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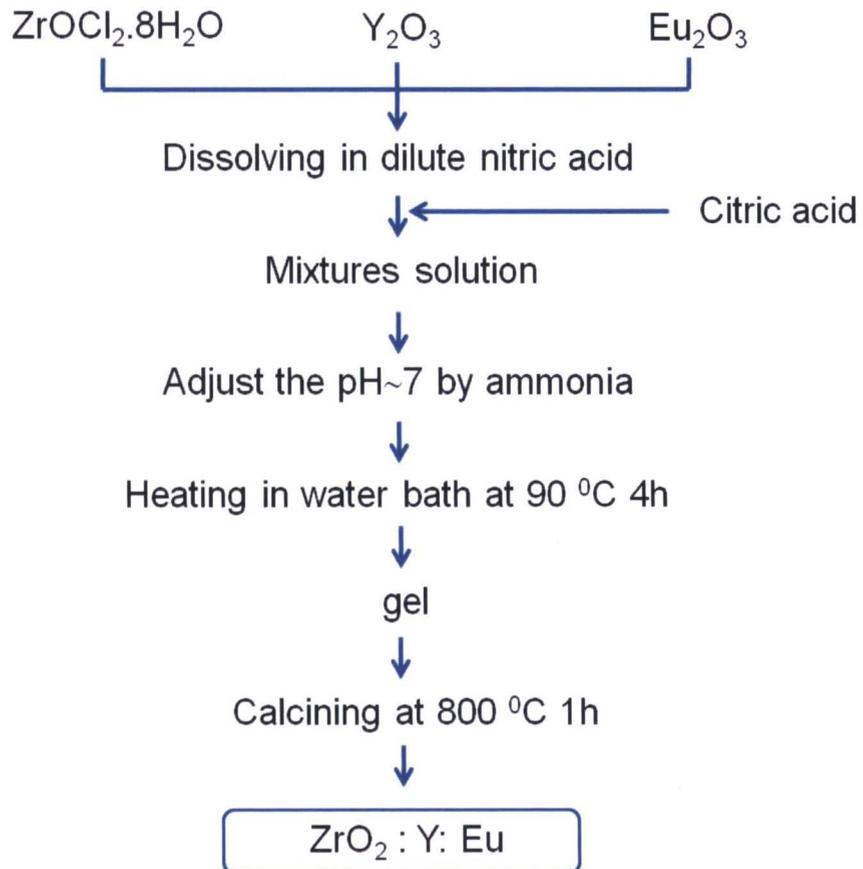
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## **APPENDIX**

## APPENDIX A

### Preparation of $ZrO_2$ : Y: Eu powder samples



## APPENDIX B

### Monoclinic phase

#### Name and formula

Reference code:	01-083-0941
ICSD name:	Zirconium Oxide
Empirical formula:	O <sub>2</sub> Zr
Chemical formula:	ZrO <sub>2</sub>

#### Crystallographic parameters

Crystal system:	Monoclinic
Space group:	P21/c
Space group number:	14
a (Å):	5.1505
b (Å):	5.2077
c (Å):	5.3164
Alpha (°):	90.0000
Beta (°):	99.2230
Gamma (°):	90.0000
Calculated density (g/cm <sup>3</sup> ):	5.81
Volume of cell (10 <sup>6</sup> pm <sup>3</sup> ):	140.75
Z:	4.00
RIR:	4.76

#### Subfiles and Quality

Subfiles:	Inorganic Alloy, metal or intermetallic Corrosion Modelled additional pattern
Quality:	Calculated (C)

#### Comments

ICSD collection code:	080047
Test from ICSD:	At least one TF implausible.

