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#####  
### CIF submission form for results of Rietveld refinements (IUCr journals) ###  
###                               Version 10 February 2005 ###  
#####
```

```
# This is an electronic "form" for submitting the results of a Rietveld  
# refinement of a model against powder diffraction data to an IUCr journal  
# as a Crystallographic Information File (CIF). Full details of the CIF  
# format are given in the paper "The Crystallographic Information File  
# (CIF): a New Standard Archive File for Crystallography" by S. R. Hall,  
# F. H. Allen and I. D. Brown [Acta Crystallogr., Sect. A, 47 (1991) 655-685].  
#  
# The current version of the powder CIF dictionary, which contains definitions
```

```
# http://www.iucr.org/iucr-top/cif/pd/index.html. Other terms are defined in  
# the core CIF dictionary at http://www.iucr.org/iucr-top/cif/core/index.html.  
#  
# Note that all fields should be numeric or character type EXCEPT those which  
# are flagged as 'text' - free-form text of any length may be included in  
# these latter fields provided the text block begins and ends with a semicolon  
# as the first character of a new line. Note also that the query marks '?'  
# are significant as placeholders, and should not be deleted where a data  
# item is not given, UNLESS the accompanying data name is also deleted.  
# Lines should not exceed 80 characters in length. The comments following a  
# hash symbol '#' may be deleted if wished.
```

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

data_global

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

1. GLOBAL DATA

```
loop_  
  _audit_conform.dict_name  
  _audit_conform.dict_version  
  _audit_conform.dict_location  
  cif_core.dic . ftp://ftp.iucr.org/pub/cif\_core.dic  
  cif_pd.dic . ftp://ftp.iucr.org/pub/cif\_pd.dic  
  
  _audit_creation_method  
; from .lst and *.dst using lst2cif (Dilanian and Izumi, 2011)  
;  
  _audit_creation_date  
  _audit_author_name      '?'  
  _audit_update_record  
; ?  
;
```

SUBMISSION DETAILS

```
  _publ_contact_author_name      '?'  
  _publ_contact_author_address  
; ?  
;
```

_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 ?

#=====

2. 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 ?

#=====

3. TITLE AND AUTHOR LIST

_publ_section_title
;
;
_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  
; ?  
;
```

Pointers to the data blocks containing information on phases

```
loop_  
  _pd_phase_block_id  
  _phase_1  
  _phase_2
```

#=====

If more than one structure is reported, sections 5-10 should be completed
per structure. For each data set, replace the '?' in the data_? line below

```
# by a unique identifier.

#=====

data_phase_1

_pd_block_id _phase_1

# 5. CHEMICAL DATA

_chemical_name_systematic
; ?
;
_chemical_name_common '?'
# Get _chemical_formula_moiety using checkCIF
_chemical_formula_moiety '?'
_chemical_formula_structural '?'
_chemical_formula_analytical '?'
_chemical_formula_sum 'Ca3 O9 Rh3'
_chemical_formula_weight 572.945
_chemical_melting_point ?
_chemical_compound_source ? # for minerals and
                             # natural products

loop_
  _atom_type_symbol
  _atom_type_description
  _atom_type_scatter_dispersion_real
  _atom_type_scatter_dispersion_imag
  _atom_type_scatter_source
Rh Rh3+ -1.0723 1.0749 'International Tables for Crystallography, Vol. C'
Ca Ca2+ 0.2288 0.3629 'International Tables for Crystallography, Vol. C'
O O- 0.0103 0.0073 'International Tables for Crystallography, Vol. C'

#=====

# 6. POWDER SPECIMEN AND CRYSTAL DATA

_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 1 21/m 1'
_symmetry_space_group_name_Hall '-P 2yb'
_symmetry_Int_Tables_number 11

loop_
  _symmetry_equiv_pos_site_id
  _symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,y+1/2,-z
3 -x,-y,-z
4 x,-y+1/2,z

_cell_length_a 12.51140(12)
_cell_length_b 3.12406(3)
_cell_length_c 8.85794(8)
_cell_angle_alpha 90
```

```

_cell_angle_beta          103.9510(6)
_cell_angle_gamma         90
_cell_volume              336.012(5)
# If checkCIF gives a different Z value, change both
# _chemical_formula_sum and _chemical_formula_weight.
_cell_formula_units_Z      2
_cell_measurement_temperature    ?

_cell_special_details
?

_exptl_crystal_density_diffn    5.6629
_exptl_crystal_density_meas     ?
_exptl_crystal_density_method   'not measured'
_exptl_crystal_F_000           534.00

# 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          transmission

_pd_spec_shape               cylinder

_pd_char_particle_morphology    ?
_pd_char_colour              ?

# 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         ?

_exptl_absorpt_coefficient_mu    11.4969
# The next four fields are normally only needed for transmission experiments.

