

## pdCIFplotter: visualizing powder diffraction data in pdCIF format

```

xdd
  local CIF_DATETIME ="2021-04-01T17:45:32";
  ...
  str
    local CIF_PHASE_ID 1
    local !CIF_Z = 2;
    ...
  str
    local CIF_PHASE_ID 2
    ...
macro ciffile { "single.cif" }
Out_pdCIF_STR(ciffile, "proc")
(i)

xdd
  local !CIF_ID 1
  local !CIF_SCAN_METHOD = "fixed";
  ...
  str
    local CIF_PHASE_ID 1
    ...
  str
    local CIF_PHASE_ID 2
    ...
  Out_pdCIF_per_xdd("many.cif", "proc")

xdd
  local !CIF_ID 2
  local !CIF_SCAN_METHOD = "cont";
  ...
  str
    local CIF_PHASE_ID 1
    ...
  str
    local CIF_PHASE_ID 2
    ...
  str
    local CIF_PHASE_ID 3
    ...
  Out_pdCIF_per_xdd("many.cif", "meas")
(ii)

num_runs 30
#list File_Name Pressure DateTime {
file_01.xye      100 "2021-04-
01T17:45:32+0800"
file_02.xye      250 "2021-04-
01T17:55:51+0800"
... }
prm CIF_ID = Run_Number;
prm CIF_PRES = Pressure(Run_Number);
prm CIF_SCAN_METHOD = "fixed";
prm CIF_DATETIME = DateTime(Run_Number);
xdd File_Name(Run_Number)
...
str
  local CIF_PHASE_ID 1
  local !CIF_CRYSTAL_SYSTEM = "cubic";
  ...
str
  local CIF_PHASE_ID 2
  local !CIF_Z = 8;
  ...
str
  local CIF_PHASE_ID 3
  local !CIF_Z = 2;
  ...
macro CIF_OUTPUT_FILE { "sequential.cif" }
Out_pdCIF(CIF_OUTPUT_FILE, "proc")
(iii)
(a)

prm CIF_ID 1
prm CIF_TEMP 293
prm CIF_PRES 101.3
prm !CIF_SCAN_METHOD = "fixed";
xdd 'eg X-ray dataset
  ...
  str
    local CIF_PHASE_ID 1
    ...
  str
    local CIF_PHASE_ID 2
    local !CIF_Z 6
    ...
  xdd 'eg neutron dataset
  ...
  str
    local CIF_PHASE_ID 1
    ...
  str
    local CIF_PHASE_ID 2
    local !CIF_Z 6
    ...
  ...
  Out_pdCIF_multi("multi.cif", "proc")
(i)

macro CIF_OUTPUT_FILE { "sequential_multi.cif" }
num_runs 30
#list File_b1 File_b2 File_b3 Temperature {
b1_01.xye b2_01.xye b3_01.xye 30
b1_02.xye b2_02.xye b3_02.xye 35
... }
prm CIF_ID = Run_Number;
prm CIF_TEMP = Temperature(Run_Number);
xdd File_b1(Run_Number)
...
str
  ...
  str
    xdd File_b2(Run_Number)
    ...
    str
      ...
      str
        xdd File_b3(Run_Number)
        ...
        str
          ...
          for xdds {
            for str 1 to 1 {
              local CIF_PHASE_ID 1
              local CIF_Z = 6;
              ...
            }
            for str 2 to 2 {
              local CIF_PHASE_ID 2
              local CIF_Z = 8;
              ...
            }
          }
        }
      Out_pdCIF_multi(CIF_OUTPUT_FILE, "meas")
      (ii)
      (b)

```

Example uses of the CIF output macros. (a) `Out_pdCIF`: (i) Simple, single diffraction pattern refinement with one crystal structure of interest and an impurity. (ii) Fitting data from two different synthesis methods, with each containing a different number of structures. (iii) Sequential refinement of in situ diffraction data. (b) `Out_pdCIF_multi`: (i) Combined refinement of two crystal structures using X-ray and neutron data. (ii) Sequential refinement of in situ diffraction data with two crystal structures across three diffraction patterns