```
##############################################################################
###     FullProf-generated CIF output file  (version: February 2008)     ###
###     Template of CIF submission form for structure report           ###
##############################################################################

# This file has been generated using FullProf.2k taking one example of
# structure report provided by Acta Cryst. It is given as a 'template' with
# filled structural items. Many other items are left unfilled and it is the
# responsibility of the user to properly fill or suppress them. In principle
# all question marks '?' should be replaced by the appropriate text or
# numerical value depending on the kind of CIF item.
# See the document: cif_core.dic (URL: http://www.iucr.org) for details.

# Please notify any error or suggestion to:
#        Juan Rodriguez-Carvajal (jrc@ill.eu)
# Improvements will be progressively added as needed.

#==============================================================================
 data_global
#==============================================================================

# PROCESSING SUMMARY (IUCr Office Use Only)

_journal_data_validation_number     ?

_journal_date_recd_electronic       ?
_journal_date_to_coeditor           ?
_journal_date_from_coeditor         ?
_journal_date_accepted              ?
_journal_date_printers_first        ?
_journal_date_printers_final        ?
_journal_date_proofs_out            ?
_journal_date_proofs_in             ?
_journal_coeditor_name              ?
_journal_coeditor_code              ?
_journal_coeditor_notes
; ?
;
_journal_techeditor_code            ?
_journal_techeditor_notes
; ?
;
_journal_coden_ASTM                 ?
_journal_name_full                  ?
_journal_year                       ?
_journal_volume                     ?
_journal_issue                      ?
_journal_page_first                 ?
_journal_page_last                  ?
_journal_paper_category             ?
_journal_suppl_publ_number          ?
_journal_suppl_publ_pages           ?
```

```
#==============================================================================

# 1. SUBMISSION DETAILS

_publ_contact_author_name           ?  # Name of author for correspondence
_publ_contact_author_address            # Address of author for correspondence
; ?
;
_publ_contact_author_email         ?
_publ_contact_author_fax          ?
_publ_contact_author_phone          ?

_publ_contact_letter
; ?
;

_publ_requested_journal          ?
_publ_requested_coeditor_name       ?
_publ_requested_category          ?  # Acta C: one of CI/CM/CO/FI/FM/FO


# Definition of non standard CIF items (Reliability indices used in FULLPROF)

loop_
_publ_manuscript_incl_extra_item
_publ_manuscript_incl_extra_info
_publ_manuscript_incl_extra_defn
#    Name                    Explanation          Standard?
#    ------                  -----------          ---------
 '_pd_proc_ls_prof_cR_factor'   'Prof. R-factor CORRECTED for background'   no
 '_pd_proc_ls_prof_cwR_factor'  'wProf.R-factor CORRECTED for background'   no
 '_pd_proc_ls_prof_cwR_expected' 'wProf.Expected CORRECTED for background'   no
 '_pd_proc_ls_prof_chi2'      'Chi-square for all considered points'     no
 '_pd_proc_ls_prof_echi2'      'Chi-2 for points with Bragg contribution'  no
#==============================================================================

# 3. TITLE AND AUTHOR LIST

_publ_section_title
; ' NaCo1'
;
_publ_section_title_footnote
;
;

# The loop structure below should contain the names and addresses of all
# authors, in the required order of publication. Repeat as necessary.

loop_
   _publ_author_name
   _publ_author_footnote
   _publ_author_address
?                   #<--'Last name, first name'
; ?
```

```
;
; ?
;

#=====================================================================

# 4. TEXT

_publ_section_synopsis
;  ?
;
_publ_section_abstract
; ?
;
_publ_section_comment
; ?
;
_publ_section_exptl_prep     # Details of the preparation of the sample(s)
                    # should be given here.
; ?
;
_publ_section_exptl_refinement
; ?
;
_publ_section_references
; ?
;
_publ_section_figure_captions