```

_exptl_absorpt_correction_type ? # include if applicable
_exptl_absorpt_process_details ? # include if applicable
_exptl_absorpt_correction_T_min ? # include if applicable
_exptl_absorpt_correction_T_max ? # include if applicable

#=====

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 'synchrotron'
_diffrn_source_target ?
_diffrn_source_type ?
_diffrn_radiation_type ?
_diffrn_measurement_device_type '?'
_diffrn_detector '?'
_diffrn_detector_type ?

_pd_meas_scan_method step # options are 'step', 'cont',
'tof', 'fixed' or
'disp' (= dispersive)

_pd_meas_special_details
; ?
;

_diffrn_radiation_wavelength 0.77462
_diffrn_radiation_monochromator ?

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

_pd_meas_number_of_points 7201
_pd_meas_2theta_range_min 3.0000
_pd_meas_2theta_range_max 75.0000
_pd_meas_2theta_range_inc 0.0100

The following three items are used for time-of-flight measurements only.

```
_pd_instr_dist_src/spec      ?
_pd_instr_dist_spec/detc     ?
_pd_meas_2theta_fixed       ?
```

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

8. REFINEMENT DATA

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_calc_method              'Rietveld Refinement'

_pd_proc_ls_profile_function  'split pseudo-Voigt function'
_pd_proc_ls_background_function 'Legendre polynomials'
_pd_proc_ls_pref_orient_corr
; ?
;
```

Replace ';' '?' with the following four lines for the March-Dollase function:

```
#; $P_k = \sum_{j=1}^{m_k} \frac{1}{m_k}
#\left( r^2 \cos^2 \alpha_j + r^{-1} \sin^2 \alpha_j \right)^{-3/2} $
#with a preferred-orientation vector, (hkl),
#and  $\langle r \rangle = 1.0(0)$ 
```

```
_pd_proc_ls_prof_R_factor    0.04721
_pd_proc_ls_prof_wR_factor    0.06228
_pd_proc_ls_prof_wR_expected  0.04119
_refine_ls_R_I_factor         0.00909
_refine_ls_R_Fsqd_factor      0.00474
_refine_ls_R_factor_all       0.00476
```

```
_refine_special_details
; ?
;
```

```
_refine_ls_matrix_type      full
_refine_ls_weighting_scheme  sigma
_refine_ls_weighting_details 1/<i>y</i>~i~
```

The following line must be commented out in the absence of H atoms.

