

data\_G00\_publ

\_pd\_block\_id

2012-01-05T09:50|G00|CoAl2O4|Overall

\_audit\_creation\_method "from EXP file using GSAS2CIF"

\_audit\_creation\_date 2012-01-05T09:50

\_audit\_author\_name CoAl2O4

\_audit\_update\_record

; 2012-01-05T09:50 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\_G00\_overall

\_refine\_ls\_shift/su\_max 1.82  
\_refine\_ls\_shift/su\_mean 1.82  
\_computing\_structure\_refinement GSAS  
\_refine\_ls\_number\_parameters 1  
\_refine\_ls\_goodness\_of\_fit\_all 1.07  
\_refine\_ls\_number\_restraints 0  
\_refine\_ls\_matrix\_type full

# pointers to the phase blocks

loop\_ \_pd\_phase\_block\_id  
2012-01-05T09:50|G00\_phase1|CoAl2O4||

# pointers to the diffraction patterns

loop\_ \_pd\_block\_diffraction\_id  
?

# Information for phase 1

data\_G00\_phase\_1

\_pd\_block\_id  
2012-01-05T09:50|G00\_phase1|CoAl2O4||

#=====

# 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	CoAl2O4
_cell_length_a	8.10559(8)
_cell_length_b	8.10559
_cell_length_c	8.10559
_cell_angle_alpha	90.0
_cell_angle_beta	90.0
_cell_angle_gamma	90.0
_cell_volume	532.543(16)
_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
Co
Co1  0.125    0.125    0.125    0.928    Uiso  0.005      8
Al
Al1  0.125    0.125    0.125    0.072    Uiso  0.005      8
Al
Al2  0.5      0.5      0.5      0.974    Uiso  0.00631   16
Co
Co2  0.5      0.5      0.5      0.036    Uiso  0.00631   16
O-
O1   0.26384(19) 0.26384(19) 0.26384(19) 1.0      Uiso  0.00788   32

```

```

loop_ _atom_type_symbol
      _atom_type_number_in_cell
      Co 8.0
      Al 16.16
      O- 32.0

```