; ?
;
_publ_section_acknowledgements
; ?
;

#=====================================================================

#=====================================================================
# If more than one structure is reported, the remaining sections should be
# completed per structure. For each data set, replace the '?' in the
# data_? line below by a unique identifier.

data_Co10Ge3O16

#=====================================================================

# 5. CHEMICAL DATA

_chemical_name_systematic
; ?
;
_chemical_name_common          ?
_chemical_formula_moiety       ?
_chemical_formula_structural   ?
_chemical_formula_analytical     ?
```

```
_chemical_formula_iupac          ?
_chemical_formula_sum            ?
_chemical_formula_weight         ?
_chemical_melting_point          ?
_chemical_compound_source        ?        # for minerals and
                                 # natural products


loop_
   _atom_type_symbol
   _atom_type_scat_length_neutron
   _atom_type_scat_source
Fe   0.94500 V.F._Sears_Neutron_News_3_26_(1992)
Ge   0.81850 V.F._Sears_Neutron_News_3_26_(1992)
O    0.58030 V.F._Sears_Neutron_News_3_26_(1992)


#==============================================================================

# 6. POWDER SPECIMEN AND CRYSTAL DATA

_symmetry_cell_setting           Monoclinic
_symmetry_space_group_name_H-M      'C 1 2/c 1'
_symmetry_space_group_name_Hall     '-C 2yc'


loop_
   _symmetry_equiv_pos_as_xyz   #<--must include 'x,y,z'
'x,y,z'
'-x,y,-z+1/2'
'-x,-y,-z'
'x,-y,z+1/2'
'x+1/2,y+1/2,z'
'-x+1/2,y+1/2,-z+1/2'
'-x+1/2,-y+1/2,-z'
'x+1/2,-y+1/2,z+1/2'


_cell_length_a                9.78478(5)
_cell_length_b                9.13685(5)
_cell_length_c                5.19364(3)
_cell_angle_alpha             90.00000
_cell_angle_beta              101.7635(4)
_cell_angle_gamma             90.00000
_cell_volume                  454.570(4)
_cell_formula_units_Z              ?
_cell_measurement_temperature      ?
_cell_special_details
; ?
;
# The next three fields give the specimen dimensions in mm.  The equatorial
# plane contains the incident and diffracted beam.

_pd_spec_size_axial          ?        # perpendicular to
                             # equatorial plane
_pd_spec_size_equat          ?        # parallel to
                             # scattering vector
                             # in transmission
```

```
_pd_spec_size_thick              ?      # parallel to
                                 # scattering vector
                                 # in reflection

# The next five fields are character fields that describe the specimen.

_pd_spec_mounting                     # This field should be
                                 # used to give details of the
                                 # container.
; ?
;
_pd_spec_mount_mode            ?      # options are 'reflection'
                                 # or 'transmission'
_pd_spec_shape                 ?      # options are 'cylinder'
                                 # 'flat_sheet' or 'irregular'
_pd_char_particle_morphology     ?
_pd_char_colour                ?      # use ICDD colour descriptions

# The following three fields describe the preparation of the specimen.
# The cooling rate is in K/min.  The pressure at which the sample was
# prepared is in kPa.  The temperature of preparation is in K.

_pd_prep_cool_rate             ?
_pd_prep_pressure              ?
_pd_prep_temperature            ?

# The next four fields are normally only needed for transmission experiments.

_exptl_absorpt_coefficient_mu       ?
_exptl_absorpt_correction_type      ?
_exptl_absorpt_process_details      ?
_exptl_absorpt_correction_T_min     ?
_exptl_absorpt_correction_T_max     ?

#=============================================================================

# 7. EXPERIMENTAL DATA

_exptl_special_details
; ?
;

# The following item is used to identify the equipment used to record
# the powder pattern when the diffractogram was measured at a laboratory
# other than the authors' home institution, e.g. when neutron or synchrotron
# radiation is used.

_pd_instr_location
; ?
;
_pd_calibration_special_details         # description of the method used