```
#_refine_ls_hydrogen_treatment ?
_refine_ls_extinction_method  none
_refine_ls_extinction_coef    ?
_refine_ls_number_parameters  80
_refine_ls_number_restraints  0
_refine_ls_number_constraints  4
```

The following item is the same as CHI, the square root of 'CHI squared'

_refine_ls_goodness_of_fit_all 1.5118

_refine_ls_restrained_S_all ?

The following item can be obtained by setting NPRINT at 2 in *.ins.

_refine_ls_shift/su_max 0.0

_refine_ls_shift/su_mean ?

_refine_diff_density_max 0.0

_refine_diff_density_min 0.0

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 3.0000

_pd_proc_2theta_range_max 74.7500

_pd_proc_2theta_range_inc 0.0100

_pd_proc_wavelength ?

loop_

_pd_phase_id

_pd_phase_block_id

_pd_phase_mass_%

1 _phase_1 85.32

2 _phase_2 14.68

Each refinement must be accompanied by a listing of the powder data

in CIF format. Each listing should be sent as a separate file consisting

of one data block containing a single powder profile. The value of

_pd_block_diffraction_id is used to associate each refinement with

its corresponding powder profile, since it must match the value

of _pd_block_id in the file containing the powder data. A template

for supplying powder data in CIF format is available by ftp at

<ftp://ftp.iucr.org/pub/rietdataform.cif> and an example is given

at <ftp://ftp.iucr.org/pub/rietdataxml.cif>.

_pd_block_diffraction_id ?

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_cell_refinement 'RIETAN-FP (Izumi and Momma, 2007)'

_computing_data_reduction ?

_computing_structure_solution ?

_computing_structure_refinement 'RIETAN-FP (Izumi and Momma, 2007)'

_computing_molecular_graphics 'VESTA (Momma and Izumi, 2008)'

_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_occupancy							
_atom_site_symmetry_multiplicity							
_atom_site_Wyckoff_symbol							
_atom_site_adp_type							
_atom_site_U_iso_or_equiv							
_atom_site_type_symbol							
O1	0.8215(6)	0.75	0.8756(10)	1	2 e Uiso	0.01267	O
O2	0.6152(6)	0.25	0.7842(9)	1	2 e Uiso	0.01267	O
O3	0.5488(6)	0.25	0.1325(9)	1	2 e Uiso	0.01267	O
O4	0.5535(6)	0.25	0.4159(10)	1	2 e Uiso	0.01267	O
O5	0.7031(6)	0.75	0.3271(10)	1	2 e Uiso	0.01267	O
O6	0.8115(6)	0.25	0.5802(9)	1	2 e Uiso	0.01267	O
O7	0.7878(6)	0.25	0.1278(9)	1	2 e Uiso	0.01267	O
