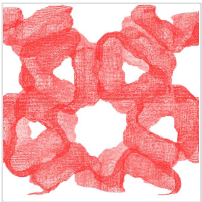

Sep 28, 2022

Calculation of MOF pore size distributions using PoreBlazer 4.0

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Jonas Sundberg: Sensors & Functional Materials

1 Works for me Share

dx.doi.org/10.17504/protocols.io.261ge671dl47/v1

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ABSTRACT

This is a brief step-by-step protocol for how to calculate and plot the pore-size distribution (PSD) of a metal-organic framework. The protocol uses the nice PoreBlazer software made by Sarkisov et. al., for in-depth information read their paper: '*Materials Informatics with PoreBlazer v4.0 and the CSD MOF Database*' *Chem. Mater.*2020, 32, 23, 9849–9867 https://doi.org/10.1021/acs.chemmater.0c03575

Disclaimer

Our protocols are primarily for internal use by students, but shared openly as we believe they might be of broader interest. But remember, this is just how we do it. Not necessarily the best, or smartest, way (but hopefully somewhat correct). Code snippets are not meant to be definite, but used as learning tools and starting points to create your own scripts. If you have comments, please e-mail us freely and direct. :)

DOI

dx.doi.org/10.17504/protocols.io.261ge671dl47/v1

PROTOCOL CITATION

Jonas Sundberg 2022. Calculation of MOF pore size distributions using PoreBlazer 4.0. **protocols.io** https://dx.doi.org/10.17504/protocols.io.261ge671dl47/v1

KEYWORDS

metal-organic frameworks, simulations, porosity, pore size distribution, MOF

CREATED

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LAST MODIFIED

Sep 28, 2022

PROTOCOL INTEGER ID

24606

SAFETY WARNINGS

Do not sit in front of the computer doing simulations for prolonged periods of time. Doing practical laboratory work is important for the progress of your project as well as mental health.

BEFORE STARTING

The protocol assumes that you have the following software packages installed and ready:

- Mercury/Cambridge Structural Database software suite
- PoreBlazer Windows binary
- Aten Molecular modelling package
- Jupyter Notebooks/JupyterLab with functional Python environment

JupyterLab with Python and Matplotlib are used for plotting the resulting data. For the less computer savvy, easiest way is to download Anaconda, and use conda to install the required packages.

Working folders

Create an appropriately (structure refcode, name or similar) named sub-folder under the directory where the '*poreblazer.exe*' executable is located. This is where you should store and save all files.

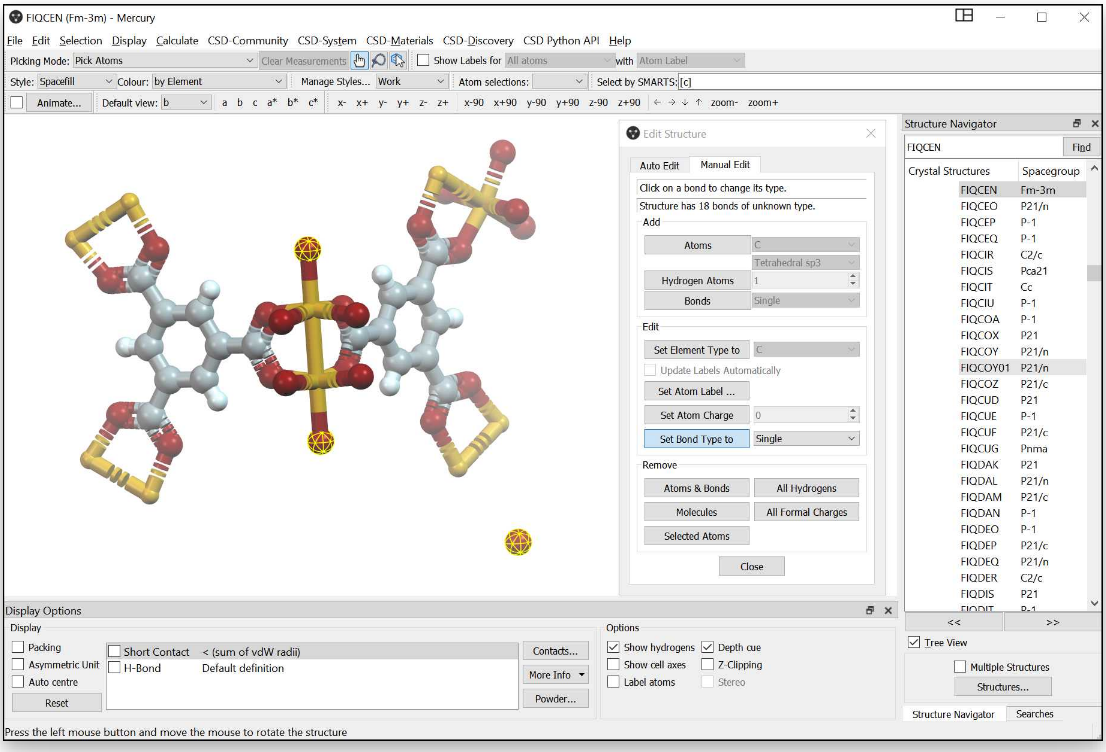
Preparation of input files

1 **Crystallographic clean-up using Mercury**

If your material has co-crystallized solvent molecule(s) it is important to remove before measuring the pore-size distribution. In this protocol we will work with HKUST-1 (CSD-refcode: FIQCEN) as an example. The crystal structure of HKUST-1 contains one co-crystallized water molecule per unit cell. Furthermore, each copper paddlewheel is coordinatively saturated by two water molecules.

1. Open the CIF-file (Ctrl+O) or use the '*Structure Navigator*' (right pane in default settings) to locate entry **FIQCEN**.
2. You will now see the asymmetric unit of the structure.
3. Select the free and bound water molecules (see figure below).
4. Select '*Edit>Edit Structure*'
5. Click '*Remove> Selected Atoms*'
6. Export the desolvated structure as cif by '*File>Save As*'; name the file '*FIQCEN_desolv.cif*'.