                                 # to calibrate the instrument
; ?
;
```

```
_diffrn_ambient_temperature          ?
_diffrn_source                'nuclear reactor'
_diffrn_radiation_type          'Constant Wavelength Neutron Diffraction'
_diffrn_radiation_wavelength        2.53600
_diffrn_source_type              ?  # Put here the diffractometer and site

_diffrn_radiation_monochromator      ?
_diffrn_measurement_device_type      ?
_diffrn_measurement_method        ?
_diffrn_detector_area_resol_mean    ?   # Not in version 2.0.1
_diffrn_detector              ?
_diffrn_detector_type            ?   # make or model of detector
_pd_meas_scan_method              ?   # options are 'step', 'cont',
                          # 'tof', 'fixed' or
                          # 'disp' (= dispersive)
_pd_meas_special_details
;  ?
;

#  The following four items give details of the measured (not processed)
#  powder pattern.  Angles are in degrees.

_pd_meas_number_of_points        3020
_pd_meas_2theta_range_min        0.95000
_pd_meas_2theta_range_max         151.89999
_pd_meas_2theta_range_inc        0.050017

#==============================================================================

# 8. REFINEMENT DATA

_refine_special_details
; ?
;

# Use the next field to give any special details about the fitting of the
# powder pattern.

_pd_proc_ls_special_details
; ?
;

# The next three items are given as text.

_pd_proc_ls_profile_function      ?
_pd_proc_ls_background_function    ?
_pd_proc_ls_pref_orient_corr
; ?
;

#  The following profile R-factors are NOT CORRECTED for background
#  The sum is extended to all non-excluded points.
#  These are the current CIF standard
```

```
_pd_proc_ls_prof_R_factor          3.7144
_pd_proc_ls_prof_wR_factor          5.0391
_pd_proc_ls_prof_wR_expected          2.2944


# The following profile R-factors are CORRECTED for background
# The sum is extended to all non-excluded points.
# These items are not in the current CIF standard, but are defined above


_pd_proc_ls_prof_cR_factor          7.2206
_pd_proc_ls_prof_cwR_factor          7.3229
_pd_proc_ls_prof_cwR_expected          3.3342


# The following items are not in the CIF standard, but are defined above


_pd_proc_ls_prof_chi2          4.8238
_pd_proc_ls_prof_echi2          5.1541


# Items related to LS refinement


_refine_ls_R_I_factor          1.1450
_refine_ls_number_reflns          106
_refine_ls_number_parameters          94
_refine_ls_number_restraints          0


# The following four items apply to angular dispersive measurements.
# 2theta minimum, maximum and increment (in degrees) are for the
# intensities used in the refinement.


_pd_proc_2theta_range_min          0.8931
_pd_proc_2theta_range_max          151.8431
_pd_proc_2theta_range_inc          0.050017
_pd_proc_wavelength          2.536000


_pd_block_diffractogram_id          ?  # The id used for the block containing
                                       # the powder pattern profile (section 11)


# Give appropriate details in the next two text fields.


_pd_proc_info_excluded_regions     ?
_pd_proc_info_data_reduction       ?


# The following items are used to identify the programs used.


_computing_data_collection          ?
_computing_structure_solution          ?
_computing_structure_refinement     FULLPROF
_computing_molecular_graphics       ?
_computing_publication_material     ?


#=============================================================================


# 9. ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS
```

```
loop_
   _atom_site_label
   _atom_site_fract_x
   _atom_site_fract_y
   _atom_site_fract_z
   _atom_site_U_iso_or_equiv
   _atom_site_occupancy
   _atom_site_adp_type          # Not in version 2.0.1
   _atom_site_type_symbol
 Fe1  0.00000    0.9083(3)  0.25000     0.0023(7)  1.00000   Uiso Fe
 Fe2  0.00000    0.2707(2)  0.25000     0.0025(8)  1.00000   Uiso Fe
 Ge1  0.30018(15) 0.0925(2)  0.2156(3)  0.0036(6)  1.00000   Uiso Ge
 O1   0.1190(2)  0.0904(3)  0.1405(4)   0.0050(7)  1.00000   Uiso O
 O2   0.3836(3)  0.2403(3)  0.3811(6)   0.0014(8)  1.00000   Uiso O
 O3   0.3587(2)  0.0659(3)  0.9132(4)   0.0031(8)  1.00000   Uiso O
```