O8	0.9118(6)	0.75	0.3879(9)	1	2 e Uiso	0.01267	O
O9	0.9890(6)	0.75	0.1170(9)	1	2 e Uiso	0.01267	O
Ca1	0.6718(2)	0.75	0.6175(3)	1	2 e Uiso	0.0111(7)	Ca
Ca2	0.6505(2)	0.75	0.9941(3)	1	2 e Uiso	0.0096(7)	Ca
Ca3	0.0521(2)	0.25	0.3318(3)	1	2 e Uiso	0.0115(7)	Ca
Rh1	0.54318(8)	0.75	0.27037(13)	1	2 e Uiso	0.0043(3)	Rh
Rh2	0.89248(9)	0.25	0.99875(12)	1	2 e Uiso	0.0045(3)	Rh
Rh3	0.19426(8)	0.75	0.64612(13)	1	2 e Uiso	0.0049(3)	Rh

#=====

#10. GEOMETRICAL PARAMETERS

_geom_special_details ?

loop_				
_geom_bond_atom_site_label_1				
_geom_bond_atom_site_label_2				
_geom_bond_distance				
_geom_bond_site_symmetry_1				
_geom_bond_site_symmetry_2				
_geom_bond_publ_flag				
O1	Rh2	1.988(5)	. 1_555	?
O1	Rh2	1.988(5)	. 1_565	?
O1	Ca1	2.584(8)	. 1_555	?
O1	Ca2	2.600(8)	. 1_555	?
O1	O9	2.61(1)	. 1_556	?
O1	Ca3	2.697(8)	. 2_656	?
O1	O7	2.84(1)	. 1_556	?
O1	O7	2.84(1)	. 1_566	?
O1	O2	2.958(9)	. 1_555	?
O1	O2	2.958(9)	. 1_565	?
O1	O6	3.02(1)	. 1_555	?

O1	O6	3.02(1)	. 1_565 ?
O2	Rh1	1.923(7)	. 2_646 ?
O2	Ca1	2.372(6)	. 1_555 ?
O2	Ca1	2.372(6)	. 1_545 ?
O2	Ca2	2.387(6)	. 1_555 ?
O2	Ca2	2.387(6)	. 1_545 ?
O2	O3	2.814(9)	. 2_646 ?
O2	O3	2.814(9)	. 2_656 ?
O2	O4	2.869(9)	. 2_646 ?
O2	O4	2.869(9)	. 2_656 ?
O2	O1	2.958(9)	. 1_555 ?
O2	O1	2.958(9)	. 1_545 ?
O3	Rh1	1.995(5)	. 1_555 ?
O3	Rh1	1.995(5)	. 1_545 ?
O3	Ca2	2.475(7)	. 2_646 ?
O3	O4	2.50(1)	. 1_555 ?
O3	Ca2	2.513(7)	. 1_554 ?
O3	Ca2	2.513(7)	. 1_544 ?
O3	O5	2.745(8)	. 1_555 ?
O3	O5	2.745(8)	. 1_545 ?
O3	O2	2.814(9)	. 2_646 ?
O3	O2	2.814(9)	. 2_656 ?
O3	O3	2.84(1)	. 2_645 ?
O3	O3	2.84(1)	. 2_655 ?
O3	O7	3.00(1)	. 1_555 ?
O4	Rh1	2.010(5)	. 1_555 ?
O4	Rh1	2.010(5)	. 1_545 ?
O4	O3	2.50(1)	. 1_555 ?
O4	Ca1	2.558(7)	. 1_555 ?
O4	Ca1	2.558(7)	. 1_545 ?
O4	O5	2.697(9)	. 1_555 ?
O4	O5	2.697(9)	. 1_545 ?
O4	O4	2.72(1)	. 2_646 ?
O4	O4	2.72(1)	. 2_656 ?
O4	Ca1	2.762(8)	. 2_646 ?
O4	O2	2.869(9)	. 2_646 ?
O4	O2	2.869(9)	. 2_656 ?
O5	Rh1	1.942(7)	. 1_555 ?
O5	Rh3	2.000(5)	. 2_646 ?
O5	Rh3	2.000(5)	. 2_656 ?
O5	O8	2.536(9)	. 1_555 ?
O5	Ca1	2.694(8)	. 1_555 ?
O5	O4	2.697(9)	. 1_555 ?
O5	O4	2.697(9)	. 1_565 ?
O5	O3	2.745(8)	. 1_555 ?
O5	O3	2.745(8)	. 1_565 ?
O5	O7	2.754(9)	. 1_555 ?
O5	O7	2.754(9)	. 1_565 ?
O5	O6	2.800(9)	. 1_555 ?
O5	O6	2.800(9)	. 1_565 ?
O5	Ca2	2.863(9)	. 1_554 ?