Citation: Jonas Sundberg Calculation of MOF pore size distributions using PoreBlazer 4.0 https://dx.doi.org/10.17504/protocols.io.261ge671dl47/v1



Click on a bond to change its type.

Structure has 18 bonds of unknown type.

Crystal Structures	Spacegroup
FIQCEN	Fm-3m
FIQCEO	P21/n
FIQCEP	P-1
FIQCEQ	P-1
FIQCIR	C2/c
FIQCIS	Pca21
FIQCIT	Cc
FIQCIU	P-1
FIQCOA	P-1
FIQCOX	P21
FIQCOY	P21/n
FIQCOY01	P21/n
FIQCOZ	P21/c
FIQCUD	P21
FIQCUE	P-1
FIQCUF	P21/c
FIQCUG	Pnma
FIQDAK	P21
FIQDAL	P21/n
FIQDAM	P21/c
FIQDAN	P-1
FIQDEO	P-1
FIQDEP	P21/c
FIQDEQ	P21/n
FIQDER	C2/c
FIQDIS	P21

☐ Packing ☐ Asymmetric Unit ☐ Auto centre

☐ Short Contact < (sum of vdW radii)
☐ H-Bond Default definition

☑ Show hydrogens ☑ Depth cue ☐ Show cell axes ☐ Z-Clipping ☐ Label atoms ☐ Stereo

☑ Tree View ☐ Multiple Structures

Press the left mouse button and move the mouse to rotate the structure

Figure 1. Screenshot of Mercury dialogue on atom removal.

FIQCEN_desolv.cif

Mercury 2020.2.0 (Build

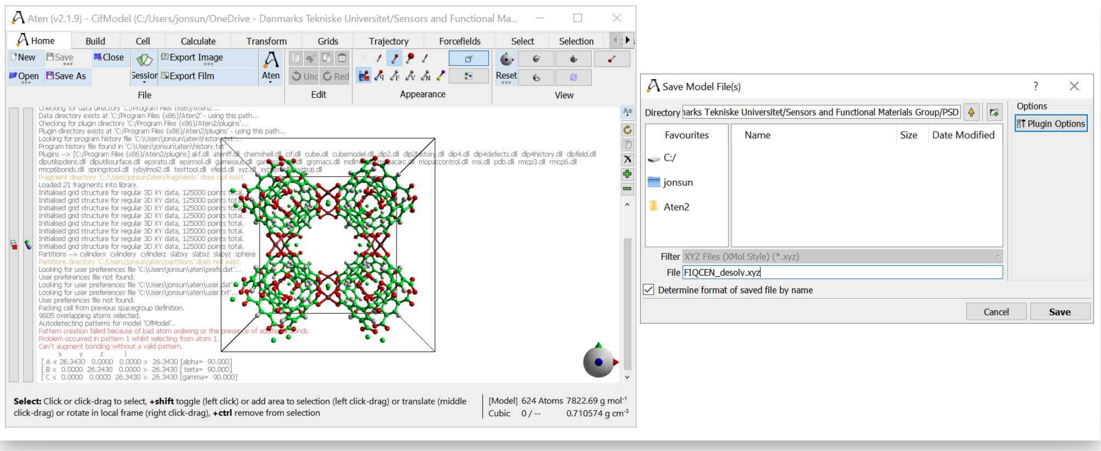
Windows 10

by CCDC

2 Use Aten to convert the CIF file to an PoreBlazer-compatible xyz input file.

> *For to me unknown reasons, direct export of CIF to XYZ in Mercury yields an incorrect structure file and erroneous PSD data.*

1. Start Aten and open the resulting CIF file by clicking the '*Open*' icon.
2. Browse to your data directory, choose '*Crystallographic Information File (CIF)*' from the '*Filter*' dropdown menu, select your file and click '*Open*'.
3. Confirm that the structure is fully desolvated.
4. Click '*Save As*', ensure that '*Determine format of saved file by name*' is selected, enter '*FIQCEN_desolv.xyz*' as filename and click '*Save*'.



```
Checking for data directory 'C:/Program Files (x86)/Aten2'...
Data directory exists at 'C:/Program Files (x86)/Aten2' - using this path...
Checking for plugin directory 'C:/Program Files (x86)/Aten2/plugins'...
Plugin directory exists at 'C:/Program Files (x86)/Aten2/plugins' - using this path...
Looking for program history file 'C:\Users\jonsun\aten\history.txt'...
Program history file found in 'C:\Users\jonsun\aten\history.txt'
Plugins --> [C:/Program Files (x86)/Aten2/plugins] akf.dll  atenff.dll  chemshell.dll  cif.dll  cube.dll  cubemodel.dll  dlp2.dll  dlp2history.dll  dlp4.dll  dlp4defects.dll  dlp4history.dll  dlpfield.dll
dlputilspdens.dll  dlputilssurface.dll  epsrato.dll  epsrmol.dll  gamessus.dll  gam[illegible].dll  gromacs.dll  mdlm[illegible]  mopacarc.dll  mopaccontrol.dll  msi.dll  pdb.dll  rmcp3.dll  rmcp6.dll
rmcp6bonds.dll  springstool.dll  sybylmol2.dll  testtool.dll  vfield.dll  xyz.dll  xyztest.dll  xyztraj.dll
Fragment directory 'C:/Users/jonsun/aten/fragments' does not exist.
Loaded 21 fragments into library.
Initialised grid structure for regular 3D XY data, 125000 points total.
Initialised grid structure for regular 3D XY data, 125000 points total.
Initialised grid structure for regular 3D XY data, 125000 points total.
Initialised grid structure for regular 3D XY data, 125000 points total.
Initialised grid structure for regular 3D XY data, 125000 points total.
Initialised grid structure for regular 3D XY data, 125000 points total.
Initialised grid structure for regular 3D XY data, 125000 points total.
Initialised grid structure for regular 3D XY data, 125000 points total.
Partitions --> cylinderx  cylindery  cylinderz  slabxy  slabxz  slabyz  sphere
Partitions directory 'C:/Users/jonsun/aten/partitions' does not exist.
Looking for user preferences file 'C:\Users\jonsun\aten\prefs.dat'...
User preferences file not found.
Looking for user preferences file 'C:\Users\jonsun\aten\user.dat'...
Looking for user preferences file 'C:\Users\jonsun\aten\user.txt'...
User preferences file not found.
Packing cell from previous spacegroup definition.
9605 overlapping atoms selected.
Autodetecting patterns for model 'CifModel'..
Pattern creation failed because of bad atom ordering or the presence of additional bonds.
Problem occurred in pattern 1 whilst selecting from atom 1.
Can't augment bonding without a valid pattern.
         x          y          z          l
 [ A < 26.3430   0.0000   0.0000 >  26.3430 [alpha=  90.000]
 [ B <  0.0000  26.3430   0.0000 >  26.3430 [ beta=  90.000]
 [ C <  0.0000   0.0000  26.3430 >  26.3430 [gamma=  90.000]
```

