

data_G10_publ

_pd_block_id

2012-01-05T09:38|G10|fco000|Overall

_audit_creation_method "from EXP file using GSAS2CIF"

_audit_creation_date 2012-01-05T09:38

_audit_author_name fco000

_audit_update_record

; 2012-01-05T09:38 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_G10_overall

_refine_ls_shift/su_max 0.06
_refine_ls_shift/su_mean 0.01
_computing_structure_refinement GSAS
_refine_ls_number_parameters 28
_refine_ls_goodness_of_fit_all 1.31
_refine_ls_number_restraints 10
_refine_ls_matrix_type full

pointers to the phase blocks

loop_ _pd_phase_block_id
2012-01-05T09:38|G10_phase1|fco000||

pointers to the diffraction patterns

loop_ _pd_block_diffraction_id
?

Information for phase 1

data_G10_phase_1

_pd_block_id
2012-01-05T09:38|G10_phase1|fco000||

#=====

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	ZnAl2O4
_cell_length_a	8.08514(10)
_cell_length_b	8.08514
_cell_length_c	8.08514
_cell_angle_alpha	90.0
_cell_angle_beta	90.0
_cell_angle_gamma	90.0
_cell_volume	528.521(20)
_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    1.0    Uiso  0.00527(20)  8
Al
Al1  0.5      0.5      0.5      1.0    Uiso  0.00279(26)  16
O-
O1   0.26446(9) 0.26446(9) 0.26446(9) 1.0    Uiso  0.0065(5)   32

```

```

loop_ _atom_type_symbol
      _atom_type_number_in_cell
      Zn 8.0
      Al 16.0
      O- 32.0

```

If you change Z, be sure to change all 3 of the following

```

_chemical_formula_sum      "Al2 O4 Zn"
_chemical_formula_weight   183.34
_cell_formula_units_Z      8

```

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      1.9530(12) .   1_555 N
Zn1  O1      1.9530(12) . 107_555 N
Zn1  O1      1.9530(12) . 111_555 N
Zn1  O1      1.9530(12) . -105_544 N
Al1  Al1     2.85853(4) .   4_556 N
Al1  Al1     2.858530(30) .  5_655 N
Al1  Al1     2.858530(30) .  6_565 N
Al1  Al1     2.85853(4) .  -4_555 N
Al1  Al1     2.858530(30) . -5_555 N
Al1  Al1     2.858530(30) . -6_555 N
Al1  O1      1.9115(6) .   4_556 N
Al1  O1      1.9115(6) .   5_655 N
Al1  O1      1.9115(6) .   6_565 N
Al1  O1      1.9115(6) .  -4_555 N
Al1  O1      1.9115(6) .  -5_555 N

```

Al1	O1	1.9115(6)	.	-6_555	N
O1	Zn1	1.9530(12)	.	1_555	N
O1	Al1	1.9115(6)	.	-4_555	N
O1	Al1	1.9115(6)	.	-5_555	N
O1	Al1	1.9115(6)	.	-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(5)	1_555	107_443 N
O1	Zn1	O1	109.4712(10)	1_555	111_443 N
O1	Zn1	O1	109.4712(5)	1_555	-105_454 N
O1	Zn1	O1	109.4712(5)	107_443	111_443 N
O1	Zn1	O1	109.4712(10)	107_443	-105_454 N
O1	Zn1	O1	109.4712(5)	111_443	-105_454 N
Al1	Al1	Al1	60.00000(30)	4_556	5_655 N
Al1	Al1	Al1	60.00000(30)	4_556	6_565 N
Al1	Al1	Al1	180.0	4_556	-4_654 N
Al1	Al1	Al1	120.00000(30)	4_556	-5_555 N
Al1	Al1	Al1	120.00000(30)	4_556	-6_645 N
Al1	Al1	O1	85.037(32)	4_556	4_556 N
Al1	Al1	O1	41.607(21)	4_556	5_655 N
Al1	Al1	O1	41.607(21)	4_556	6_565 N
Al1	Al1	O1	94.963(32)	4_556	-4_564 N
Al1	Al1	O1	138.393(21)	4_556	-5_465 N
Al1	Al1	O1	138.393(21)	4_556	-6_555 N
Al1	Al1	Al1	60.0000(6)	5_655	6_565 N
Al1	Al1	Al1	120.00000(30)	5_655	-4_654 N
Al1	Al1	Al1	180.0	5_655	-5_555 N
Al1	Al1	Al1	120.0000(6)	5_655	-6_645 N
Al1	Al1	O1	41.607(21)	5_655	4_556 N
Al1	Al1	O1	85.037(32)	5_655	5_655 N
Al1	Al1	O1	41.607(21)	5_655	6_565 N
Al1	Al1	O1	138.393(21)	5_655	-4_564 N
Al1	Al1	O1	94.963(32)	5_655	-5_465 N
Al1	Al1	O1	138.393(21)	5_655	-6_555 N
Al1	Al1	Al1	120.00000(30)	6_565	-4_654 N
Al1	Al1	Al1	120.0000(6)	6_565	-5_555 N
Al1	Al1	Al1	180.0	6_565	-6_645 N
Al1	Al1	O1	41.607(21)	6_565	4_556 N
Al1	Al1	O1	41.607(21)	6_565	5_655 N
Al1	Al1	O1	85.037(32)	6_565	6_565 N
Al1	Al1	O1	138.393(21)	6_565	-4_564 N
Al1	Al1	O1	138.393(21)	6_565	-5_465 N
Al1	Al1	O1	94.963(32)	6_565	-6_555 N
Al1	Al1	Al1	60.00000(30)	-4_654	-5_555 N
Al1	Al1	Al1	60.00000(30)	-4_654	-6_645 N
Al1	Al1	O1	94.963(32)	-4_564	4_556 N