\# Note: if the displacement parameters were refined anisotropically
\# the U matrices should be given as for single-crystal studies.

\#===

\# 10. DISTANCES AND ANGLES / MOLECULAR GEOMETRY

_geom_special_details   ?

```
loop_
   _geom_bond_atom_site_label_1
   _geom_bond_atom_site_label_2
   _geom_bond_site_symmetry_1
   _geom_bond_site_symmetry_2
   _geom_bond_distance
   _geom_bond_publ_flag
   ? ? ? ? ? ?

loop_
   _geom_contact_atom_site_label_1
   _geom_contact_atom_site_label_2
   _geom_contact_distance
   _geom_contact_site_symmetry_1
   _geom_contact_site_symmetry_2
   _geom_contact_publ_flag
   ? ? ? ? ? ?

loop_
_geom_angle_atom_site_label_1
_geom_angle_atom_site_label_2
_geom_angle_atom_site_label_3
_geom_angle_site_symmetry_1
_geom_angle_site_symmetry_2
_geom_angle_site_symmetry_3
_geom_angle
_geom_angle_publ_flag
? ? ? ? ? ? ? ?
```

```
loop_
_geom_torsion_atom_site_label_1
_geom_torsion_atom_site_label_2
_geom_torsion_atom_site_label_3
_geom_torsion_atom_site_label_4
_geom_torsion_site_symmetry_1
_geom_torsion_site_symmetry_2
_geom_torsion_site_symmetry_3
_geom_torsion_site_symmetry_4
_geom_torsion
_geom_torsion_publ_flag
? ? ? ? ? ? ? ? ? ?

loop_
_geom_hbond_atom_site_label_D
_geom_hbond_atom_site_label_H
_geom_hbond_atom_site_label_A
_geom_hbond_site_symmetry_D
_geom_hbond_site_symmetry_H
_geom_hbond_site_symmetry_A
_geom_hbond_distance_DH
_geom_hbond_distance_HA
_geom_hbond_distance_DA
_geom_hbond_angle_DHA
_geom_hbond_publ_flag
? ? ? ? ? ? ? ? ? ? ?

#======================================================================

#======================================================================
# Additional structures (last six sections and associated data_? identifiers)
# may be added at this point.
#======================================================================

data_Co10Ge3O16

#======================================================================

# 5. CHEMICAL DATA

_chemical_name_systematic
; ?
;
_chemical_name_common           ?
_chemical_formula_moiety        ?
_chemical_formula_structural    ?
_chemical_formula_analytical     ?
_chemical_formula_iupac         ?
_chemical_formula_sum           ?
_chemical_formula_weight         ?
_chemical_melting_point         ?
_chemical_compound_source        ?     # for minerals and
                        # natural products
```

```
loop_
   _atom_type_symbol
   _atom_type_scat_length_neutron
   _atom_type_scat_source
```

#===

6. POWDER SPECIMEN AND CRYSTAL DATA

```
_symmetry_cell_setting            Cubic
_symmetry_space_group_name_H-M       'F d -3 m'
_symmetry_space_group_name_Hall      '-F 4vw 2vw 3'
```

```
loop_
   _symmetry_equiv_pos_as_xyz   #<--must include 'x,y,z'
'x,y,z'
'x,-y+1/4,-z+1/4'
'-x+1/4,y,-z+1/4'
'-x+1/4,-y+1/4,z'
'y,z,x'
'-y+1/4,-z+1/4,x'
'y,-z+1/4,-x+1/4'
'-y+1/4,z,-x+1/4'
'z,x,y'
'-z+1/4,x,-y+1/4'
'-z+1/4,-x+1/4,y'
'z,-x+1/4,-y+1/4'
'y,x,z'
'-y+1/4,x,-z+1/4'
'y,-x+1/4,-z+1/4'
'-y+1/4,-x+1/4,z'
'z,y,x'
'-z+1/4,-y+1/4,x'
'-z+1/4,y,-x+1/4'
'z,-y+1/4,-x+1/4'
'x,z,y'
'x,-z+1/4,-y+1/4'
'-x+1/4,-z+1/4,y'
'-x+1/4,z,-y+1/4'
'-x,-y,-z'
'-x,y+3/4,z+3/4'
'x+3/4,-y,z+3/4'
'x+3/4,y+3/4,-z'
'-y,-z,-x'
'y+3/4,z+3/4,-x'
'-y,z+3/4,x+3/4'
'y+3/4,-z,x+3/4'
'-z,-x,-y'
'z+3/4,-x,y+3/4'
'z+3/4,x+3/4,-y'
'-z,x+3/4,y+3/4'
'-y,-x,-z'
'y+3/4,-x,z+3/4'
'-y,x+3/4,z+3/4'
```

