

# FOCUS MANUAL

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## 1. Installation

Download the FOCUS package from [https://github.com/stefsmeets/focus\\_package/releases](https://github.com/stefsmeets/focus_package/releases)

It is recommended to install the pre-compiled versions for Windows 7+ (32 bit) OS X (Intel x64) or Linux (debian x64).

1. Unzip or extract using `tar -xvzf focus-osx.tar.gz`
2. Install with python:  
`python setup.py install`

After the installation step, setup will ask to move sginfo/focus to a directory on the system path. Afterwards, the whole directory can be removed. The scripts have been tested to work on recent versions of OS X (10.8+), Ubuntu 12.04 LTS x64, and Windows 7-10.

**Note:** Windows users need to install Python 2.7 (<https://www.python.org/downloads/>) and Visual C++ Redistributable for Visual Studio 2015 (<https://www.microsoft.com/en-us/download/details.aspx?id=48145> => `vc_redist.x86.exe`)

## 2. FOCUS installation from source

The FOCUS package comes with several useful tools for working with and analyzing FOCUS output. FOCUS and KRIBER are written in C and should therefore be compatible with any C compiler. Additionally, FOCUS requires Scons (2.4.1), fftw (3.3.2), libtbx (20000) and Python2.x (2.7) for compilation. More recent versions of libtbx cause the installation to fail.

DLS76 was written in FORTRAN and should be compiled using gfortran.

It is recommended that the installation scripts provided (see above) be used to compile FOCUS, or at least be used as a guide.

### 2.1.1. Overview of dependencies

#### **FOCUS**

gcc  
Scons  
libtbx  
fftw

#### **Kriber**

gcc

#### **DLS76**

gfortran

#### **install scripts**

curl  
svn

Curl and SVN are used in the install scripts to download the required packages, such as Scons (curl), libtbx (svn) and fftw (curl), from the internet.

This installation script (build\_all.sh) will download and compile dependencies, and compile FOCUS and related programs in 4 steps by calling the following scripts:

1. focus\_build\_script.sh  
Downloads and compiles FFTW 3.3.2, libtbx, scons 2.4.1 and FOCUS (focus/focus\_build\_script)  
requires curl and svn
2. make  
Compiles and sets up KRIBER (src/dls76/makefile)
3. make  
Compiles and sets up DLS76 (src/kriber/makefile)
4. python setup.py install  
Moves all executables/scripts into to a directory on your system path

### 2.1.2. OS X

For OS X, C-compilers are available via the Command Line Tools for Xcode (type xcode-select install in the terminal to initiate installation). Curl and Python come pre-installed, svn is part of the Command Line Tools.

gfortran is available via <http://hpc.sourceforge.net/> or a package manager like brew (<http://brew.sh>).

### 2.1.3. Linux/Unix

Most Linux distributions come with their own compiler suite, otherwise compilers are usually available via the package manager or <http://gcc.gnu.org> . Python usually also comes preinstalled, but is otherwise available from the packages manager or <http://www.python.org>

SVN and Curl did not come preinstalled on the system used for testing the installation procedure (Ubuntu 12.04), but both were available via the package manager.

The installation script was tested successfully on Ubuntu 12.04 LTS x64.

#### 2.1.4. *Compiling*

After compiling, all the files necessary to run FOCUS are in the `./focus_package` directory.

Install with python:

```
python setup.py install
```

### 3. The FOCUS input file

A template for the input file can always be generated directly using:

```
focus > template.inp
```

The template generated has sensible defaults for solving zeolite structures. Of course, some parameters are more sample specific than others. Some of the parameters in the template can be ignored or removed (e.g. all the profile related ones from GenerateFWHM to NormalizeSurface).

A sample input file that solves a structure readily has been provided in the directory `./manuals/example/`

The parameters relevant for structure solution are discussed below.

#### **Formatting:**

#hash	denotes numerical values. #N is usually used for integers and #d for distances in Å.
\$dollar	denotes an arbitrary string
x/y	denotes a choice of keywords
(parentheses)	denote optional input
[Square brackets]	indicate repeated input.

#### 3.1.1. *Title*

##### **Title \$title**

Set a title for the calculation. It is recorded in the output file.

#### 3.1.2. *SpaceGroup*

##### **SpaceGroup \$spgr**

Spacegroup for the supplied data.