Select: Click or click-drag to select, **+shift** toggle (left click) or add area to selection (left click-drag) or translate (middle click-drag) or rotate in local frame (right click-drag), **+ctrl** remove from selection

[Model] 624 Atoms 7822.69 g mol-1
Cubic 0 / -- 0.710574 g cm-3

Directory ıarks Tekniske Universitet/Sensors and Functional Materials Group/PSD

Filter XYZ Files (XMol Style) (*.xyz)

File FIQCEN_desolv.xyz

☑ Determine format of saved file by name

Figure 2. Interface of Aten after loading of CIF and 'Save as' dialogue.

FIQCEN_desolv.xyz

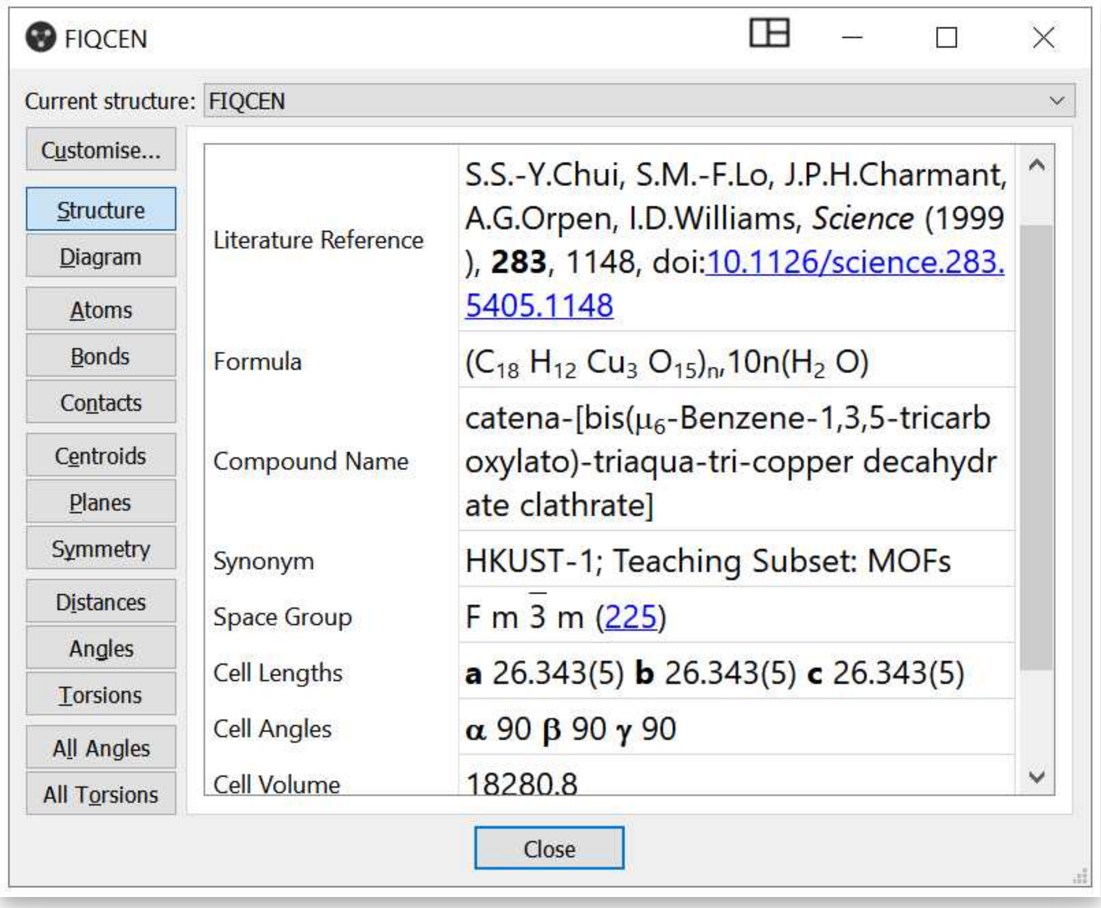
Aten 2.1.9

Windows 10

source by TGA Youngs

3 **Create a PoreBlazer input files:**

1. In your working directory, create and save a '*input.dat*' file in Notepad (or other text editor).
2. The first line should contain the xyz filename, e.g. '*FIQCEN_desolv.xyz*'
3. The second and third line contains unit cell dimensions (cell lengths and angles).
4. To obtain these, go back to Mercury. With your structure loaded, select '*Structure Information*' from the More Info' drop down menu (bottom pane).
5. The unit cell dimensions are provided under the '*Structure*' tab.
6. Enter the cell lengths (tab separated) on the second line.
7. Enter the cell angles (tab separated) on the third line.
8. In addition to the '*input.dat*' file, the PoreBlazer requires force field data. Default values are provided by PoreBlazer and should typically not be modified. Either copy the '*defaults.dat*' and '*UFF.dat*' files from the source distribution or use the values provided below.



