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

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

1. SUBMISSION DETAILS

```
_publ_contact_author_name      'Alan Woodland, cif by D.M.Trots' #
_publ_contact_author_address    # Address of author for correspondence
; 'Institut fuer Geowissenschaften, Uni Frankfurt, 60438 Frankfurt'
;
_publ_contact_author_email      'woodland@em.uni-frankfurt.de'
_publ_contact_author_fax        '++49 (0)69 798-40121'
_publ_contact_author_phone      '++49 (0)69 798-40119'
```

```
_publ_requested_journal        'Submitted to American Mineralogist'
```

3. TITLE AND AUTHOR LIST

```
_publ_section_title
; 'In situ observation of the breakdown of Fe3O4 to Fe4O5 and Fe2O3 at HP/HT'
;
```

```
# 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
'A. Woodland et al.'  #<--'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
; ?
;
;
```

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```
# 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_Fe4O5
```

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

5. CHEMICAL DATA

```
_chemical_name_systematic
; ?
;
_chemical_name_common      'Fe4O5'
```

```

_chemical_formula_moiety      ?
_chemical_formula_structural  'Fe16O20'
_chemical_formula_analytical  'Fe4O5'
_chemical_formula_iupac       Fe4O5
_chemical_formula_sum         'Fe4 O5'
_chemical_formula_weight      303.388
_chemical_melting_point       ?
_chemical_compound_source      'Multianvil in-situ experiment'
_exptl_crystal_density_diffrn 5.82
                                # natural products

```

```

loop_
  _atom_type_symbol
  _atom_type_scatter_Cromer_Mann_a1
  _atom_type_scatter_Cromer_Mann_b1
  _atom_type_scatter_Cromer_Mann_a2
  _atom_type_scatter_Cromer_Mann_b2
  _atom_type_scatter_Cromer_Mann_a3
  _atom_type_scatter_Cromer_Mann_b3
  _atom_type_scatter_Cromer_Mann_a4
  _atom_type_scatter_Cromer_Mann_b4
  _atom_type_scatter_Cromer_Mann_c
  _atom_type_scatter_dispersion_real
  _atom_type_scatter_dispersion_imag
  _atom_type_scatter_source
fe  11.76950  4.76110  7.35730  0.30720  3.52220  15.35350
    2.30450  76.88050  1.03690  0.24400  0.54500
International Tables for Crystallography Vol.C(1991) Tables_6.1.1.4_and_6.1.1.5
o   3.04850  13.27710  2.28680  5.70110  1.54630  0.32390
    0.86700  32.90890  0.25080  0.00300  0.00400
International Tables for Crystallography Vol.C(1991) Tables_6.1.1.4_and_6.1.1.5

```

#=====

6. POWDER SPECIMEN AND CRYSTAL DATA

```

_symmetry_cell_setting      Orthorhombic
_symmetry_space_group_name_H-M  'C m c m'
_symmetry_space_group_name_Hall  '-C 2c 2'

```

```

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

```

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

_cell_length_a 2.87366(8)
_cell_length_b 9.6940(3)
_cell_length_c 12.4116(4)
_cell_angle_alpha 90.00000
_cell_angle_beta 90.00000
_cell_angle_gamma 90.00000
_cell_volume 345.751(18)
_cell_formula_units_Z 4
_cell_measurement_temperature ?
_cell_special_details
; ?
;
_pd_char_colour 'black'

#=====

7. EXPERIMENTAL DATA

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.

_diffrn_radiation_wavelength 0.375518
_diffrn_source 'ID27 at ESRF'
_diffrn_radiation_type synchrotron
_diffrn_measurement_device_type 'Paris-Edinburgh pressure cell '

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

_pd_meas_number_of_points 1455
_pd_meas_2theta_range_min 5.00141
_pd_meas_2theta_range_max 25.28605
_pd_meas_2theta_range_inc 0.013961

#=====

8. REFINEMENT DATA

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 4.6645

_pd_proc_ls_prof_wR_factor	7.4262
_pd_proc_ls_prof_wR_expected	8.9672
_refine_ls_goodness_of_fit_all	0.69

Items related to LS refinement

_refine_ls_R_I_factor	3.7738
_refine_ls_number_reflns	204
_refine_ls_number_parameters	32
_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	5.0014
_pd_proc_2theta_range_max	25.2860
_pd_proc_2theta_range_inc	0.013961
_pd_proc_wavelength	0.375518

The following items are used to identify the programs used.

_computing_structure_refinement	FULLPROF
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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	0.00000	0.00000	0.030(2)	1.00000	Uiso Fe
Fe2	0.00000	0.2619(5)	0.1176(3)	0.0317(11)	1.00000	Uiso Fe
Fe3	0.00000	0.5079(6)	0.25000	0.040(2)	1.00000	Uiso Fe
O1	0.00000	0.165(2)	0.25000	0.019(6)	1.00000	Uiso O
O2	0.00000	0.3577(15)	0.5485(14)	0.036(5)	1.00000	Uiso O
O3	0.00000	0.0937(17)	0.6448(11)	0.026(4)	1.00000	Uiso O

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

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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

Fe1 Fe2 . . 2.9281(54) ?

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

Fe1 O3 O3 . . . 180 ?