#### 3.1.3. *UnitCell*

##### **UnitCell #a #b #c #al #be #ga**

Dimensions of the unit cell in Å and angles in degrees. Parameters can be given in shortened form, i.e. by specifying only *a* for a cubic system.

### 3.1.4. *AtomType*

#### **AtomType +/- node/nodebridge/\* \$label #N (#occ) (#U) (#scattering factor)**

The AtomType parameter defines the cell contents of the structure to be solved, as determined by a chemical analysis or estimated by other means. One AtomType line for each type of atom needs to be specified. The first item after the keyword AtomType is either "+" or "-". All atoms specified with an AtomType line are used in the calculation of F000 (the Fourier magnitude at the origin of reciprocal space), but only atoms with the "+" marker are considered in the atom and/or the framework fragment recycling procedures. The next item is a "class label", Node, NodeBridge, or " ", which determines how FOCUS should treat this atom type. The latter is for non-framework atoms. Nodes are typically T atoms and NodeBridge denotes bridging (O) atoms. For the following item, an "atom label" and the number of atoms of this type per unit cell should be supplied. The rest is optional.

For a typical zeolite, such as ZSM-5, the AtomType parameters look like this:

```
AtomType + Node    Si    96
AtomType - NodeBridge O    192
```

Also possible - but not used here - is the definition of the occupancy factor to be used in the recycling (default: 1.0), the isotropic temperature factor (default: 0.035), and a "scattering factor label" (default: derived from the preceding atom label).

For example, the line

```
AtomType - * Ow 20 1.25 0.05 O
```

Describes an oxygen with an occupancy of 1.25 and an isotropic temperature factor of 0.05 Å<sup>2</sup>, which is a commonly used approximation for water molecules in zeolite channels. The scattering factor used is that of oxygen, and 20 water per unit cell are expected. However, experience has shown that recycling extra framework atoms is not efficient, nor necessary, and for the calculation of F000 it would be sufficient to supply one AtomType line for oxygen and one for hydrogen using the default occupancy and temperature factors.

### 3.1.5. *Chemistry*

#### **Chemistry MinDistance/MaxDistance \$NodeType1 \$label1 \$NodeType2 \$label2 #d**

The Chemistry lines define the expected connectivity of the atom types specified before. This is related to the atom recycling procedure. The Chemistry lines define the individual minimum and/or maximum distances for each pair of atom types which are used in the atom recycling procedure. Following Chemistry MinDistance/MaxDistance are two pairs of "class label" and "atom label" as defined on AtomType lines, and the minimum distance for this pair of atom types in the same units as the lattice constants, usually Å. It should be noted that bonding is not considered in atom recycling mode. The minimum distances apply to all pairs of atoms, whether they are bonded or not.

For ZSM-5, this section could look like this:

```
Chemistry MinDistance Node    Si    Node    Si    2.6
Chemistry MinDistance NodeBridge O    Node    Si    1.4
Chemistry MinDistance NodeBridge O    NodeBridge O    2.3
```

Specification of the MaxDistance is also possible in the same way. Note: if there is a "-" on the AtomType line as for

AtomType - NodeBridge O 192

this atom type is not used in the atom recycling procedure. Therefore it would be sufficient to supply only the first Chemistry line for Si--Si.

### 3.1.6. MaxPotentialAtoms

#### **MaxPotentialAtoms #N**

This parameter gives the maximum number of peaks which are considered in the assignment algorithm.

Example: MaxPotentialAtoms 130

With this value, if the algorithm tries to assign a silicon atom to one of the peaks in the asymmetric unit, but is not able to find a valid position among the peaks in the asymmetric unit which generate the 130 highest peaks in the unit cell, the silicon is not assigned at all.

### 3.1.7. MaxRecycledAtoms

#### **MaxRecycledAtoms #N**

MaxRecycledAtoms prescribes the maximum number of atoms in the unit cell that are actually assigned and is forced to be smaller or equal to MaxPotentialAtoms.

### 3.1.8. FwSearchMethod

#### **FwSearchMethod FwTracking/AltFwTracking**

The value can be either FwTracking or AltFwTracking, which are simple backtracking and "colored" backtracking, respectively. The latter is only useful in case of strict alternation of the T atoms, for example in case of a germanosilicate.

### 3.1.9. MaxPeaksFwSearch

#### **MaxPeaksFwSearch #N**

In the atom recycling procedure, only complete frameworks are sought, and MaxPeaksFwSearch defines the maximum number of peaks in the unit cell that are used in the backtracking procedure.

