

data_G05_publ

_pd_block_id

2012-01-05T09:45|G05|GfCo050|Overall

_audit_creation_method "from EXP file using GSAS2CIF"

_audit_creation_date 2012-01-05T09:45

_audit_author_name GfCo050

_audit_update_record

; 2012-01-05T09:45 Initial CIF as created by GSAS2CIF

;

#=====

this information describes the project, paper etc. for the CIF

Acta Cryst. Section C papers and editorial correspondence is generated

from the information in this section

#

#

(from) CIF submission form for Rietveld refinements (Acta Cryst. C)

Version 14 December 1998

#

#=====

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

#

#=====

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
; ?
;

```

```

#=====
# 5. OVERALL REFINEMENT & COMPUTING DETAILS

```

```

_refine_special_details
; ?
;
_pd_proc_ls_special_details
; ?
;

```

The following items are used to identify the programs used.

```

_computing_molecular_graphics  ?
_computing_publication_material ?

```

```

_refine_ls_weighting_scheme    ?
_refine_ls_weighting_details   ?
_refine_ls_hydrogen_treatment  ?
_refine_ls_extinction_method   ?
_refine_ls_extinction_coef     ?
_refine_ls_number_constraints   ?

```

```

_refine_ls_restrained_S_all    ?
_refine_ls_restrained_S_obs    ?

```

```

#=====
# 6. SAMPLE PREPARATION DATA

```

(In the unusual case where multiple samples are used in a single
Rietveld study, this information should be moved into the phase
blocks)

The following three fields describe the preparation of the material.
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 ?

_pd_char_colour ? # use ICDD colour descriptions
data_G05_overall

_refine_ls_shift/su_max 0.08
_refine_ls_shift/su_mean 0.01
_computing_structure_refinement GSAS
_refine_ls_number_parameters 27
_refine_ls_goodness_of_fit_all 1.12
_refine_ls_number_restraints 0
_refine_ls_matrix_type full

pointers to the phase blocks
loop_ _pd_phase_block_id
2012-01-05T09:45|G05_phase1|GfCo050||
pointers to the diffraction patterns
loop_ _pd_block_diffraction_id
?

Information for phase 1
data_G05_phase_1

_pd_block_id
2012-01-05T09:45|G05_phase1|GfCo050||

#=====

7. CHEMICAL, STRUCTURAL AND CRYSTAL DATA

_pd_char_particle_morphology ?

_chemical_name_systematic
; ?
;
_chemical_name_common ?
_chemical_formula_moiety ?
_chemical_formula_structural ?
_chemical_formula_analytical ?
_chemical_melting_point ?
_chemical_compound_source ? # for minerals and
natural products
_symmetry_space_group_name_Hall ?

_exptl_crystal_F_000 ?
_exptl_crystal_density_diffn ?
_exptl_crystal_density_meas ?
_exptl_crystal_density_method ?

_cell_measurement_temperature ?

_cell_special_details
; ?

;

_geom_special_details ?