```

# If you change Z, be sure to change all 3 of the following
_chemical_formula_sum      "Al0.50 Co0.25 O"
_chemical_formula_weight   44.36
_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
Co1  O1      1.9492(27) .   1_555 N
Co1  O1      1.9492(27) . 107_555 N
Co1  O1      1.9492(27) . 111_555 N
Co1  O1      1.9492(27) . -105_544 N
Al1  O1      1.9492(27) .   1_555 N
Al1  O1      1.9492(27) . 107_555 N
Al1  O1      1.9492(27) . 111_555 N
Al1  O1      1.9492(27) . -105_544 N
Al2  Al2     2.865760(30) .   4_556 N
Al2  Al2     2.865760(20) .   5_655 N
Al2  Al2     2.865760(20) .   6_565 N

```

Al2	Al2	2.865760(30)	. -4_555	N
Al2	Al2	2.865760(20)	. -5_555	N
Al2	Al2	2.865760(20)	. -6_555	N
Al2	Co2	2.865760(30)	. 4_556	N
Al2	Co2	2.865760(20)	. 5_655	N
Al2	Co2	2.865760(20)	. 6_565	N
Al2	Co2	2.865760(30)	. -4_555	N
Al2	Co2	2.865760(20)	. -5_555	N
Al2	Co2	2.865760(20)	. -6_555	N
Al2	O1	1.9208(14)	. 4_556	N
Al2	O1	1.9208(14)	. 5_655	N
Al2	O1	1.9208(14)	. 6_565	N
Al2	O1	1.9208(14)	. -4_555	N
Al2	O1	1.9208(14)	. -5_555	N
Al2	O1	1.9208(14)	. -6_555	N
Co2	Al2	2.865760(30)	. 4_556	N
Co2	Al2	2.865760(20)	. 5_655	N
Co2	Al2	2.865760(20)	. 6_565	N
Co2	Al2	2.865760(30)	. -4_555	N
Co2	Al2	2.865760(20)	. -5_555	N
Co2	Al2	2.865760(20)	. -6_555	N
Co2	Co2	2.865760(30)	. 4_556	N
Co2	Co2	2.865760(20)	. 5_655	N
Co2	Co2	2.865760(20)	. 6_565	N
Co2	Co2	2.865760(30)	. -4_555	N
Co2	Co2	2.865760(20)	. -5_555	N
Co2	Co2	2.865760(20)	. -6_555	N
Co2	O1	1.9208(14)	. 4_556	N
Co2	O1	1.9208(14)	. 5_655	N
Co2	O1	1.9208(14)	. 6_565	N
Co2	O1	1.9208(14)	. -4_555	N
Co2	O1	1.9208(14)	. -5_555	N
Co2	O1	1.9208(14)	. -6_555	N
O1	Co1	1.9492(27)	. 1_555	N
O1	Al1	1.9492(27)	. 1_555	N
O1	Al2	1.9208(14)	. -4_555	N
O1	Al2	1.9208(14)	. -5_555	N
O1	Al2	1.9208(14)	. -6_555	N
O1	Co2	1.9208(14)	. -4_555	N
O1	Co2	1.9208(14)	. -5_555	N
O1	Co2	1.9208(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	Co1	O1	109.4712(4)	1_555 . 107_433 N
O1	Co1	O1	109.4712(7)	1_555 . 111_433 N
O1	Co1	O1	109.4712(4)	1_555 . -105_444 N

O1	Co1	O1	109.4712(4)	107_433	.	111_433	N
O1	Co1	O1	109.4712(7)	107_433	.	-105_444	N
O1	Co1	O1	109.4712(4)	111_433	.	-105_444	N
O1	Al1	O1	109.4712(4)	1_555	.	107_433	N
O1	Al1	O1	109.4712(7)	1_555	.	111_433	N
O1	Al1	O1	109.4712(4)	1_555	.	-105_444	N
O1	Al1	O1	109.4712(4)	107_433	.	111_433	N
O1	Al1	O1	109.4712(7)	107_433	.	-105_444	N
O1	Al1	O1	109.4712(4)	111_433	.	-105_444	N
O1	Al2	O1	83.12(10)	4_556	.	5_655	N
O1	Al2	O1	83.12(10)	4_556	.	6_565	N
O1	Al2	O1	180.0	4_556	.	-4_554	N
O1	Al2	O1	96.88(10)	4_556	.	-5_455	N
O1	Al2	O1	96.88(10)	4_556	.	-6_545	N
O1	Al2	O1	83.12(10)	5_655	.	6_565	N
O1	Al2	O1	96.88(10)	5_655	.	-4_554	N
O1	Al2	O1	180.0	5_655	.	-5_455	N
O1	Al2	O1	96.88(10)	5_655	.	-6_545	N
O1	Al2	O1	96.88(10)	6_565	.	-4_554	N
O1	Al2	O1	96.88(10)	6_565	.	-5_455	N
O1	Al2	O1	180.0	6_565	.	-6_545	N
O1	Al2	O1	83.12(10)	-4_554	.	-5_455	N
O1	Al2	O1	83.12(10)	-4_554	.	-6_545	N
O1	Al2	O1	83.12(10)	-5_455	.	-6_545	N
O1	Co2	O1	83.12(10)	4_556	.	5_655	N
O1	Co2	O1	83.12(10)	4_556	.	6_565	N
O1	Co2	O1	180.0	4_556	.	-4_554	N
O1	Co2	O1	96.88(10)	4_556	.	-5_455	N
O1	Co2	O1	96.88(10)	4_556	.	-6_545	N
O1	Co2	O1	83.12(10)	5_655	.	6_565	N
O1	Co2	O1	96.88(10)	5_655	.	-4_554	N
O1	Co2	O1	180.0	5_655	.	-5_455	N
O1	Co2	O1	96.88(10)	5_655	.	-6_545	N
O1	Co2	O1	96.88(10)	6_565	.	-4_554	N
O1	Co2	O1	96.88(10)	6_565	.	-5_455	N
O1	Co2	O1	180.0	6_565	.	-6_545	N
O1	Co2	O1	83.12(10)	-4_554	.	-5_455	N
O1	Co2	O1	83.12(10)	-4_554	.	-6_545	N
O1	Co2	O1	83.12(10)	-5_455	.	-6_545	N
Co1	O1	Al1	0.0	1_555	.	1_555	N
Co1	O1	Al2	120.53(7)	1_555	.	-4_564	N
Co1	O1	Al2	120.53(7)	1_555	.	-5_465	N
Co1	O1	Al2	120.53(7)	1_555	.	-6_555	N
Co1	O1	Co2	120.53(7)	1_555	.	-4_554	N
Co1	O1	Co2	120.53(7)	1_555	.	-5_455	N
Co1	O1	Co2	120.53(7)	1_555	.	-6_545	N
Al1	O1	Al2	120.53(7)	1_555	.	-4_564	N
Al1	O1	Al2	120.53(7)	1_555	.	-5_465	N
Al1	O1	Al2	120.53(7)	1_555	.	-6_555	N
Al1	O1	Co2	120.53(7)	1_555	.	-4_554	N
Al1	O1	Co2	120.53(7)	1_555	.	-5_455	N
Al1	O1	Co2	120.53(7)	1_555	.	-6_545	N
Al2	O1	Al2	96.49(9)	-4_564	.	-5_465	N
Al2	O1	Al2	96.49(9)	-4_564	.	-6_555	N

Al2	O1	Co2	0.0	-4_554	.	-4_554	N
Al2	O1	Co2	96.49(9)	-4_554	.	-5_455	N
Al2	O1	Co2	96.49(9)	-4_554	.	-6_545	N
Al2	O1	Al2	96.49(9)	-5_465	.	-6_555	N
Al2	O1	Co2	96.49(9)	-5_455	.	-4_554	N
Al2	O1	Co2	0.0	-5_455	.	-5_455	N
Al2	O1	Co2	96.49(9)	-5_455	.	-6_545	N
Al2	O1	Co2	96.49(9)	-6_545	.	-4_554	N
Al2	O1	Co2	96.49(9)	-6_545	.	-5_455	N
Al2	O1	Co2	0.0	-6_545	.	-6_545	N
Co2	O1	Co2	96.49(9)	-4_554	.	-5_455	N
Co2	O1	Co2	96.49(9)	-4_554	.	-6_545	N
Co2	O1	Co2	96.49(9)	-5_455	.	-6_545	N

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