Current structure: FIQCEN

Literature Reference	S.S.-Y.Chui, S.M.-F.Lo, J.P.H.Charmant, A.G.Orpen, I.D.Williams, *Science* (1999), **283**, 1148, doi:10.1126/science.283.5405.1148
Formula	$(C_{18} H_{12} Cu_3 O_{15})_n,10n(H_2 O)$
Compound Name	catena-[bis(μ_6-Benzene-1,3,5-tricarboxylato)-triaqua-tri-copper decahydrate clathrate]
Synonym	HKUST-1; Teaching Subset: MOFs
Space Group	F m $\bar{3}$ m (225)
Cell Lengths	**a** 26.343(5) **b** 26.343(5) **c** 26.343(5)
Cell Angles	**α** 90 **β** 90 **γ** 90
Cell Volume	18280.8

Figure 3. Unit cell dimensions of HKUST-1/FIQCEN as provided by Mercury.

input.dat

```
FIQCEN_desolv.xyz
26.343 26.343 26.343
90 90 90
```

run.bat

```
..\poreblazer.exe < input.dat > results.txt
```

defaults.dat

```
UFF.atoms
2.58, 10.22, 298, 12.8
3.314
500
0.2
20.0, 0.25
21908391
0
```

Citation: Jonas Sundberg Calculation of MOF pore size distributions using PoreBlazer 4.0
https://dx.doi.org/10.17504/protocols.io.261ge671dl47/v1

```

! Default forcefield: UFF
! Helium atom sigma (A), helium atom epsilon (K), temperature (K),
cutoff distance (A)
! Nitrogen atom sigma (A)
! Number of samples per atom for the surface area calculation
! 0.2: Cubelet size (A)
! Largest anticipated pore diameter (A), size of the bin for PSD
(A)
! Random number seed
! Visualization options: 1 -xyz, 2 - grd, 3 - both; 0 - none

! Do not change these values unless you know what you are doing
```

UFF.atoms

```
98
C       3.431   52.8    12.0
O       3.118   30.2    16.0
H       2.571   22.14   1.0
N 3.261 34.70 14.007
F 2.997 25.14 18.998
Na 2.658 15.09 22.99
Mg 2.691 55.82 24.305
Al 4.008 253.94 26.982
Si 3.826 202.15 28.085
P 3.695 153.37 30.974
S 3.595 137.78 32.06
Cl 3.516 114.15 35.45
K 3.396 17.60 39.098
Ca 3.028 119.68 40.078
Sc 2.936 9.55 44.956
Ti 2.829 8.55 47.867
V 2.801 8.05 50.942
Cr 2.693 7.54 51.996
Mn 2.638 6.54 54.938
Fe 2.594 6.54 55.845
Co 2.559 7.04 58.933
Ni 2.525 7.54 58.693
Cu 3.114 2.51 63.546
Zn      2.462   62.38   65.39
Zr 2.783 34.70 91.224
Mo 2.719 28.16 95.96
Re 2.632 33.19 186.21
Be 2.446 42.74 9.0121831
B 3.638 90.51 10.811
```

Citation: Jonas Sundberg Calculation of MOF pore size distributions using PoreBlazer 4.0
https://dx.doi.org/10.17504/protocols.io.261ge671dl47/v1

```
Zn 2.462 62.35 65.39
Ga 3.905 208.69 69.723
Ge 3.813 190.58 72.64
As 3.769 155.38 74.9216
Se 3.746 146.33 78.96
Br 3.732 126.22 79.904
Rb 3.665 20.11 85.4678
Sr 3.244 118.17 87.62
Y 2.980 36.21 88.9059
Nb 2.820 29.67 92.9064
Tc 2.671 24.14 98
Ru 2.640 28.16 101.07
Rh 2.609 26.65 102.9055
Pd 2.583 24.14 106.42
Ag 2.805 18.10 107.8682
Cd 2.537 114.65 112.411
In 3.976 301.21 114.818
Sn 3.913 285.12 118.71
Sb 3.938 225.78 121.76
Te 3.982 200.14 127.6
In 4.009 170.47 126.9045
Cs 4.024 22.63 132.9055
Ba 3.299 183.04 137.327
La 3.138 8.55 138.9055
Ce 3.168 6.54 140.116
Pr 3.213 5.03 140.9077
Nd 3.185 5.03 144.24
Pm 3.160 4.53 145
Sm 3.136 4.02 150.36
Eu 3.112 4.02 151.964
Gd 3.001 4.53 157.25
Tb 3.074 3.52 158.9253
Dy 3.054 3.52 162.5
Ho 3.037 3.52 164.9303
Er 3.021 3.52 167.259
Tm 3.006 3.02 168.9342
Yb 2.989 114.65 173.04
Lu 3.243 20.62 174.967
Hf 2.798 36.21 178.49
Ta 2.824 40.73 180.9479
W 2.734 33.69 183.84
Re 2.632 33.19 186.207
Os 2.780 18.61 190.23
Ir 2.530 36.71 192.217
Pt 2.454 40.23 195.078
Au 2.934 19.61 196.9665
Hg 2.410 193.60 200.59
```