'y+3/4,x+3/4,-z'
'-z,-y,-x'
'z+3/4,y+3/4,-x'
'z+3/4,-y,x+3/4'
'-z,y+3/4,x+3/4'
'-x,-z,-y'
'-x,z+3/4,y+3/4'
'x+3/4,z+3/4,-y'
'x+3/4,-z,y+3/4'
'x+1/2,y+1/2,z'
'x+1/2,-y+3/4,-z+1/4'
'-x+3/4,y+1/2,-z+1/4'
'-x+3/4,-y+3/4,z'
'y+1/2,z+1/2,x'
'-y+3/4,-z+3/4,x'
'y+1/2,-z+3/4,-x+1/4'
'-y+3/4,z+1/2,-x+1/4'
'z+1/2,x+1/2,y'
'-z+3/4,x+1/2,-y+1/4'
'-z+3/4,-x+3/4,y'
'z+1/2,-x+3/4,-y+1/4'
'y+1/2,x+1/2,z'
'-y+3/4,x+1/2,-z+1/4'
'y+1/2,-x+3/4,-z+1/4'
'-y+3/4,-x+3/4,z'
'z+1/2,y+1/2,x'
'-z+3/4,-y+3/4,x'
'-z+3/4,y+1/2,-x+1/4'
'z+1/2,-y+3/4,-x+1/4'
'x+1/2,z+1/2,y'
'x+1/2,-z+3/4,-y+1/4'
'-x+3/4,-z+3/4,y'
'-x+3/4,z+1/2,-y+1/4'
'-x+1/2,-y+1/2,-z'
'-x+1/2,y+1/4,z+3/4'
'x+1/4,-y+1/2,z+3/4'
'x+1/4,y+1/4,-z'
'-y+1/2,-z+1/2,-x'
'y+1/4,z+1/4,-x'
'-y+1/2,z+1/4,x+3/4'
'y+1/4,-z+1/2,x+3/4'
'-z+1/2,-x+1/2,-y'
'z+1/4,-x+1/2,y+3/4'
'z+1/4,x+1/4,-y'
'-z+1/2,x+1/4,y+3/4'
'-y+1/2,-x+1/2,-z'
'y+1/4,-x+1/2,z+3/4'
'-y+1/2,x+1/4,z+3/4'
'y+1/4,x+1/4,-z'
'-z+1/2,-y+1/2,-x'
'z+1/4,y+1/4,-x'
'z+1/4,-y+1/2,x+3/4'
'-z+1/2,y+1/4,x+3/4'
'-x+1/2,-z+1/2,-y'

