

***** BaZrO3 a Simple Cubic *****

PARAMETERS

A= 4.2000 B= 4.2000 C= 4.2000
 AF= 90.000 BT= 90.000 GM= 90.000
 NUVW= 8 NSY= 1 NL= 6
 SY: 1-CUBIC; 2-TETRA; 3-ORTH; 4-HEX; 5-MONO; 6-TRIC
 LT: 1-F; 2-I; 3-C; 4-B; 5-A; 6-P; 7-R;

K	U	V	W	H1	K1	L1	H2	K2	L2	R2/R1	R3/R1	FAI	D1	D2
1	1	1	1	0	-1	1	1	0	-1	1.000	1.000	120.00	2.970	2.970
2	6	5	2	-1	2	-2	-2	2	1	1.000	1.054	63.61	1.400	1.400
3	5	3	1	-1	1	2	1	-2	1	1.000	1.291	99.59	1.715	1.715
4	1	0	0	0	1	0	0	0	1	1.000	1.414	90.00	4.200	4.200
5	4	2	1	-1	2	0	0	-1	2	1.000	1.095	113.58	1.878	1.878
6	8	3	1	-1	2	2	0	-1	3	1.054	1.106	65.06	1.400	1.328
7	7	6	2	-2	2	1	0	-1	3	1.054	1.374	83.95	1.400	1.328
8	4	3	2	-1	0	2	1	-2	1	1.095	1.342	79.48	1.878	1.715
9	5	2	1	0	-1	2	1	-2	-1	1.095	1.483	90.00	1.878	1.715
10	7	5	4	2	-2	-1	1	1	-3	1.106	1.247	72.45	1.400	1.266
11	8	5	1	-1	2	-2	-1	1	3	1.106	1.247	107.55	1.400	1.266
12	8	7	5	-1	-1	3	2	-3	1	1.128	1.243	71.20	1.266	1.122
13	7	6	4	-2	1	2	0	-2	3	1.202	1.247	68.30	1.400	1.165
14	2	1	1	0	-1	1	1	-1	-1	1.225	1.581	90.00	2.970	2.425
15	5	4	3	-1	2	-1	-2	1	2	1.225	1.354	74.21	1.715	1.400
16	6	4	1	-1	1	2	1	-2	2	1.225	1.472	82.18	1.715	1.400
17	8	7	2	-2	2	1	1	-2	3	1.247	1.374	105.50	1.400	1.122
18	8	7	3	-1	2	-2	-2	1	3	1.247	1.453	100.26	1.400	1.122
19	8	6	5	-2	1	2	1	-3	2	1.247	1.528	95.11	1.400	1.122
20	7	3	1	-1	2	1	0	-1	3	1.291	1.528	82.58	1.715	1.328
21	3	2	1	-1	1	1	0	-1	2	1.291	1.414	75.04	2.425	1.878
22	6	2	1	0	-1	2	1	-2	-2	1.342	1.414	107.35	1.878	1.400
23	5	4	2	0	-1	2	2	-2	-1	1.342	1.673	90.00	1.878	1.400
24	7	4	1	-1	2	-1	-1	1	3	1.354	1.683	90.00	1.715	1.266
25	7	3	2	-1	1	2	1	-3	1	1.354	1.472	104.25	1.715	1.266
26	6	3	1	-1	2	0	0	-1	3	1.414	1.483	106.43	1.878	1.328
27	6	3	2	-1	2	0	-1	0	3	1.414	1.612	81.87	1.878	1.328
28	1	1	0	0	0	-1	-1	1	0	1.414	1.732	90.00	4.200	2.970
29	8	3	2	-1	2	1	0	-2	3	1.472	1.683	96.50	1.715	1.165
30	6	5	4	-1	2	-1	-2	0	3	1.472	1.683	96.50	1.715	1.165
31	7	2	1	0	-1	2	1	-3	-1	1.483	1.673	82.25	1.878	1.266
32	7	5	1	-1	1	2	2	-3	1	1.528	1.528	109.11	1.715	1.122
33	7	5	3	-1	2	-1	-2	1	3	1.528	1.732	83.74	1.715	1.122
34	2	2	1	-1	1	0	0	-1	2	1.581	1.581	108.43	2.970	1.878
35	6	4	3	-1	0	2	2	-3	0	1.612	1.673	104.36	1.878	1.165
36	8	2	1	0	-1	2	1	-3	-2	1.673	1.844	96.86	1.878	1.122
37	6	5	3	-1	0	2	2	-3	1	1.673	1.949	90.00	1.878	1.122
38	7	4	2	0	-1	2	2	-3	-1	1.673	1.844	83.14	1.878	1.122
39	8	5	2	-1	2	-1	-2	2	3	1.683	1.683	72.72	1.715	1.019
40	8	6	1	-1	1	2	2	-3	2	1.683	1.871	95.68	1.715	1.019
41	3	1	1	0	-1	1	1	-1	-2	1.732	1.732	106.78	2.970	1.715
42	4	3	1	-1	1	1	1	-2	2	1.732	1.826	101.10	2.425	1.400
43	7	6	5	-1	2	-1	-3	1	3	1.780	1.871	79.20	1.715	.964
44	8	4	1	-1	2	0	0	-1	4	1.844	1.897	102.53	1.878	1.019
45	8	4	3	-1	2	0	-1	-1	4	1.897	2.049	96.05	1.878	.990