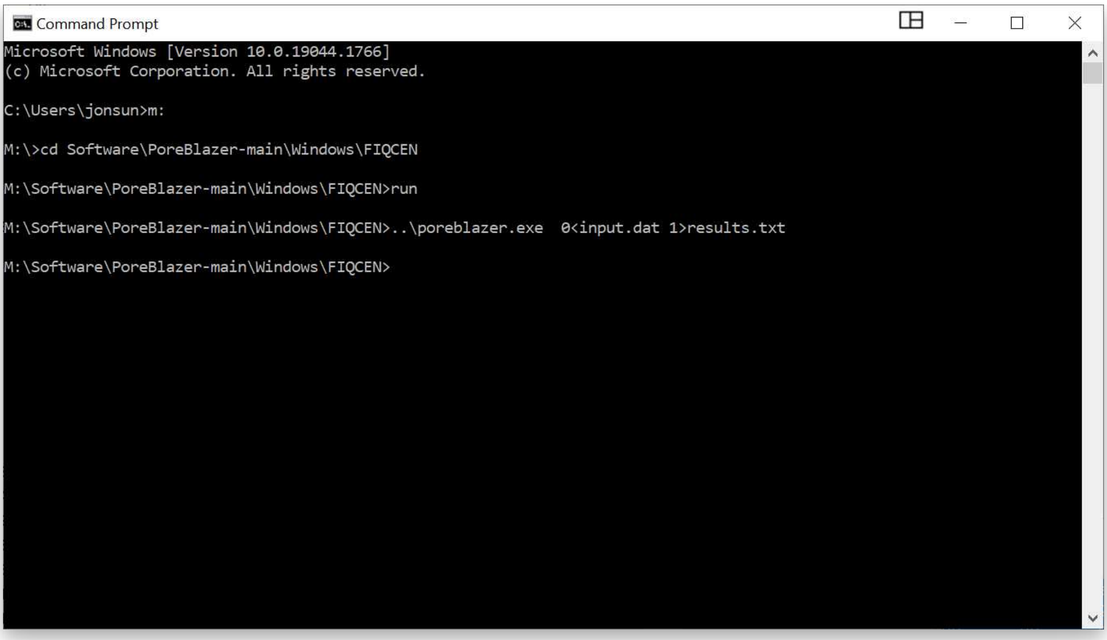
```
Tl 3.873 341.94 204.3833
Pb 3.828 333.39 207.2
Bi 3.893 260.48 208.9804
Po 4.195 163.43 209
At 4.232 142.81 210
Rn 4.245 124.71 222
Ra 3.276 203.15 226
Ac 3.099 16.59 227
Th 3.025 13.07 232
Pa 3.050 11.06 231
U 3.025 11.06 238
Np 3.050 9.55 237
Pu 3.050 8.05 244
Am 3.012 7.04 243
Cm 2.963 6.54 247
Bk 2.975 6.54 247
Cf 2.952 6.54 251
Es 2.939 6.03 252
Fm 2.927 6.03 257
Md 2.917 5.53 258
No 2.894 5.53 259
Lw 2.883 5.53 262

! name of framework atom, diameter (LJ sigma) in A, epsilon in K, mol weight
```

Simulation and plotting/presentation of results

4 **Execute PoreBlazer:**

1. Start the Windows command prompt by pressing Windows+R and entering '*cmd*' followed by clicking '*Ok*'.
2. Change directory to enter the working folder containing the input files.
3. Execute '*run.bat*', wait a few seconds and voila!



```
Microsoft Windows [Version 10.0.19044.1766]
(c) Microsoft Corporation. All rights reserved.

C:\Users\jonsun>m:

M:\>cd Software\PoreBlazer-main\Windows\FIQCEN

M:\Software\PoreBlazer-main\Windows\FIQCEN>run

M:\Software\PoreBlazer-main\Windows\FIQCEN>..\poreblazer.exe  0<input.dat 1>results.txt

M:\Software\PoreBlazer-main\Windows\FIQCEN>
```

Figure 4. Command prompt, showing execution of the PB binary called from run.bat

The software should generate the following files:

- '*results.txt*';
- '*summary.dat*'; Contains a brief summary of the results, including pore-limiting and largest cavity diameter, total and network accessible surface area.
- '*Total_psd.txt*' + '*Total_psd_cumulative.txt*'; Total pore-size distribution and
- '*Network-accessible_psd.txt*' + '*Network-accessible_psd_cumulative.txt*'; network accessible pore-size distribution

An archive containing both input and output files as described in this protocol is attached below. A more detailed description of the output can be found at https://github.com/SarkisovGitHub/PoreBlazer

PoreBlazer 4.0
Windows 10
source by Lev Sarkisov

PSD_FIQCEN_input_output.zip

5 Plotting of single PSD data

This section assumes that you are working with the Anaconda platform for accessing Jupyter Notebooks. Adjust accordingly if not. :)

Citation: Jonas Sundberg Calculation of MOF pore size distributions using PoreBlazer 4.0 https://dx.doi.org/10.17504/protocols.io.261ge671dl47/v1

1. Start JupyterLab by initiating an 'Anaconda prompt' and entering the command '*jupyter lab*'
2. Use the left-pane browser to locate your working directory containing the output from PoreBlazer.
3. Create new launcher by clicking the '+' symbol and choose a Python 3 Notebook.
4. Rename the '*untitled.ipynb*' to '*DATE-REFCODE_PSD_Plots.ipynb*', e.g. '*220927-FIQCEN_PSD_Plots.ipynb*'
5. Add the following code snippets to cells of the notebook (**example notebook is attached below**).
6. Press Ctrl+Enter to execute each cell in order.

