

data_G02_publ

_pd_block_id
2012-01-05T09:48|G02|GfCo075|Overall

_audit_creation_method "from EXP file using GSAS2CIF"
_audit_creation_date 2012-01-05T09:48
_audit_author_name GfCo075
_audit_update_record
; 2012-01-05T09:48 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_G02_overall

_refine_ls_shift/su_max 0.88
_refine_ls_shift/su_mean 0.88
_computing_structure_refinement GSAS
_refine_ls_number_parameters 1
_refine_ls_goodness_of_fit_all 1.02
_refine_ls_number_restraints 0
_refine_ls_matrix_type full

pointers to the phase blocks

loop_ _pd_phase_block_id
2012-01-05T09:48|G02_phase1|GfCo075||

pointers to the diffraction patterns

loop_ _pd_block_diffraction_id
?

Information for phase 1

data_G02_phase_1

_pd_block_id
2012-01-05T09:48|G02_phase1|GfCo075||

#=====

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	Zn025Co075Al2O4
_cell_length_a	8.10011(13)
_cell_length_b	8.10011
_cell_length_c	8.10011
_cell_angle_alpha	90.0
_cell_angle_beta	90.0
_cell_angle_gamma	90.0
_cell_volume	531.462(26)
_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    0.25    Uiso  0.00476    8
Co
Co1  0.125    0.125    0.125    0.701    Uiso  0.00476    8
Al
Al1  0.125    0.125    0.125    0.049    Uiso  0.00476    8
Al
Al2  0.5      0.5      0.5      0.9755   Uiso  0.00575   16
Co
Co2  0.5      0.5      0.5      0.0245   Uiso  0.00575   16
O-
O1   0.26397(20) 0.26397(20) 0.26397(20) 1.0      Uiso  0.00801   32

```

```

loop_ _atom_type_symbol
      _atom_type_number_in_cell
      Zn 2.0
      Co 6.0
      Al 16.0
      O- 32.0

```