46	7	6	3	0	-1	2	3	-3	-1	1.949	2.098	84.11	1.878	.964
47	8	7	6	-1	2	-1	-3	0	4	2.041	2.198	94.68	1.715	.840
48	8	5	4	-1	0	2	2	-4	1	2.049	2.280	90.00	1.878	.917
49	5	3	2	-1	1	1	0	-2	3	2.082	2.160	80.79	2.425	1.165
50	8	6	3	0	-1	2	3	-3	-2	2.098	2.236	95.47	1.878	.895
51	3	2	2	0	-1	1	2	-2	-1	2.121	2.121	76.37	2.970	1.400
52	4	1	1	0	-1	1	1	-2	-2	2.121	2.345	90.00	2.970	1.400
53	5	4	1	-1	1	1	1	-2	3	2.160	2.380	90.00	2.425	1.122
54	3	3	1	-1	1	0	0	-1	3	2.236	2.236	102.92	2.970	1.328
55	2	1	0	0	0	-1	-1	2	0	2.236	2.449	90.00	4.200	1.878
56	8	7	4	-1	0	2	3	-4	1	2.280	2.408	95.03	1.878	.824
57	3	3	2	-1	1	0	-1	-1	3	2.345	2.550	90.00	2.970	1.266
58	5	1	1	0	-1	1	1	-3	-2	2.646	2.646	79.11	2.970	1.122
59	6	5	1	-1	1	1	1	-2	4	2.646	2.708	82.76	2.425	.917
60	7	4	3	-1	1	1	0	-3	4	2.887	2.944	83.37	2.425	.840
61	5	2	2	0	-1	1	2	-3	-2	2.915	2.915	80.13	2.970	1.019
62	4	4	1	-1	1	0	0	-1	4	2.915	2.915	99.87	2.970	1.019
63	4	3	3	0	-1	1	3	-2	-2	2.915	3.082	90.00	2.970	1.019
64	7	5	2	-1	1	1	1	-3	4	2.944	3.109	90.00	2.425	.824
65	6	1	1	0	-1	1	1	-3	-3	3.082	3.240	90.00	2.970	.964
66	3	1	0	0	0	-1	-1	3	0	3.162	3.317	90.00	4.200	1.328
67	4	4	3	-1	1	0	-1	-2	4	3.240	3.240	98.88	2.970	.917
68	5	3	3	0	-1	1	3	-2	-3	3.317	3.317	98.67	2.970	.895
69	5	5	1	-1	1	0	0	-1	5	3.606	3.606	97.97	2.970	.824
70	7	1	1	0	-1	1	1	-4	-3	3.606	3.606	82.03	2.970	.824
71	3	2	0	0	0	-1	-2	3	0	3.606	3.742	90.00	4.200	1.165
72	5	5	2	-1	1	0	-1	-1	5	3.674	3.808	90.00	2.970	.808
73	4	1	0	0	0	-1	-1	4	0	4.123	4.243	90.00	4.200	1.019
74	4	3	0	0	0	-1	-3	4	0	5.000	5.099	90.00	4.200	.840
75	5	1	0	0	0	-1	-1	5	0	5.099	5.196	90.00	4.200	.824