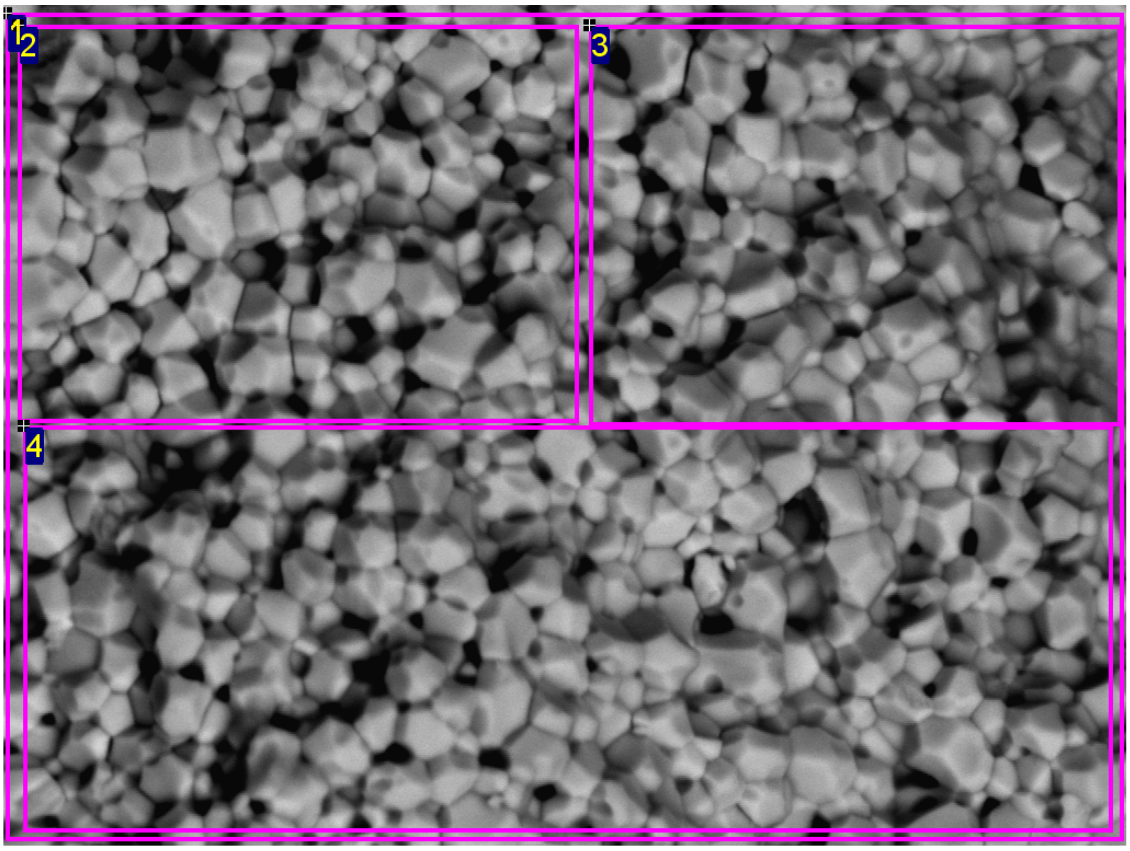
Supplementary Information



Element	O	Zr	Ce
1	64.63	31.11	4.27
2	64.78	31.17	4.05
3	62.66	32.97	4.36
4	64.60	31.39	4.02
Average	64.17	31.66	4.17
Standard error	1.01	0.89	0.17
Maximum	64.78	32.97	4.36
Minimum	62.66	31.11	4.02

All results in atomic percent.

Figure S1. EDAX data concerning the $Zr_{0.91}Ce_{0.09}O_2$ (normal composition) sample.