'-x+1/2,z+1/4,y+3/4'
'x+1/4,z+1/4,-y'
'x+1/4,-z+1/2,y+3/4'
'x+1/2,y,z+1/2'
'x+1/2,-y+1/4,-z+3/4'
'-x+3/4,y,-z+3/4'
'-x+3/4,-y+1/4,z+1/2'
'y+1/2,z,x+1/2'
'-y+3/4,-z+1/4,x+1/2'
'y+1/2,-z+1/4,-x+3/4'
'-y+3/4,z,-x+3/4'
'z+1/2,x,y+1/2'
'-z+3/4,x,-y+3/4'
'-z+3/4,-x+1/4,y+1/2'
'z+1/2,-x+1/4,-y+3/4'
'y+1/2,x,z+1/2'
'-y+3/4,x,-z+3/4'
'y+1/2,-x+1/4,-z+3/4'
'-y+3/4,-x+1/4,z+1/2'
'z+1/2,y,x+1/2'
'-z+3/4,-y+1/4,x+1/2'
'-z+3/4,y,-x+3/4'
'z+1/2,-y+1/4,-x+3/4'
'x+1/2,z,y+1/2'
'x+1/2,-z+1/4,-y+3/4'
'-x+3/4,-z+1/4,y+1/2'
'-x+3/4,z,-y+3/4'
'-x+1/2,-y,-z+1/2'
'-x+1/2,y+3/4,z+1/4'
'x+1/4,-y,z+1/4'
'x+1/4,y+3/4,-z+1/2'
'-y+1/2,-z,-x+1/2'
'y+1/4,z+3/4,-x+1/2'
'-y+1/2,z+3/4,x+1/4'
'y+1/4,-z,x+1/4'
'-z+1/2,-x,-y+1/2'
'z+1/4,-x,y+1/4'
'z+1/4,x+3/4,-y+1/2'
'-z+1/2,x+3/4,y+1/4'
'-y+1/2,-x,-z+1/2'
'y+1/4,-x,z+1/4'
'-y+1/2,x+3/4,z+1/4'
'y+1/4,x+3/4,-z+1/2'
'-z+1/2,-y,-x+1/2'
'z+1/4,y+3/4,-x+1/2'
'z+1/4,-y,x+1/4'
'-z+1/2,y+3/4,x+1/4'
'-x+1/2,-z,-y+1/2'
'-x+1/2,z+3/4,y+1/4'
'x+1/4,z+3/4,-y+1/2'
'x+1/4,-z,y+1/4'
'x,y+1/2,z+1/2'
'x,-y+3/4,-z+3/4'
'-x+1/4,y+1/2,-z+3/4'

```
'-x+1/4,-y+3/4,z+1/2'
'y,z+1/2,x+1/2'
'-y+1/4,-z+3/4,x+1/2'
'y,-z+3/4,-x+3/4'
'-y+1/4,z+1/2,-x+3/4'
'z,x+1/2,y+1/2'
'-z+1/4,x+1/2,-y+3/4'
'-z+1/4,-x+3/4,y+1/2'
'z,-x+3/4,-y+3/4'
'y,x+1/2,z+1/2'
'-y+1/4,x+1/2,-z+3/4'
'y,-x+3/4,-z+3/4'
'-y+1/4,-x+3/4,z+1/2'
'z,y+1/2,x+1/2'
'-z+1/4,-y+3/4,x+1/2'
'-z+1/4,y+1/2,-x+3/4'
'z,-y+3/4,-x+3/4'
'x,z+1/2,y+1/2'
'x,-z+3/4,-y+3/4'
'-x+1/4,-z+3/4,y+1/2'
'-x+1/4,z+1/2,-y+3/4'
'-x,-y+1/2,-z+1/2'
'-x,y+1/4,z+1/4'
'x+3/4,-y+1/2,z+1/4'
'x+3/4,y+1/4,-z+1/2'
'-y,-z+1/2,-x+1/2'
'y+3/4,z+1/4,-x+1/2'
'-y,z+1/4,x+1/4'
'y+3/4,-z+1/2,x+1/4'
'-z,-x+1/2,-y+1/2'
'z+3/4,-x+1/2,y+1/4'
'z+3/4,x+1/4,-y+1/2'
'-z,x+1/4,y+1/4'
'-y,-x+1/2,-z+1/2'
'y+3/4,-x+1/2,z+1/4'
'-y,x+1/4,z+1/4'
'y+3/4,x+1/4,-z+1/2'
'-z,-y+1/2,-x+1/2'
'z+3/4,y+1/4,-x+1/2'
'z+3/4,-y+1/2,x+1/4'
'-z,y+1/4,x+1/4'
'-x,-z+1/2,-y+1/2'
'-x,z+1/4,y+1/4'
'x+3/4,z+1/4,-y+1/2'
'x+3/4,-z+1/2,y+1/4'
```