Import the required packages

```
# Load pandas for data import/processing + Matplotlib for plotting
import pandas as pd
import matplotlib.pyplot as plt
#Import scipy to do peak fitting
from scipy.signal import find_peaks
```

Define and load data

```
# Load NA PSD data
data1 = "./Network-accessible_psd.txt"
na_psd = pd.read_csv(data1, header=None,  skiprows=1,sep='\s+')
na_psd.columns = ['Derivative distribution function','d (Å)']

# Load total PSD data
data2 = "./Total_psd.txt"
tot_psd = pd.read_csv(data2, header=None,  skiprows=1,sep='\s+')
tot_psd.columns = ['Derivative distribution function','d (Å)']
```

Plotting of network accessible pore size distribution

```
def cm2inch(value):
    return value/2.54

# Initiate plot and define classic style, and 16:9 ratio.
plt.figure()
plt.style.use('classic')
plt.rcParams["figure.figsize"] = (cm2inch(19.2),cm2inch(10.8))
plt.minorticks_on()
plt.grid()

# Label axes
plt.xlabel('d (Å)')
plt.ylabel('Derivate distribution function')
```

```
#Plot NA PSD
plt.plot(na_psd['Derivative distribution function'],na_psd['d
(Å)'],color="#8b0000")

# Export as png, change to svg if necessary.
plt.savefig('FIQCEN_desolv_NA_PSD.png', dpi=300,
bbox_inches='tight',transparent="True", pad_inches=0)
```

Plotting of total accessible pore size distribution

```
def cm2inch(value):
    return value/2.54

# Initiate plot and define classic style, and 16:9 ratio.
plt.figure()
plt.style.use('classic')
plt.rcParams["figure.figsize"] = (cm2inch(19.2),cm2inch(10.8))
plt.minorticks_on()
plt.grid()

# Label axes
plt.xlabel('d (Å)')
plt.ylabel('Derivate distribution function')

#Plot total PSD
plt.plot(tot_psd['Derivative distribution function'],tot_psd['d
(Å)'],color="#457ca4")

# Export as png, change to svg if necessary.
plt.savefig('FIQCEN_desolv_tot_PSD.png', dpi=300,
bbox_inches='tight',transparent="True", pad_inches=0)
```

Adjust file names, resolution and size after needs, e.g. change to .svg to generate vector graphics for publication.

Citation: Jonas Sundberg Calculation of MOF pore size distributions using PoreBlazer 4.0
https://dx.doi.org/10.17504/protocols.io.261ge671dl47/v1

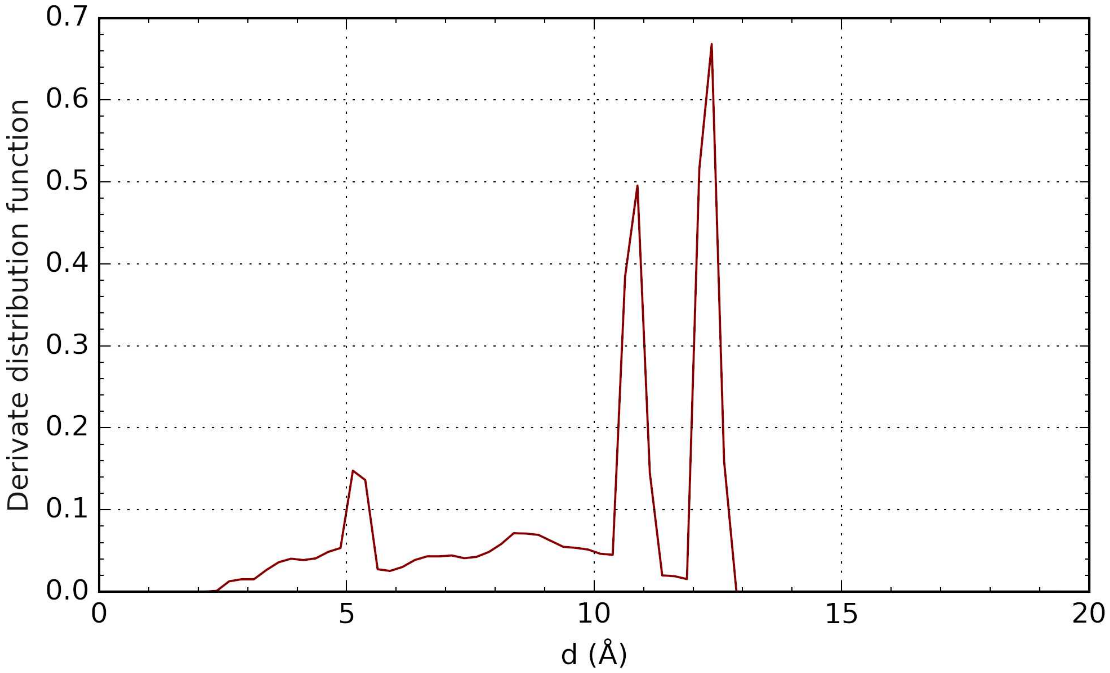


Figure 5. Example network accessible PSD plot of FIQCEN.

220927-FIQCEN_PSD_plots.ipynb

6 Plotting of multiple PSD series as overlay

1. Create a working directory for storage of all PSD data, e.g. '*PSDs*'
2. Make a copy of each single PSD datafile and rename it to REFCODE_NA_PSD.txt' (or 'REFCODE_tot_PSD.txt' if plotting total PSD). Note:
3. Move all uniquely named data files into the working directory.
4. Create a new Python 3 notebook in Jupyter Lab as described previously.
5. Add the following code snippets to cells, and execute (**example notebook is attached below**).

Import required packages

```
# Load pandas for data processing, matplotlib for plotting
import pandas as pd
import matplotlib.pyplot as plt
```

This snippet basically imports *all* data from a specific subfolder, plots and labels them incrementally. Very basic, but effective. The legend is labelled based on filename, export as SVG and modify text to more appropriate names (or modify the code).