Al1	Al1	O1	138.393(21)	-4_564 .	5_655 N
Al1	Al1	O1	138.393(21)	-4_564 .	6_565 N
Al1	Al1	O1	85.037(32)	-4_564 .	-4_564 N
Al1	Al1	O1	41.607(21)	-4_564 .	-5_465 N
Al1	Al1	O1	41.607(21)	-4_564 .	-6_555 N
Al1	Al1	Al1	60.0000(6)	-5_555 .	-6_645 N
Al1	Al1	O1	138.393(21)	-5_465 .	4_556 N
Al1	Al1	O1	94.963(32)	-5_465 .	5_655 N
Al1	Al1	O1	138.393(21)	-5_465 .	6_565 N
Al1	Al1	O1	41.607(21)	-5_465 .	-4_564 N
Al1	Al1	O1	85.037(32)	-5_465 .	-5_465 N
Al1	Al1	O1	41.607(21)	-5_465 .	-6_555 N
Al1	Al1	O1	138.393(21)	-6_555 .	4_556 N
Al1	Al1	O1	138.393(21)	-6_555 .	5_655 N
Al1	Al1	O1	94.963(32)	-6_555 .	6_565 N
Al1	Al1	O1	41.607(21)	-6_555 .	-4_564 N
Al1	Al1	O1	41.607(21)	-6_555 .	-5_465 N
Al1	Al1	O1	85.037(32)	-6_555 .	-6_555 N
O1	Al1	O1	82.78(5)	4_556 .	5_655 N
O1	Al1	O1	82.78(5)	4_556 .	6_565 N
O1	Al1	O1	180.0	4_556 .	-4_564 N
O1	Al1	O1	97.22(5)	4_556 .	-5_465 N
O1	Al1	O1	97.22(5)	4_556 .	-6_555 N
O1	Al1	O1	82.78(5)	5_655 .	6_565 N
O1	Al1	O1	97.22(5)	5_655 .	-4_564 N
O1	Al1	O1	180.0	5_655 .	-5_465 N
O1	Al1	O1	97.22(5)	5_655 .	-6_555 N
O1	Al1	O1	97.22(5)	6_565 .	-4_564 N
O1	Al1	O1	97.22(5)	6_565 .	-5_465 N
O1	Al1	O1	180.0	6_565 .	-6_555 N
O1	Al1	O1	82.78(5)	-4_564 .	-5_465 N
O1	Al1	O1	82.78(5)	-4_564 .	-6_555 N
O1	Al1	O1	82.78(5)	-5_465 .	-6_555 N
Zn1	O1	Al1	120.301(32)	1_555 .	-4_654 N
Zn1	O1	Al1	120.301(32)	1_555 .	-5_555 N
Zn1	O1	Al1	120.301(32)	1_555 .	-6_645 N
Al1	O1	Al1	96.79(4)	-4_654 .	-5_555 N
Al1	O1	Al1	96.79(4)	-4_654 .	-6_645 N
Al1	O1	Al1	96.79(4)	-5_555 .	-6_645 N

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