

Oscillatory- and sector-zoned pyrochlore from carbonatites of the Kerimasi volcano, Gregory rift, Tanzania

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Supplementary materials

Table S1.

The analyses of the pyrochlore-group minerals were carried out at The Natural history Museum, London using a Cameca SX50 electron microprobe. The following beam conditions were employed:

Accelerating voltage: 20kV

Beam Current: 10nA

Spot Size: 1µm

The Following standards and counting times were used:

Element	X-ray line	Standard	Peak counting time (s)
F	ka	Barium Fluoride (synthetic)	30
Na	ka	Sodium Niobate (synthetic)	10
Mg	ka	Magnesium Oxide (synthetic)	20
Al	ka	Aluminium Oxide (synthetic)	20
Si	ka	Wollastonite	20
Ca	ka	Wollastonite	20
K	ka	Potassium Bromide	20
Ti	ka	Rutile	20
Mn	ka	Manganese Titanium Oxide (synthetic)	20
Fe	ka	Haematite	20
Sr	ka	Strontium Titanium Oxide (synthetic)	30
Y	la	Yttrium Glass (synthetic)	30
Zr	la	Zirconium Oxide (synthetic)	30
Nb	la	Sodium Niobate (synthetic)	30
Ba	la	Barium Fluoride (synthetic)	30
La	la	Lanthanum Glass (synthetic)	30
Ce	la	Cerium Glass (synthetic)	30
Pr	la	Praseodymium Glass (synthetic)	60
Nd	la	Neodymium Glass (synthetic)	60
Sm	la	Samarium Glass (synthetic)	60
Hf	la	Hafnium (synthetic)	60
Ta	la	Tantalum (synthetic)	60
W	la	Tungsten (synthetic)	60
Pb	ma	Galena	60
Th	ma	Monazite	60
U	mb	Uranium Oxide (Depleted synthetic)	60

Background counting times (upper and lower) were half the peak times. Data reduction was performed using the internal PAP [1] matrix correction software of Cameca. Peak overlaps were determined by analysing the above standards as unknowns and deriving empirical correction factors [2].

Fluorine was determined using the F Ka X-ray line peak measurement. A large multi-layer (W/Si) pseudocrystal (Cameca - LPC0) diffracting crystal (this crystal has a 2d spacing of 44.4 Angstroms) was used on a spectrometer with a thin polypropylene spectrometer window. The Pulse Height analysis was set to differential mode with a window set to remove high order interferences (eg. P and Ca). Peak overlaps from interfering element lines such as Ce were corrected in software from measured values obtained from standards using the Cameca software interference peak overlap routine. The standard used was Topaz. There was no discernible peak shift between the standard and Pyrochlore. Measurements of count rate Vs time have been previously obtained to determine that there is no change in count rate (F ka) from the standard over the time used for calibration (30s on peak, 15s on each background position).

[1] Pouchou, J-L and Pichoir, F. (1986) Basic expression of "PAP" computation for quantitative empa, in JD Brown and RH Packwood, ed, 11th Intl Congress on X-ray Optics and Microanalysis, p. 249+

[2] Roeder, P. (1985) Electron-microprobe analysis of minerals for rare-earth elements: use of calculated peak-overlap corrections. Canadian Mineralogist, 23, 263-271.

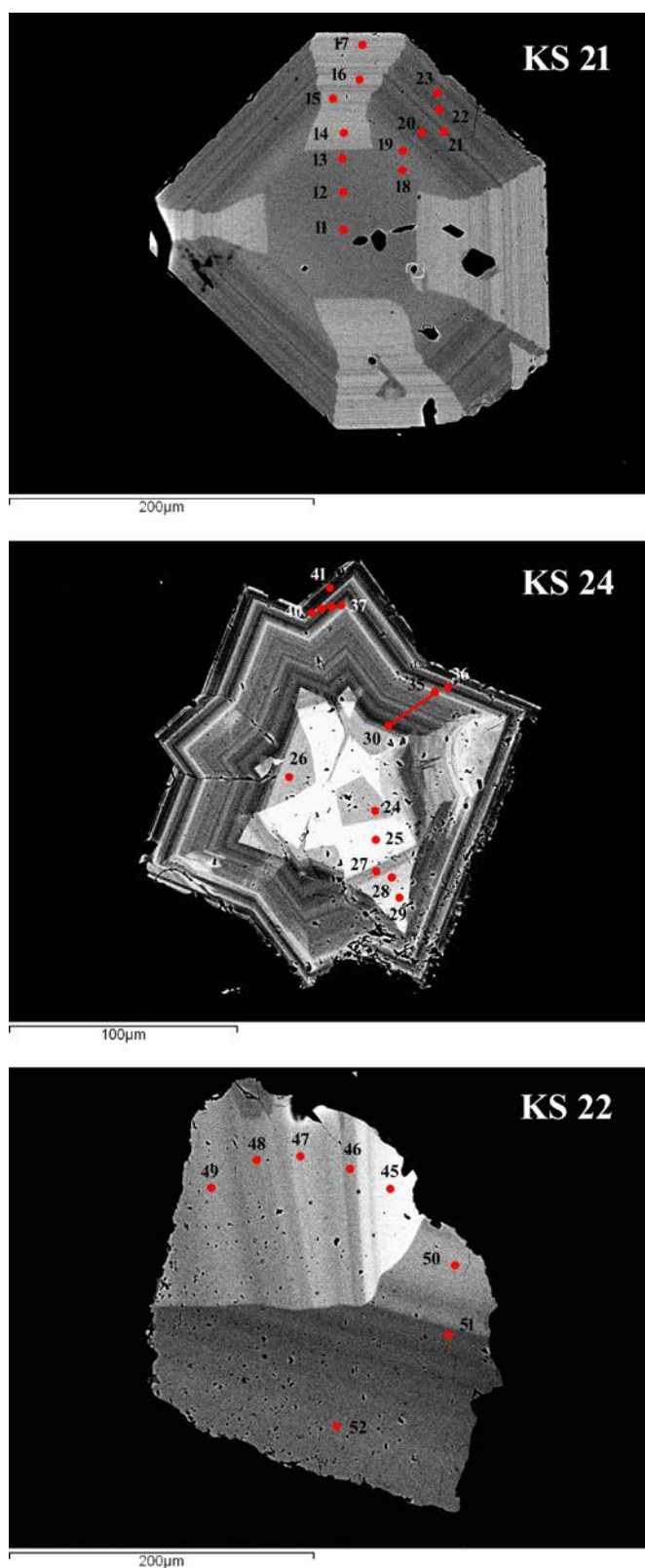
Table S2. Powder XRD data and unit-cell parameters for pyrochlore.