```

# If you change Z, be sure to change all 3 of the following
_chemical_formula_sum      "Al0.50 Co0.19 O Zn0.06"
_chemical_formula_weight   44.63
_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
Zn1   O1      1.9497(28) .    1_555 N
Zn1   O1      1.9497(28) .  107_555 N
Zn1   O1      1.9497(28) .  111_555 N
Zn1   O1      1.9497(28) . -105_544 N
Co1   O1      1.9497(28) .    1_555 N
Co1   O1      1.9497(28) .  107_555 N
Co1   O1      1.9497(28) .  111_555 N
Co1   O1      1.9497(28) . -105_544 N

```

Al1	O1	1.9497(28)	. 1_555 N
Al1	O1	1.9497(28)	. 107_555 N
Al1	O1	1.9497(28)	. 111_555 N
Al1	O1	1.9497(28)	. -105_544 N
Al2	Al2	2.86382(5)	. 4_556 N
Al2	Al2	2.863820(30)	. 5_655 N
Al2	Al2	2.863820(30)	. 6_565 N
Al2	Al2	2.86382(5)	. -4_555 N
Al2	Al2	2.863820(30)	. -5_555 N
Al2	Al2	2.863820(30)	. -6_555 N
Al2	Co2	2.86382(5)	. 4_556 N
Al2	Co2	2.863820(30)	. 5_655 N
Al2	Co2	2.863820(30)	. 6_565 N
Al2	Co2	2.86382(5)	. -4_555 N
Al2	Co2	2.863820(30)	. -5_555 N
Al2	Co2	2.863820(30)	. -6_555 N
Al2	O1	1.9186(14)	. 4_556 N
Al2	O1	1.9186(14)	. 5_655 N
Al2	O1	1.9186(14)	. 6_565 N
Al2	O1	1.9186(14)	. -4_555 N
Al2	O1	1.9186(14)	. -5_555 N
Al2	O1	1.9186(14)	. -6_555 N
Co2	Al2	2.86382(5)	. 4_556 N
Co2	Al2	2.863820(30)	. 5_655 N
Co2	Al2	2.863820(30)	. 6_565 N
Co2	Al2	2.86382(5)	. -4_555 N
Co2	Al2	2.863820(30)	. -5_555 N
Co2	Al2	2.863820(30)	. -6_555 N
Co2	Co2	2.86382(5)	. 4_556 N
Co2	Co2	2.863820(30)	. 5_655 N
Co2	Co2	2.863820(30)	. 6_565 N
Co2	Co2	2.86382(5)	. -4_555 N
Co2	Co2	2.863820(30)	. -5_555 N
Co2	Co2	2.863820(30)	. -6_555 N
Co2	O1	1.9186(14)	. 4_556 N
Co2	O1	1.9186(14)	. 5_655 N
Co2	O1	1.9186(14)	. 6_565 N
Co2	O1	1.9186(14)	. -4_555 N
Co2	O1	1.9186(14)	. -5_555 N
Co2	O1	1.9186(14)	. -6_555 N
O1	Zn1	1.9497(28)	. 1_555 N
O1	Co1	1.9497(28)	. 1_555 N
O1	Al1	1.9497(28)	. 1_555 N
O1	Al2	1.9186(14)	. -4_555 N
O1	Al2	1.9186(14)	. -5_555 N
O1	Al2	1.9186(14)	. -6_555 N
O1	Co2	1.9186(14)	. -4_555 N
O1	Co2	1.9186(14)	. -5_555 N
O1	Co2	1.9186(14)	. -6_555 N

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
O1      Zn1      O1      109.4712(6)    1_555 .   107_433 N
O1      Zn1      O1      109.4712(12)   1_555 .   111_433 N
O1      Zn1      O1      109.4712(6)    1_555 .  -105_444 N
O1      Zn1      O1      109.4712(6)   107_433 .   111_433 N
O1      Zn1      O1      109.4712(12)   107_433 . -105_444 N
O1      Zn1      O1      109.4712(6)   111_433 . -105_444 N
O1      Co1      O1      109.4712(6)    1_555 .   107_433 N
O1      Co1      O1      109.4712(12)   1_555 .   111_433 N
O1      Co1      O1      109.4712(6)    1_555 .  -105_444 N
O1      Co1      O1      109.4712(6)   107_433 .   111_433 N
O1      Co1      O1      109.4712(12)   107_433 . -105_444 N
O1      Co1      O1      109.4712(6)   111_433 . -105_444 N
O1      Al1      O1      109.4712(6)    1_555 .   107_433 N
O1      Al1      O1      109.4712(12)   1_555 .   111_433 N
O1      Al1      O1      109.4712(6)    1_555 .  -105_444 N
O1      Al1      O1      109.4712(6)   107_433 .   111_433 N
O1      Al1      O1      109.4712(12)   107_433 . -105_444 N
O1      Al1      O1      109.4712(6)   111_433 . -105_444 N