_cell_length_a	8.40018(10)
_cell_length_b	8.40018(10)
_cell_length_c	8.40018(10)
_cell_angle_alpha	90.00000
_cell_angle_beta	90.00000
_cell_angle_gamma	90.00000
_cell_volume	592.742(12)
_cell_formula_units_Z	?

```
_cell_measurement_temperature        ?
_cell_special_details
; ?
;
# The next three fields give the specimen dimensions in mm.  The equatorial
# plane contains the incident and diffracted beam.

_pd_spec_size_axial              ?      # perpendicular to
                                 # equatorial plane
_pd_spec_size_equat              ?      # parallel to
                                 # scattering vector
                                 # in transmission
_pd_spec_size_thick              ?      # parallel to
                                 # scattering vector
                                 # in reflection

# The next five fields are character fields that describe the specimen.

_pd_spec_mounting                       # This field should be
                                 # used to give details of the
                                 # container.
; ?
;
_pd_spec_mount_mode              ?      # options are 'reflection'
                                 # or 'transmission'
_pd_spec_shape                   ?      # options are 'cylinder'
                                 # 'flat_sheet' or 'irregular'
_pd_char_particle_morphology     ?
_pd_char_colour                  ?      # use ICDD colour descriptions

# The following three fields describe the preparation of the specimen.
# The cooling rate is in K/min.  The pressure at which the sample was
# prepared is in kPa.  The temperature of preparation is in K.

_pd_prep_cool_rate               ?
_pd_prep_pressure                ?
_pd_prep_temperature             ?

# The next four fields are normally only needed for transmission experiments.

_exptl_absorpt_coefficient_mu       ?
_exptl_absorpt_correction_type      ?
_exptl_absorpt_process_details      ?
_exptl_absorpt_correction_T_min     ?
_exptl_absorpt_correction_T_max     ?

#=========================================================================

# 7. EXPERIMENTAL DATA

_exptl_special_details
; ?
;
```

```
# The following item is used to identify the equipment used to record
# the powder pattern when the diffractogram was measured at a laboratory
# other than the authors' home institution, e.g. when neutron or synchrotron
# radiation is used.

_pd_instr_location
; ?
;
_pd_calibration_special_details        # description of the method used
                          # to calibrate the instrument
; ?
;

_diffrn_ambient_temperature        ?
_diffrn_source                'nuclear reactor'
_diffrn_radiation_type        'Constant Wavelength Neutron Diffraction'
_diffrn_radiation_wavelength        2.53600
_diffrn_source_type            ?  # Put here the diffractometer and site

_diffrn_radiation_monochromator     ?
_diffrn_measurement_device_type     ?
_diffrn_measurement_method        ?
_diffrn_detector_area_resol_mean    ?  # Not in version 2.0.1
_diffrn_detector            ?
_diffrn_detector_type            ?  # make or model of detector
_pd_meas_scan_method            ?  # options are 'step', 'cont',
                     # 'tof', 'fixed' or
                     # 'disp' (= dispersive)
_pd_meas_special_details
; ?
;

#  The following four items give details of the measured (not processed)
#  powder pattern.  Angles are in degrees.

_pd_meas_number_of_points        0
_pd_meas_2theta_range_min        0.95000
_pd_meas_2theta_range_max        151.89999
_pd_meas_2theta_range_inc        0.050017

#========================================================================

# 8. REFINEMENT DATA

_refine_special_details
; ?
;

# Use the next field to give any special details about the fitting of the
# powder pattern.

_pd_proc_ls_special_details
; ?
;
```

The next three items are given as text.

_pd_proc_ls_profile_function   ?
_pd_proc_ls_background_function   ?
_pd_proc_ls_pref_orient_corr
; ?
;

The following profile R-factors are NOT CORRECTED for background
The sum is extended to all non-excluded points.
These are the current CIF standard

_pd_proc_ls_prof_R_factor   3.7144
_pd_proc_ls_prof_wR_factor   5.0391
_pd_proc_ls_prof_wR_expected   2.2944

The following profile R-factors are CORRECTED for background
The sum is extended to all non-excluded points.
These items are not in the current CIF standard, but are defined above

_pd_proc_ls_prof_cR_factor   7.2206
_pd_proc_ls_prof_cwR_factor   7.3229
_pd_proc_ls_prof_cwR_expected   3.3342

The following items are not in the CIF standard, but are defined above

_pd_proc_ls_prof_chi2   4.8238
_pd_proc_ls_prof_echi2   5.1541

Items related to LS refinement

_refine_ls_R_I_factor   0.9540
_refine_ls_number_reflns   14
_refine_ls_number_parameters   94
_refine_ls_number_restraints   0

The following four items apply to angular dispersive measurements.
2theta minimum, maximum and increment (in degrees) are for the
intensities used in the refinement.

_pd_proc_2theta_range_min   0.8931
_pd_proc_2theta_range_max   151.8431
_pd_proc_2theta_range_inc   0.050017
_pd_proc_wavelength   2.536000

_pd_block_diffractogram_id   ? # The id used for the block containing
                          # the powder pattern profile (section 11)

Give appropriate details in the next two text fields.