### 3.1.10.

#### MaxPeaksFwFragmentSearch

#### **MaxPeaksFwFragmentSearch #N**

In framework fragment recycling mode, MaxPeaksFwFragmentSearch determines the maximum number of peaks. Since the fragment search is significantly slower than the search for complete frameworks only, it is sometimes necessary to set MaxPeaksFwFragmentSearch to a smaller value than MaxPeaksFwSearch in order to retain reasonable computing times.

### 3.1.11.

#### MinNodeDistance

#### **MinNodeDistance #d**

The MinNodeDistance and MaxNodeDistance parameters establish the lower and upper limits for the node-node distances which are used in the preparation of the lists of potential node-node bonds. In this case, a tolerance of 0.5 Å around the "ideal" distance of 3.1 Å is set:

MinNodeDistance 2.6  
MaxNodeDistance 3.6

This is usually a good starting point for aluminosilicates. In case that no solutions are found, increasing the upper limit may help.

3.1.12.

MaxNodeDistance

**MaxNodeDistance #d**

See MinNodeDistance.

3.1.13.

MaxSymNodes

**MaxSymNodes #N**

MinSymNodes and MaxSymNodes set the lower and upper limits for the number of framework nodes per unit cell. While MinSymNodes just prevents frameworks with too low a density from being evaluated and printed and can usually be left at 0, MaxSymNodes cuts complete branches of the search tree. On the one hand, this can reduce the computing time for frameworks with a well-established low density, but on the other, one has to be careful not to prescribe a value that is too small. Normally, the choice for MaxSymNodes is based on the consideration that the number of T-sites per 1000 Å<sup>3</sup> in a zeolite must be less than 20.

3.1.14.

MinSymNodes

**MinSymNodes #N**

See MaxSymNodes.

3.1.15.

NodeType

**NodeType #Nbonds #Natoms [\$symaxis ...]**

The NodeType keyword defines the number of bonds for a given node type, the maximum number of nodes of this type in the asymmetric unit and a list of the symmetry elements which can not be occupied by a node of this type.

For example, by default, this NodeType should always be specified:

```
NodeType 4 * -6 -3 -1 4 6
```

In the example, only one node type with tetrahedral connectivity is defined. The asterisk "\*" specifies that an unlimited number of nodes in the asymmetric unit can be of this type. The following numbers "-6 -3 -1 4 6" specify that this node type cannot be on a six- or threefold rotoinversion axis, an inversion center, or a four- or sixfold rotation axis.

**Multiple NodeTypes can be specified, for example adding: NodeType 3 1 -6 -3 -1 4 6**

tells FOCUS that there is a single Q<sup>3</sup> T atom in the asymmetric unit that is not on any of the specified axes of symmetry. If such information is known, it should be specified, as it can mean the difference between solving the structure and finding no solutions at all.

However, adding NodeTypes means that the algorithm has to check every possible atom position for given connectivities, which will exponentially increase the time taken for the framework search.

3.1.16.

MinLoopSize

### **MinLoopSize #N**

Example: MinLoopSize 4

Supplying a value greater than three for MinLoopSize has two consequences: when atoms are recycled and only complete frameworks are sought, frameworks which have loops with less than MinLoopSize members are rejected (that just means they are not printed). In framework fragment recycling mode, the fragments which are candidates for the "largest fragment" for recycling are checked for MinLoopSize. Unfortunately, the present implementation of the loop size test is very time consuming. The time spent for the fragment search increases by roughly 40%. In this example, MinLoopSize was therefore kept at its default value of three, although four is perhaps more appropriate for high silica frameworks. (However, the structure of the high silica ZSM-18 (MEI) does contain 3-rings).

3.1.17.

MaxLoopSize

### **MaxLoopSize #N**

Example: MaxLoopSize 24

MaxLoopSize is less critical than MinLoopSize and just specifies the maximum loop size up to which the LC algorithm advances. The default value of 24 is sufficient for all known zeolite topologies. For loops with more than MaxLoopSize members, a "0" is printed. Cases where smaller values would result in a speed gain for the price of having some zeros in the LC are hardly imaginable.

3.1.18.