O6	Rh3	1.989(8)	. 2_646 ?
O6	Ca3	2.306(6)	. 2_646 ?
O6	Ca3	2.306(6)	. 2_656 ?

O6	Ca1	2.426(6)	. 1_555 ?
O6	Ca1	2.426(6)	. 1_545 ?
O6	O5	2.800(9)	. 1_555 ?
O6	O5	2.800(9)	. 1_545 ?
O6	O8	2.819(9)	. 1_555 ?
O6	O8	2.819(9)	. 1_545 ?
O6	O1	3.02(1)	. 1_555 ?
O6	O1	3.02(1)	. 1_545 ?
O7	Rh2	1.935(8)	. 1_554 ?
O7	Rh3	1.961(8)	. 2_646 ?
O7	Ca2	2.411(6)	. 1_554 ?
O7	Ca2	2.411(6)	. 1_544 ?
O7	O5	2.754(9)	. 1_555 ?
O7	O5	2.754(9)	. 1_545 ?
O7	O1	2.84(1)	. 1_554 ?
O7	O1	2.84(1)	. 1_544 ?
O7	O8	2.904(9)	. 1_555 ?
O7	O8	2.904(9)	. 1_545 ?
O7	O9	2.98(1)	. 1_555 ?
O7	O9	2.98(1)	. 1_545 ?
O7	O3	3.00(1)	. 1_555 ?
O8	Rh3	2.025(5)	. 2_646 ?
O8	Rh3	2.025(5)	. 2_656 ?
O8	Ca3	2.415(8)	. 2_656 ?
O8	Ca3	2.488(6)	. 1_655 ?
O8	Ca3	2.488(6)	. 1_665 ?
O8	O5	2.536(9)	. 1_555 ?
O8	O9	2.79(1)	. 1_555 ?
O8	O6	2.819(9)	. 1_555 ?
O8	O6	2.819(9)	. 1_565 ?
O8	O7	2.904(9)	. 1_555 ?
O8	O7	2.904(9)	. 1_565 ?
O9	Rh2	2.094(5)	. 1_554 ?
O9	Rh2	2.094(5)	. 1_564 ?
O9	Ca3	2.441(6)	. 1_655 ?
O9	Ca3	2.441(6)	. 1_665 ?
O9	O1	2.61(1)	. 1_554 ?
O9	O9	2.66(1)	. 2_755 ?
O9	O8	2.79(1)	. 1_555 ?
O9	O7	2.98(1)	. 1_555 ?
O9	O7	2.98(1)	. 1_565 ?
Ca1	O2	2.372(6)	. 1_555 ?
Ca1	O2	2.372(6)	. 1_565 ?
Ca1	O6	2.426(6)	. 1_555 ?
Ca1	O6	2.426(6)	. 1_565 ?
Ca1	O4	2.558(7)	. 1_555 ?
Ca1	O4	2.558(7)	. 1_565 ?
Ca1	O1	2.584(8)	. 1_555 ?
Ca1	O5	2.694(8)	. 1_555 ?
Ca1	O4	2.762(8)	. 2_656 ?
Ca2	O2	2.387(6)	. 1_555 ?
Ca2	O2	2.387(6)	. 1_565 ?
Ca2	O7	2.411(6)	. 1_556 ?
Ca2	O7	2.411(6)	. 1_566 ?

Ca2	O3	2.475(7)	.	2_656	?
Ca2	O3	2.513(7)	.	1_556	?
Ca2	O3	2.513(7)	.	1_566	?
Ca2	O1	2.600(8)	.	1_555	?
Ca2	O5	2.863(9)	.	1_556	?
Ca2	Rh1	3.062(3)	.	1_556	?
Ca3	O6	2.306(6)	.	2_646	?
Ca3	O6	2.306(6)	.	2_656	?
Ca3	O8	2.415(8)	.	2_646	?
Ca3	O9	2.441(6)	.	1_455	?
Ca3	O9	2.441(6)	.	1_445	?
Ca3	O8	2.488(6)	.	1_455	?
Ca3	O8	2.488(6)	.	1_445	?
Ca3	O1	2.697(8)	.	2_646	?
Rh1	O2	1.923(7)	.	2_656	?
Rh1	O5	1.942(7)	.	1_555	?
Rh1	O3	1.995(5)	.	1_555	?
Rh1	O3	1.995(5)	.	1_565	?
Rh1	O4	2.010(5)	.	1_555	?
Rh1	O4	2.010(5)	.	1_565	?
Rh1	Ca2	3.062(3)	.	1_554	?
Rh2	O7	1.935(8)	.	1_556	?
Rh2	O1	1.988(5)	.	1_555	?
Rh2	O1	1.988(5)	.	1_545	?
Rh2	O9	2.094(5)	.	1_546	?
Rh2	O9	2.094(5)	.	1_556	?
Rh3	O7	1.961(8)	.	2_656	?
Rh3	O6	1.989(8)	.	2_656	?
Rh3	O5	2.000(5)	.	2_646	?
Rh3	O5	2.000(5)	.	2_656	?
Rh3	O8	2.025(5)	.	2_646	?
Rh3	O8	2.025(5)	.	2_656	?