The following item identifies the program(s) used (if appropriate).

_computing_structure_solution ?

#=====

8. Phase information from GSAS

_pd_phase_name	Zn050Co050Al2O4
_cell_length_a	8.09491(7)
_cell_length_b	8.09491
_cell_length_c	8.09491
_cell_angle_alpha	90.0
_cell_angle_beta	90.0
_cell_angle_gamma	90.0
_cell_volume	530.440(14)
_symmetry_cell_setting	cubic
_symmetry_space_group_name_H-M	"F d -3 m"

loop_ _symmetry_equiv_pos_site_id _symmetry_equiv_pos_as_xyz

- 1 +x,+y,+z
- 2 +z,+x,+y
- 3 +y,+z,+x
- 4 +x+1/4,+y+1/4,-z
- 5 -z,+x+1/4,+y+1/4
- 6 +y+1/4,-z,+x+1/4
- 7 -z+1/4,+x+1/2,-y+3/4
- 8 -y+3/4,-z+1/4,+x+1/2
- 9 +y+1/2,-z+1/4,-x+3/4
- 10 -x+3/4,+y+1/2,-z+1/4
- 11 -z+1/4,-x+3/4,+y+1/2
- 12 +x+1/2,-y+3/4,-z+1/4
- 13 +y,+x,+z
- 14 +z,+y,+x
- 15 +x,+z,+y
- 16 +y+1/4,+x+1/4,-z
- 17 -z,+y+1/4,+x+1/4
- 18 +x+1/4,-z,+y+1/4
- 19 -z+1/4,+y+1/2,-x+3/4
- 20 -x+3/4,-z+1/4,+y+1/2
- 21 +x+1/2,-z+1/4,-y+3/4
- 22 -y+3/4,+x+1/2,-z+1/4
- 23 -z+1/4,-y+3/4,+x+1/2
- 24 +y+1/2,-x+3/4,-z+1/4
- 1 -x,-y,-z
- 2 -z,-x,-y
- 3 -y,-z,-x
- 4 -x+3/4,-y+3/4,+z
- 5 +z,-x+3/4,-y+3/4
- 6 -y+3/4,+z,-x+3/4
- 7 +z+3/4,-x+1/2,+y+1/4
- 8 +y+1/4,+z+3/4,-x+1/2

-9 -y+1/2,+z+3/4,+x+1/4
 -10 +x+1/4,-y+1/2,+z+3/4
 -11 +z+3/4,+x+1/4,-y+1/2
 -12 -x+1/2,+y+1/4,+z+3/4
 -13 -y,-x,-z
 -14 -z,-y,-x
 -15 -x,-z,-y
 -16 -y+3/4,-x+3/4,+z
 -17 +z,-y+3/4,-x+3/4
 -18 -x+3/4,+z,-y+3/4
 -19 +z+3/4,-y+1/2,+x+1/4
 -20 +x+1/4,+z+3/4,-y+1/2
 -21 -x+1/2,+z+3/4,+y+1/4
 -22 +y+1/4,-x+1/2,+z+3/4
 -23 +z+3/4,+y+1/4,-x+1/2
 -24 -y+1/2,+x+1/4,+z+3/4
 101 +x,+y+1/2,+z+1/2
 102 +z,+x+1/2,+y+1/2
 103 +y,+z+1/2,+x+1/2
 104 +x+1/4,+y+3/4,-z+1/2
 105 -z,+x+3/4,+y+3/4
 106 +y+1/4,-z+1/2,+x+3/4
 107 -z+1/4,+x,-y+1/4
 108 -y+3/4,-z+3/4,+x
 109 +y+1/2,-z+3/4,-x+1/4
 110 -x+3/4,+y,-z+3/4
 111 -z+1/4,-x+1/4,+y
 112 +x+1/2,-y+1/4,-z+3/4
 113 +y,+x+1/2,+z+1/2
 114 +z,+y+1/2,+x+1/2
 115 +x,+z+1/2,+y+1/2
 116 +y+1/4,+x+3/4,-z+1/2
 117 -z,+y+3/4,+x+3/4
 118 +x+1/4,-z+1/2,+y+3/4
 119 -z+1/4,+y,-x+1/4
 120 -x+3/4,-z+3/4,+y
 121 +x+1/2,-z+3/4,-y+1/4
 122 -y+3/4,+x,-z+3/4
 123 -z+1/4,-y+1/4,+x
 124 +y+1/2,-x+1/4,-z+3/4
 -101 -x,-y+1/2,-z+1/2
 -102 -z,-x+1/2,-y+1/2
 -103 -y,-z+1/2,-x+1/2
 -104 -x+3/4,-y+1/4,+z+1/2
 -105 +z,-x+1/4,-y+1/4
 -106 -y+3/4,+z+1/2,-x+1/4
 -107 +z+3/4,-x,+y+3/4
 -108 +y+1/4,+z+1/4,-x
 -109 -y+1/2,+z+1/4,+x+3/4
 -110 +x+1/4,-y,+z+1/4
 -111 +z+3/4,+x+3/4,-y
 -112 -x+1/2,+y+3/4,+z+1/4
 -113 -y,-x+1/2,-z+1/2
 -114 -z,-y+1/2,-x+1/2

-115 $-x, -z+1/2, -y+1/2$
 -116 $-y+3/4, -x+1/4, +z+1/2$
 -117 $+z, -y+1/4, -x+1/4$
 -118 $-x+3/4, +z+1/2, -y+1/4$
 -119 $+z+3/4, -y, +x+3/4$
 -120 $+x+1/4, +z+1/4, -y$
 -121 $-x+1/2, +z+1/4, +y+3/4$
 -122 $+y+1/4, -x, +z+1/4$
 -123 $+z+3/4, +y+3/4, -x$
 -124 $-y+1/2, +x+3/4, +z+1/4$