Citation: Jonas Sundberg Calculation of MOF pore size distributions using PoreBlazer 4.0
https://dx.doi.org/10.17504/protocols.io.261ge671dl47/v1

Multi-data import and overlay plotting

```
#This is a multtiplot script, taking all files from a specific
directory and plotting as overlay.
# Get list of datafiles, modify data_path accordingly if needed
import os
data_path = r'./PSDs/'
data = []
for path in os.listdir(data_path):
    # check if current path is a file
    if os.path.isfile(os.path.join(data_path, path)):
        data.append(path)
print(data)

# Setup plot
def cm2inch(value):
    return value/2.54

plt.figure()
plt.style.use('classic')
plt.rcParams["figure.figsize"] = (cm2inch(19.2),cm2inch(10.8))
plt.minorticks_on()
plt.grid()

plt.xlabel('d (Å)')
plt.ylabel('Derivative distribution function')

#Setup colorscheme, colorblind-friendly palette taken from
https://yoshke.org/blog/colorblind-friendly-diagrams. Modify as
wanted.
colors =
['#000000','#E69F00','#56B4E9','#009E73','#F0E442','#0072B2','#D55E
00','#CC79A7']

#MinMax
#plt.xlim(500, 2000)

# Do the actual plotting
int = 1
for fname in data:
    df = pd.read_csv(data_path+fname,index_col=False,header=None,
skiprows=1,sep='\s+')
    df.columns = ['Derivative distribution function','d (Å)']

    X=df['d (Å)']
    Y=df['Derivative distribution function']

    # Prepare plot with incremental coloring
    plt.plot(Y,X,color=colors[int],label=fname)
    plt.legend(fontsize=8)
    int = int+1

# Export figure, modify filename and settings if needed.
plt.savefig('220927-PSD_NA_Overlay.png', dpi=300,
bbox_inches='tight',transparent="True", pad_inches=0)
```

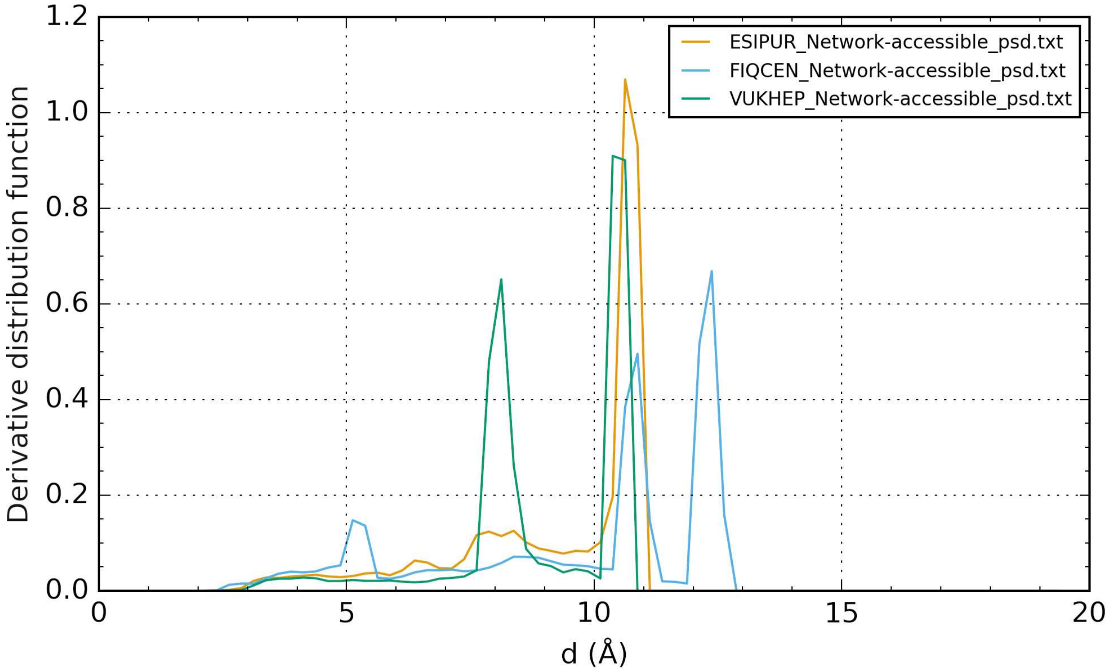


Figure 6. Example of overlay plot of multiple PSDs.

7 Bonus: Summary clean-up and Excel export

This is just a short code-snippet to reformat the multiple 'summary.dat' output file into a slightly more user friendly edition. :)

1. Create a secondary working subfolder called '*Summaries*'
2. Make a copy of each 'summary.dat' named '*REFCODE_summary.dat*' and copy into the 'Summaries' subfolder.
3. In the parent directory, create a new Jupyter Notebook and add the following code to a cell:

```
# Load pandas for data processing
import pandas as pd
```

Citation: Jonas Sundberg Calculation of MOF pore size distributions using PoreBlazer 4.0
https://dx.doi.org/10.17504/protocols.io.261ge671dl47/v1

```
# Load single summary.dat
data1 = "./summary.dat"
# Summary.dat is a bit funky, so read using regex with min 2 spaces
as separator.
summary = pd.read_csv(data1, header=None, index_col=None,
skiprows=1, sep='\s{2,}',names=
['Parameter','Value'],engine='python')
#na_psd.columns = ['Derivative distribution function','d (Å)']

# Get original xyz source from summary.dat
with open(data1) as f:
    source_xyz = f.readline()
    # Strip newline character
    source_xyz = source_xyz.strip()

summary.rename(columns = {'Value':source_xyz}, inplace = True)

# Generate list for renaming of indeces
parameters = ['Volume (Å)',
'Mol. Weight (g/mol)',
'Density (g/cm3)',
'Pore-limiting diameter (Å)',
'Largest cavity diameter (Å)',
'Dimensionality','Total properties',
'Total accessible surface area (Å2)',
'Total accessible surface area (m2/cm3)',
'Total accessible surface area (m2/g)',
'Total properties',
'Total helium pore volume (Å3)',
'Total helium pore volume (cm3/g)',
'Total geometric pore volume (Å3)',
'Total geometric pore volume (cm3/g)',
'Total probe-occupiable pore volume (Å3)',
'Total probe-occupiable pore volume (cm3/g)',
'Total volume fraction (%)',
'Network accessible',
'Network accessible surface area (Å2)',
'Network accessible surface area (m2/cm3)',
'Network accessible surface area (m2/g)',
'Network accessible',
'Network accessible helium pore volume (Å3)',
'Network accessible helium pore volume (cm3/g)',
'Network accessible geometric pore volume (Å3)',
'Network accessible geometric pore volume (cm3/g)',
'Network accessible probe-occupiable pore volume (Å3)',
'Network accessible probe-occupiable pore volume (cm3/g)',
```

