201 H N Ammonium NH4+ derivative
202 H N Ammonia NH3 derivative
301 H O SP3 C (alcohols etc)
302 H O Carboxylic acids
303 H O Other SP2 C (Phenols etc)
311 Water
401 Nitro group

Atom types
The following tables show the default atom types available. If additions need to be made, modifications can be
done in the subroutine SETMAS.
Atom type from input file
FDAT/SHELX
Convert to DMAREL
atom type labelling
Atom type Atomic mass
H
H
H
D
HE
LI
BE
B
C
C
N
N
O
O
F
NE
NA
MG
AL
SI
P
SI
CL
AR
K
I
CA
FE
CU
ZN
BR
HYD
HHD

HPD
DEU
HEL
LIT
BER
BOR
CAR
CCR
NIT
NNT
OXY
OOY
FLU
NEO
NAR
MGN
ALU
SIL
PHO
SUL
CLR
AR
POT
IOD
CIM
FER
CUP
ZIN
BRO
HY
HH
HP
DE
HE
LI
BE
BO
CA
CC
NI
NN
OX
OO
FL
NE
NA
MG
AL
SI
PH
SU
CL
AR
PO
IO
CI

FE
CU
ZI
BR
1.0079
1.0079
1.0079
2.014
4.003
6.939
9.012
10.811
12.011
12.011
14.0067
14.0067
15.9994
15.9994
18.9984
20.183
22.99
24.312
26.982
28.086
30.974
32.064
35.453
35.4527
39.948
39.102
126.9
40.08
55.85
63.54
65.37

6. Example of input file (formic acid)

This example was run using option (ii) b. using an FDAT filename that is the same as the refcod. Please visit

this web site for further details. http://www.ucl.ac.uk/~uccahht/neighmanual/formic.html

Input files

cutoff

FORMAC01.axis

FORMAC01.fdat

FORMAC01.punch

pote.dat

Output files

FORMAC01.ccl

FORMAC01.nem

FORMAC01.nnl

FORMAC01.mac

FORMAC01.dmain

fort.7

fort.8

fort.10

fort.20

fort.21

fort.22

DMAREL

The following only provide a quick guide to the program DMAREL, for full details of the capabilities of the

program, please refer to the DMAREL manual.

Input files

FORMAC01.dmain

fort.20 (from NEIGBOURS output)

Output files

FORMAC01.out

fort.8 - Lattice vectors and molecule coordinates of minimised structure

fort.12 - summary file

fort.13 - spf file

fort.14 - empty file, please ignore

fort.15 - FDAT file

fort.16 - SHELX file

fort.30 - Crystal information,

graphic - graphic output

7. Anisotropic potentials

Changes to the input dataset:

To input the anisotropic short range parameters

```
BUCK NI CODA CL CODA
10549.321 0.264206 28.490 0.0 70.0
ANIS NI CODA CL CODA
0 0 1 0 1 -0.022080
0 0 0 1 1 0.026758
0 0 2 0 2 0.004878
0 0 0 2 2 -0.101149
ENDS
```

`ANIS` should follow immediately after the parameters for the `BUCK` part.

The lines after `ANIS` are

k1 k2 l1 l2 j rho

RHO(0) is read in in the above example as the first parameter of the `BUCK` potential; this value is EXP(ALPHA

* RHO(0)).

You can read it in as rho(0) by supplying a line after anis

0 0 0 0 0 rho(o), in which case you will get a warning message.

The second parameter after `BUCK` _____ , the third is the Van der Waals parameter.

To convert from anisotropic to isotropic, just remove `ANIS` and the lines following it.

On the output file, the first parameter of the `BUCK` potential is reset to zero and the correct value of rho(0) is

printed out even if it was not input.

At present to input a potential between two species that are the same you need to supply both of the identical

interactions.

```
BUCK CL CODA CL CODA
15555.674 0.271759 57.363 0.0 70.0
ANIS CL CODA CL CODA
0 0 0 1 1 0.026758
0 0 1 0 1 0.026758
0 0 0 2 2 -0.101149
0 0 2 0 2 -0.101149
ENDS
```

Note: This can be set up automatically using NEIGHBOURS.

Input of the axis system for the anisotropic atoms

This must be put in after the molecular axes (`MOLX`) but before the following `ENDS`

```
ANIS
..
..
CLR1 CODA
Z LINE CAR1 CODA CLR1 CODA 1
X PLANE CAR1 CODA NIT1 CODA 1 NIT3 CODA 1
..
```

```
..
NIT1 CODA
Z BIEX NIT1 CODA CAR1 CODA 1 CAR2 CODA 1
X PLANE NIT1 CODA CAR1 CODA 1 CAR2 CODA 1
..
..
ENDS
```

Format:

Record 1

Species on which the anisotropic axis is to lie

Record 2

First axis, format

`[X,Y,Z] [LINE,BIEX,BIIN]` species1 species 2 separation(1-2) [species 3 separation(1-3)]

LINE is as for molecular axes; the species in line do not have to contain the species on which you are constructing the axis. `BIEX BIIN` are external and internal bisector of a bond angle. The species are in the

order centre of bond end 1 separation 1 end 2 separation 2 so the bond angle is 2-1-3.

Record 3

Second axis which must be a plane, same format as for `MOLX`. The sequence is terminated by an `ENDS` record;

note that this will give you two `ENDS` records in a row. The calculated anisotropic axes are printed out.

Note: This needs to be set up by modifying the dmain file manually.