```

loop_
  _geom_angle_atom_site_label_1
  _geom_angle_atom_site_label_2
  _geom_angle_atom_site_label_3
  _geom_angle
  _geom_angle_site_symmetry_1
  _geom_angle_site_symmetry_2
  _geom_angle_site_symmetry_3
  _geom_angle_publ_flag
O3      O4      O1      133.3(3)    1_555 . 1_555 ?
O3      O4      O2      167.6(4)    1_555 . 1_555 ?

```

```

#=====

```

```

data_phase_2

_pd_block_id  _phase_2

#11. CHEMICAL DATA

_chemical_name_systematic

```

```

; ?
;
_chemical_name_common      '?'
# Get _chemical_formula_moiety using checkCIF
_chemical_formula_moiety    '?'
_chemical_formula_structural  '?'
_chemical_formula_analytical  '?'
_chemical_formula_sum        "
_chemical_formula_weight     134.904
_chemical_melting_point      ?
_chemical_compound_source    ?   # for minerals and
                                # natural products

loop_
  _atom_type_symbol
  _atom_type_description
  _atom_type_scatter_dispersion_real
  _atom_type_scatter_dispersion_imag
  _atom_type_scatter_source
Rh Rh3+ -1.0723 1.0749 'International Tables for Crystallography, Vol. C'
Ca Ca2+ 0.2288 0.3629 'International Tables for Crystallography, Vol. C'
O O- 0.0103 0.0073 'International Tables for Crystallography, Vol. C'

#=====
#12. POWDER SPECIMEN AND CRYSTAL DATA

_symmetry_cell_setting      cubic
_symmetry_space_group_name_H-M  'P a -3'
_symmetry_space_group_name_Hall  '-P 2ac 2ab 3'
_symmetry_Int_Tables_number     205

loop_
  _symmetry_equiv_pos_site_id
  _symmetry_equiv_pos_as_xyz
1  x,y,z
2  -x+1/2,-y,z+1/2
3  -x,y+1/2,-z+1/2
4  x+1/2,-y+1/2,-z
5  z,x,y
6  z+1/2,-x+1/2,-y
7  -z+1/2,-x,y+1/2
8  -z,x+1/2,-y+1/2
9  y,z,x
10 -y,z+1/2,-x+1/2
11 y+1/2,-z+1/2,-x
12 -y+1/2,-z,x+1/2
13 -x,-y,-z
14 x+1/2,y,-z+1/2
15 x,-y+1/2,z+1/2
16 -x+1/2,y+1/2,z
17 -z,-x,-y
18 -z+1/2,x+1/2,y
19 z+1/2,x,-y+1/2
20 z,-x+1/2,y+1/2

```

21 -y,-z,-x
22 y,-z+1/2,x+1/2
23 -y+1/2,z+1/2,x
24 y+1/2,z,-x+1/2

_cell_length_a 4.8440(1)

_cell_length_b 4.8440(1)

_cell_length_c 4.8440(1)

_cell_angle_alpha 90

_cell_angle_beta 90

_cell_angle_gamma 90

_cell_volume 113.66(1)

If checkCIF gives a different Z value, change both

_chemical_formula_sum and _chemical_formula_weight.

_cell_formula_units_Z 4

_cell_measurement_temperature ?

_cell_special_details

?

_exptl_crystal_density_diffn 7.8837

_exptl_crystal_density_meas ?

_exptl_crystal_density_method 'not measured'

_exptl_crystal_F_000 244.00

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 transmission

_pd_spec_shape cylinder

_pd_char_particle_morphology ?

_pd_char_colour ?

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 ?

_exptl_absorpt_coefficient_mu 16.9001

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

_exptl_absorpt_correction_type ? # include if applicable
_exptl_absorpt_process_details ? # include if applicable
_exptl_absorpt_correction_T_min ? # include if applicable
_exptl_absorpt_correction_T_max ? # include if applicable

#=====

#13. 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 'synchrotron'
_diffrn_source_target ?
_diffrn_source_type ?
_diffrn_radiation_type ?
_diffrn_measurement_device_type '?'
_diffrn_detector '?'
_diffrn_detector_type ?

_pd_meas_scan_method step # options are 'step', 'cont',
'tof', 'fixed' or
'disp' (= dispersive)

_pd_meas_special_details
; ?
;

_diffrn_radiation_wavelength 0.77462
_diffrn_radiation_monochromator ?

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

_pd_meas_number_of_points 7201
_pd_meas_2theta_range_min 3.0000
_pd_meas_2theta_range_max 75.0000
_pd_meas_2theta_range_inc 0.0100

The following three items are used for time-of-flight measurements only.

_pd_instr_dist_src/spec ?
_pd_instr_dist_spec/detc ?
_pd_meas_2theta_fixed ?

#=====

#14. REFINEMENT DATA

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_calc_method 'Rietveld Refinement'

_pd_proc_ls_profile_function 'split pseudo-Voigt function'
_pd_proc_ls_background_function 'Legendre polynomials'
_pd_proc_ls_pref_orient_corr
; ?
;

Replace '; ?' with the following four lines for the March-Dollase function:

#; $P_k = \sum_{j=1}^{m_k} \frac{1}{m_k}$
$\left(r^2 \cos^2 \alpha_j + r^{-1} \sin^2 \alpha_j \right)^{-3/2}$
#with a preferred-orientation vector, (hkl),
#and $\langle r \rangle = 1.0(0)$

_pd_proc_ls_prof_R_factor 0.04721
_pd_proc_ls_prof_wR_factor 0.06228
_pd_proc_ls_prof_wR_expected 0.04119
_refine_ls_R_I_factor 0.00651
_refine_ls_R_Fsqd_factor 0.00466
_refine_ls_R_factor_all 0.00466

_refine_special_details
; ?
;

_refine_ls_matrix_type full
_refine_ls_weighting_scheme sigma
_refine_ls_weighting_details 1/ $\langle y \rangle \sim i \sim$

The following line must be commented out in the absence of H atoms.