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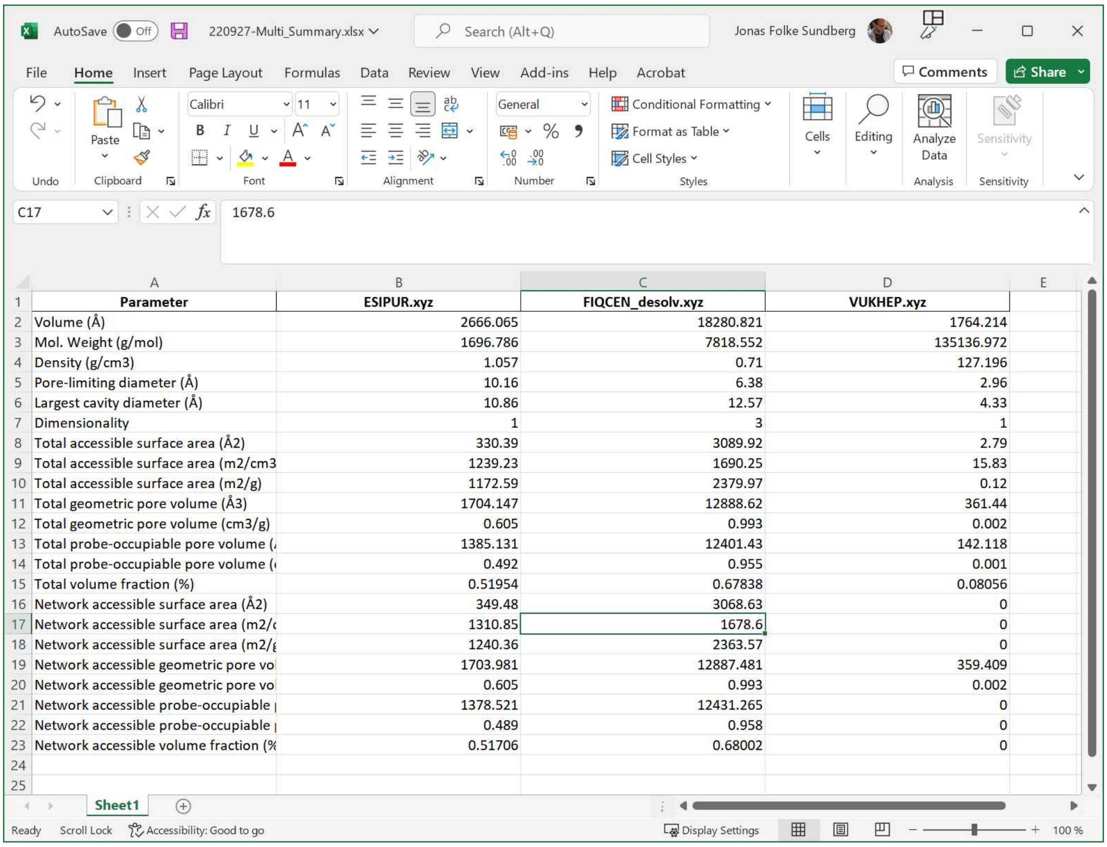
```
'Network accessible volume fraction (%)']

# Update parameter list with slightly more userfriendly text
int = 0
for index, row in summary.iterrows():
    summary.loc[int, ['Parameter']] = [parameters[int]]
    int = int+1

# Drop rows with NaN values
summary = summary.dropna()

# Export as Excel file.
summary.to_excel('220927-Multi_Summary.xlsx', index=False)
```



	A	B	C	D
1	Parameter	ESIPUR.xyz	FIQCEN_desolv.xyz	VUKHEP.xyz
2	Volume (Å)	2666.065	18280.821	1764.214
3	Mol. Weight (g/mol)	1696.786	7818.552	135136.972
4	Density (g/cm3)	1.057	0.71	127.196
5	Pore-limiting diameter (Å)	10.16	6.38	2.96
6	Largest cavity diameter (Å)	10.86	12.57	4.33
7	Dimensionality	1	3	1
8	Total accessible surface area (Å2)	330.39	3089.92	2.79
9	Total accessible surface area (m2/cm3	1239.23	1690.25	15.83
10	Total accessible surface area (m2/g)	1172.59	2379.97	0.12
11	Total geometric pore volume (Å3)	1704.147	12888.62	361.44
12	Total geometric pore volume (cm3/g)	0.605	0.993	0.002
13	Total probe-occupiable pore volume (	1385.131	12401.43	142.118
14	Total probe-occupiable pore volume (	0.492	0.955	0.001
15	Total volume fraction (%)	0.51954	0.67838	0.08056
16	Network accessible surface area (Å2)	349.48	3068.63	0
17	Network accessible surface area (m2/c	1310.85	1678.6	0
18	Network accessible surface area (m2/g	1240.36	2363.57	0
19	Network accessible geometric pore vo	1703.981	12887.481	359.409
20	Network accessible geometric pore vo	0.605	0.993	0.002
21	Network accessible probe-occupiable	1378.521	12431.265	0
22	Network accessible probe-occupiable	0.489	0.958	0
23	Network accessible volume fraction (%	0.51706	0.68002	0
24				
25				

Figure 7. Example of multi-summary Excel output.

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