EvenLoopSizesOnly

### **EvenLoopSizesOnly On/Off**

If EvenLoopSizesOnly is turned Off, this means that all loop sizes greater than or equal to MinLoopSize are allowed. The EvenLoopSizesOnly option was introduced for the search for frameworks where a strict alternation of two atom types is expected. In these cases, only even loop sizes are possible. A special problem arises for aluminophosphates. Since the scattering powers of Al, and P are only slightly different, it is often not possible to determine the true space group from the powder profile. Only after the structure is known, can one introduce the strict Al-P alternation, which in many cases reduces the symmetry. For this situation, EvenLoopSizesOnly provides a more robust alternative to AltFwTracking.

It has to be noted that in framework fragment search mode the impact of EvenLoopSizesOnly on the computing time requirements is similar to setting MinLoopSize to a value greater than three. However, since loop sizes have to be computed only once per framework or framework fragment, MinLoopSize greater than three does not result in more time consumption if EvenLoopSizesOnly is switched On.

3.1.19.

Check3DimConnectivity

**Check3DimConnectivity On/Off**

If On, a filter procedure is called for each framework topology found. Only 3-dimensionally connected frameworks can pass this filter, layer or chain structures are rejected.

3.1.20.

IdealT\_NodeDistance

**IdealT\_NodeDistance #d**

specifies the "ideal" node-node distance for four-connected nodes. This is the basic value for the geometrical tests and is normally set to 3.1 Å for aluminosilicates.

3.1.21.

CheckTetrahedralGeometry

**CheckTetrahedralGeometry Off/Normal/Hard**

This parameter adds to the geometrical tests and checks for Tetrahedral connectivity of the framework. In most cases, this can be set to Normal. Turning this parameter Off tends to result in unrealistic frameworks. For high silica and Si-Al frameworks such as Dodecasil-1H, the Hard test is appropriate.

3.1.22.

RandomInitialization

**RandomInitialization Time/#seed**

Defines the "seed" value for a portable pseudo random number generator, which is used to generate the starting phases. The special value Time tells FOCUS to use the machine time for the automatic determination of the seed value, which is then printed on the output file. This integer value - like any positive integer value - can be resupplied with RandomInitialization in order to rerun FOCUS with different output options or for testing or debugging purposes.

3.1.23.

FeedBackCycles

**FeedBackCycles [ #Natom #Nfw ... ... ]**

Example: FeedBackCycles 1 1 1 1 1 1 1 1 1 1

This keyword is followed by an arbitrarily long sequence of nonnegative integers (including zero). The first integer specifies the number of times the atom recycling procedure is to be used in one trial, the second integer is for the number of framework fragment recycling loops, the third again for atom recycling, and so on. In the example, ten cycles with alternation of atom and framework fragment recycling are requested. Experience has shown that a simple alternation of atom recycling and framework fragment recycling, as in the example, is usually the most efficient approach.

3.1.24.

FeedBackBreakIf

**FeedBackBreakIf PhaseDiff < 5.00 % and DeltaR < 1.00 %**

The recycling is prematurely terminated if both the phase set and the RF residual value have converged. Another special situation is, when no fragment which can be recycled is found. In this case, a trial continues with atom recycling (but the cycle is still counted as framework fragment recycling cycle).

3.1.25.

Grid\_xyz

**Grid\_xyz #Nx #Ny #Nz**

Sets grid for the electron density map is defined such that a resolution of about 1/3 Å is achieved. One has also to take care that all symmetry elements pass through grid points. In its present form, FOCUS does not automatically generate an appropriate grid, but it does refuse to work with grid sizes that do not conform to this requirement. For example, in space group P-1 the grid sizes for all directions have to be a multiple of two, in order to have all inversion centers laying on a grid point. In the case of space group *P6/mmm*, the grid size in the *z*-direction has to be a multiple of two, and the grid sizes for the *x*- and *y*-direction have to be a multiple of six.

3.1.26.

eDensityCutOff

**eDensityCutOff #cutoff (%)**

Default: eDensityCutOff 1 %

specifies the lower cut-off value for the peak search in the electron density maps. This specification can either be an absolute value, e.g. eDensityCutOff 1.0, or relative to the maximum value of the whole map, as is in the default. The overall maximum value of MaxPotentialAtoms, MaxPeaksFwSearch, and MaxPeaksFwFragmentSearch is the maximum number of peaks in the unit cell which are put on the peaklist by the peaksearch procedure. However, if there are less than this number of peaks with a maximum peak height above the value set by eDensityCutOff, the list will contain fewer peaks.