O1      Al2      O1      83.05(11)    4_556 .   5_655 N
O1      Al2      O1      83.05(11)    4_556 .   6_565 N
O1      Al2      O1      180.0    4_556 .  -4_554 N
O1      Al2      O1      96.95(11)   4_556 .  -5_455 N
O1      Al2      O1      96.95(11)   4_556 .  -6_545 N
O1      Al2      O1      83.05(11)   5_655 .   6_565 N
O1      Al2      O1      96.95(11)   5_655 .  -4_554 N
O1      Al2      O1      180.0    5_655 .  -5_455 N
O1      Al2      O1      96.95(11)   5_655 .  -6_545 N
O1      Al2      O1      96.95(11)   6_565 .  -4_554 N
O1      Al2      O1      96.95(11)   6_565 .  -5_455 N
O1      Al2      O1      180.0    6_565 .  -6_545 N
O1      Al2      O1      83.05(11)  -4_554 .  -5_455 N
O1      Al2      O1      83.05(11)  -4_554 .  -6_545 N
O1      Al2      O1      83.05(11)  -5_455 .  -6_545 N
O1      Co2      O1      83.05(11)    4_556 .   5_655 N
O1      Co2      O1      83.05(11)    4_556 .   6_565 N
O1      Co2      O1      180.0    4_556 .  -4_554 N
O1      Co2      O1      96.95(11)   4_556 .  -5_455 N
O1      Co2      O1      96.95(11)   4_556 .  -6_545 N
O1      Co2      O1      83.05(11)   5_655 .   6_565 N
O1      Co2      O1      96.95(11)   5_655 .  -4_554 N
O1      Co2      O1      180.0    5_655 .  -5_455 N
O1      Co2      O1      96.95(11)   5_655 .  -6_545 N
O1      Co2      O1      96.95(11)   6_565 .  -4_554 N
O1      Co2      O1      96.95(11)   6_565 .  -5_455 N
O1      Co2      O1      180.0    6_565 .  -6_545 N
O1      Co2      O1      83.05(11)  -4_554 .  -5_455 N
O1      Co2      O1      83.05(11)  -4_554 .  -6_545 N
O1      Co2      O1      83.05(11)  -5_455 .  -6_545 N
Zn1     O1       Co1      0.0    1_555 .   1_555 N

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Zn1	O1	Al1	0.0	1_555	.	1_555	N
Zn1	O1	Al2	120.48(7)	1_555	.	-4_554	N
Zn1	O1	Al2	120.48(7)	1_555	.	-5_455	N
Zn1	O1	Al2	120.48(7)	1_555	.	-6_545	N
Zn1	O1	Co2	120.48(7)	1_555	.	-4_554	N
Zn1	O1	Co2	120.48(7)	1_555	.	-5_455	N
Zn1	O1	Co2	120.48(7)	1_555	.	-6_545	N
Co1	O1	Al1	0.0	1_555	.	1_555	N
Co1	O1	Al2	120.48(7)	1_555	.	-4_554	N
Co1	O1	Al2	120.48(7)	1_555	.	-5_455	N
Co1	O1	Al2	120.48(7)	1_555	.	-6_545	N
Co1	O1	Co2	120.48(7)	1_555	.	-4_554	N
Co1	O1	Co2	120.48(7)	1_555	.	-5_455	N
Co1	O1	Co2	120.48(7)	1_555	.	-6_545	N
Al1	O1	Al2	120.48(7)	1_555	.	-4_554	N
Al1	O1	Al2	120.48(7)	1_555	.	-5_455	N
Al1	O1	Al2	120.48(7)	1_555	.	-6_545	N
Al1	O1	Co2	120.48(7)	1_555	.	-4_554	N
Al1	O1	Co2	120.48(7)	1_555	.	-5_455	N
Al1	O1	Co2	120.48(7)	1_555	.	-6_545	N
Al2	O1	Al2	96.55(10)	-4_554	.	-5_455	N
Al2	O1	Al2	96.55(10)	-4_554	.	-6_545	N
Al2	O1	Co2	0.0	-4_554	.	-4_554	N
Al2	O1	Co2	96.55(10)	-4_554	.	-5_455	N
Al2	O1	Co2	96.55(10)	-4_554	.	-6_545	N
Al2	O1	Al2	96.55(10)	-5_455	.	-6_545	N
Al2	O1	Co2	96.55(10)	-5_455	.	-4_554	N
Al2	O1	Co2	0.0	-5_455	.	-5_455	N
Al2	O1	Co2	96.55(10)	-5_455	.	-6_545	N
Al2	O1	Co2	96.55(10)	-6_545	.	-4_554	N
Al2	O1	Co2	96.55(10)	-6_545	.	-5_455	N
Al2	O1	Co2	0.0	-6_545	.	-6_545	N
Co2	O1	Co2	96.55(10)	-4_554	.	-5_455	N
Co2	O1	Co2	96.55(10)	-4_554	.	-6_545	N
Co2	O1	Co2	96.55(10)	-5_455	.	-6_545	N

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