```
#_refine_ls_hydrogen_treatment    ?
_refine_ls_extinction_method      none
_refine_ls_extinction_coef        ?
_refine_ls_number_parameters      80
_refine_ls_number_restraints      0
_refine_ls_number_constraints     4
```

The following item is the same as CHI, the square root of 'CHI squared'

```
_refine_ls_goodness_of_fit_all    1.5118
```

```
_refine_ls_restrained_S_all      ?
```

The following item can be obtained by setting NPRINT at 2 in *.ins.

```
_refine_ls_shift/su_max          0.0
_refine_ls_shift/su_mean         ?
```

```
_refine_diff_density_max         0.0
_refine_diff_density_min         0.0
```

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        3.0000
_pd_proc_2theta_range_max        74.7500
_pd_proc_2theta_range_inc        0.0100
_pd_proc_wavelength               ?
```

loop_

```
  _pd_phase_id
  _pd_phase_block_id
  _pd_phase_mass_%
1  _phase_1  85.32
2  _phase_2  14.68
```

Each refinement must be accompanied by a listing of the powder data

in CIF format. Each listing should be sent as a separate file consisting

of one data block containing a single powder profile. The value of

_pd_block_diffraction_id is used to associate each refinement with

its corresponding powder profile, since it must match the value

of _pd_block_id in the file containing the powder data. A template

for supplying powder data in CIF format is available by ftp at

<ftp://ftp.iucr.org/pub/rietdataform.cif> and an example is given

at <ftp://ftp.iucr.org/pub/rietdataxml.cif>.

```
_pd_block_diffraction_id         ?
```

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_cell_refinement 'RIETAN-FP (Izumi and Momma, 2007)'
_computing_data_reduction ?
_computing_structure_solution ?
_computing_structure_refinement 'RIETAN-FP (Izumi and Momma, 2007)'
_computing_molecular_graphics 'VESTA (Momma and Izumi, 2008)'
_computing_publication_material ?

#=====

#15. ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS

loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_symbol
_atom_site_adp_type
_atom_site_U_iso_or_equiv
_atom_site_type_symbol
O10 0.351(1) 0.351(1) 0.351(1) 1 8 c Uiso 0.013(4) O
Rh4 0 0 0 1 4 a Uiso 0.0042(5) Rh

#=====

#16. GEOMETRICAL PARAMETERS

_geom_special_details ?

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

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