 201 $+x+1/2, +y, +z+1/2$
 202 $+z+1/2, +x, +y+1/2$
 203 $+y+1/2, +z, +x+1/2$
 204 $+x+3/4, +y+1/4, -z+1/2$
 205 $-z+1/2, +x+1/4, +y+3/4$
 206 $+y+3/4, -z, +x+3/4$
 207 $-z+3/4, +x+1/2, -y+1/4$
 208 $-y+1/4, -z+1/4, +x$
 209 $+y, -z+1/4, -x+1/4$
 210 $-x+1/4, +y+1/2, -z+3/4$
 211 $-z+3/4, -x+3/4, +y$
 212 $+x, -y+3/4, -z+3/4$
 213 $+y+1/2, +x, +z+1/2$
 214 $+z+1/2, +y, +x+1/2$
 215 $+x+1/2, +z, +y+1/2$
 216 $+y+3/4, +x+1/4, -z+1/2$
 217 $-z+1/2, +y+1/4, +x+3/4$
 218 $+x+3/4, -z, +y+3/4$
 219 $-z+3/4, +y+1/2, -x+1/4$
 220 $-x+1/4, -z+1/4, +y$
 221 $+x, -z+1/4, -y+1/4$
 222 $-y+1/4, +x+1/2, -z+3/4$
 223 $-z+3/4, -y+3/4, +x$
 224 $+y, -x+3/4, -z+3/4$
 -201 $-x+1/2, -y, -z+1/2$
 -202 $-z+1/2, -x, -y+1/2$
 -203 $-y+1/2, -z, -x+1/2$
 -204 $-x+1/4, -y+3/4, +z+1/2$
 -205 $+z+1/2, -x+3/4, -y+1/4$
 -206 $-y+1/4, +z, -x+1/4$
 -207 $+z+1/4, -x+1/2, +y+3/4$
 -208 $+y+3/4, +z+3/4, -x$
 -209 $-y, +z+3/4, +x+3/4$
 -210 $+x+3/4, -y+1/2, +z+1/4$
 -211 $+z+1/4, +x+1/4, -y$
 -212 $-x, +y+1/4, +z+1/4$
 -213 $-y+1/2, -x, -z+1/2$
 -214 $-z+1/2, -y, -x+1/2$
 -215 $-x+1/2, -z, -y+1/2$
 -216 $-y+1/4, -x+3/4, +z+1/2$
 -217 $+z+1/2, -y+3/4, -x+1/4$
 -218 $-x+1/4, +z, -y+1/4$
 -219 $+z+1/4, -y+1/2, +x+3/4$
 -220 $+x+3/4, +z+3/4, -y$

-221 $-x, +z+3/4, +y+3/4$
-222 $+y+3/4, -x+1/2, +z+1/4$
-223 $+z+1/4, +y+1/4, -x$
-224 $-y, +x+1/4, +z+1/4$
301 $+x+1/2, +y+1/2, +z$
302 $+z+1/2, +x+1/2, +y$
303 $+y+1/2, +z+1/2, +x$
304 $+x+3/4, +y+3/4, -z$
305 $-z+1/2, +x+3/4, +y+1/4$
306 $+y+3/4, -z+1/2, +x+1/4$
307 $-z+3/4, +x, -y+3/4$
308 $-y+1/4, -z+3/4, +x+1/2$
309 $+y, -z+3/4, -x+3/4$
310 $-x+1/4, +y, -z+1/4$
311 $-z+3/4, -x+1/4, +y+1/2$
312 $+x, -y+1/4, -z+1/4$
313 $+y+1/2, +x+1/2, +z$
314 $+z+1/2, +y+1/2, +x$
315 $+x+1/2, +z+1/2, +y$
316 $+y+3/4, +x+3/4, -z$
317 $-z+1/2, +y+3/4, +x+1/4$
318 $+x+3/4, -z+1/2, +y+1/4$
319 $-z+3/4, +y, -x+3/4$
320 $-x+1/4, -z+3/4, +y+1/2$
321 $+x, -z+3/4, -y+3/4$
322 $-y+1/4, +x, -z+1/4$
323 $-z+3/4, -y+1/4, +x+1/2$
324 $+y, -x+1/4, -z+1/4$
-301 $-x+1/2, -y+1/2, -z$
-302 $-z+1/2, -x+1/2, -y$
-303 $-y+1/2, -z+1/2, -x$
-304 $-x+1/4, -y+1/4, +z$
-305 $+z+1/2, -x+1/4, -y+3/4$
-306 $-y+1/4, +z+1/2, -x+3/4$
-307 $+z+1/4, -x, +y+1/4$
-308 $+y+3/4, +z+1/4, -x+1/2$
-309 $-y, +z+1/4, +x+1/4$
-310 $+x+3/4, -y, +z+3/4$
-311 $+z+1/4, +x+3/4, -y+1/2$
-312 $-x, +y+3/4, +z+3/4$
-313 $-y+1/2, -x+1/2, -z$
-314 $-z+1/2, -y+1/2, -x$
-315 $-x+1/2, -z+1/2, -y$
-316 $-y+1/4, -x+1/4, +z$
-317 $+z+1/2, -y+1/4, -x+3/4$
-318 $-x+1/4, +z+1/2, -y+3/4$
-319 $+z+1/4, -y, +x+1/4$
-320 $+x+3/4, +z+1/4, -y+1/2$
-321 $-x, +z+1/4, +y+1/4$
-322 $+y+3/4, -x, +z+3/4$
-323 $+z+1/4, +y+3/4, -x+1/2$
-324 $-y, +x+3/4, +z+3/4$

ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS


