

```
#####
###   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_scatter_length_neutron
  _atom_type_scatter_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              9.79931(4)
_cell_length_b              9.14906(4)
_cell_length_c              5.19908(2)
_cell_angle_alpha           90.00000
_cell_angle_beta            101.8908(3)
_cell_angle_gamma           90.00000
_cell_volume                456.119(3)
_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         3059
_pd_meas_2theta_range_min         1.00000
_pd_meas_2theta_range_max         153.89999
_pd_meas_2theta_range_inc         0.050016

#=====

# 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	3.3574
_pd_proc_ls_prof_wR_factor	4.5551
_pd_proc_ls_prof_wR_expected	4.1124

# 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	6.8142
_pd_proc_ls_prof_cwR_factor	7.3347
_pd_proc_ls_prof_cwR_expected	6.6219

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

_pd_proc_ls_prof_chi2	1.2268
_pd_proc_ls_prof_echi2	1.2455

# Items related to LS refinement

_refine_ls_R_I_factor	1.4241
_refine_ls_number_reflns	107
_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	0.9533
_pd_proc_2theta_range_max	153.8532
_pd_proc_2theta_range_inc	0.050016
_pd_proc_wavelength	2.536000

\_pd\_block\_diffraction\_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  0.9081(3) 0.25000  0.0048(6) 1.00000  Uiso Fe
Fe2  0.00000  0.2703(2) 0.25000  0.0055(8) 1.00000  Uiso Fe
Ge1  0.30029(14) 0.09232(19) 0.2162(2) 0.0057(5) 1.00000  Uiso Ge
O1   0.11913(20) 0.0906(3) 0.1405(4) 0.0082(6) 1.00000  Uiso O
O2   0.3840(3)  0.2401(3) 0.3820(6) 0.0062(8) 1.00000  Uiso O
O3   0.35886(19) 0.0649(3) 0.9144(4) 0.0063(7) 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_scatter_length_neutron
  _atom_type_scatter_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	8.40861(9)
_cell_length_b	8.40861(9)
_cell_length_c	8.40861(9)
_cell_angle_alpha	90.00000
_cell_angle_beta	90.00000
_cell_angle_gamma	90.00000
_cell_volume	594.529(11)
_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           1.00000
_pd_meas_2theta_range_max            153.89999
_pd_meas_2theta_range_inc            0.050016
```

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

## # 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 3.3574  
\_pd\_proc\_ls\_prof\_wR\_factor 4.5551  
\_pd\_proc\_ls\_prof\_wR\_expected 4.1124

# 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 6.8142  
\_pd\_proc\_ls\_prof\_cwR\_factor 7.3347  
\_pd\_proc\_ls\_prof\_cwR\_expected 6.6219

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

\_pd\_proc\_ls\_prof\_chi2 1.2268  
\_pd\_proc\_ls\_prof\_echi2 1.2455

# Items related to LS refinement

\_refine\_ls\_R\_I\_factor 1.4174  
\_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 0.9533  
\_pd\_proc\_2theta\_range\_max 153.8532  
\_pd\_proc\_2theta\_range\_inc 0.050016  
\_pd\_proc\_wavelength 2.536000

\_pd\_block\_diffraction\_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 0.00609 0.99988 Uani Fe  
O1 0.24660 0.24660 0.24660 0.00620 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 0.00609 0.00609 0.00609 0.00039 0.00039 0.00039 Fe  
O1 0.00620 0.00620 0.00620 -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  
# !@#\$%^&\*()\_+{ }:"~<>?|\-=[];'`.,/