3.1.27.

MinPfl

**MinPfl #N**

Default: MinPfl 17

MinPfl ("minimum number of points for interpolation") defines the minimum number of grid points with a positive electron density value surrounding a grid peak position. If the actual number is fewer than MinPfl, no interpolation for the peak position is carried out and the coordinates of the grid point are retained.

3.1.28.

CatchDistance

**CatchDistance #d**

Default: CatchDistance 0.5

CatchDistance is the minimum distance a peak has to have to all of its symmetrically equivalent peaks (self-distance). For self-distances smaller than CatchDistance, a procedure is activated, which moves the peak onto the symmetry element which is responsible for the close contact.

3.1.29.

eD\_PeaksSortElement

**eD\_PeaksSortElement Grid\_eD/Maximum/Integral.**

Defines how the peaks are sorted.

3.1.30.

Lambda

**Lambda #d/\$code**

Sets the wavelength either in Å or one of the codes for the internally stored wavelengths.

CrA1: 2.28970	CrA2: 2.29361	Cr: 2.2909
FeA1: 1.93604	FeA2: 1.93998	Fe: 1.9373
CuA1: 1.54056	CuA2: 1.54439	Cu: 1.5418
MoA1: 0.70930	MoA2: 0.71359	Mo: 0.7107
AgA1: 0.55941	AgA2: 0.56380	Ag: 0.5608

3.1.31.

FobsMin\_d

**FobsMin\_d #d**

Sets the minimum d-spacing for the reflections to be used in Å.

3.1.32.

FobsScale

**FobsScale #N**

Defines the scale factor.

3.1.33.

SigmaCutOff

**SigmaCutOff #cutoff**

This is normally set to 3. If standard deviations are available, reflections with an intensity smaller than SigmaCutOff times their standard deviation can be excluded.

3.1.34.

OverlapFactor

**OverlapFactor #of**

Usually, a good value for the overlap factor is 0.3. Together with the individual FWHM for each reflection is used to determine the overlap groups, which are then processed according to OverlapAction.

3.1.35.

OverlapAction

**OverlapAction NoAction/EqualF2/EqualMF2**

NoAction specifies that no action should be taken if reflections are in the same overlap groups. In case of EqualF2, overlapped reflections are equipartitioned to have equal structure factor amplitudes and in case of EqualMF2, the reflections are equipartitioned based on the structure factor amplitude times multiplicity. In case of electron diffraction, this value should be set to NoAction, while for powder diffraction data, EqualMF2 is usually the most appropriate.

3.1.36.

ReflectionUsage

**ReflectionUsage #N**

This parameter specifies the number of reflections that are actually used. This can be absolute, for example ReflectionUsage 80 will select the 80 highest reflections, or it can be relative, as in the example. In the latter case, reflections are selected in descending order of (equipartitioned) intensity times multiplicity (M.F ) until the prescribed percentage of the

total sum of M.F over all input reflections is accumulated. Usually, no more than 400 reflections are necessary.

3.1.37.

### ScatteringFactorTable

#### **ScatteringFactorTable xray/electron**

This parameter specifies whether given structure factor amplitudes are from an electron or X-ray diffraction experiment.

3.1.38.

### ScatteringFactor

#### **ScatteringFactor \$label**

Custom scattering factors can be specified by supplying a list of  $\sin(\theta)/\lambda$  with corresponding scattering factor values. The list should start with the keyword and the label for this particular scatterer, and end with &. The label can then be used the Chemistry and AtomType keywords for example. As an example using the conventional X-ray scattering factors for silicon:

ScatteringFactor \$label

```
0.00 13.99892
0.05 13.43532
0.10 12.13342
0.15 10.76817
0.20 9.67481
0.25 8.85950
0.30 8.22972
0.35 7.69734
0.40 7.20320
0.45 6.71934
0.50 6.23962
0.55 5.76816
0.60 5.31198
0.65 4.87773
0.70 4.47063
0.75 4.09426
0.80 3.75063
0.85 3.44035
0.90 3.16292
0.95 2.91693
1.00 2.70033
```

&

3.1.39.

