The data in this archive relate to the paper

A K Soper, I. Skarmoutsos, J. Klos, J. Samios and S. Marinakis. (2019) “A study of Ar-N_2 supercritical mixtures using neutron scattering, molecular dynamics simulations and quantum mechanical scattering calculations”, J. Mol. Liq.

The main items are the EPSR input files, whose files have xxxmix1 (for 49 bar) or xxxmix2 (for 98 bar) in their filenames. For pure Ar xxx=ar, and for pure N2 xxx=n2. For the mixtures, xxx=arn22575 (for x=0.25), xxx=arn25050 (for x=0.5) and xxx=arn27525 (x=0.75). (Se Table 1 below for details.) Generally they will have the extension .EPSR.xxx, except the .ato files, which contain the molecular and atomic coordinates in a particular form, and the .pcof files, which contain the coefficients used to generate the empirical contribution to the interatomic potential. Note that in this case there was no empirical potential refinement so the empirical potentials are all zero. Instead the Lennard-Jones parameters were adjusted to give the best possible fits to all the datasets.

Table 1: x_{N_2}-T_{exp}-P_{exp} state points employed in the neutron scattering measurements. The REFPROP [51] was used to calculate the density, $\rho_{REFPROP}$, and the $Q = 0$ limit of the structure factor, $F(0) = (\rho k_B T \kappa_T - 1)$ (1) where ρ is the atomic number density and κ_T is the isothermal compressibility, corresponding to the experimental conditions, and the critical point (T_c, P_c, and ρ_c (kg/m^3)).

x_{N_2}	T_{exp} [K]	P_{exp} [bar]	$\rho_{REFPROP}$ [kg/m^3]	F(0)	T_c [K]	P_c [bar]	ρ_c [kg/m^3]
0.00	154.1	48.9±0.5	288.29	4.4	150.69	48.63	535.60
		97.8±1.0	910.61	-0.3			
0.25	147.7	48.9±0.5	342.63	13.5	144.64	45.74	478.98
		97.8±1.0	813.71	-0.1			
0.50	141.2	48.7±0.4	488.95	15.9	138.44	42.18	423.60
		96.9±1.1	728.29	-0.1			
0.75	134.8	48.9±0.1	509.84	4.8	132.28	38.22	368.57
		92.2±4.9	644.33	0.0			
1.00	128.4	49.4±0.6	484.62	2.3	126.19	33.96	313.30
		94.0±4.7	575.37	-0.1			

There are two .zip files, namely **ArN2cm-singlelj-q.zip** and **ArN2cm-singleljmod-q.zip**. The first is the best fit to the data obtained with the specified Lennard-Jones parameters, while the second file uses the Lennard-Jones parameters that were used in the MD simulations. (See paper for more details.)

A full description of the EPSR file structure and names can be found in the EPSR manual which can be downloaded from this location:-

http://purl.org/net/epubs/work/56239

The EPSR code and binaries can be downloaded from here:

https://www.isis.stfc.ac.uk/Pages/Empirical-Potential-Structure-Refinement.aspx

Note that the current version of EPSR is EPSR25, but the data were run with EPSR26 (t currently released). However EPSR has always been upwards and downwards

compatible, so that the new simulation files should run with the earlier versions of the program – with some caveats. Equally the above EPSR manual may not be quite up to date and a more up to date version is available with the code and binaries download.

The fits to the scattering data are in the .f01 files, and the associated site-site g(r)s are in the .g01 files. The data that were fitted are stored in the .t01 files.

These are multicolumn files with two columns for each dataset or g(r) and the label at the top of each even column indicates which dataset or site-site term that column relates to. The first column in these files is either Q or r. The even columns are then the actual fits or g(r)s respectively, while the remaining odd columns give the RMS deviation of individual configurations away from the mean value. They are strictly not error bars since the systematic errors in these experiments are hard to quantify. A number of other EPSR files are presented and these can be interrogated if desired – see the above manual for more information. One useful example is the running coordination number for each site-site term, which is in the .z01 file. Note that in this latter file, the odd columns are NOT the RMS deviation, but instead represent the running coordination number of the opposite atom pair. For example if the even column represents the atom pair O – H, then the next odd column represents the atom pair H – O, since these two coordination numbers may not be the same, even though the corresponding site-site terms are identical.

In addition the results of other EPSR analysis programs may be available, such as the triangle angle distributions and the spherical harmonic coefficients (to calculate spatial density functions) and some files for these other programs may be available. Note that the archive may contain some historic data and files that can be safely ignored.