**References**

Primary reference: Calculated from ICSD using POWD-12++,  
(1997)

Structure: Bondars, B., Heidemane, G., Grabis, J., Laschke,  
K., Boysen, H., Schneider, J., Frey, F., J. Mater.  
Sci., 30, 1621, (1995)

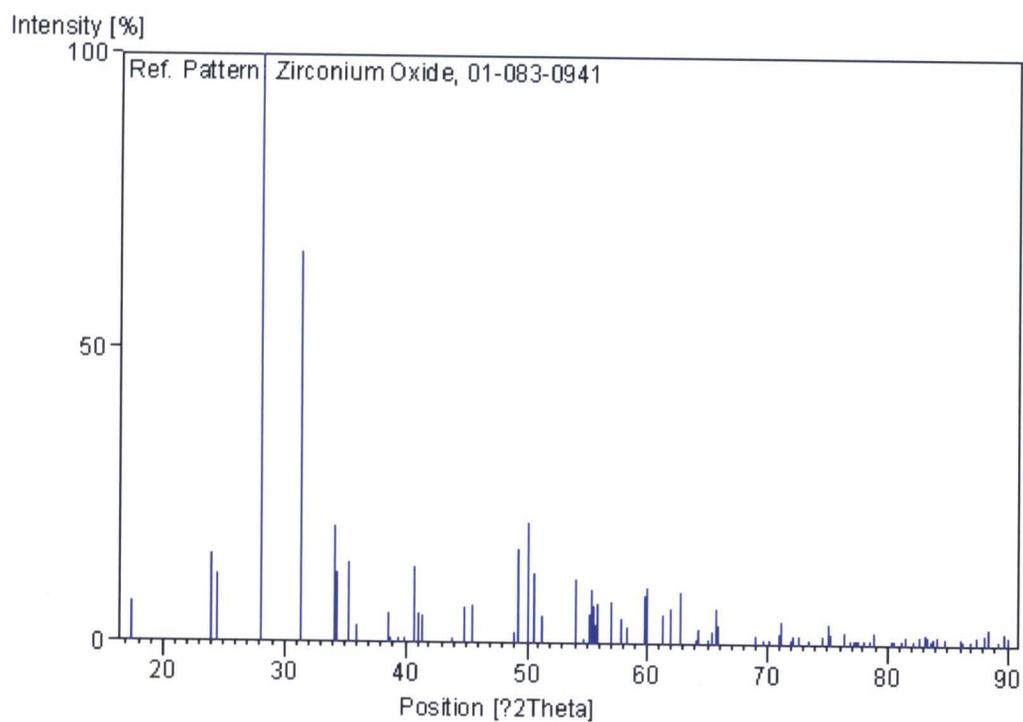
**Peak list**

No.	h	k	l	d [Å]	2Theta[deg]	I [%]
1	1	0	0	5.08391	17.430	7.0
2	0	1	1	3.69645	24.056	15.2
3	1	1	0	3.63785	24.449	11.8
4	-1	1	1	3.16447	28.177	100.0
5	1	1	1	2.84104	31.463	66.7
6	0	0	2	2.62384	34.144	20.0
7	0	2	0	2.60385	34.415	12.1
8	2	0	0	2.54196	35.280	13.9
9	-1	0	2	2.50068	35.882	2.9
10	0	2	1	2.33250	38.567	5.2
11	1	2	0	2.31756	38.826	0.4
12	2	1	0	2.28435	39.414	0.8
13	-1	1	2	2.25425	39.962	0.5
14	-2	1	1	2.21449	40.711	13.1
15	1	0	2	2.19278	41.132	5.2
16	-1	2	1	2.17969	41.391	4.6
17	1	2	1	2.06499	43.805	0.1
18	1	1	2	2.02093	44.811	6.3
19	-2	0	2	1.99223	45.493	6.5
20	-2	1	2	1.86072	48.910	1.9
21	0	2	2	1.84823	49.263	16.2
22	2	2	0	1.81892	50.111	20.8