### Reflections

The last part of the input file is a listing of the extracted Fourier magnitudes. The data are given as reflection indices hkl, observed relative Fourier magnitude, the estimated standard deviation of the Fourier magnitude and the FWHM as derived from the refined profile parameters. If estimated standard deviations are not available, asterisks can be supplied instead. The reflection list should always end with the word "End". For example:

```
# h k l Fobs Sigma FWHM
0 2 1 4.02 * 0.0535
0 4 0 2.75 * 0.0534
1 1 0 4.91 * 0.0534
End
```

## 4. KRIBER

Kriber can be used to analyze the results of the FOCUS output file. Kriber expects a strudat file to be present in the current directory. A strudat can be created from the FOCUS output file by using the focus2strudat script (See below).

The strudat file contains a listing of all the frameworks reported by FOCUS (i.e. the ones in the fo2hist output).

The main commands of interest are:

help	Prints out a summary of all commands.
reacs	This command is used to read in a framework from the strudat file. The user is then prompted for the framework to load, which is any framework in the strudat file (without the *).
dis	Show all entries in the strudat file.
addo	O atoms are added in the expected positions between T atoms.
wricif	Save the current framework to a cif file named 'structure.cif'.
dett	Calculate the coordination sequence of the current framework.
wriid	Write an input file for DLS named 'dlsinp' (See below).
exit	Exit the program.

## 5. DLS76

DLS can be used to perform distance least squares calculations on the framework. The easiest way to generate an input file for DLS is by running Kriber with the 'addo' command and then the 'wriid' command. Then, DLS can be run on the resulting 'dlsinp' file.

## 6. EXTRAS

### *6.1.1.fo2hist*

Fo2hist is essential for the analysis of the FOCUS output file. It will parse the FOCUS output file, count all identical frameworks, and report the histogram of solutions to the terminal. The idea is that the framework with the most occurrences is the correct one. Fo2hist takes multiple files.

All coordination sequences are referenced against a database of known frameworks (see ascii file coseq). Fo2hist will show a note when a match is found. In the output, the first column gives the framework name of the first occurrence in the FOCUS output file, the second column the number of occurrences of this framework and the third column the percentage.

Example: `fo2hist focus.out`

In case fo2hist recognizes the framework type, the framework type code will be given.

### 6.1.2. *multifocal*

*multifocal* is a python program written to make it easier to run several focus runs in parallel, and thus to speed up the structure solution process. The help file can be accessed with the `-h` command line parameter.

The program can run a single input file in parallel, or run several input files at the same time. The number of processes to run can be specified via the `-p` flag, and the number of trials per process via `-n`

Example: `multifocal focus.inp -p8 -n1000`

This will spawn 8 FOCUS processes, each performing 1000 trials.

There is a 1 second delay between the start of every process on the same input file, in order to avoid having the same seed for the random number generator, which is based on system time.

### 6.1.3. *fo2cif*

This script automatically converts all the frameworks in a focus output file to cif format. It uses `focus2strudat` and then `strudat2cif`.

Example: `fo2cif focus.out`

### 6.1.4. *fo2strudat*

Converts the given focus file to a strudat file, ready to be used with Kriber.

Example: `fo2strudat focus.out`

### 6.1.5. *strudat2cif*

Convert all frameworks in a strudat file to cif format. This script calls Kriber for parsing and writing the cif file via the `wricif` command. Any command line argument specified will be passed on directly to Kriber, which can be useful to generate cif files of framework structures with oxygens added.

For example: `strudat2cif addo`

Will read every framework from the strudat file, add oxygens in the expected positions and write a cif file.

### 6.1.6. *dlsall*

Run DLS76 on all frameworks in the strudat file. Frameworks that minimize with an *R*-value of lower than 0.01 are converted to a cif file via KRIBER. This threshold can be changed via an optional command line argument:

`dlsall 0.1`

will convert all frameworks with an *R*-value of lower than 0.1 to cif files.

### 6.1.7. *cdlsall*

*cdlsall* works in the same way as *dlsall*, but will instead perform a cell-DLS refinement on all frameworks in the *strudat* file.

## 7. Example

This example shows the general workflow when using FOCUS using the example in the example directory.

Create a template input file:

```
focus > template.inp
```

Not all of the input parameters in the template are relevant for structure solution, but those that are have been discussed in the FOCUS input file chapter.

In this case, a working example file has been supplied for the DOH framework (*doh.inp*).

