Table S1. Atom coordinates, isotropic parameters of atomic displacements in the crystal structure of parakeldyshite.

Site	*x*	*y*	*z*	U(iso)
Zr1	1.21851(5)	0.70978(4)	0.22894(3)	2.19(10)
Si1	0.22568(16)	0.64653(12)	0.64655(9)	3.42(17)
Si2	0.68180(15)	1.06181(12)	0.16476(9)	3.26(17)
Na1	0.2352(2)	0.34482(18)	0.99840(14)	7.2(3)
Na2	0.2575(2)	1.12304(19)	0.40236(14)	10.6(3)
O1	0.8833(4)	0.8726(3)	0.1611(2)	5.1(4)
O2	0.4681(4)	0.4914(3)	0.7063(2)	7.1(4)
O3	0.2823(4)	0.8825(3)	0.6661(2)	5.3(4)
O4	0.1627(4)	0.7143(3)	0.4594(2)	6.2(4)
O5	0.2913(4)	0.7210(3)	0.9868(2)	4.6(4)
O6	-0.0220(4)	0.5660(3)	0.7538(2)	5.2(4)
O7	0.3974(4)	-0.0056(3)	1.1790(2)	4.6(4)

Table S2. Selected bond lengths in the crystal structure of parakeldyshite.

Zr1 – O1	2.051(2)	Na1 – O1	2.443(2)
– O2	2.057(2)	– O2	2.725(2)
– O4	2.047(2)	– O5	2.491(2)
– O5	2.128(2)	– O5	2.573(3)
– O6	2.139(2)	– O5	2.913(3)
– O7	2.090(2)	– O6	2.584(2)
<Zr1–O>	2.085	– O6	2.629(2)
		– O7	2.471(2)
Si1 – O2	1.601(2)	<Na1–O>	2.604
– O3	1.672(2)		
– O4	1.610(2)	Na2 – O2	2.913(2)
– O6	1.626(2)	– O3	2.359(2)
<Si1–O>	1.627	– O3	2.539(3)
		– O4	2.665(2)
Si2 – O1	1.600(2)	– O4	2.830(2)
– O3	1.669(2)	– O6	2.384(2)
– O5	1.625(2)	– O7	2.447(2)
– O7	1.626(2)	<Na2–O>	2.591

<Si2–O>	1.630

Table S3. Anisotropic parameters of atomic displacements in the crystal structure of parakeldyshite (Å^2 10^{-3}).

Site	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Zr1	1.38(16)	2.64(15)	2.57(15)	-0.88(10)	0.34(10)	-0.31(10)
Si1	2.8(4)	3.9(4)	3.6(4)	-1.2(3)	0.2(3)	-0.3(3)
Si2	2.7(4)	3.8(4)	3.6(4)	-1.5(3)	0.3(3)	-0.9(3)
Na1	7.9(7)	6.2(5)	7.0(5)	-1.6(4)	-1.5(5)	0.7(5)
Na2	8.8(7)	11.1(6)	9.1(6)	-0.2(5)	1.4(5)	1.7(5)
O1	3.3(11)	5.9(9)	6.0(10)	-1.7(8)	0.0(8)	-0.4(8)
O2	6.1(11)	6.2(9)	8.1(10)	-1.2(8)	-0.6(8)	0.6(8)
O3	7.0(11)	5.0(9)	3.6(9)	-0.7(8)	-0.2(8)	-1.8(8)
O4	6.6(11)	6.9(9)	5.6(10)	-2.8(8)	-0.9(8)	-0.2(8)
O5	5.1(11)	4.9(9)	3.6(9)	-1.2(8)	0.9(8)	-1.1(8)
O6	3.7(11)	5.0(9)	6.7(9)	-1.4(8)	0.7(8)	-1.3(8)
O7	2.0(11)	6.0(9)	5.6(9)	-1.9(8)	1.5(8)	-1.3(8)

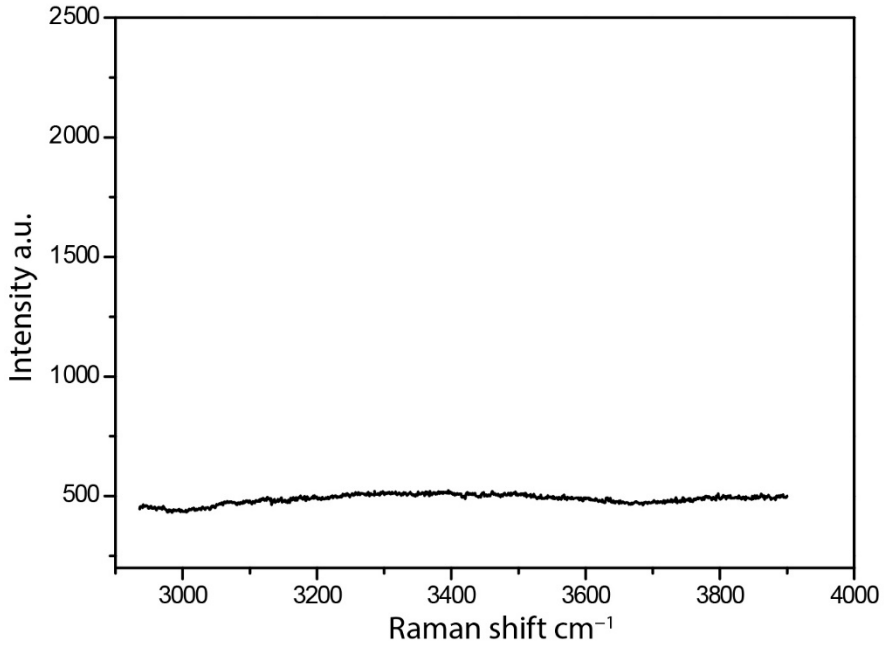

Figure S1. Raman spectrum of parakeldyshite in the range 2950-3900 cm^{-1}.