

This data repository contains all the Gudrun and EPSR input and output data files used to produce the paper “Adsorption of simple gases into the porous glass MCM-41” by Alan K Soper and Daniel T Bowron. The relevant ISIS experiment number is RB1800005.

It is divided into two folders, Gudrun and EPSR.

The Gudrun folder contains a single folder, MCM41GasAdsorption, which is the complete folder as existed on my computer. The Gudrun input files for the final production runs are called CD4absmint-ver4.txt, D2absmint-ver4.txt, N2absmint-ver4.txt, O2absmint-ver4.txt. Provided you download the relevant .nxs files from the ISIS raw data website, this is all you need to recreate or modify what I did for the paper. Gudrun is a standalone executable which is available from the ISIS Disordered Materials website.

The EPSR folder also has a single folder, mcm41-2021, which itself contains five subfolders, CD4, D2, Dry, N2 and O2. These each contain all the EPSR input files that are needed to recreate the graphs shown in the paper. The actual names of those files can be found in the EPSR script file run-best-alternate.txt which is in the top mcm41-2021 folder. Note that a # at the beginning of a line means that command will be skipped when the script is run. If the # is removed, the command will be executed. The EPSR file names are also referred in the .plt files in that same folder, which were used to produce the Gnuplot figures, but note that the folder path given in these .plt files will not be correct if the files are unzipped on another computer or disk. EPSRfitsQspace-ver2.plt refers to Fig. 6, EPSRfitsrspace-ver2.plt refers to Fig. 7, EPSRRadialDensities.plt refers to Fig. 7, EPSR-low-high-comparison.plt refers to Fig. 9, and EPSR-0ep.plt refers to Fig. 13.

The simulations were run with EPSR26 which is also available from the ISIS Disordered Materials website.