To start, run FOCUS on the input file:

```
focus doh.inp 100 > doh.out
```

The number 100 here specifies how many trials FOCUS should start. In the case of this simple structure, 100 trials is enough. This should take about 10-20 seconds. However, more complex problems can take several hours, or sometimes days to solve. The output file, *doh.out*, can be analyzed using the 'fo2hist' program:

```
fo2hist doh.out
```

In this case, the framework is known and fo2hist will identify the correct framework as DOH:

```
>> fo2hist doh.out
doh.out
fw      #      %   Natoms   ftc
F0003   297  0.705     4   DOH
F0019    66  0.157     4   -
F0000    47  0.112     4   -
F0037    3   0.007     5   -
F0205    3   0.007     4   -
F0035    2   0.005     4   -
F0255    2   0.005     4   -
F0340    1   0.002     3   -
Total: 421
```

In case of an unknown structure, it is useful to look at all frameworks in more detail. To do so, a CIF file can be created by using fo2cif:

```
fo2cif doh.out
```

This creates a cif file for every framework reported in the fo2hist output. In this case, Fw0000 is the correct framework. When it is decided to use this framework for refinement, the framework structure can be optimized using distance least-squares with the program DLS76. The easiest way to generate a DLS input file is by using Kriber. First, a *strudat* file should be created (in this case a *strudat* file is already available, as fo2cif will write one) with *focus2strudat*:

```
foc2strudat doh.out
```

Then running Kriber:

```
kriber
```

And issuing the following commands:

```
reacs  
Fw0000  
addo  
wriid  
exit
```

'reacs' will tell the program to read a structure, in this case Fw0000, 'addo' will add oxygens in the expected bridging positions and 'wriid' will write a DLS76 input file called 'dlsinp'.

Finally, run DLS76:

```
dls76 dlsinp
```

This will generate 2 files, dlsout with the results of the least-squares refinement and nfilea.inp with the atomic parameters. The easiest way to use the new atomic parameters is to replace them in an existing CIF file, for example one written using the command 'wricif' in Kriber. Alternatively, the program **dlsall** can be used:

```
>> dlsall 0.1  
Threshold = 0.1  
  
framework      Rval  
Fw0000          0.0239 ** >> Wrote file Fw0000_dls.cif  
Fw0003          0.0166 ** >> Wrote file Fw0003_dls.cif  
Fw0019          0.0187 ** >> Wrote file Fw0019_dls.cif  
Fw0035          0.0256 ** >> Wrote file Fw0035_dls.cif  
Fw0037          0.0324 ** >> Wrote file Fw0037_dls.cif  
Fw0205          0.0273 ** >> Wrote file Fw0205_dls.cif  
Fw0255          0.0136 ** >> Wrote file Fw0255_dls.cif  
Fw0340          0.0225 ** >> Wrote file Fw0340_dls.cif
```

This generates dls-optimized cif files directly.

## 8. Further reading

For further information, please consult the following literature:

Smeets, S; McCusker, L. B.; Baerlocher, C.; Mugnaioli, E. & Kolb, U.  
Using FOCUS to solve zeolite structures from three-dimensional electron diffraction data  
Journal of Applied Crystallography, 2013, 46(4), 1017–1023  
<http://dx.doi.org/10.1107/S0021889813014817>

Grosse-Kunstleve, R. W.; McCusker, L. B. & Baerlocher, C.  
Powder Diffraction Data and Crystal Chemical Information Combined in an Automated  
Structure Determination Procedure for Zeolites  
Journal of Applied Crystallography, 1997, 30, 985-995  
<http://dx.doi.org/10.1107/S0021889897005013>

Grosse-Kunstleve, R. W.  
Zeolite Structure Determination from Powder Data: Computer-based Incorporation of Crystal  
Chemical Information  
PhD thesis, ETH Zurich, 1996  
<http://cci.lbl.gov/~rwgk/Dissertation/Dissertation.pdf>

Grosse-Kunstleve, R. W.; McCusker, L. B. & Baerlocher, C.  
Powder Diffraction Data and Crystal Chemical Information Combined in an Automated  
Structure Determination Procedure for Zeolites  
Journal of Applied Crystallography, 1997, 30, 985-995  
<http://dx.doi.org/10.1107/S0021889897005013>

Grosse-Kunstleve, R. W.; McCusker, L. B. & Baerlocher, C.  
Zeolite structure determination from powder diffraction data: applications of the it FOCUS  
method  
Journal of Applied Crystallography, 1999, 32, 536-542  
<http://dx.doi.org/10.1107/S0021889899003453>