_pd_proc_info_excluded_regions   ?
_pd_proc_info_data_reduction   ?

The following items are used to identify the programs used.

```
_computing_data_collection        ?
_computing_structure_solution      ?
_computing_structure_refinement    FULLPROF
_computing_molecular_graphics      ?
_computing_publication_material    ?
```

#===

9. ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS

```
loop_
   _atom_site_label
   _atom_site_fract_x
   _atom_site_fract_y
   _atom_site_fract_z
   _atom_site_U_iso_or_equiv
   _atom_site_occupancy
   _atom_site_adp_type          # Not in version 2.0.1
   _atom_site_type_symbol
 Ge1  0.12500   0.12500   0.12500   0.00458   1.00000   Uani Ge
 Fe1  0.50000   0.50000   0.50000   0.00608   0.99988   Uani Fe
 O1   0.24660   0.24660   0.24660   0.00618   0.99994   Uani O
```

```
loop_
   _atom_site_aniso_label
   _atom_site_aniso_U_11
   _atom_site_aniso_U_22
   _atom_site_aniso_U_33
   _atom_site_aniso_U_12
   _atom_site_aniso_U_13
   _atom_site_aniso_U_23
   _atom_site_aniso_type_symbol
 Ge1  0.00458   0.00458   0.00458   0.00000   0.00000   0.00000   Ge
 Fe1  0.00608   0.00608   0.00608   0.00039   0.00039   0.00039   Fe
 O1   0.00618   0.00618   0.00618  -0.00150  -0.00150  -0.00150   O
```

Note: if the displacement parameters were refined anisotropically
the U matrices should be given as for single-crystal studies.

#===

10. DISTANCES AND ANGLES / MOLECULAR GEOMETRY

```
_geom_special_details          ?
```

```
loop_
   _geom_bond_atom_site_label_1
   _geom_bond_atom_site_label_2
   _geom_bond_site_symmetry_1
   _geom_bond_site_symmetry_2
   _geom_bond_distance
   _geom_bond_publ_flag
```

```
    ? ? ? ? ? ?

loop_
    _geom_contact_atom_site_label_1
    _geom_contact_atom_site_label_2
    _geom_contact_distance
    _geom_contact_site_symmetry_1
    _geom_contact_site_symmetry_2
    _geom_contact_publ_flag
    ? ? ? ? ? ?

loop_
_geom_angle_atom_site_label_1
_geom_angle_atom_site_label_2
_geom_angle_atom_site_label_3
_geom_angle_site_symmetry_1
_geom_angle_site_symmetry_2
_geom_angle_site_symmetry_3
_geom_angle
_geom_angle_publ_flag
? ? ? ? ? ? ? ?

loop_
_geom_torsion_atom_site_label_1
_geom_torsion_atom_site_label_2
_geom_torsion_atom_site_label_3
_geom_torsion_atom_site_label_4
_geom_torsion_site_symmetry_1
_geom_torsion_site_symmetry_2
_geom_torsion_site_symmetry_3
_geom_torsion_site_symmetry_4
_geom_torsion
_geom_torsion_publ_flag
? ? ? ? ? ? ? ? ? ? ?

loop_
_geom_hbond_atom_site_label_D
_geom_hbond_atom_site_label_H
_geom_hbond_atom_site_label_A
_geom_hbond_site_symmetry_D
_geom_hbond_site_symmetry_H
_geom_hbond_site_symmetry_A
_geom_hbond_distance_DH
_geom_hbond_distance_HA
_geom_hbond_distance_DA
_geom_hbond_angle_DHA
_geom_hbond_publ_flag
? ? ? ? ? ? ? ? ? ? ? ?


#===========================================================================

#===========================================================================
# Additional structures (last six sections and associated data_? identifiers)
# may be added at this point.
```

#==

The following lines are used to test the character set of files sent by
network email or other means. They are not part of the CIF data set.
abcdefghijklmnopqrstuvwxyzABCDEFGHIJKLMNOPQRSTUVWXYZ0123456789
!@#$%^&*()_+{}:"~<>?|\-=[];`,./