23	-1	2	2	1.80362	50.565	12.0
24	-2	2	1	1.78305	51.191	4.7
25	2	0	2	1.69497	54.061	10.9
26	1	2	2	1.67726	54.679	0.5
27	2	2	1	1.66069	55.271	5.1
28	0	1	3	1.65818	55.362	9.2
29	-1	1	3	1.65219	55.580	6.6
30	0	3	1	1.64807	55.731	3.5
31	1	3	0	1.64278	55.926	6.8
32	3	1	0	1.61091	57.133	7.2
33	-1	3	1	1.59143	57.898	4.4
34	-2	2	2	1.58224	58.266	3.0
35	1	3	1	1.54510	59.807	8.3
36	-3	0	2	1.54051	60.004	9.5
37	1	1	3	1.51025	61.334	5.2
38	-2	1	3	1.49677	61.947	6.0
39	3	1	1	1.47853	62.797	8.8
40	0	2	3	1.45200	64.080	1.1
41	-1	2	3	1.44797	64.279	2.6
42	2	3	0	1.43353	65.006	0.8
43	-1	3	2	1.42600	65.392	2.2
44	2	2	2	1.42052	65.676	6.1
45	-2	3	1	1.41577	65.924	3.4
46	1	3	2	1.36104	68.939	1.8
47	1	2	3	1.34957	69.608	0.6
48	-2	2	3	1.33992	70.183	0.5
49	3	2	1	1.32585	71.040	1.9
50	-1	0	4	1.32263	71.239	4.2
51	0	0	4	1.31192	71.911	0.9
52	-2	3	2	1.30877	72.111	1.5
53	0	4	0	1.30192	72.550	1.5
54	-3	1	3	1.28696	73.531	0.4

55	4	0	0	1.27098	74.611	1.6
56	0	4	1	1.26362	75.121	3.7
57	1	4	0	1.26123	75.288	2.1
58	-4	1	1	1.24595	76.376	2.2
59	-1	4	1	1.23754	76.990	0.3
60	4	1	0	1.23474	77.197	0.8
61	0	3	3	1.23215	77.389	0.8
62	-1	3	3	1.22968	77.573	0.7
63	1	0	4	1.22374	78.021	0.9
64	-2	1	4	1.21579	78.629	0.5
65	3	3	0	1.21262	78.875	2.2
66	2	2	3	1.19423	80.334	0.4
67	1	1	4	1.19094	80.602	0.3
68	-3	2	3	1.18313	81.245	0.5
69	-1	2	4	1.17922	81.571	1.6
70	0	2	4	1.17161	82.215	0.5
71	1	3	3	1.16768	82.552	1.6
72	0	4	2	1.16625	82.675	0.6
73	4	1	1	1.16142	83.095	2.1
74	2	4	0	1.15878	83.326	1.6
75	-1	4	2	1.15479	83.679	0.4
76	3	3	1	1.15283	83.854	1.4
77	-2	4	1	1.14934	84.167	1.7
78	4	2	0	1.14218	84.817	1.2
79	-3	0	4	1.12863	86.080	1.2
80	-2	2	4	1.12713	86.223	0.5
81	1	4	2	1.11947	86.959	0.3
82	2	4	1	1.11451	87.443	1.7
83	1	2	4	1.10752	88.137	2.1
84	3	1	3	1.10428	88.463	3.0
85	2	0	4	1.09639	89.268	0.9
86	-4	1	3	1.09203	89.721	2.4



**Stick Pattern**

## APPENDIX C

### Tetragonal phase

#### Name and formula

Reference code:	01-081-1544
ICSD name:	Zirconium Oxide
Empirical formula:	O <sub>1.95</sub> Zr
Chemical formula:	ZrO <sub>1.95</sub>

#### Crystallographic parameters

Crystal system:	Tetragonal
Space group:	P42/nmc
Space group number:	137
a (Å):	3.6067
b (Å):	3.6067
c (Å):	5.1758
Alpha (°):	90.0000
Beta (°):	90.0000
Gamma (°):	90.0000
Calculated density (g/cm <sup>3</sup> ):	6.04
Volume of cell (10 <sup>6</sup> pm <sup>3</sup> ):	67.33
Z:	2.00
RIR:	10.26

#### Subfiles and Quality

Subfiles:	Inorganic Alloy, metal or intermetallic Corrosion Modelled additional pattern
Quality:	Calculated (C)