CELREF Version 3. 11/19/2015 4:51:05 PM

Initial values : (Refinement keys on 2nd line)

Zero	Lambda	a	b	c	alpha	beta	gamma	volume
0.000	1.54060	3.6435	3.6435	5.2437	90.00	90.00	90.00	69.61
0	0	1	0	1	0	0	0	

H	K	L	2Th(obs)	2Th_obs-shift	2Th(Calc)	diff.
0	1	1	29.8530	29.8530	29.8368	0.0162
0	0	2	34.1928	34.1928	34.1712	0.0216
1	1	0	34.8102	34.8102	34.7939	0.0163
1	1	2	49.5779	49.5779	49.5659	0.0120
0	2	0	50.0452	50.0452	50.0274	0.0178
0	1	3	58.5162	58.5162	58.5220	-0.0058
1	2	1	59.3894	59.3894	59.3450	0.0444
2	0	2	61.9643	61.9643	61.9797	-0.0154
0	0	4	71.9643	71.9643	71.9738	-0.0095
2	2	0	73.4051	73.4051	73.4506	-0.0455

Sqrt(Sum(2Th O-C)**2)/(Nref-Npar)) : 0.0271

Sqrt(Sum(2Th O-C)**2)/Nref) : 0.0242

Final values : (Standard errors on 2nd line)

Zero	Lambda	a	b	c	alpha	beta	gamma	volume
0.000	1.54060	3.6440	3.6440	5.2433	90.00	90.00	90.00	69.63
0.0000	0.00000	0.0015	0.0000	0.0003	0.000	0.000	0.000	0.029

H	K	L	2Th(obs)	2Th_obs-shift	2Th(Calc)	diff.
0	1	1	29.8530	29.8530	29.8345	0.0185
0	0	2	34.1928	34.1928	34.1736	0.0192
1	1	0	34.8102	34.8102	34.7886	0.0216
1	1	2	49.5779	49.5779	49.5637	0.0142
0	2	0	50.0452	50.0452	50.0196	0.0256
0	1	3	58.5162	58.5162	58.5237	-0.0075
1	2	1	59.3894	59.3894	59.3367	0.0527
2	0	2	61.9643	61.9643	61.9744	-0.0101
0	0	4	71.9643	71.9643	71.9794	-0.0151
2	2	0	73.4051	73.4051	73.4381	-0.0330

Sqrt(Sum(2Th O-C)**2)/(Nref-Npar)) : 0.0280

Sqrt(Sum(2Th O-C)**2)/Nref) : 0.0251

```
#------------------------------------------------------------------------------
-
#$Date: 2015-09-18 21:29:51 +0000 (Fri, 18 Sep 2015) $
#$Revision: 158024 $
#$URL: file:///home/coder/svn-repositories/cod/cif/2/30/05/2300544.cif $
#------------------------------------------------------------------------------
-
#
# This file is available in the Crystallography Open Database (COD),
# http://www.crystallography.net/. The original data for this entry
# were provided by IUCr Journals, http://journals.iucr.org/.
#
# The file may be used within the scientific community so long as
# proper attribution is given to the journal article from which the
# data were obtained.
#
data_2300544
loop_
_publ_author_name
'Winterer, M.'
'Delaplane, R.'
'McGreevy, R.'
_publ_section_title
;
 X-ray diffraction, neutron scattering and EXAFS spectroscopy of
 monoclinic zirconia: analysis by Rietveld refinement and reverse Monte
 Carlo simulations
;
_journal_name_full               'Journal of Applied Crystallography'
_journal_page_first              434
_journal_page_last               442
_journal_volume                  35
_journal_year                    2002
_chemical_formula_sum            'O2 Zr'
_chemical_name_systematic        'Zr O2'
_space_group_IT_number           14
_symmetry_space_group_name_Hall  '-P 2ybc'
_symmetry_space_group_name_H-M   'P 1 21/c 1'
_cell_angle_alpha                90
_cell_angle_beta                 99.164
_cell_angle_gamma                90
_cell_formula_units_Z            4
_cell_length_a                   5.1487
_cell_length_b                   5.2023
_cell_length_c                   5.3231
_cell_volume                     140.760
```

```
_citation_journal_id_ASTM        JACGAR
_cod_data_source_file            Winterer_JACGAR_2002_309.cif
_cod_data_source_block           O2Zr1
_cod_original_cell_volume        140.7599
_cod_chemical_formula_sum_orig   'O2 Zr1'
_cod_database_code               2300544
loop_
_symmetry_equiv_pos_as_xyz
x,y,z
-x,y+1/2,-z+1/2
-x,-y,-z
x,-y-1/2,z-1/2
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_U_iso_or_equiv
O2 O-2 0.449 0.7559 0.4792 1 0.0
Zr1 Zr+4 0.2762 0.0397 0.209 1 0.0
O1 O-2 0.0694 0.3315 0.3463 1 0.0
```