Name and formula

Reference code: 01-073-0958

ICSD name: Zirconium Oxide

Empirical formula: OZr_3
Chemical formula: Zr_3O

Crystallographic parameters

Crystal system: Rhombohedral
Space group: R32
Space group number: 155

a (Å):   5,5630
b (Å):   5,5630
c (Å):   31,1850
Alpha (°):   90,0000
Beta (°):   90,0000
Gamma (°):   120,0000

Calculated density (g/cm^3):   6,91
Volume of cell (10^6 pm^3):   835,77
Z: 12,00

RIR: 11,83

Subfiles and Quality

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

Comments

ICSD collection code: 023402
Test from ICSD: At least one TF missing.
                       No R value given.

References

Primary reference: *Calculated from ICSD using POWD-12++, (1997)*
Structure: Dubertret, A., Lehr, P., *C. R. Seances Acad. Sci., Ser. C* **268**, 501, (1969)

Peak list

No.	h	k	l	d [Å]	2Theta[deg]	I [%]
1	0	0	3	10,39500	8,499	0,1
2	1	0	1	4,76118	18,621	0,1
3	0	1	2	4,60295	19,267	0,4
4	1	0	4	4,09831	21,667	0,1
5	0	1	5	3,81268	23,312	0,8

6	0	0	9	3,46500	25,689	0,1
7	1	0	7	3,27086	27,243	0,5
8	0	1	8	3,03038	29,451	0,1
9	1	1	0	2,78148	32,155	19,1
10	0	0	12	2,59875	34,484	23,5
11	1	1	6	2,45238	36,613	100,0
12	0	1	11	2,44334	36,754	58,7
13	2	0	2	2,38059	37,759	0,2
14	0	2	4	2,30148	39,108	0,1
15	2	0	5	2,24706	40,096	0,1
16	1	1	9	2,16907	41,603	0,1
17	1	0	13	2,14737	42,043	0,1
18	0	2	7	2,11892	42,635	0,1
19	2	0	8	2,04915	44,161	0,1
20	0	1	14	2,02185	44,790	0,1
21	1	1	12	1,89891	47,864	16,8
22	2	0	11	1,83568	49,622	0,1
23	2	1	1	1,81781	50,143	0,1
24	1	2	2	1,80861	50,416	0,1
25	2	1	4	1,77318	51,496	0,1
26	1	2	5	1,74793	52,296	0,1
27	0	1	17	1,71434	53,401	0,1
28	0	2	13	1,69976	53,896	0,1
29	2	1	7	1,68554	54,388	0,1
30	1	1	15	1,66524	55,107	0,1
31	1	2	8	1,64978	55,668	0,1
32	2	0	14	1,63543	56,199	0,1
33	3	0	0	1,60589	57,328	15,8
34	2	1	10	1,57247	58,664	0,1
35	1	0	19	1,55363	59,446	0,1
36	1	2	11	1,53210	60,367	0,1
37	0	2	16	1,51519	61,113	0,1
38	1	1	18	1,47056	63,177	14,8
39	1	2	14	1,40980	66,239	0,1
40	2	2	0	1,39074	67,267	1,6
41	3	0	12	1,36610	68,647	13,1
42	2	2	6	1,34347	69,971	10,1
43	1	3	4	1,31698	71,592	0,1
44	3	1	5	1,30653	72,254	0,1
45	0	0	24	1,29938	72,715	2,1
46	1	3	7	1,27985	74,008	0,1
47	3	1	8	1,26398	75,096	0,1
48	2	2	12	1,22619	77,836	2,6
49	3	1	11	1,20866	79,184	0,1
50	4	0	1	1,20352	79,589	0,1
51	0	4	2	1,20084	79,803	0,1
52	3	0	18	1,17725	81,736	1,6
53	0	1	26	1,16389	82,880	0,1
54	4	0	7	1,16267	82,986	0,1
55	0	4	8	1,15074	84,041	0,1
56	3	1	14	1,14584	84,483	0,1
57	4	0	10	1,12353	86,567	0,1
58	2	1	22	1,11854	87,049	0,1
59	0	4	11	1,10852	88,037	0,1
60	0	2	25	1,10769	88,120	0,1
61	3	2	1	1,10455	88,436	0,1
62	2	3	2	1,10248	88,645	0,1
63	3	2	4	1,09430	89,485	0,1

Stick Pattern

Ref. Pattern: Zirconium Oxide, 01-073-0958