#### Comments

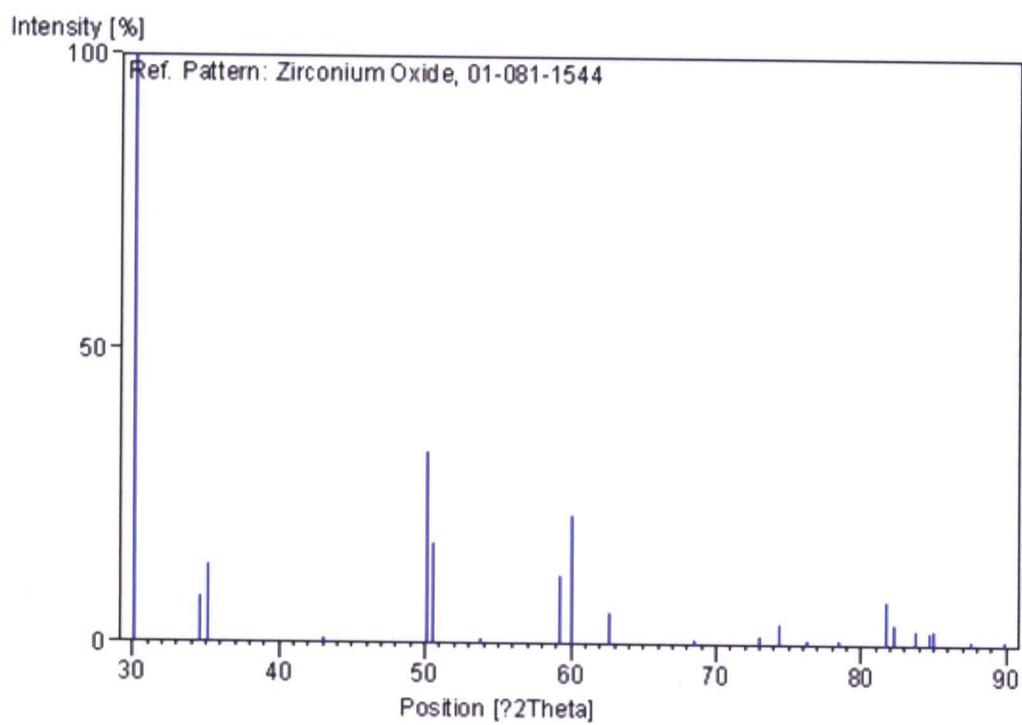
ICSD collection code:	072949
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**References**

- Primary reference: Calculated from ICSD using POWD-12++,  
(1997)
- Structure: Martin, U., Boysen, H., Frey, F., Acta  
Crystallogr., Sec. B: Structural Science, 49, 403,  
(1993)

**Peak list**

No.	h	k	l	d [Å]	2Theta[deg]	I [%]
1	1	0	1	2.95911	30.177	100.0
2	0	0	2	2.58790	34.634	8.0
3	1	1	0	2.55032	35.160	13.5
4	1	0	2	2.10263	42.981	0.9
5	1	1	2	1.81649	50.182	32.6
6	2	0	0	1.80335	50.574	17.3
7	2	0	1	1.70294	53.787	0.1
8	1	0	3	1.55637	59.331	11.5
9	2	1	1	1.53992	60.029	22.0
10	2	0	2	1.47956	62.749	5.5
11	2	1	2	1.36885	68.490	0.2
12	0	0	4	1.29395	73.069	1.7
13	2	2	0	1.27516	74.325	3.9
14	2	0	3	1.24664	76.326	0.1
15	1	0	4	1.21794	78.464	0.2
16	2	1	3	1.17824	81.653	7.6
17	3	0	1	1.17106	82.262	3.8
18	1	1	4	1.15392	83.757	2.7
19	2	2	2	1.14384	84.665	2.2
20	3	1	0	1.14054	84.968	2.8
21	3	1	1	1.11382	87.511	0.1
22	3	0	2	1.09032	89.900	0.1

**Stick Pattern**

## APPENDIX D

### Cubic phase

#### Name and formula

Reference code:	01-081-1550
ICSD name:	Zirconium Oxide
Empirical formula:	O <sub>2.12</sub> Zr
Chemical formula:	ZrO <sub>2.12</sub>

#### Crystallographic parameters

Crystal system:	Cubic
Space group:	Fm-3m
Space group number:	225
a (Å):	5.1291
b (Å):	5.1291
c (Å):	5.1291
Alpha (°):	90.0000
Beta (°):	90.0000
Gamma (°):	90.0000
Calculated density (g/cm <sup>3</sup> ):	6.16
Volume of cell (10 <sup>6</sup> pm <sup>3</sup> ):	134.93
Z:	4.00
RIR:	9.52

#### Subfiles and Quality

Subfiles:	Inorganic Alloy, metal or intermetallic Corrosion Modelled additional pattern
Quality:	Calculated (C)

#### Comments

ICSD collection code:	072955
Test from ICSD:	At least one SOF implausible.