LL 444				KS 21				<i>hkl</i>
<i>I_{obs}</i>	<i>I_{calc}</i>	<i>d_{obs}</i> , Å	<i>d_{calc}</i> , Å	<i>I_{obs}</i>	<i>I_{calc}</i>	<i>d_{obs}</i> , Å	<i>d_{calc}</i> , Å	
33	17	6.09	6.03	58	38	6.03	6.00	111
18	15	3.142	3.146	43	30	3.133	3.132	311
100	100	3.009	3.012	100	100	3.010	2.999	222
21	20	2.602	2.609	32	17	2.598	2.597	400
-	-	-	-	2	1	2.116	2.120	422
20	5	2.004	2.008	15	9	1.9983	1.9992	333
42	51	1.8403	1.8447	76	56	1.8361	1.8364	440
-	-	-	-	8	5	1.7554	1.7559	531
-	-	-	-	2	2	1.6397	1.6425	620
26	39	1.5682	1.5731	67	41	1.5647	1.5661	622
6	9	1.5041	1.5062	15	9	1.4972	1.4994	444
-	-	-	-	6	4	1.4560	1.4546	551
4	3	1.3600	1.3585	9	7	1.3512	1.3524	731
3	6	1.3037	1.3044	7	7	1.2972	1.2985	800
-	-	-	-	1	1	1.2226	1.2242	822
8	13	1.1931	1.1970	13	14	1.1908	1.1916	662
6	10	1.1631	1.6667	12	10	1.1606	1.1614	840
-	-	-	-	1	1	1.1424	1.1402	911
-	-	-	-	2	2	1.0889	1.0890	931
4	8	1.0629	1.0650	8	9	1.0592	1.0602	844
<i>a</i> = 10.4152(1) Å				<i>a</i> = 10.3763(1) Å				

Table S3. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for LL 441 and KS 23.

sample	site	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
LL 441	<i>A</i>	0.0143(7)	0.0143(7)	0.0143(7)	−0.002.1(2)	−0.002.1(2)	−0.002.1(2)
KS 23	<i>A</i>	0.0149(4)	0.0149(4)	0.0149(4)	−0.0030(1)	−0.0030(1)	−0.0030(1)
LL 441	<i>B</i>	0.0118(4)	0.0118(4)	0.0118(4)	0.0009(1)	−0.0009(1)	0.0009(1)
KS 23	<i>B</i>	0.0118(1)	0.0118(1)	0.0118(1)	0.00067(5)	−0.00067(5)	0.00067(5)
LL 441	<i>O</i>	0.020(2)	0.014(1)	0.014(1)	0.005(1)	0	0
KS 23	<i>O</i>	0.0154(6)	0.0118(4)	0.0118(4)	0.0046(4)	0	0
LL 441	<i>Z</i>	0.026(2)	0.026(2)	0.026(2)	0	0	0
KS 23	<i>Z</i>	0.0146(5)	0.0146(5)	0.0146(5)	0	0	0

Supplementary Figure 1a. Back-scattered electron images of the sector zoned pyrochlore crystals from the Kisete crater showing positions of spot analyses.



Supplementary Figure 1b. Back-scattered electron image of the oscillatory zoned pyrochlore crystal from the Loluni crater showing positions of spot analyses (sample LL 445).