```

loop_
  _atom_site_type_symbol
  _atom_site_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_occupancy
  _atom_site_thermal_displace_type
  _atom_site_U_iso_or_equiv
  _atom_site_symmetry_multiplicity
Zn
Zn1  0.125    0.125    0.125    0.5      Uiso  0.00521    8
Co
Co1  0.125    0.125    0.125    0.464    Uiso  0.00521    8
Al
Al1  0.125    0.125    0.125    0.036    Uiso  0.00521    8
Al
Al2  0.5      0.5      0.5      0.982    Uiso  0.00449   16
Co
Co2  0.5      0.5      0.5      0.018    Uiso  0.00449   16
O-
O1   0.26415(12) 0.26415(12) 0.26415(12) 1.0      Uiso  0.00532   32

```

```

loop_ _atom_type_symbol
      _atom_type_number_in_cell
      Zn 4.0
      Co 4.0
      Al 16.0
      O- 32.0

```

```

# If you change Z, be sure to change all 3 of the following
_chemical_formula_sum      "Al0.50 Co0.13 O Zn0.13"
_chemical_formula_weight   45.03
_cell_formula_units_Z      32

```

MOLECULAR GEOMETRY

```

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
 ? ? ? ? ? ? ? ?
 #--eof--eof--eof--eof--eof--eof--eof--eof--eof--eof--eof--eof--eof--eof--eof--eof--#