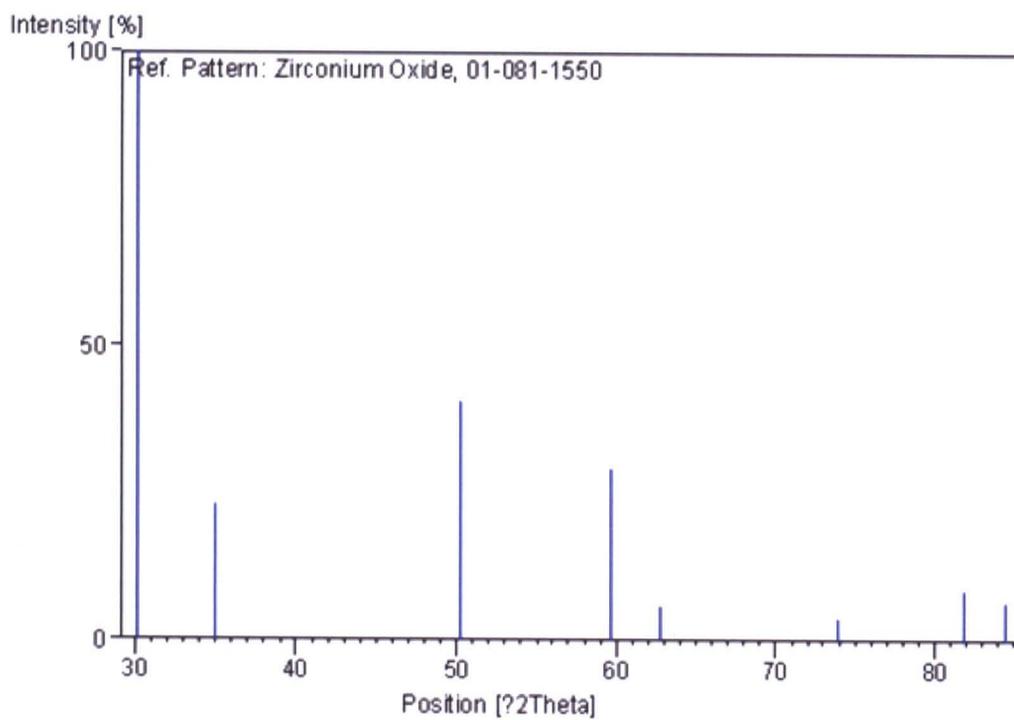
**References**

- Primary reference: Calculated from ICSD using POWD-12++,  
(1997)
- Structure: Martin, U., Boysen, H., Frey, F., Acta  
Crystallogr., Sec. B: Structural Science, 49, 403,  
(1993)

**Peak list**

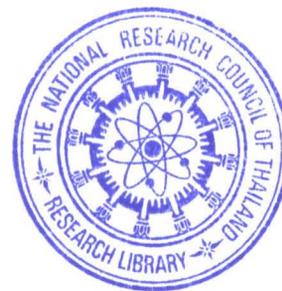
No.	h	k	l	d [Å]	2Theta[deg]	I [%]
1	1	1	1	2.96129	30.155	100.0
2	2	0	0	2.56455	34.959	23.2
3	2	2	0	1.81341	50.273	40.5
4	3	1	1	1.54648	59.749	29.1
5	2	2	2	1.48064	62.698	5.8
6	4	0	0	1.28228	73.844	3.8
7	3	3	1	1.17670	81.783	8.5
8	4	2	0	1.14690	84.387	6.4

## Stick Pattern



## **BIOGRAPHY**

## BIOGRAPHY



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